CWI Tract 72

Modeling one dimensional pattern formation by anti-diffusion

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1980 Mathematics Subject Classification: 60J60, 60J70, 35B32, 65CXX, 90A16, 92A40.
ISBN 90 6196 389 3
NUGI-code: 811

Acknowledgement

In the year 1982 a small study group on pattern formation and bifurcation was formed at the Erasmus University Rotterdam. I am grateful to prof. dr. M. Hazewinkel for inviting me to join this group. His broad ideas were always stimulating and encouraging. I also owe much to prof. dr. B. Leynse and prof. dr. J.H.P. Paelinck. This interdisciplinary study was only possible by their continuous interest and valuable suggestions on so different topics as germ formation, crystallization and migration.
Moreover, I thank the Centre for Mathematics and Computer Science for the opportunity to publish this monograph in their series CWI Tracts and all those at the Centre who have contributed to its technical realization.

This study was supported by the Netherlands Organization for Scientific Research (NWO).

CONTENTS

CHAPTER I

PATTERN FORMATION

I.1 Introduction

In the world around us most diverse forms and shapes can be observed. Many are caused by man himself not only in a continuous process of innovation and technical application restructuring his natural environment but also in a less objective way in the constitution of social forms in which individual life takes part. But, just as biological life forms, much of the structures are produced by nature in the form of some ordering in time and space. The cooperation of elementary components produces an entity with an individual, recognizable structure which is more or less stable and reproducible. A structure has properties and fulfill laws which can not be derived from the constituents alone.

In science the naive immediate experiences are ordered in a systematic way. The main research of natural science was directed towards the laws which constitute structures and their functional relationships. In recent years, the research of I. Prigogine and H. Haken has initiated a shift in attention to the natural aspects of the emergence of structure on macroscopic level in multi particle systems.

A complete mathematical characterization of such a system, say one liter of ethyl alcohol would entail the specification of coordinates and momenta for each molecule in the sample, plus additional variables describing the internal state of each molecule. At least 10^{23} numbers

(atomic, *microscopic* coordinates) are needed to describe this system! However, structures are observed *macroscopically* on scales which are slow and coarse compared to the atomic scale of time and distance. Only those few particular (combinations of) atomic coordinates which survive time and spatial averaging are macroscopically observable. Some sciences, e.g. mechanics, are concerned with the study of one or more of these surviving coordinates, other are concerned with the macroscopic consequences of multiple actions on microscopic level, e.g. thermodynamics. But as a consequence of the coarseness of macroscopic observations, the microscopic coordinates do not appear explicitly in a macroscopic description of the system. In that case processes are characterized by macroscopic quantities i.e. temperature, particle density (e.g. Callen, 1985).

Under certain conditions multi particle systems perform a well organized collective motion or function which results in ordered phenomena on a macroscopic scale. Structure formation is conceived of as the transition between an disordered state and an ordered one. The disordered state is characterized by random or non-identifiable behavior. The transition between those states is called *pattern formation.*

Prigogine's and Haken's ideas add up to a theory of change which is not only relevant for physical and related chemical and biological systems but also for the understanding of systems where the physical aspects are not decisive for the determination of structural laws. Such a common denominator seems hardly likely. Already in physics, the Newtonian model offers total determinism and thermodynamics a movement towards a final uniform state.

Newtonian determinism means no essential difference in going backward or forward in time: the time evolution is fixed, each stage is unambiguously determined by the (complete description of the) initial state. In the disorder movement of gas molecules complete information on all possible states is present. On macroscopic scale all those disorder (chaotic) states look the same. If the movement becomes less chaotic, a pattern could be detected. Different time paths can give rise to the same ordered structure: the initial state is not uniquely reachable by reversing time. Such a time *irreversible* process is not

possible in a Newtonian world.

The second law of thermodynamics provides a time arrow for physical processes, however just in the direction of disorder. This applies only for *isolated* systems which have no exchange of matter and energy with their environment. It is precisely in non-isolated physical systems that processes occur which resemble pattern formation; e.g. in biological- and social systems. In the latter case, the time evolution is in the direction of higher ordered structures. The same development can take place in physical systems. A continuous influx of energy and/or matter provide conditions under which pattern formation can take place (see below, paragraph 2). A particular aspect is that those conditions do not specify the pattern itself. The observed form can not be deduced uniquely from the external influences only. It looks as if the elements organize themselves to react coherently to changes in the environment. This aspect of the process is labelled *self-organization.* From all possible reactions, one particular form is chosen throughout the whole system. The emergence of structure in itself and the multiplicity of ordered structures which can arise in a self-organizing way are two of the fascinating aspects of this type of pattern formation.

In Prigogine's theory and in Haken's approach, denoted by the term *synergetics*, the basic conditions for such a process are: a non-isolated system, many subsystems, intrinsic fluctuations. (An introduction to the work of Prigogine can be found in Prigogine and Stengers (1984) and to the work of Haken in Haken (1981)). The impossibility of a complete microscopic description of multi particle systems (continuously extended systems as fluids), the fundamental uncertainty with respect to position and velocity, as well as other considerations, has given rise to a statistical approach. The system is subdivided in ensembles; the elements belonging to an ensemble are assumed to be indistinguishable. This so called *mezoscopic* scale is large compared to microscopic distance- and time scales but small compared to those of the observed macroscopic pattern.

The evolving macroscopic patterns are a consequence of microscopic interactions. Based on the assumption that micro behavior is a scaled down version of the macro one, pattern formation is now described as a

spatial and/or time redistribution of some macroscopic quantities defined for the ensembles, e.g. temperature, particle density and concepts such as phase. Apart from intrinsic fluctuations, the mezoscopic approach generates spontaneously more 'fluctuations' since not all microscopic elements will be in the same (averaged) state. Those fluctuations test continuously the stability of some distribution (macroscopic pattern) and can induce a transition to a new pattern if stability is lost.
These conditions are apparently present in social systems: inter-dependence of different groups, fluctuations as a manifestation of individual behavior deviating from average group behavior, the openness to innovation and information. With the introduction of statistical mechanical concepts, Prigogine's methods and Haken's synergetics are used in the study of change and ordering in social systems, see e.g. Weidlich and Haag, 1983.
Before part of Prigogine's theory and Haken's synergetic approach will be exposed in paragraph I.3, some examples of pattern formation processes will be given in the next paragraph. The examples are selected on the basis of a criterion of elementary conditions and no attempt has been made to bring all pattern formation processes under the common denominator of self-organization.

I.2 Examples

The first examples are typical for pattern formation induced by lowering of the temperature and removal of energy from the system.

Physics, phase transitions at low temperature

The most obvious example is water vapor. At elevated temperature its molecules move freely without mutual correlation. A liquid drop is formed when temperature is lowered; molecular motion becomes highly correlated. Finally, at still lower temperature, at the freezing point, water is transformed into ice crystals. The molecules are now arranged in fixed order.

The different aggregate states are called phases and the change of one phase to the other is called a phase transition. Though the same kind of molecules are involved, the mechanical, optical, electrical, thermal properties of the three phases differ wildly.

A similar type of ordering occurs in ferromagnets. At the atomic level, the magnet may visualized as being composed of many elementary atomic magnets, called spins. At high temperature, the spins point in random directions. When added up, their magnetic moments (practically) cancel each other and no magnetization results. Below a critical temperature, the elementary magnets may line up, giving rise to magnetization.

In some alloys physical properties such as elasticity are changed under the influence of external forces (stress) (Falk, 1983, 1984). Spatial differentiation by binary phase decomposition is applied in the so-called WORM, write once, read many, optical disk drives used as high capacity data storage devices. The state of the memory is given in terms of the properties belonging to one of the phases.

In superconductors below a certain temperature electrical resistance vanishes completely and abruptly (Berggren and Huberman, 1978). (For a general reference on phase transition, see Domb and Green, 1972-1976).

Physics, Fluids

Fluid dynamics provides beautiful examples of pattern formation. A standard type is given by Bénard instability (convection instability). Here a thin layer of fluid is heated from below such that the bottom of the layer has a constant and uniform temperature; similarly, heat is withdrawn at the top of the layer in such a way that the temperature there is also constant and uniform but lower than at the bottom. The fluid is subject to gravity only and incompressible.

The most important feature of the model is that only one property, density, is directly altered by the temperature difference. Due to this temperature difference (temperature gradient) a vertical flux of heat is created. For a small temperature gradient, this heat transport occurs at the particle *(microscopical)* level and no fluid motion is observable, that means no *macroscopic* motion is visible. When the

temperature gradient is increased, suddenly at a critical temperature gradient a macroscopic motion of the fluid sets in.
The fundamental unit of this pattern consists of two long rolls which rotate in opposite directions; in each unit, the fluid rises in the center along one side of a roll, cools down at the upper surface and sinks at the periphery along the other side of the roll. As the temperature gradient increases, more complicated patterns arise, such as the Bénard cells: see Haken (1978) for more details. Convective systems can be observed in nature: atmospheric convection where cloud streets or mare's tails (long straight streaks of cirrus clouds) are produced by cells of the roll type extending over thousands of square kilometers. On a much smaller scale, the drying of lacquer (varnish) shows convective patterns, see e.g. Velarde e.a. (1980).

A related phenomenon is the so-called Taylor instability. In an experimental setup liquid is filled in between two coaxial cylinders. The outer cylinder is kept fixed while the inner cylinder can be rotated. At slow rotation speeds, the fluid forms coaxial streamlines: by means of the friction between fluid and cylinder, the fluid is carried along with the inner cylinder. When the rotation speed is increased, a new kind of motion appears: the fluid motion becomes *organized* in the form of rolls such that the fluid moves outwards and inwards in horizontal periodical ordered layers. At a second critical speed value, the rolls start to oscillate with one basic frequency, at higher speed with two frequencies, eventually at still higher speed chaotic motion sets in (Haken, 1978).

Chemistry

Temporal, spatial and spatio-temporal reactions: usually, when reactants are brought together and well stirred, a homogeneous end product arises. However, some reactions show specific patterns. In Chapter IX an example of a spatial precipitation pattern, Liesegang rings, will be given. Temporal oscillating systems date from an accidental discovery in 1958 by the Russian chemist B.P. Belousov. A few years after its publication, A.M. Zhabotinsky modified slightly Belousov's recipe and started a systematic study of the reaction which is now commonly called the Belousov-Zhabotinsky reaction (see Epstein e.a., 1983).

In Belousov's experiment, citric acid and sulfuric acid is dissolved in water with potassium bromate and a cerium salt. Oscillations are clearly visible as the cerium changes back and forth from an oxidized state (yellow) to a less oxidized state which is colorless. The reaction is maintained by an influx of new reactants from the external environment with at the same time removal of final products (see e.g. Winfree e.a., 1984).

Biology

Animal grouping: insect swarming, fish schooling. The interior of an insect swarm consists of a number of subswarms, each moving in a random direction. Insects at the leading, peripheral and rear edges show a consistent orientation inwards to the centre of the swarm. This behavior at the edges provides a mechanism to keep the swarm together. The swarming activity depends on the external factors such as animals, human beings and special ground conditions.
Fish schooling is more organized: neighboring fish orient themselves similarly. Moreover there seems to exist a critical density below which no aggregation takes place (Okubo, 1980).

Pattern formation in algal cell cultures: swimming micro organisms may spontaneously form regular convection patterns. Local stimuli affect their orientation and speed. Reaction to a light source is a common occurrence which is called positive phototaxis if the swimming direction is towards the light source; regulation of speed is called kinesis (Okubo, 1980).

Termite nests (chemotactic interaction): from a multitude of disorderly movements arises the construction of walls and pillars. Initially termites move randomly, dropping small quantities of earth mixed with a hormonal substance by which they are attracted. Above some threshold, deviations in the concentration induce a preferential direction such that more earth and hormones becomes accumulated at those points amplifying the initial critical fluctuation. The termites start to interfere with each other and start building large structures (see e.g. Courtois, 1985).

Slime mold aggregation: intercellular interaction depends on the

stage of the cell's life cycle. Immediately following germination, the cells disperse as if acting under mutual repulsion. When a source of food (bacteria) is present, the cells move toward it with a high positive chemotactic coefficient. After exhausting their food supply, the amoebae first tend to distribute themselves uniformly over the space; later they begin to aggregate in a number of "collecting points". At each center a slug forms, migrates and eventually forms a multicellular fruiting body. This final process is understood as follows. The single cells are capable of spontaneous emission of a certain kind of molecules (cAMP) in the form of pulses into their surroundings. These pulses can be amplified by the cells themselves and the single cells can measure the direction of the gradient. In this way, higher concentrated areas can be detected and the cells migrate towards them (Keller e.a., 1970; Hagan e.a., 1981).

A similar mechanism is found in morphogenesis. Cell differentiation is assumed to be dependent on the position of the cell in a morphogenetic field which is generated by the gradient of a characteristic substance. This chemical gradient provides each cell with a different chemical environment which induces a spatially differentiated evolution (Turing, 1952).

The nervous system seems to process information in terms of competitively and cooperatively correlated interactions of neurons. The brain processes information in a parallel manner by neural excitation and self-organization (the network hypothesis). In the case of vision, the contour of a spatial structure is projected on the retina where the information is transmitted by correlated nerve pulses. Just like its original is build of interrelated elements, it is the cohesion between the elementary nerve pulses which reveals the original structure. Adjustments in the pattern recognition process occur in a self-learning way (Amari, 1982; Rinzel, 1977).

Geology.

Distribution of minerals or pore space in rocks.

Metamorphic layering: if pressures and temperatures are intermediate between those at the surface and the molten state, rocks can become segregated into bands, under the combined effects of stress,

dissolution, crystal growth and transport of mineral dissolution products along grain boundaries (McBirney e.a., 1979).

Stylolites (crenated fracture lines): if a porous rock is subjected to an overall stress, grains in a region of higher porosity will be subjected to higher stress and hence be more soluble; in such areas the porosity increases whereas grains in lower porosity areas will grow. The self-enhancing process causes cementation of regions which are separated by dissolution seams (Ortoleva, 1979,1984).

Dendritic growth, snowflake patterns: branching growth of an solidifying crystal. When a crystal solidifies outward from an initial seed, the process does not generate a smooth boundary: any part of the boundary that gets in front of its neighbors gains an advantage in picking up new water molecules and therefore grows much faster. Tips or dendrites are formed, moving rapidly outward and giving birth to subbranches (Langer, 1982).

Other examples are: stalactites, downward growth of calcium carbonate formed at the roof of a cave by trickling of water containing calcium compounds. Stalagmites: upward growth on the floor. Deviations from a (more or less) flat surface are enhanced since the enlarged boundary will contain more water and, by evaporation, grows faster. On the roof, the gravitation has a positive effect: the water seeks the lowest level. On the floor, gravitation has a smoothing effect which can be overcome by fast evaporation.

Convective patterns (see Bénard convection): convection in oceans is caused by heating of the water by solar radiation which penetrates a few tens of meters. On the surface the water is cooled by evaporation and conduction. Since heat is introduced at a level below which it is removed, a layer of water, several meters deep, can become unstable and give rise to convection.

Convection in the earth's mantle: the heat that drives the circulation is liberated not at a boundary but rather throughout the volume of the material, mainly as a result of the decay of radioactive elements. A temperature gradient is formed because heat is lost from the system only on the surface so that temperature increases with depth. Observable effects of this convection are the creation of a chain of rifts in the sea floor and the drift of the continents across

the surface of the earth (see references in Velarde e.a., 1980).

Economics

Spatial distribution of populations. Regional growth or stagnation, urban development, intra-urban redistribution generates a macro-structure based on micro behavior. During the initial growth phase the area is attractive and can accept additional population, but if carried far enough, the influx of people overcrowds the area, reduces the attractiveness, reduces the population inflow, and increases the outflow until population growth stops. By this process population rises and falls to maintain the attractiveness of the area in balance with that of the surrounding environment.
Shifts in manufacturing procedures, transport costs, mobility can cause redistribution of capital and labour with its consequences for the attractiveness of an area and the overall migration pattern. A prosperous area generates new industry, managers and skilled labor beyond those who can remain employed within the city area. These men and enterprises leave to start nuclei of rising economic activity at other places which are perturbations of the existing distribution (Forrester, 1970,1974).

Product cycles: life cycles of interacting commodities. Perturbations in product structures are brought about by innovations. The application of technological inventions can start the development of a new product or the rationalization of existing manufacturing procedures. A successful installment of a new industrial branch can have positive cooperative effects on the general welfare in the form of lower unemployment and attraction of production of related commodities. However the extension of production with new products is more costly than extension by rationalization which goes along with a reduction of labour costs per product. If the firms want to keep their profit margins, product rationalization leads to either higher production at lower selling prices or lower production at the same old prices. The willingness to undertake investments and the availability of capital resources depends on the (expected development of the) macro state of the economy. With a shift to lower production, rationalization reduces employment and linked with that, spending-power. In such a situation

expansion by new products becomes more difficult.
The interdependence of micro behavior and macro structure does not necessarily give rise to collective changes from, say, full-employment to under-employment. The economic state can stay close to equilibrium; only in response to large fluctuations with collective, cooperative behavior on the microscale (and external factors), a transition to a new state will occur.
In the model of Mensch (Mensch e.a., 1985) two different types of product dynamics are distinguished: intrinsic dynamics describing the "natural" fate of the product as a technological maturing process and evolution of its market share and interaction dynamics describing the life cycle of a product as it is influenced by interaction with competing commodities of different stages of maturity. This interaction process can lead to a synchronization such that clusters of products adapt to the same development stage. If this clustering is effective it will give rise to the self-organization of temporal structures in the form of groups of products at the same maturity level, and furthermore, it explains collective behavior between different industrial branches with its macroscopic effects. The decisions taken on the basis of expected development generate an autocatalytic process. Very subjective expectations can give rise to singular phenomena such as the Dutch "tulip mania" in the eighteenth century. Azariadis (1981) terms such expectations as self-fulfilling prophecies.

I.3 Order by fluctuations

The phenomena alluded to above have some specific features in common. The pattern formation is not merely a transformation or deformation. The structure obtains properties which can not be derived uniquely from the foregoing stages. There does not exist a one-to-one mapping between the states before and after the change in external conditions; the system has undergone a *structural change*. In some cases structures are maintained in a dynamic way by a continuous influx of energy, e.g. fluid dynamics; others are first generated dynamically and

then fixed by solidification, e.g. precipitation patterns, crystal growth and morphogenesis (cell differentiation).

All examples mentioned above concern systems with many elementary components. Moreover, the transition to an other state is triggered by intrinsic fluctuations. Consider for instance a parcel of fluid in the Bénard instability. Because of the elevated temperature at the bottom, a parcel has a density less than the average density of the entire layer. But as long as the parcel remains in place nothing will happen: it is surrounded by fluid of the same density and so has neutral floating power (buoyancy). All forces, viscosity and buoyancy with heat diffusion, are in balance: the system is and stays in *equilibrium.*

But molecules of a fluid are constantly in motion, so any small displacement can happen. Suppose now that the parcel is given a slight upward motion. The parcel becomes surrounded by cooler and denser fluid: as a result of positive floating power it tends to rise, and so on. Thus an initial upward movement is enhanced in an *autocatalytic* way by the density gradient which is caused by the temperature gradient. Similar reasoning applies to a parcel at the top.

If thermal diffusion is fast enough, the buoyant force will be so small that it compensates the viscous drag and the heat input is carried through the layer in a purely conductive way without any specific flow pattern; the initial state is not altered significantly, the system stays in a state of *near-equilibrium.*

However with sufficiently high density differences between fluid parcel and its environment, the viscous drag can not cancel the upward buoyancy; the initial upward displacement of the parcel is now amplified by the density gradient and this amplification, in turn, gives rise to forces which cause further upward movement. As long as the fluid moves faster than it loses heat by diffusion, the movement can be sustained. The initial small deviations are enhanced as a result of the buoyancy and the system evolves to a state *far-from-equilibrium.* The continuous influx of heat at the bottom and simultaneous withdrawal at the top keeps the system away from equilibrium. In the far-from-equilibrium state the forces acting on the system's elements are not in balance, on the contrary those forces give rise to an autocatalytic reaction which keeps the system far away from equilibrium.

This Bénard instability is a typical example of a *dissipative* structure: the added energy is converted into a vertical movement, the "remainders" are removed at the top. This process can only be sustained under the continuous influx of energy (or matter in other cases). In biological systems such a dissipative mechanism is obvious. The human body has a temperature higher than its environment. The metabolism inherent to dissipative structures transforms matter into energy to keep the system in a state far-from-equilibrium.

Such systems must be distinguished from *conservative* (Hamiltonian) systems which do not waste energy or matter (or charge, or momentum). Similar conditions to those in dissipative structures prevail. However the pattern formation in most conservative systems is initiated by removal of energy and, in contrast with a dissipative evolution as in the Bénard instability, there exists a new equilibrium state towards which the system tends. The phase transition phenomena mentioned in paragraph I.2 are examples of such processes (phase transition at thermal equilibrium). The spatial structure of atoms in a molecule are the result only of forces acting on the elementary components at the given temperature.

So the two processes differ quite substantially with respect to the interpretation of the final state: equilibrium versus far-from-equilibrium. A second aspect is that, e.g. in crystals, the position of the particles is fixed (or almost fixed) whereas in Bénard instability the pattern is fixed indeed, but the position of the particles is not. In general, dissipative structures have more degrees of freedom than conservative structures.

In mathematical terms: the steady states of the dynamical equation(s) define the pattern, but far from equilibrium those states are not equilibrium solutions of the underlying physical reactions. A simple example of a non-linear autocatalytic reaction scheme taken from Nicolis and Prigogine (1977), page 170, can illustrate the processes mentioned above. Suppose a substance A is converted into a substance B via an intermediate X which can autocatalyze its own production; the reaction scheme is

$$A + 2X \underset{k_2}{\overset{k_1}{\rightleftarrows}} 3X \qquad \text{(I.1a)}$$

$$X \underset{k_4}{\overset{k_3}{\rightleftarrows}} B \qquad \text{(I.1b)}$$

The system is open to interaction with infinite reservoirs of reactant A and B so that the concentrations of A and B are kept constant in the system. The rate equation of X is:

$$\frac{dX}{dt} = -k_2X^3 + k_1AX^2 - k_3X + k_4B \qquad \text{(I.2)}$$

Now, this equation can have different steady state solutions which are equilibrium solutions if the reactions (I.1a) and (I.1b) are in equilibrium; that is if X satisfies the following conditions:

$$k_1AX^2 = k_2X^3 \qquad \text{(I.3a)}$$

$$k_3X = k_4B \qquad \text{(I.3b)}$$

Assuming the reaction rates k_i to be fixed, then only (the concentrations of) A and B determine the number of solutions of (I.2) (and the stability properties). To make the point clear, all k_i are taken equal: an equilibrium solution exists if A = B, and in this case it is also the only steady state solution of (I.2).
But suppose the initial equilibrium is at B = 0.01 = A. Now the system is moved away from equilibrium by putting more A into the system and holding B at 0.01. Of course the equilibrium conditions of (I.3) are no longer fulfilled but still the equation will have only one solution if A is small (near-equilibrium state). No structural change will happen until A crosses the threshold at which equation (I.3) has three positive steady state solutions (with at the same time an exchange of stability). The system will branch into one of the two new structures. Important is that those new structures are only present under far-from-equilibrium conditions (e.g. A = 2.0).

So far the degree of ordering is not quantified. In the 19th century the quantity *entropy* was introduced in thermodynamics. When heat Δq at temperature T is added reversibly, entropy increases according to the

formula $\Delta S = \Delta q/T$ where S denotes entropy. This thermodynamic notion of entropy can be expressed in statistical mechanical terms.

Consider independent but distinguishable particles. At a fixed temperature, for a closed system, the particles are in some way distributed over the possible energy levels. One particular ordering of the particles is called a *complexion*. Let the number of all possible complexions be denoted by N, then the entropy S of the system can be written as: $S = k_b \ln N$, where k_b is the Boltzmann constant.

It was pointed out by Boltzmann that entropy was really a measure of disorder and order. The temperature is an average quantity (in kinetic gas theory it is identified with the average kinetic energy of particles). The temperature does not alter by bringing together two systems with the same temperature. (Temperature is an *intensive* variable, just as concentration and density.) However, the entropy will be larger since the number of possible positions, and with that the uncertainty about the positions of particles, increases. (Entropy is an *extensive* variable.) So the two notions are complementary: the entropy measures the number of possible states, the temperature describes the deviations from the average state.

The notion of entropy is strongly connected with the so-called *second law of thermodynamics*: in an isolated system the entropy increases monotonically until it reaches its maximum in a state known as *thermal equilibrium*. At a given temperature, the number of complexions becomes maximal which gives maximal uncertainty about the possible position of a particle in (phase) space. This rules out the possibility of pattern formation in isolated systems. The principle of maximum entropy defines the most probable state of the isolated system as the state with maximum entropy.

Consider now a system which is in equilibrium, but which can exchange energy with the environment (a *closed* system in Prigogine's terms; systems exchanging not only energy but also matter are called *open* systems). The system will tend to get to its lowest energy level; the (total) energy U will become as small as possible. On the other hand entropy will try to become as large as possible (second law). These are opposite directions: lowering energy will diminish the number of complexions (possible energy levels) which decreases entropy. In

thermodynamics the so-called *free energy* potential which quantifies the state of the system, expresses both tendencies. This free energy functional, more specific the Helmholtz free energy functional, is defined as

$$F = U - T \cdot S. \tag{I.4}$$

where F denotes the free energy, U total energy, T temperature and S entropy.

At equilibrium F is minimal, which for an isolated system coincides with S maximal since U will not change. At a given temperature T, the probability that a system is in a state of energy ε is given by the Boltzmann distribution function:

$$P(\varepsilon) = \frac{1}{Z}\exp(-\varepsilon/k_b T) \tag{I.5a}$$

where Z is the partition function:

$$Z = \sum_{\varepsilon} \exp(-\varepsilon/k_b T) \tag{I.5b}$$

(Z is not only some normalization factor, but links free energy with entropy, temperature, pressure etc.).

With increasing temperature, the contribution of entropy to the free energy becomes comparable with that of the energy U to F, and according to (I.5) the various energy levels become equally populated. However with decreasing temperatures, the entropy contribution diminishes and only low levels of energy are occupied to a non negligible extent. So for a non-isolated system, there exists a possibility to form low entropy, ordered structures provided T is low. This is called the *Boltzmann ordering principle*: the most probable state is defined as the state with minimal free energy. It is responsible for pattern formation properties in phase transitions, like in the case of the vapor-water-ice cycle. Equilibrium structures, as are most conservative systems, are characterized by Boltzmann ordering.

This type of low temperature pattern formation does not fit with pattern formation in far-from-equilibrium processes. In Bénard instability, heat influx brings ordering. For non-isolated systems in a non-equilibrium state, Prigogine has formulated a new, nonequilibrium ordering principle. The entropy change dS during time interval dt is

expressed as the sum of two contributions $dS = d_eS + d_iS$, where d_eS is the entropy flux due to exchanges with the outer world, and d_iS is the entropy production due to processes inside the system, such as diffusion, heat conduction; the second law implies $d_iS \geq 0$ and $d_iS = 0$ in equilibrium, hence such processes are *irreversible*. With the external "production" d_eS the system can attain a steady state with a lower entropy than the initial one, and this state can be maintained provided that $d_eS = -d_iS < 0$. As a consequence, such a situation can only occur under non-equilibrium conditions since at thermal equilibrium both d_iS and d_eS would vanish.

Note that for instance in Bénard instability, the imposed temperature gradient induces a supplementary ordering in the system which means a lowering of entropy; also the cAMP gradient in slime mold aggregation gives rise to a spatial ordering. In Prigogine's theory, the final state is now defined as the state with minimal entropy production; see for relation between statistical mechanics and thermodynamics e.g. Powles, 1968; for thermodynamics e.g. Buckingham, 1972; for far-from-equilibrium processes Prigogine e.a. 1967, 1968 and Nicolis and Prigogine, 1977).

So far the notions have been given in a thermodynamical context. Social systems are most highly open systems. Such systems show not only cooperative aspects but also autocatalytic effects. Multiplier effects are well known in economics, cooperation in producing and merchandising goods is practically a necessary condition.

In the works of Haken with his accent on cooperation (and the physical concept of phase transition), physical pattern formation processes and structure evolution in social systems are brought under the common denominator of *synergetics*. (For a general introduction see Haken, 1978, 1981; also Weidlich and Haag, 1983.) The basic notions are (again): multiple elements, randomness (based on ignorance or intrinsic fluctuations), openness and cooperation translated in terms of autocatalytic growth processes.

In physical systems entropy is a measure of order and disorder and for isolated systems, based on the principle of maximum entropy, it provides a way of determining the most probable configuration. This concept resembles strongly the Shannon information entropy which is

defined as the expected information included in an (encoded) message. The uncertainty in a message depends on the amount of information conveyed by this message. The Shannon information entropy is defined as

$$S = - \sum P(m)\log(P(m)) \qquad (I.6)$$

where the sum is over all messages. Maximal uncertainty coincides with equal probability for all messages; hence maximal uncertainty goes along with maximal entropy (Hamming, 1980). The name of entropy for the quantity defined in (I.6) is not chosen arbitrarily; by way of the Boltzmann distribution function P (I.5a) the statistical entropy can be formulated as in (I.6), in terms of summation over all energy levels. This concept of information entropy as a measure of uncertainty is used in the social sciences (Theil, 1967). In a similar way, the more physical interpretation in the sense that the most probable configuration of a system is that with maximal entropy, is applied to non-physical systems. In regional science, entropy maximization as a selection procedure amidst the numerous possible spatial states, has lead to the general formulation of so-called gravity models (Nijkamp and Paelinck, 1974).

It is a surprise that the result of fluctuations and interaction is a coherent, *stable* pattern. In Bénard instability only a differentiation in vertical direction is induced by the temperature gradient. A fluid parcel cannot move simultaneously upward and downward, so some selection must take place but why in a spatial coherent way? How does the system evolve from the chaotic phase to the ordered phase? How does the system select a specific *mode*? By which factors does the system (or its elements) organize itself in the observed mode? How is *cooperation* between the elements established? These are questions which arise in relation to self-organization. A mathematical system description can provide insight in the formal mechanism of pattern formation.

I.4 Implementation

All the systems which have been mentioned so far are generally composed of very many subsystems. Accordingly, these systems must be described by many variables. For implementation it is important to choose the variables on the adequate level of description. In the paragraphs above temperature and density were used; as mentioned there, these are average quantities which can only be formulated for sets of elements, for example a liquid. Individual atoms or molecules are found at the *microscopic* level; the appropriate variables would be their positions, velocities and mutual interactions.

At the *mezoscopic* level the liquid is described by *ensembles* of many atoms or molecules. Such ensembles are assumed to be large compared to scales on microscopic level but small compared to the evolving *macroscopic* pattern. The mezoscopic scales allow for averaging out individual behavior and the introduction of such quantities as temperature, density, mean local velocity. At the same time a mezoscopic description introduces (supplementary) randomness into the system description (and reduces entropy since its assumes that particles belonging to the same ensemble are indistinguishable).

Moreover, in physical systems the concept of ensembles allows for the merging of trajectories (time-paths) since exact position (and velocity) of particles is unknown. By Liouville's theorem, at the microscopic level the entropy is a conserved quantity for an isolated system. Defining the system in average quantities over ensembles, the entropy, or rather minus the Boltzmann H-function, formulated as in (I.6), is a monotone increasing function of time (Kac and Logan, 1979). (The thermodynamic entropy is this coarse-grain entropy.)

The macroscopic level is the observer's level where the pattern is unveiled. In the study of pattern formation processes, one looks at the evolution from a chaotic, uniform state to a ordered, non-uniform state. On the macroscopic level, this evolution is observed as a change in symmetry properties of the system. The initial state has complete symmetry, the final state has less symmetry. At the *symmetry-breaking* point, fluctuations drive the system away from the unstable uniform solution, or in general the reference state, and *branches* (or jumps) to

another, mostly not uniquely given less symmetric state.

With spatial interaction between the ensembles, the evolution is modeled by partial differential equations. The symmetry-breaking property must allow for a change in quantitative (symmetric and non-symmetric) and qualitative (stability) properties of the solutions of the model at some specific parameter values.

Those values are denoted as *bifurcation points*; at such a point, the curve which represents solutions in the parameter space, branches (*bifurcates*). The structural change in mathematical properties at the bifurcation point, resembles the structural change of the system studied at the onset of pattern formation. In bifurcation theory one studies when and how, for a given model, changes in the properties of solutions occur. Perturbations in stability theory play somewhat the role of fluctuations generated by a mezoscopic description.

Multiplicity of solutions, autocatalytic reaction in self-organizing systems, far-from-equilibrium conditions, also present at the transition from one equilibrium state to another, make non-linear modeling necessary. Only at near-equilibrium, linear approximations are valid.

Even very simple non-linear evolution equations can show a richness and complexity in pattern formation which resembles "almost" the abundance of forms in nature. Or in the words of P. Ortoleva: 'In nonlinear partial differential systems almost anything can happen. And what is beautiful is that it does. However depressing this thought might be to those who like simple generalizations, it also serves to point out the beauty and great variation of the manifestations of the nonlinear in the bio-, geo- and other spheres around us.' (Ortoleva, 1979). It may be one of the reasons why it seems so "easy" to apply non-linear dynamics to social science: the multiplicity and complexity of outcomes, possibly simulated by computer, seems to resemble analogous properties of social systems.

The mathematical model which is formulated and studied in the following chapters, is based on the reduction of spatial pattern formation to spatial separated subsystems which cooperate to form a common spatial structure. Moreover, apart from the non ordered mixed state, the ensembles (groups) can only be in one of two possible states; the

pattern is characterized by a binary phenomenon: the upward- and downward movement of water in Bénard instability, precipitation and non-precipitation, conglomeration areas and rural areas, orientation of elementary magnets, the decomposition of a market in firms which are in the excess-supply "phase" and which are in the excess-demand "phase". In the mixed phase no pattern is observed, the two states are randomly distributed (or not even present) over the given domain.

Pattern formation means now a decomposition of the (spatial) domain in separate sectors or groups of ensembles where all mezoscopic elements belong to the same phase. In the formulation of H.J. Maresquelle: 'eine Erscheinung E (entweder Konvektionssaüle, oder Amöbenaggregation) kann überall vorkommen; doch, wenn einmal irgendwo E vorhanden ist, wird E in der nächsten Nähe unmöglich. Jedes E-bezirk wird von einer "non E"-Hemmungszone umgeben.', (Maresquelle, 1977). Structure is now a binary system E - non E. The same structure is found in Conway's well-known Game-of-Life of Conway or in general in cellular automata (see e.g. Wolfram, 1983; Vichniac, 1986). Here the rules of life and death are made without reference to any specific, say physical property. The approach is purely formal.

A second way is found in models which give the evolution of the E - non E structure as the time evolution of the average E density of ensembles (groups, cells). In general, the models are taken to be continuous in time and space. For example, Meinhardt and Gierer in modeling chemical, biological (and even economic) processes, distinguish between a substance which activates growth and a substance which inhibits growth (see e.g. Meinhardt, 1977; Gierer, 1979; Mimura, 1982). The evolution of the density of the substances, called activator and inhibitor, is given in the form of reaction-diffusion equations:

$$\frac{\partial u}{\partial t} = D\Delta u + f(u) \qquad (I.7)$$

with $u = (u_1, u_2)$, $D = (d_{ij})$ being a diagonal matrix with $d_{ii} > 0$ and Δ the Laplace operator in the spatial domain. The nonlinear reaction term $f(u)$ models growth and decay of the substances; the diffusion term models spatial interaction (as in slime mold aggregation where the cAMP gradient induces spatial inhomogeneities). The pattern (the "E-profile") is given by the distribution of the activator substance over the spatial domain.

Already in 1952 Turing has pointed out the importance of reaction-diffusion equations with respect to modeling morphogenetic processes (Turing, 1952). The models developed by Meinhardt and Gierer resemble the so-called Brusselator and Oregonator of the Brussels school of Prigogine used in simulating far-from-equilibrium phenomena (see e.g. Nicolis and Prigogine, 1977).

The problem is that it is not always possible to discriminate between a inhibitor and activator substance; phase transition is formulated in terms of the concentration of particles in one of the phases; city growth is initiated by attracting people and stopped at overpopulation; the pattern of a river delta results from erosion power as a function of the stream width. Only one variable is involved which is synonymous with the local density of Maresquelle's E-phenomenon.

In this case, pattern formation is conceived of as a process in which space becomes divided in areas with either a high or low frequency of the E phenomenon. If it is assumed (in this context) that particle density is constant, then the observed pattern can be described by the density of particles which are in state E. We will denote those particles as mass. The disordered state is characterized by an uniform distribution of mass, and pattern formation can now be seen as a mass redistribution process.

Spatial decomposition will take place due to the following specific conditions:

a) an autocatalytic mechanism such that "mass" will increase at locations which have already initially a higher mass density;

b) neighbouring particles tend to evolve to the same state;

c) a conservation condition, which implies that not all particles can be in the same state at the same time.

The conditions a and b may be initiated by environmental changes.

In Chapter II a specific evolution equation is derived, based on Thom's river basin model (Thom, 1976). The time evolution of the positions of N watersheds (particles) is described in a formal way.

By assuming that N is large, the model is transformed into a continuous one which gives the time evolution of a mezoscopic variable, the local particle density $u(x,t)$. The evolution equation is:

$$\frac{\partial u}{\partial t} = \Delta\left[\phi(u) - \gamma\Delta u\right], \quad \gamma > 0 \tag{I.8}$$

Equation (I.8) is a mass conserving evolution with only nearest neighbor interactions. The autocatalytic effects can be obtained by negative diffusion which, instead of smoothing out, gives a clustering of mass (see Chapter II, § 3). The system (I.8) is denoted by the name of anti-diffusion. It depends on the specification of ϕ (and on the level of u) whether diffusion or anti-diffusion occur. A phase transition can be initiated by environmental changes, so in general the specification of ϕ will include some parameters which represent environmental conditions.

Although derived in a quite different context, this equation is a particular form of a phase transition model based on the minimization of the Ginzburg-Landau free energy functional which defines free energy (I.4) as a function of particle density only, see Chapter III, § 4.

In Chapter IV a stochastic formulation is given in the form of a Markov process. The deterministic evolution equation derived in Chapter II, is the most probable path equation of this stochastic process. By defining different spatial interactions, a whole class of mass conserving evolution equations can be found, e.g. diffusion- or migration-like mass exchange processes.

Existence and stability of non-trivial solutions are investigated in Chapter V. To find an answer to the question how the system will evolve if the uniform distribution is unstable, some bifurcation analysis is applied in chapter VI. Although all systems belonging to the class of evolution equations defined in chapter IV have the same properties with respect to existence and stability of stationary solutions, their transient behavior can be different. In chapter VII it is proven that every non-trivial, non-monotone stationary solution of this class of evolution equations is unstable. This conclusion is not valid for the discrete versions.

Numerical simulations (discrete system) are reported in chapter VIII. We have followed the time evolution of a randomly disturbed uniform initial state. By applying the so-called simulated annealing procedure, it is possible to simulate a stochastic time evolution. In both cases, deterministic and stochastic time evolution, the final patterns are (in general) non constant, non monotone functions.

In chapter IX we give a review of a periodic precipitation phenomenon, the so-called Liesegang rings. Two mathematical models are exposed, one being based on the anti-diffusion equation. Numerical simulations of both models are reported.

A model for (human) migration is introduced in chapter X. In contrast with the anti-diffusion equation (I.8), mass redistribution (migration) in unit time is not restricted to mass exchange between neighboring locations only, but still the same two phases can be distinguished: smoothing out of people ("diffusion", the uniform distribution is stable), and clustering of people ("anti-diffusion", the uniform distribution is unstable). The parameters of this migration model are estimated using Dutch migration data (1970-1985); the estimated parameter values show a change which can be interpreted as a transition in the migration pattern from "diffusion" to "anti-diffusion".

CHAPTER II

THOM'S RIVER BASIN MODEL

II.1 Introduction

In Thom (1976) the following situation is described. Rain is steadily falling on a sandy hill; at the top brooklets form and disappear almost continuously. Down the hill, the slope is gentler and erosion is less severe: the pattern of watersheds and brooklets becomes more stable. Surviving brooks compete with each other for the available space. The result will be an almost regular pattern at the bottom of the hill. Such patterns can be observed in nature, e.g. in Death Valley, California (USA):

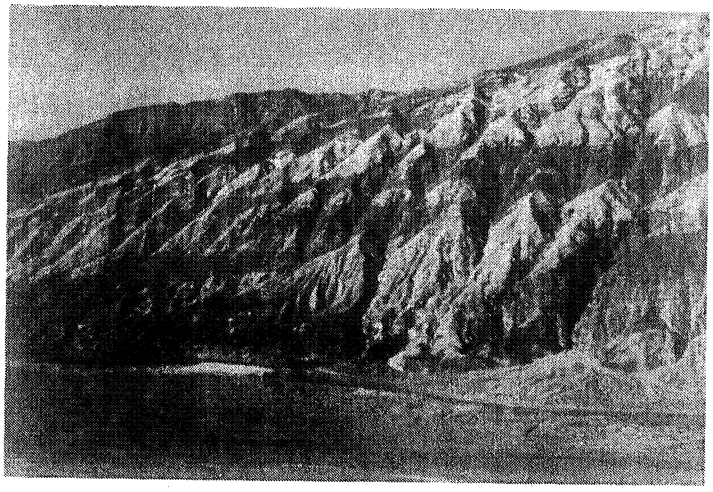


Figure II.1: Drainage pattern in Death Valley, California (USA)

The model proposed by Thom is written in terms of the position $s_n(t)$ of the n-th watershed at time t ($s_{n-1} < s_n < s_{n+1}$). Suppose the eroding power of a stream is proportional to its basin width a_n, $a_n = s_n - s_{n-1}$, then the position s_n is governed by the following differential equation:

$$\dot{s}_n = -c(s_{n+1} - s_n) + c(s_n - s_{n-1}), \quad c > 0 \qquad (II.1)$$

where $\dot{}$ denotes derivatives with respect to time t and c is a proportionality factor.
Since erosion power will be less than proportional at greater values of the basin width a, the proportionality factor c is a function of a. A first, reasonable looking, graph of c as function of the basin width a could be as depicted in figure (II.2).

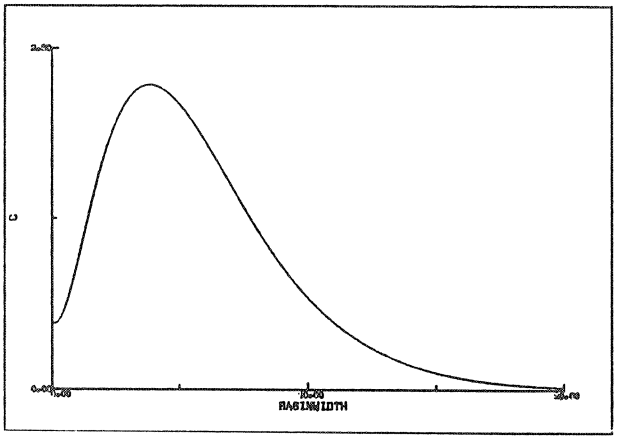


Figure II.2: Graph of c as function of the basin width a.

This function c(a) also incorporates the idea that a certain water mass is needed for effective erosion.

Any equidistant distribution with basin width a_o for all streams is a stationary solution of (II.1). By performing some linear stability analysis the character of the equations becomes more clear. Consider two streams with watersheds at +a and -a and at u near 0 on $\mathbb{R}$. Taking

Taylor expansions of c(a-u) and c(a+u) around a, the time evolution of u becomes:

$$\dot{u} = 2(c(a) + ac'(a))u + u^2(\ldots) + \ldots \qquad (II.2)$$

For $c(a) + ac'(a) < 0$ and u small, u will tend to zero: the system is stable. With c as in figure (II.2), there will be a basin width a_c such that $c(a_c) + a_c c'(a_c) = 0$ and for $a > a_c$ stability will be obtained.
On the contrary, if the stream width is in the range where $c(a) + ac'(a) > 0$, broader streams will grow at the cost of smaller ones. The deviation u will not tend to zero.
Since smaller streams coincide with higher density of the watersheds, local maxima of the watershed spatial distribution function will grow when the system is unstable with respect to uniform distributions. Thus an uniform unstable distribution, randomly disturbed, will tend in time to a non-uniform distribution. If the uniform solution is unstable then equation (II.1) models a pattern formation process.
Now, as mentioned in chapter I with respect to self-organization, at least two questions are open: (i) how does a more or less regular spacing of the watersheds with a characteristic distance a_o arise from the initially uniform, unstable situation, and (ii) how does the model select between different possible a_o's. Indeed, what is observed e.g. in the Death Valley pictures alluded to above, is a characteristic wave pattern for the watersheds. The "equilibrium restoring force" for a spacing a_o is $c(a_o) + a_o c'(a_o)$ and one could argue that there would be a natural tendency towards a spacing with a_o such that $-(c(a_o) + a_o c'(a_o))$ is maximal. Other arguments favor the largest a_o for which $c(a_o) + a_o c'(a_o)$ is still negative (the so called marginal stability hypothesis).
As formulated, the model describes the evolution for a fixed, time independent number of watersheds. It is unequal to the arising or disappearance of watersheds. In the following section a continuous model will be derived resulting in the time evolution of a mass density function. In such a multi-particle system, local maxima will represent watersheds. Redistribution of mass goes along with "growth or destruction of watersheds".

II.2 The small amplitude continuous scaling limit of Thom's river basin equation

In a multi-particle system the transition from a discrete model to a continuous model assumes that the discrete values are values of continuous, slowly varying functions in time and space. Two different identification procedures are used below. The first method identifies the subindex n with a fixed, time independent spatial location $x = n \cdot l$, where l is the grid length.
The second one is based on the observation that the inverse of the basin width a is equal to a scaled watershed density. Otherwise stated: the basin width a is identified with specific volume as used in thermodynamics (Widom, 1972). In both cases the scaling parameter l is essential in justifying the deletion or inclusion of terms in the final equation: a fourth order derivative term must be included. This term is analogous to the viscosity terms in standard reaction-diffusion equations; in thermodynamics it is just the van der Waals-Korteweg addition to usual visco-thermoelastic stress (Widom, 1972).

II.2.1 Density approach

Assume some quantity of mass is distributed on a spatial domain I and identify s_n with values of a cumulative distribution function at fixed positions denoted by the subindex n.
Let there exist a density function σ_n such that

$$\sigma_n(t) = s_n(t) - s_{n-1}(t) \qquad (II.3)$$

(Without restriction the assumption can be made that σ is the deviation from some (non-stable) uniform density $\rho_n = \rho_o$ for each n).
Let $\phi(a) = ac(a)$, then using (II.1) and (II.3) one finds:

$$\dot{\sigma}_n = -\phi(\sigma_{n+1}) + 2\phi(\sigma_n) - \phi(\sigma_{n-1}) \qquad (II.4)$$

Observe that for any reasonable function F of n

$$\exp(s\frac{\partial}{\partial n})F(n) = F(n+s) \qquad (II.5)$$

so

$$\dot{\sigma}_n = -\phi(\exp(\frac{\partial}{\partial n})\sigma_n) + 2\phi(\sigma_n) - \phi(\exp(-\frac{\partial}{\partial n})\sigma_n) \qquad (II.6)$$

Expand ϕ in a MacLaurin series: $\phi(s) = \phi(0) + \phi'(0)s + \frac{1}{2}\phi''(0)s^2 + \ldots$ to find

$$\dot{\sigma}_n = -\phi'(0)\left\{ \frac{\partial^2\sigma}{\partial n^2} + \frac{1}{12}\frac{\partial^4\sigma}{\partial n^4} + \ldots \right\} - \frac{1}{2}\phi''(0)\left\{ \frac{\partial^2\sigma^2}{\partial n^2} + \ldots \right\} + -\frac{1}{6}\phi'''(0)\left\{ \frac{\partial^2\sigma^3}{\partial n^2} + \ldots \right\} \qquad (II.7)$$

where one uses: $\frac{\partial^2\sigma^2}{\partial n^2} = 2\sigma\frac{\partial^2\sigma}{\partial n^2} + 2\left(\frac{\partial\sigma}{\partial n}\right)^2$ and $\frac{\partial^2\sigma^3}{\partial n^2} = 3\sigma^2\frac{\partial^2\sigma}{\partial n^2} + 6\sigma\left(\frac{\partial\sigma}{\partial n}\right)^2$.

Now write $x = l\cdot n$ with l a scaling parameter; so $\frac{\partial}{\partial n} = l\frac{\partial}{\partial x}$ and rescale σ as $l\cdot u$ to obtain to the fourth order in l

$$\frac{\partial u}{\partial t} = -\phi'(0)\left\{ l^2\frac{\partial^2 u}{\partial x^2} + \frac{1}{12}l^4\frac{\partial^4 u}{\partial x^4} \right\} - \frac{1}{2}l^3\,\phi''(0)\frac{\partial^2 u^2}{\partial x^2} - \frac{1}{6}l^4\,\phi'''(0)\frac{\partial^2 u^3}{\partial x^2} \qquad (II.8)$$

Observing that for an unstable uniform density $\phi'(0)$ will be positive (see equation (II.2)); without restriction $\phi'(0)l^2$ can be taken equal to 1 and the final equation becomes:

$$\frac{\partial u}{\partial t} = \frac{\partial^2}{\partial x^2}\left\{ -u + r_1 u^2 + r_2 u^3 \right\} - \gamma\frac{\partial^4 u}{\partial x^4} \qquad (II.9)$$

with $\gamma > 0$, $r_1 \sim 1$ and $r_2 \sim l^2$. No-flux boundary conditions are supplied to complete the system.

Note that the sign of the coefficients of the linear terms $\frac{\partial^2 u}{\partial x^2}$, $\frac{\partial^4 u}{\partial x^4}$ and so on, will always have the same sign.

II.2.2 Basin width as specific volume

The second approach is based on the observation that the inverse of the basin width a is proportional to the watershed density.

Let $v_n(t) = \dot{s}_n(t)$, $a_n(t) = s_n(t) - s_{n-1}(t)$.

Let $\phi(a) = ac(a)$ then (II.1) becomes:

$$v_n(t) = -\phi(a_{n+1}) + \phi(a_n) \tag{II.10}$$

Let v and a be functions defined on $I \times \mathbb{R}^+$, $I = [0,L] \subset \mathbb{R}$ such that (Whitman, 1974):

$$v(s_n(t),t) = v_n(t) \tag{II.11a}$$

$$a\left(\frac{s_n(t) + s_{n-1}(t)}{2}, t\right) = a_n(t) \tag{II.11b}$$

Denoting the partial derivative with respect to s_n by $\frac{\partial}{\partial n}$, one finds

$$a_{n+1}(t) = \exp\left(\frac{1}{2}a_{n+1}\frac{\partial}{\partial n}\right)a(s_n,t) \tag{II.12a}$$

$$a_n(t) = \exp\left(-\frac{1}{2}a_n\frac{\partial}{\partial n}\right)a(s_n,t) \tag{II.12b}$$

and the following approximations are obtained:

$$a_{n+1} - a_n = a\frac{\partial a}{\partial n} + \frac{1}{6}a^3\frac{\partial^3 a}{\partial n^3} + \ldots \tag{II.13a}$$

$$a_{n+1} + a_n = 2a + \frac{1}{2}a^2\frac{\partial^2 a}{\partial n^2} + \ldots \tag{II.13b}$$

Now use (II.12a,b) and (II.13a,b) to find:

$$\frac{\partial a}{\partial t} + \frac{\partial a}{\partial n}\cdot v = \frac{da}{dt} \approx \frac{\dot{a}_{n+1} + \dot{a}_n}{2} = \frac{v(s_{n+1},t) - v(s_{n-1},t)}{2} \approx \frac{\partial v}{\partial n}\cdot a$$

So the continuity equation for a becomes:

$$\frac{\partial a}{\partial t} = a^2\frac{\partial(\frac{v}{a})}{\partial n} \tag{II.14}$$

Given the definition of the function a, a mass (watershed) distribution function ρ can be defined:

$$\rho(x,t) = \frac{1}{a(x,t)} \tag{II.15}$$

which reduces (II.14) to the standard mass continuity equation.

Take a_o such that $\phi'(a_o) > 0$ (unstable equidistant distribution) and expand ϕ as a MacLaurin series in $a = a_o$, to get:

$$v(s_n,t) = -\phi'(a_o)(a_{n+1}-a_n) - \tfrac{1}{2}\phi''(a_o)(a_{n+1}-a_n)(a_{n+1}+a_n-2a_o)+$$

$$- \tfrac{1}{6}\phi'''(a_o)(a_{n+1}-a_n)(a_{n+1}^2+a_{n+1}a_n+a_n^2-3a_o(a_{n+1}+a_n)+3a_o^2) - \ldots \qquad (II.16)$$

Use (II.13a,b) to find:

$$v(s_n,t) = -\phi'(a_o)\left[a\frac{\partial a}{\partial n} + \tfrac{1}{6}a^3\frac{\partial^3 a}{\partial n^3}\ldots\right] - \tfrac{1}{2}\phi''(a_o)\left[2a(a-a_o)\frac{\partial a}{\partial n} +\right.$$

$$\left. + \tfrac{1}{3}a^3(a-a_o)\frac{\partial^3 a}{\partial n^3}\ldots\right] - \tfrac{1}{6}\phi'''(a_o)\left[3a(a-a_o)^2\frac{\partial a}{\partial n} + \tfrac{1}{2}a^3(a-a_o)^2\frac{\partial^3 a}{\partial n^3}\ldots\right] \qquad (II.17)$$

Let

$$\rho_o = \frac{1}{a_o} \text{ and } u(x,t) = \rho(x,t) - \rho_o$$

then by (II.15)

$$a-a_o \sim -\frac{1}{\rho_o^2}u \text{ and } a^3 \sim a_o^3 - 3\frac{1^3 u}{\rho_o^4}.$$

Write $x = l\cdot s_n$ so that again $\frac{\partial}{\partial n} = l\frac{\partial}{\partial x}$. Using (II.14) with (II.17) and neglecting all terms of higher than seventh order in l, the final equation is of the form (after additional time scaling):

$$\frac{\partial u}{\partial t} = \frac{\partial^2}{\partial x^2}\left[-u + r_1u^2 + r_2u^3\right] - \gamma\frac{\partial^4 u}{\partial x^4} \qquad (II.18a)$$

where is made use of the fact that $\phi'(a_o) < 0$ and hence $\gamma > 0$.
The equation is supplemented by the zero mass flux boundary condition

$$-\frac{\partial}{\partial x}\left[-u + r_1u^2 + r_2u^3 - \gamma\frac{\partial^2 u}{\partial x^2}\right] = 0, \qquad (II.18b)$$

the natural boundary condition

$$\left.\frac{\partial u}{\partial x}\right|_{x=0,L} = 0 \qquad (II.18c)$$

and the initial condition

$$u(x,0) = u_o(x), \quad 0 < x < L \qquad (II.18d)$$

From (II.18c) it follows that (II.18b) can be replaced by

$$\left.\frac{\partial^3 u}{\partial x^3}\right|_{x=0,L} = 0 \qquad (II.18e)$$

By writing (II.18a) as $\frac{\partial u}{\partial t} = \frac{\partial^2}{\partial x^2}\left[-u + r_1 u^2 + r_2 u^3 - \gamma\frac{\partial^2 u}{\partial x^2}\right]$, the identification of $\gamma\frac{\partial^4 u}{\partial x^4}$ as a viscoelasticity term is obvious since (II.18a) is a reaction-diffusion equation with the local action distributed by diffusion.

II.3 Anti-diffusion

Neglecting non-linear terms in (II.18a), the equation is reduced to

$$\frac{\partial u}{\partial t} = -\frac{\partial^2 u}{\partial x^2} - \gamma\frac{\partial^4 u}{\partial x^4} \qquad \text{(II.19)}$$

Thus for γ small (or zero), the equation is the negative of a standard Fickian diffusion equation: the mass flow is along the gradient of u. In contradiction to Fickian diffusion, local maxima of u will therefore grow rather than flatten out. For this reason, the name of *anti-diffusion* was attached to this equation (Hazewinkel et al., 1986). The time evolution is a mass redistribution by mass transport only. With no-flux boundary conditions mass conservation is achieved.

The general structure of the system described by equations like the anti-diffusion equation, is a multi-particle system with a time scale where specific individual micro action can be averaged out. All particles are assumed to have the same properties and accordingly react identically to a given environment. The micro activities determine the macro structure and as far as observables are concerned the model can be formulated in macroscopic variables only. Note that working with a scaling limit contains the idea that the micro behavior is a scaled down version of the macro one.

In most cases the system behavior will depend on the environment, as expressed by exogenous environmental variables, such as temperature, pH, governmental action. Changes in the environment can cause loss of stability of the current distribution and evolution towards a new equilibrium will occur. Environmental dependence is formulated by a functional relationship between those environmental variables and the

coefficients of the non-diffusion term, especially the linear term (see chapter III).

The general framework of equation (II.18), the anti-diffusion system (AD), is the time evolution of a (probability) density function u defined on some event space E; then (II.18) will describe a system where the probability of an event E_o will increase in time if initially the probability of E_o was higher than that of neighboring events (neglecting competition). The evolution is directed to increase the occurrence of situations which are already more likely. The density u will become more and more concentrated around local maxima. The time evolution is self-fulfilling. Thresholds on growth are supplied by the non-linear terms. The fourth order viscosity term connects the evolution in neighboring points: events, phenomena which are closely related will have an almost similar probability to occur.

The name anti-diffusion is used as a description of the macroscopic mass redistribution process only: as in a standard Fickian diffusion process only nearest neighbor interactions are considered, see equation (II.4); the difference is that action leads to mass clustering.

In the context of chemical-physical clustering mechanism the evolution equation (II.18) is well known under the name Cahn-Hilliard equation (see also chapter IX). Secondly, animal grouping and migration is modeled with an anti-diffusion term. The inclusion is motivated by phenomenological similarity between clustering in biological and chemical systems (Cohen et al., 1981). In the same context Okubo (1980) distinguishes between neutral diffusion (Fickian) and density dependent diffusion; the last type is subdivided in attractive (anti-diffusion) and repulsive diffusion (where the coefficient of u is positive).

II.4 Other examples of anti-diffusion equations

The first example is derived from Langer (1982) where the growth of solidification patterns in an eutectic environment is studied. The eutectic growing is characterized by the coexistence of two solid

phases denoted by α and β. The solidification front advances in the liquid phase in the form of parallel plates of the two solid phases (see figure II.3).

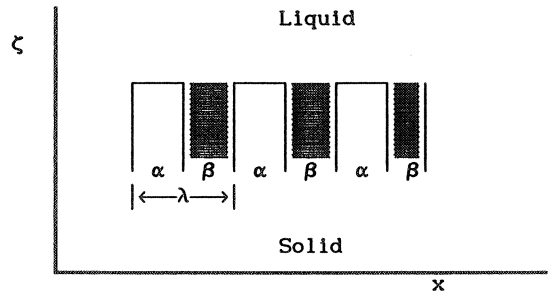


Figure II.3: Schematic illustration of eutectic growing with solid phases a and b.

The two solid phases compete for the space and the system's characteristic quantities are the widths λ_α of the α-phase and λ_β of the β-phase. Langer's model is formulated in the lamellar spacing λ defined as $\lambda = \lambda_\alpha + \lambda_\beta$ which should be compared with the basin width a of Thom's river basin model. Roughly the analogy is: λ = width of river, λ = width of stretch of dry land between rivers; so that $\lambda + \lambda$ width of drainage basin of a river.

The advancement velocity v of the solidification front depends on the temperature G, assumed to be constant, and the supercooling grade ΔT at the liquid-solid interface; ΔT depends on λ. The relation is formulated as follows:

$$G \cdot \zeta = -\Delta T(\lambda) \qquad \text{(II.20)}$$

where $\zeta(x,t)$ is the profile of an initially undeformed solidification front.

Let $y(x,t)$ be the sideways (horizontal) displacement of lamellae positioned at x, then:

$$\lambda(x,t) = \lambda_o\left(1 + \frac{\partial y}{\partial x}\right) \qquad \text{(II.21)}$$

where λ_o is the original uniform spacing.

Now the assumption is made that lamellae must grow in a direction locally perpendicular to the solidification front $\zeta(x,t)$ which gives:

$$\frac{\partial y}{\partial t} = -v \frac{\partial \zeta}{\partial x}, \quad v > 0. \tag{II.22}$$

Combining (II.20), (II.21) and (II.22) gives the equation for λ:

$$\frac{\partial \lambda}{\partial t} = \lambda_o \frac{v}{G} \frac{\partial^2}{\partial x^2} \Delta T(\lambda) \tag{II.23}$$

The functional form of $\Delta T(\lambda)$ is given as follows:

$$\Delta T(\lambda) = \alpha \left(\frac{\lambda}{\lambda_s} + \frac{\lambda_s}{\lambda} \right) \tag{II.24}$$

where λ_s is some stable spacing ($\alpha > 0$) (Langer, 1982). Since

$$\frac{\partial \Delta T(\lambda)}{\partial \lambda}\Big|_{\lambda=\lambda_o} = \frac{\alpha}{\lambda_s} \left(1 - \frac{\lambda_s^2}{\lambda_o^2} \right)$$

the equation (II.23) behaves like an anti-diffusion form if $\lambda_o < \lambda_s$.

The second example stems from Haken (1983). In Haken's approach, the cooperative aspects of pattern formation are translated in competition between the modes implemented by the *slaving principle:* linearly unstable modes (*order parameters)* slave the linearly stable modes by expressing those stable modes as functions of the unstable ones. Those relations are obtained by assuming that stable modes are in equilibrium and can be found as a solution of the non-linear evolution equations of those modes (*adiabatic approximation*) (Haken, 1978, 1983).
For Bénard instability the eigenvalues λ of the unstable modes k are given as:

$$\lambda = a - (k_o^2 + (ik_c + \nabla)^2)^2 \tag{II.25}$$

where variable a measures the distance from critical temperature and k_c is the critical mode ($k_o = |k_c|$). The inclusion of the gradient operator ∇ is motivated by taking into account finite band width excitations (Haken, 1983).
Given (II.25) the leading term in the evolution equation of an unstable mode u_{k_c} is given by

$$\dot{u}_{k_c} = \left[a - (k_o^2 + (ik_c + \nabla)^2)^2 \right] u_{k_c} + \ldots \tag{II.26}$$

The function Ψ is defined as follows

$$\Psi(x) = \sum_{k_c} e^{ik_c \cdot x} u_{k_c}(x) \qquad (II.27)$$

where the sum is taken over all critical k vectors which have the same absolute value k_o but point in different directions.
Using the transformation:

$$e^{ik_c \cdot x}\left[(k_o^2 + (ik_c + \nabla)^2)^2\right] = \left[k_o^2 + \nabla^2\right]^2 e^{ik_c \cdot x}$$

where $\nabla^2 = \Delta$ is the Laplace operator, the first order approximation of the time evolution of Ψ is

$$\frac{\partial}{\partial t}\Psi = \left[a - \left(k_o^2 + \nabla^2\right)^2\right]\Psi \qquad (II.28)$$

Since the coefficient of the diffusion term is $-2k_o^2$, the equation (II.27) is clearly an anti-diffusion form with a fourth order derivative term. The equation is supplemented with a quadratic and a cubic term in Ψ derived from the second and third order approximation term in the time evolution of u_{k_c} (II.26):

$$\frac{\partial}{\partial t}\Psi = \left[a - \left(k_o^2 + \nabla^2\right)^2\right]\Psi + A\Psi^2 - B\Psi^3 \qquad (II.29)$$

with A and B positive constants.

In the same context of Bénard instability, Swift and Hohenberg have derived an evolution equation similar to (II.29). They consider a fluid bounded by infinite horizontal plates separated by a distance l and at temperatures T_1 and $T_1 + \Delta T$, respectively (Swift and Hohenberg, 1977). Let $T(x,y,z;t)$ be the temperature; the deviation $\theta(x,y,z;t)$ of the temperature given for an uniform gradient $\Delta T/l$, is defined by

$$\theta(x,y,z;t) = T - T_1 - (\Delta T/l)z \qquad (II.30)$$

The important variables are: $\theta(x,y,z;t)$ and the z component of the fluid velocity, denoted by $u_z(x,y,z;t)$; the so called Swift-Hohenberg model is formulated in a variable w as a linear combination of the lowest vertical modes of the Fourier transforms of θ and u_z.

The final one-dimensional equation is written as

$$\frac{\partial w}{\partial t} = -2\frac{\partial^2 w}{\partial x^2} - \gamma_1 \frac{\partial^4 w}{\partial x^4} - (1 - \varepsilon)w - w^3, \quad 0 < \varepsilon < 1, \ \gamma_1 > 0 \qquad (II.31)$$

(See Swift and Hohenberg (1977) and Saarloos (1987).) We shall return to the Swift-Hohenberg equation (II.31) in chapter VII and compare it with the anti-diffusion system (II.18a).

CHAPTER III

GENERAL PROPERTIES OF THE ANTI-DIFFUSION EQUATION

III.1 Introduction

For the anti-diffusion system as defined in chapter II, equation (II.18a-b), some general properties can be derived by comparing the system with a standard reaction-diffusion system of the form:

$$\frac{\partial u}{\partial t} = -\left[-u + r_1 u^2 + r_2 u^3 - \gamma \frac{\partial^2 u}{\partial x^2}\right], \quad \gamma > 0 \qquad \text{(III.1)}$$

with no-flux boundary conditions.
The main difference is the mass-conserving property of the anti-diffusion system which restricts the solution space essentially.
Since the anti-diffusion equation is a one variable system, it can be formulated as a gradient system. In the second part, a Lyapunov functional is defined, which is similar to the Ginzburg-Landau free energy functional.

III.2 A priori bounds for stationary solutions for r_2 positive

Let the spatial domain be $I = [0,L] \subset \mathbb{R}$. The evolution equations which interest us together with the boundary conditions are

$$\frac{\partial u}{\partial t} = \frac{\partial^2}{\partial x^2}\left[\phi(u) - \gamma\frac{\partial^2 u}{\partial x^2}\right], \quad \gamma > 0 \tag{III.2a}$$

and

$$\frac{\partial u}{\partial x}\Big|_{x=0,L} = \frac{\partial^3 u}{\partial x^3}\Big|_{x=0,L} = 0 \tag{III.2b}$$

with

$$\phi(u) = -u + r_1 u^2 + r_2 u^3 \tag{III.2c}$$

Mass conservation is expressed by

$$\int_0^L \frac{\partial u}{\partial t}\, dx = 0 \text{ thus } \int_0^L u(x,t)dx = \int_0^L u(x,0)dx = M_o.$$

Regarding u as a deviation from some uniform density $\rho(x,0) = \rho_o$, M_o equals zero. Thus the initial condition $u(x,0) = u_o$ is such that

$$\int_0^L u_o(x)dx = 0 \tag{III.2d}$$

A stationary solution u(x) of (III.2) will satisfy

$$\phi(u) - \gamma\frac{\partial^2 u}{\partial x^2} = \alpha x + \beta \tag{III.3a}$$

But given the boundary conditions (III.2b), $\alpha = 0$ and β satisfies:

$$\frac{1}{L}\int \phi(u)\, dx = \beta \tag{III.3b}$$

Thus stationary solutions are similar to stationary solutions of a standard reaction diffusion equation:

$$\frac{\partial u}{\partial t} = -\left\{\phi(u) - \gamma\frac{\partial^2 u}{\partial x^2}\right\} \tag{III.4}$$

except that for (III.4) β is always equal to zero. The only constant solution of (III.2a-d) is the null solution $u = 0$, see (III.2d). Equation (III.4) is not mass-conserving, so non-zero constant solutions are possible. These differences play an essential role in the proof of stability of non-constant solutions, see chapter VII.

Similarity and difference between stationary solutions of (III.3) and (III.4) are elucidated by using the characterization exposed in Fife (1979). Writing

$$f(u) = \int_0^u \phi(s)ds \tag{III.5}$$

equation (III.3a) can be integrated once to obtain the equivalent equation

$$f(u) - \frac{1}{2}\gamma u_x^2 = \beta u + \alpha_1, \qquad \text{(III.6a)}$$

where β is defined in (III.3b) and

$$\alpha_1 = -\frac{1}{2}\gamma u_x^2\Big|_{x=x_o} \qquad \text{(III.6b)}$$

where the derivative of u is evaluated at x_o with $u(x_o) = 0$ $(u_x = \frac{\partial u}{\partial x})$.

Definition III.1:

The set S_h consists of nonzero length line segments in the (u,f)-plane which satisfy:

i) the line segment is horizontal,

ii) the line segment lies strictly under the graph of f, except at its endpoints;

iii) each finite endpoint must lie on the graph. (III.7a)

For a reaction-diffusion system (III.4), defined on $\mathbb{R}$, the following theorem gives a characterization of nonconstant stationary solutions:

Theorem III.2 (Fife, 1979):

There is a one-one correspondence between segments in S_h and the nonconstant solutions of (III.4) defined on $\mathbb{R}$, modulo shifts in x and reversals of sign. The correspondence is such that the segment in S_h overlays an interval on the u-axis which is the range of the corresponding solution. □

Definition III.3:

The set S_a consists of nonzero length line segments in the (u,f)-plane which satisfy:

i) the line segment lies strictly under the graph of f, except at its endpoints;

ii) each finite endpoint must lie on the graph. (III.7b)

The proof of theorem III.2 in Fife (1979), page 91-92, is directly applicable for solutions of (III.3) by writing $\psi(u) = \phi(u) - \beta$ and

applying the proof to the equation $\psi(u) - \gamma\frac{\partial^2 u}{\partial x^2} = 0$ with the set S_a of line segments lying under the graph of f. Note that the set S_a is containing all (not only horizontal) line segments.

In figure III.1 we have depicted the graph of $f(u) = \int_0^u \phi(s)ds$ with $\phi(u) = -u + 3u^2 + u^3$; S_a contains the line segments in the area OAB.

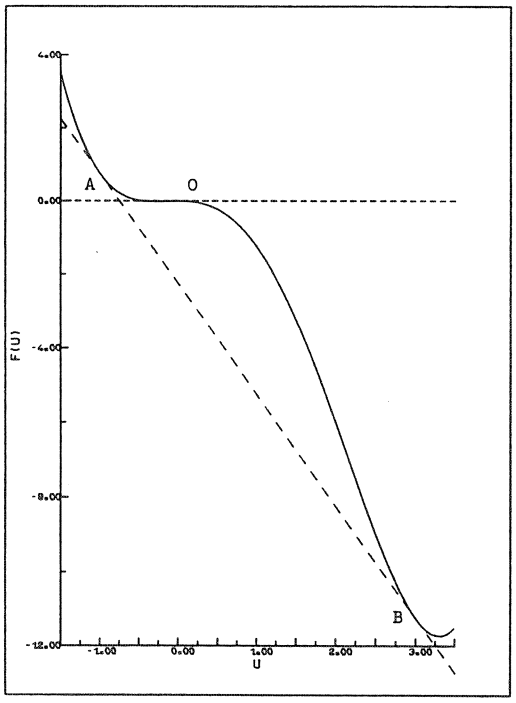


Figure III.1
Graph of f(u).
Bounded stationary solutions are represented by line segments lying in the area OAB.

By property i) of (III.7b) no internal point of the range of a solution can be a maximum or a minimum.

The one-one correspondence between line segments and nonconstant stationary solutions is lost if the systems are defined only for $x \in [0,L] \subset \mathbb{R}$. However, stationary solutions of a system with no-flux boundary conditions can be extended beyond x = 0 and x = L as an even function in x = 0 respectively x = L. Continued extensions this way will yield a periodic function which is a solution of the system

defined on $\mathbb{R}$. The line segment corresponding uniquely with this function is already determined by the original no-flux solution: the line segment is given by the right hand side of (III.6a) with α_1 and β given by (III.6b) and (III.3b) respectively. If the original function is bounded then the maximum value and minimum value satisfy $f(u) = \beta u + \alpha_1$ and hence define the endpoints of the line segment. If the original function is unbounded then the extended one is unbounded also.

Consider figure III.1: all bounded stationary solutions of (III.2) defined on [0,L] with no-flux boundary conditions, are represented uniquely by line segments S_a, lying in the area AOB where AB is the common tangent to the graph of f. In this way a priori bounds u_o and u_1 can be calculated; they may only be attained by solutions of systems defined on $\mathbb{R}$ (Fife, 1979). Since $f(u_1) - f(u_o) = \phi(u_o)(u_1 - u_o)$, the bounds u_o and u_1 are determined by the so called Maxwell equal area condition: if $u_o < u_2 < u_1$ with $\phi(u_2) = \phi(u_o) = \phi(u_1)$ then

$$\int_{u_o}^{u_2} \phi(u) - \phi(u_o)\, du = -\int_{u_2}^{u_1} \phi(u) - \phi(u_o)\, du$$

(In first-order phase transitions, the Maxwell equal area condition is the condition for the spatial coexistence of two phase; the two phases are equally attractive (Widom, 1972).)

For $\phi(u)$ as defined in (III.5) u_o and u_1 are given as the solution of the equations:

$$\phi(u_o) = \phi(u_1) \;\&\; \phi'(u_o) = \phi'(u_1) \;\&\; \phi(u) = -u + r_1u^2 + r_2u^3$$
with $u_o \neq u_1$. (III.8)

As a summary, the following corollary is formulated:

Corollary III.4

If the evolution equation $\frac{\partial u}{\partial t} = \frac{\partial^2}{\partial x^2}\left[-u + r_1u^2 + r_2u^3\right] - \gamma\frac{\partial^4 u}{\partial x^4}$ with $r_2 > 0$, $\gamma > 0$, defined on $I = [0,L] \subset \mathbb{R}$ with no-flux boundary conditions and initial condition $\int_0^L u(x,0)dx = 0$, has a stationary solution u, then this solution u is characterized by a line segment in the set S_a (III.7b); a priori bounds on bounded stationary solutions are given by u_o and u_1 defined in (III.8).□

III.3 A Lyapunov functional for the anti-diffusion equation

Consider the functional V defined on the space of functions u:

$$V(u) = \int_0^L f(u) + \tfrac{1}{2}\gamma u_x^2 \, dx \qquad \text{(III.9)}$$

where f(u) is defined in (III.5). The time evolution of V is

$$\frac{dV}{dt} = \int_0^L \phi(u)u_t + \gamma u_x u_{xt} \, dx \qquad \text{(III.10)}$$

where $u_t = \frac{\partial u}{\partial t}$, $u_{xt} = \frac{\partial^2 u}{\partial x \partial t}$.

By partial integration and using the boundary conditions (III.2b) one obtains:

$$\frac{dV}{dt} = \int_0^L \left\{ \phi(u) - \gamma \frac{\partial^2 u}{\partial x^2} \right\} u_t \, dx$$

And, again by partial integration:

$$\frac{dV}{dt} = -\int_0^L \left[\frac{\partial}{\partial x} \left\{ \phi(u) - \gamma \frac{\partial^2 u}{\partial x^2} \right\} \right]^2 dx \qquad \text{(III.11)}$$

Thus, given the evolution equation (III.2),

$$\frac{dV}{dt} \leq 0 \qquad \text{(III.12a)}$$

and

$$\frac{dV}{dt} = 0 \iff \frac{\partial}{\partial x} \left\{ \phi(u) - \gamma \frac{\partial^2 u}{\partial x^2} \right\} = 0 \text{ almost everywhere} \qquad \text{(III.12b)}$$

The right hand side of (III.12b) defines precisely the stationary solutions of (III.2a-b) (see (III.3)). Thus the time evolution is characterized by minimization of V; i.e. V is a Lyapunov functional for the anti-diffusion system (III.2) (just as it is a Lyapunov functional for the reaction diffusion system (III.4)). Now the idea is that

i) if V attains its minimum for some feasible u, this u will be a stable stationary solution of (III.2) since, by (III.12a), for small deviations the system will be driven back to this minimum;

ii) the stationary solutions are ordered in time in the following sense: a stationary solution u_2 is reachable (in forward time) from the stationary solution u_1 only if $V(u_2) < V(u_1)$.

If the system is (re)written such that $u(x) = 0$ for all x is a solution, then instability of this null solution implies that V does not attain a minimum at $u \equiv 0$. So, if it is possible to prove that V attains a minimum, the existence of a stable nonconstant stationary solution is proven; non constancy follows from the fact that the solution space is restricted to functions with $\int_0^L u(x)dx = 0$.
In chapter V an exact formulation will be given, here the result is stated somewhat loosely:

for $\phi(u) = -u + r_1u^2 + r_2u^3$, with $r_2 > 0$, V attains its minimum for square integrable functions with (generalized) partial derivatives of first order $\frac{\partial u}{\partial x}$ which are also square integrable.

If $\gamma = 0$, the graph of a solution u consists of line segments with

$$u(\cdot) = u_1 \text{ or } u(\cdot) = u_2 \text{ or } u(\cdot) = u_3$$
$$\phi(u_1) = \phi(u_2) = \phi(u_3) = \beta$$

with the condition $\int_0^L u(x,\cdot)dx = 0$ (III.13)

Consider such a solution u with "spatial distribution" λ_1, λ_2 and λ_3 ($\lambda_i \geq 0$, $i = 1,2,3$); the value λ_n denotes the total length of the domain where $u = u_n$. This domain may well consist of several disjoint intervals so that $\lambda_n = \int \chi_A(x)dx$, where $A = \{x \mid u(x) = u_n\}$ and χ is the indicator function.
Hence the stationary solutions given in (III.13) can be written as:

$$\phi(u_i) = \phi(u_j) \text{ for all } i,j = 1,..,3 \quad \text{(III.14a)}$$

$$\lambda_1u_1 + \lambda_2u_2 + \lambda_3u_3 = 0 \quad \text{(III.14b)}$$

$$\lambda_1 + \lambda_2 + \lambda_3 = L \quad \text{(III.14c)}$$

For this configuration, the value of V is

$$V(u) = \sum_{n=1}^{3} \lambda_n f(u_n) \quad \text{(III.15)}$$

Hence V(u) is given by the ordinate of a point lying in the convex polytope with vertices $(u_n, f(u_n))$, $n = 1,2,3$. (points P, Q and R in figure III.2) and by (III.14b) that point must be on the line $u = 0$.

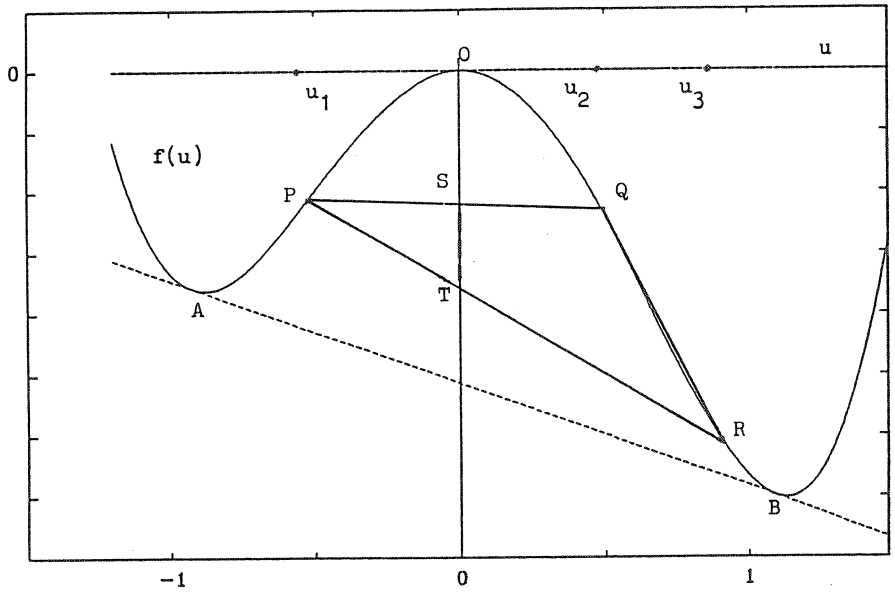


Figure III.2: Graph of f(u). The functional value V of a solution (u_1,u_2,u_3) is given by the ordinate of a point on ST (γ = 0).

From the condition $\sum \lambda_n u_n = 0$ it follows directly that for any 'non-binary' solution there exists a binary solution with endpoints on the branches OA, OB respectively, which has a V value less or equal to the V value of the non-binary solution. A 'binary' solution is of course one with just two values.

For any binary solution with $u = u_1$ or $u = u_2$, the V value is given by the intersection of the line u = 0 and the line segment connecting $(u_1,f(u_1))$ and $(u_2,f(u_2))$. Hence the lowest value of V is attained by the intersection of the line u = 0 and the common tangent AB at the graph of f, see figure III.2. This lowest value is the minimum of V (and thus stable).

For those piece wise constant solutions at $\gamma = 0$ the volume fractions are well described by the condition $\int_0^L u(x,\cdot)dx = 0$. However the spatial configuration is arbitrary. The discontinuities do not necessary disqualify such solutions but they are irrelevant for the description of pattern formation as self-organisation with an internally dictated non-random frequency; in particular all frequencies occur and higher

frequencies are favored. This does not fit in well with the physico-chemical idea that neighboring particles show some cohesion in behavior with respect to one another. Viscosity! Hence we are mainly interested in the case $\gamma > 0$.

For $\gamma \neq 0$ we can write the functional value V of a stationary solution u, by using (III.6a-b) as

$$V(u) = \int \gamma u_x^2 + \alpha_1 \, dx \qquad \text{(III.16)}$$

Note that α_1 is given by the intersection in the u-f plane of the line segment corresponding with the stationary solution and the line u = 0; e.g.: suppose the line segment PQ in figure III.2 represents a stationary solution then α_1 is the ordinate of point S. For γ fixed, and fixed α_1, the lowest V value is attained by functions with the smallest variation. This seems to suggest that minimal solutions are monotone. Since $\frac{d}{dt}V(u) < 0$ if u is not a stationary solution, this would result in u eventually going to a monotone solution. We will return to this question in chapter V and in chapter VII.

III.4 The Ginzburg-Landau free energy functional

In the previous chapter two examples of anti-diffusion equations were mentioned. This was rather meagre since there exists a wide range of physico-chemical applications which are based on an evolution minimizing the same functional V as defined in (III.10), whether for conserving systems or not. In that case V is called the Ginzburg-Landau functional which describes the free energy of the systems as function of the concentration u. In this context, f(u) in equation (III.10) is called the free energy density function; it defines the free energy of a homogeneous system with density u. The gradient term in (III.10) is called the gradient energy and it takes account of spatial inhomogeneities.

Based on this free energy functional, phase transitions are modeled. With no mass conservation, the evolution equation is a

reaction-diffusion equation as (III.1), see chapter IV. But especially phase decomposition in binary mixtures where $u(x,t)$ is a perturbation of the concentration of one of the phases, is modeled by the anti-diffusion equation, in this context better known as the Cahn-Hilliard equation (Cahn, 1958, 1966, 1968; Novick-Cohen et al., 1984; Coutsias et al., 1984). See Widom (1972) for an extensive review and discussion of the validity of the functional relationship between free energy and mass density.

As mentioned in chapter I, paragraph 3, thermal equilibrium structures are defined by the minima of the free energy. The dependence of the equilibrium state (e.g. vapor, liquid or crystal phase) on environmental parameters (e.g. temperature) is obtained by making the coefficient of the quadratic term of $f(u)$ (linear term of $\phi(u)$) a function of those parameters. For example, temperature dependence is incorporated in the anti-diffusion equation by setting:

$$\phi(u) = -r_o(T)u + r_1u^2 + r_2u^3, \qquad \text{(III.17)}$$

where $r_o(T) = (T_c - T)/T_c$ with T_c the critical temperature. For high temperature the coefficient of u is positive and the diffusion term is as a standard Fickian diffusion term. At the critical temperature T_c, the (linear) diffusion becomes negative. If the viscosity coefficient γ is small, the system will be unstable with respect to any perturbation and decomposition in high and low density areas will set in (see spinodal decomposition, chapter IX).

CHAPTER IV

A STOCHASTIC MODEL

IV.1 Introduction

For a one variable (one order parameter) system defined on a spatial domain, the state of the system is given by the density function of the order parameter; this parameter shall be denoted as mass. Elements of the system are named particles. Observable structures are equivalent with a profiled density function.
Assuming a multi-particle, open system, structures are the result of particle-particle and particle-environment interactions which take place on the microscopic level. The environment is mostly given in the form of macroscopic variables such as temperature, pH etc.. The stability of a structure will depend on these macroscopic quantities. At the loss of stability, transitions of one structure to another are initiated by fluctuations. Most complex systems have an intrinsic mechanism allowing to test for stability continuously: thermodynamic fluctuations, Brownian motion.
If fluctuations are incorporated in the system description, the state is no longer given by the density function but by the probability distribution of the densities. Denoting the density by ρ, the probability function is given as $P(\rho,t)$ and $P(\rho,t)d\rho$ defines the probability that at time t the density ρ lies between ρ and $\rho + d\rho$.
In this chapter it is assumed that the variation in time of P is governed by a Markovian master equation. The connection between the

microscopic and the macroscopic level is achieved by assuming that the (transition) probability of a particle to move from one spot to another depends on a similar functional $V(\rho)$ as defined in chapter III, equation (III.9). It will be shown that, assuming the existence of such a V, the functional form itself is hardly restrictive with respect to the system specification.
Under some restrictions on the probability function P, the mean value and the most probable path equation are derived. Both resulting equations are similar and define a class of evolution equations which contain as a special case the anti-diffusion equation derived in chapter II.

IV.2 Stochastic formulation

A multi-particle system is considered with mass distributed over a one dimensional spatial domain. Let $\rho(x,t)$ be the mass density at any time t and any position x. The evolution of ρ is seen as a stochastic process based on individual stochastic behavior and described by a markovian master equation. The system is divided into N mezoscopic equidistant cells which are much larger than the microscopic length scale (size of a particle) and much smaller than any macroscopic length scale (size of the total system). A similar discretization is performed on the time scale such that individual particle kinetics can be neglected: the population of a cell may be seen as a sum of identically distributed independent random variables .
Let ρ_n be the mass density in cell n. Then $P(\rho_1,\ldots,\rho_N,t)$ is the probability density function of $(\rho_1,\ldots,\rho_N)$. On a macroscopic scale the centres of the cells form a continuum and if in the following continuous functional notations are used (e.g. $P(\rho(x),t)$, they must be understood as the large N limit of a function of N variables.
The master equation for P is:

$$\tau\frac{\partial P(\rho,t)}{\partial t} = -\sum_{\delta(x)} W\{\rho(x) \to \rho(x) + \delta(x)\}P(\rho(x),t) + \\ + \sum_{\delta(x)} W\{\rho(x) - \delta(x) \to \rho(x)\}P(\rho(x)-\delta(x),t) + \qquad \text{(IV.1a)}$$

where $W\{\rho(x) \to \rho(x) + \delta(x)\}d\delta \equiv W\{\rho_1,..,\rho_N \to \rho_1+\delta_1,..,\rho_N+\delta_N\}d\delta_1..d\delta_N$ is the probability that in unit time the density change in cell n lies between δ_n and $\delta_n + d\delta_n$, n = 1,...N. If $P(\rho + \delta, t + \Delta t|\rho, t)$ is the probability that the system be in state $\rho + \delta$ at time $t + \Delta t$ if the system was in state ρ at time t then

$$W\{\rho \to \rho + \delta\} = \frac{\partial}{\partial \Delta t} P(\rho + \delta, t + \Delta t|\rho, t)_{|\Delta t=0} \qquad \text{(IV.1b)}$$

To make W explicit the following assumptions are used:

a). There exists a quantity $V(\rho)$ which characterizes the macroscopic structure ρ of the system at any time t.

b). Changes in ρ which increase V are less likely than those which decrease it.

c). Small changes are more likely than larger ones.

d). All changes can be superimposed. (IV.2)

Then a possible form for W is :

$$W\{\rho(x) \to \rho(x) + \delta(x)\} = \alpha \exp\left[-\int \frac{\delta^2(x)dx}{\Delta}\right] \times$$
$$\exp\left[-\frac{\beta}{2}\left\{V(\rho(x)+\delta(x)) - V(\rho(x))\right\}\right] \qquad \text{(IV.3)}$$

(α, β, Δ are positive constants) (Metiu et al., 1979).

The formulation (IV.3) is not a necessary consequence of the assumptions but it makes the equations tractable. A drawback is that the range of δ is not restricted; the possibility that ρ becomes negative is not excluded. For large particle systems formulation (IV.3) is an adequate approximation with Δ small. (See chapter VIII, section 5 where a simulated annealing procedure is applied with truncated normal error terms.)

Note that by assumption b), the time evolution is characterized by minimizing V. First we describe V.

Let $\hat{f}$ be the contribution to V per unit volume, thus

$$V(\rho) = \int \hat{f}(\rho)dx \qquad \text{(IV.4)}$$

($\hat{f}$ is called a generalized potential (Novick-Cohen et al., 1984).) To include spatial inhomogeneities, $\hat{f}$ will be assumed to depend not only

on the density ρ but also on its higher derivatives; expanding $\hat{f}$ in Taylor series in these higher derivatives around the uniform (average) density, gives

$$\hat{f} = \hat{f}(\rho,0,\ldots,0) + \sum_i L_i\left(\frac{\partial\rho}{\partial x_i}\right) + \sum_{i,j} K^1_{i,j}\left(\frac{\partial^2\rho}{\partial x_i \partial x_j}\right) + \frac{1}{2}\sum_{i,j} K^2_{i,j}\left(\frac{\partial\rho}{\partial x_i}\frac{\partial\rho}{\partial x_j}\right) + \ldots \qquad \text{(IV.5a)}$$

where

$$L_i = \partial\hat{f}(\rho,0,\ldots,0)/\partial(\partial\rho/\partial x_i),$$
$$K^1_{i,j} = \partial\hat{f}(\rho,0,\ldots,0)/\partial(\partial^2\rho/\partial x_i\partial x_j),$$
$$K^2_{i,j} = \partial\hat{f}(\rho,0,\ldots,0)/\partial(\partial\rho/\partial x_i)\partial(\partial\rho/\partial x_j). \qquad \text{(IV.5b)}$$

($\hat{f}(\rho,0,\ldots,0)$ is the contribution of uniform density per unit volume to the potential V).

Assume the media are isotropic, i.e. there is no preferred direction, then $L_i = 0$ and the $K_{i,j}$'s are multiples of the Kronecker delta $\delta_{i,j}$ (Novick-Cohen et al., 1984). Thus $\hat{f}$ can be written as

$$\hat{f}(\rho,\nabla\rho,\Delta\rho,\ldots) = f(\rho) + K_1\Delta\rho + \tfrac{1}{2}K_2(\nabla\rho)^2 + \ldots \qquad \text{(IV.6)}$$

Neglecting higher order terms in (IV.6), V is found as

$$V(\rho) = \int_\Omega f(\rho) + K_1\Delta\rho + \tfrac{1}{2}K_2(\nabla\rho)^2\,dx \qquad \text{(IV.7a)}$$

where Ω is the spatial domain. The natural boundary condition is

$$\frac{\partial\rho}{\partial\nu} = 0 \text{ on the boundary of } \Omega \qquad \text{(IV.7b)}$$

where ν is the unit normal to the boundary.

By Green's identity, the boundary condition (IV.7b) implies that the contribution of the Laplacian term Δ vanishes in (IV.7a) (John, 1982). Hence (IV.7a) is reduced to

$$V(\rho) = \int_\Omega f(\rho) + \tfrac{1}{2}\gamma(\nabla\rho)^2\,dx \qquad \text{(IV.8)}$$

where $\gamma = K_2$. If $\gamma > 0$ then the formation of spatial inhomogeneities has its costs. In physico-chemical literature equation (IV.8) is called the Ginzburg-Landau free energy functional (see chapter III and IX).

Apart from isotropy the definition of V does not involve any constraints on the system. Of course assumption a) that V as a global

quantity, expressed in ρ only, characterizes the phases of the system, is more restrictive; at the least this assumes that the system is 'homogeneous' with respect to all parameters of the system since f depends only on ρ and does not vary with the local cells.
Inclusion of specific cell qualities can be accommodated by letting f also depend on $x \in \Omega$. In the following Ω is supposed to be decomposed into a disjoint union such that $f(\rho,x)$ can be assumed to depend only on ρ for $x \in \Omega_i$ all i. Let $f_i(\rho) = f(\rho,x)$ for $x \in \Omega_i$. Let $\chi_i(x)$ be the indicator function of Ω_i, then V can be written as:

$$V(\rho) = \int_\Omega \sum_i \left[\chi_i(x) f_i(\rho)\right] + \tfrac{1}{2}\gamma(\nabla\rho)^2 \, dx \qquad \text{(IV.9)}$$

(In order to avoid burdening the notation too much, in the following V is used as defined in (IV.8).)

IV.3 Mass kinetics

The next set of assumptions involve restrictions on the mass kinetics. The changes in $\rho^T = (\rho_1,\ldots,\rho_N)$ are given by the array $\delta^T = (\delta_1,\ldots,\delta_N) \in \mathbb{R}^N$.
There are essential two ways to introduce specific mass kinetics. Explicit formulation of the mass flows between cells, see section IV.5, or implicit formulation by a global restriction on δ. In this paragraph the second approach is followed by comparing a model with unrestricted changes to one with restrictions.

Let the unconstrained model be formulated by a mass distribution array $\sigma^T = (\sigma_1,\ldots,\sigma_N) \in \mathbb{R}^N$ with mass changes $\varepsilon^T = (\varepsilon_1,\ldots,\varepsilon_N) \in \mathbb{R}^N$.
Consider also two types of symmetric positive NxN matrices K:

A) $K = \left(K(n,m)\right)$ is strictly positive; especially $K(n,m) = \delta(n-m)$ with δ the Dirac delta function (K is identity matrix).

B) $K = \left(K(n,m)\right)$ with $\sum_{n=1}^{N} K(n,m) = 0$.

Now we relate the two models as follows:

$$\delta = K\varepsilon \tag{IV.10a}$$

$$\rho = \mathcal{K}\sigma = K\sigma + M_{\rho} \tag{IV.10b}$$

where M_{ρ} is zero if K is of type A and $M_{\rho} = \sum_{n=1}^{N} \rho_n$ if K is of type B. Note that the positivity condition of K ensures that δ changes which increase V are less likely than changes which decrease V if the same holds for changes ε. By (IV.10a) it follows that $\sum_{n=1}^{N} \delta_n = 0$ if K is of type B. Hence we refer to the constrained model as case B and consequently to the unconstrained model as case A.

For a continuous formulation, the operator K will be defined as:

$$K\varepsilon = \int K(x,y)\varepsilon(y)dy \tag{IV.11}$$

where K(x,y) is symmetric and positive; type A: $K(x,y) = \delta(x-y)$, the Dirac delta function, and for type B $\int K(x,y)dx = 0$; The formulation above is different from Metiu et al., (1979) where the inverse of K is involved which need not to exist in all cases.

The properties of the unconstrained and constrained model (case B) are related as follows. Denote the probability density function P in case B by P_{ρ} and for case A by P_{σ}; similar the transition probability density function $W(\rho \to \rho + \delta)$ with $W_{\delta}(\delta,\rho)$ for case B and $W_{\varepsilon}(\varepsilon,\sigma) = W(\sigma \to \sigma + \varepsilon)$ for unconstrained changes ε.

The complete original of $A \subseteq \mathbb{R}^N$ under a transformation $\mathcal{F}$ is denoted as $\mathcal{F}^{-1}(A)$. Using theorem 6.8 in Kingman and Taylor (1983) one finds:

$$\int_R f(\rho)P_{\rho}(\rho)d\rho = \int_S f(\mathcal{K}\sigma)P_{\sigma}(\sigma)d\sigma \tag{IV.12a}$$

where $S = \mathcal{K}^{-1}(R)$, and with $E = K^{-1}(D)$,

$$\int_D g(\delta)W_{\delta}(\delta,\rho)d\delta = \int_E g(K\varepsilon)W_{\varepsilon}(\varepsilon,\rho)d\varepsilon \tag{IV.12b}$$

IV.4 Mean value equations

Given the probability density function $P(\rho_1,\ldots,\rho_N)$ the mean-value of ρ^T, is defined as

$$\bar{\rho}^T = (\bar{\rho}_1,\ldots,\bar{\rho}_N) = \int \rho P(\rho,t)d\rho \qquad \text{(IV.13a)}$$

Consequently the time evolution of $\bar{\rho}^T$, which is called the mean value equation, is

$$\frac{\partial}{\partial t}\bar{\rho} = \int \rho\frac{\partial P}{\partial t}\, d\rho \qquad \text{(IV.13b)}$$

Let $P = P_\rho = P(\rho)$ with ρ defined in (IV.10b). Then using (IV.1) one finds:

$$\tau\frac{\partial}{\partial t}\bar{\rho} = \int_R \left[-\int_D \rho W\{\rho \to \rho+\delta\}P_\rho(\rho,t)d\delta + \int_D \rho W\{\rho-\delta \to \rho\}P_\rho(\rho-\delta,t)d\delta\right]d\rho \qquad \text{(IV.14a)}$$

where $R = \left\{\rho \in \mathbb{R}^N \middle| \sum_{n=1}^{N} \rho_n = M_\rho\right\}$ and $D = \left\{\delta \in \mathbb{R}^N \middle| \sum_{n=1}^{N} \delta_n = 0\right\}$.

Since

$$\int\left[\sum_\delta \rho W\{\rho - \delta \to \rho\}P(\rho-\delta)\right]d\rho = \int\left[\sum_\delta \{\rho + \delta\}W\{\rho \to \rho + \delta\}P(\rho)\right]d\rho$$

the righthand side of (IV.14a) can be written as:

$$\int_R\int_D \left(\delta\, W\{\rho \to \rho + \delta\}P_\rho(\rho,t)\right)d\delta d\rho \qquad \text{(IV.14b)}$$

Using (IV.12a) one finds for (IV.14b):

$$\tau\frac{\partial}{\partial t}\bar{\rho} = \int_S\int_D\left(\delta W\{\mathcal{K}\sigma \to \mathcal{K}\sigma + \delta\}P_\sigma(\sigma,t)\right)d\delta d\sigma =$$

$$= \int_S\int_D\left(\delta W_\delta(\delta,\mathcal{K}\sigma)P_\sigma(\sigma,t)\right)d\delta d\sigma \qquad \text{(IV.15a)}$$

where $S = \mathcal{K}^{-1}(R)$ and thus $S = \mathbb{R}^N$. Apply (IV.12b) to (IV.15a) to get:

$$\tau\frac{\partial}{\partial t}\bar{\rho} = \int_S\int_E\left(K\varepsilon W_\varepsilon(\varepsilon,\mathcal{K}\sigma)P_\sigma(\sigma,t)\right)d\varepsilon d\sigma \qquad \text{(IV.15b)}$$

where $E = K^{-1}(D)$ and so $E = \mathbb{R}^N$.

Commonly used in the derivation of a closed form of the mean value

equations (IV.14a) is the approximation of $\int_\rho W\{\rho \to \rho + \delta\}P(\rho,t)d\rho$ by $W\{\bar{\rho} \to \bar{\rho} + \delta\}$ where $\bar{\rho}$ is the mean value of ρ (Weidlich and Haag, 1983; Kanaroglou et al., 1986a, 1986b). The approximation is only valid if P is unimodal and symmetric which rather contradicts the long run behavior of P in bifurcating systems with multiple solutions. But the use of this approximation is motivated by the argument that in most cases, especially in the field of socio-economic systems, the environmental parameters which define the qualitative and quantitative properties of the system, are changing long before the system can reach its final state (Weidlich and Haag, 1983). Using this approximation gives:

$$\int_S \int_E \left(K\varepsilon W_\varepsilon(\varepsilon, \mathcal{K}\sigma)P_\sigma(\sigma,t)\right)d\varepsilon d\sigma = \int_E K\varepsilon W_\varepsilon(\varepsilon, \mathcal{K}\bar{\sigma})d\varepsilon \qquad (IV.16)$$

where $\bar{\sigma}$ is the mean of σ.

From (IV.12a) it is obvious by taking $f(\rho) = \rho$ that $\bar{\rho} = \mathcal{K}\bar{\sigma}$; thus $W_\varepsilon(\varepsilon, \mathcal{K}\bar{\sigma}) = W_\varepsilon(\varepsilon, \bar{\rho})$ where W_ε is evaluated at $\bar{\rho}$ and use equation (IV.2a) to find:

$$W_\varepsilon(\varepsilon, \mathcal{K}\bar{\sigma}) = \alpha \exp\left[-\int \frac{\varepsilon^2(x)dx}{\Delta}\right] \cdot \exp\left[-\frac{\beta}{2}\left\{V(\bar{\rho}(x)+\varepsilon(x)) - V(\bar{\rho}(x))\right\}\right] \qquad (IV.17)$$

Since Δ is taken small only small values of ε are allowed to contribute to the sum (integral) over ε; therefore it is reasonable to expand V in a power series of ε and to retain only the first order approximation:

$$V(\bar{\rho} + \varepsilon) - V(\bar{\rho}) = \langle \frac{\delta V}{\delta \bar{\rho}}, \varepsilon \rangle$$

where $\frac{\delta V}{\delta \rho} = (\frac{\delta V}{\delta \rho_1}, \ldots, \frac{\delta V}{\delta \rho_N})^T$, the derivative of V and $\langle \cdot, \cdot \rangle$ is the standard Euclidean inner product. Then the integration over ε in (IV.16) can be performed to find the 'expected' value of $K\varepsilon$. This results in the following evolution equations (see appendix C):

$$\tau \frac{\partial}{\partial t}\rho = -M\left(K\frac{\delta V}{\delta \rho}\right) \qquad (IV.18a)$$

where M, the mobility constant, is positive ($M = \frac{1}{2}\beta(2\pi\Delta)^{N/2}\Delta$). In (IV.18a) the upper bar denoting mean values is omitted.

Using the continuous form of K, equation (IV.18a) is written as:

$$\tau\frac{\partial\rho}{\partial t} = -M\int K(x,y)\frac{\delta V}{\delta\rho}\,dy \qquad \text{(IV.18b)}$$

supplemented with no-flux boundary conditions.
For a one dimensional spatial domain, the variation term

$$<\frac{\delta V}{\delta\rho},\varepsilon>_0 = \int \frac{\delta V}{\delta\rho}(x)\varepsilon(x)dx$$

is given by:

$$<\frac{\delta V}{\delta\rho},\varepsilon>_0 = \int\phi(\rho)\varepsilon(x) + \gamma\rho_x\varepsilon_x dx \qquad \text{(IV.19a)}$$

where $\phi(\rho) = df(\rho)/d\rho$ (see appendix E) ($\rho_x = \frac{\partial\rho}{\partial x}$, $\varepsilon_x = \frac{\partial\varepsilon}{\partial x}$); with no-flux boundary conditions we can write (IV.19a) as

$$<\frac{\delta V}{\delta\rho},\varepsilon>_0 = \int\left\{\phi(\rho) - \gamma\frac{\partial^2\rho}{\partial x^2}\right\}\varepsilon(x)dx \qquad \text{(IV.19b)}$$

and hence

$$\frac{\delta V}{\delta\rho} = \phi(\rho) - \gamma\frac{\partial^2\rho}{\partial x^2} \qquad \text{(IV.19c)}$$

IV.5 Most probable path equations

The most probable path equations are defined as follows (Metiu et al., 1979; Haken, 1978):
The conditional probability $G(\rho,t|\rho^0,t^0)$ that the density profile ρ changes from $\rho^0(x)$ to $\rho(x)$ in the time interval $t - t^0$, is defined as:

$$P(\rho,t) = \int G(\rho,t|\rho^0,t^0)P(\rho^0,t)d\rho^0 \qquad \text{(IV.20)}$$

The most probable path is defined as the path leading from ρ^0 to ρ such that G is maximal. In appendix C it is shown that $G(\rho,t|\rho^0,t^0)$ can be written as a path integral. The final result for a path from ρ^0 to ρ via changes of the form $\delta = K\varepsilon$, the restricted case with $\rho = K\sigma$ at any time, is

$$G(\rho,t|\rho^0,t^0) = \int_{\rho} \exp\left[-\int_0^t\left\{<\tau\dot{\rho}(t') - E(\delta),Q_\delta^{-1}(\tau\dot{\rho}(t') - E(\delta))>\right\}\right]\mathcal{D}'(\rho) \qquad \text{(IV.21)}$$

where $E(\delta) = \int \delta W\{\rho \to \rho + \delta\}d\delta$ and $Q_\delta = \int (\delta\delta^T)W\{\rho \to \rho + \delta\}d\delta$.

The time integral is essentially a summation over time interval Δt's generating a time sequence $t^0, t^1, t^2, \ldots, t^L$ with $L.\Delta t = t - t^0$; consequently $\dot{\rho}_n$ means $(\rho_n^{j+1} - \rho_n^j)/\Delta t$ where the upper index j gives the time indication. The symbol $\int \mathcal{D}'(\rho)$ denotes the path integral defined as the limit of the multiple integral $\int d\rho^{L-1} \ldots d\rho^0$. The consequence of this result (IV.21) is that G consists of the weighted sum of all successive path sections leading from ρ^0 to ρ. The weights are maximal if $\tau\dot{\rho}(t') - E(\delta)$ is zero (Q_δ is strictly positive).

Calculating the mean-value $E(\delta)$ as $KE(\varepsilon)$ where $E(\varepsilon)$ is the mean value of the unrestricted changes ε, the evolution equations are given by:

$$\tau\dot{\rho}_n = -M\left(K\frac{\delta V}{\delta \rho}\right)_n \quad , \; n = 1,..N \tag{IV.22}$$

where K is symmetric and positive. (See appendix C.)

This result is equivalent to the mean value equation (IV.18a). Since the mean value equation was derived under the condition that P is unimodal and symmetric in the maximum of P, the mean value time path coincides with the most probable time path if this condition holds.

IV.6 Migration dynamics

In the foregoing sections equal grid spacing was assumed. In the case of population migration, the spatial domain will be subdivided in areas with no equal spacing. Suppose the spatial domain is divided in L subspaces with area A_l, $l = 1,..,L$. As a consequence not only the density array $(\rho_1,..,\rho_L)$ must be considered but also the array of population numbers $(n_1,..,n_L)$ with n_l the population number of area l and $\rho_l = n_l/A_l$, $l = 1,..,L$.

Let furthermore δ_{ij} be the change in population of area i caused by the flow between area i and area j; hence $\delta_{ji} = -\delta_{ij}$. Suppose the changes δ_{ij} with $i < j$, $j = 1,..,N$, are independent. Such a change in the population causes density changes denoted by ρ_{ij} and defined as $\rho_{ij} = \delta_{ij}/A_i$ with $\rho_{ji} = -\delta_{ij}/A_j$, $i,j = 1,..,L$.

Let the transition probability W_{ij} of a change from $(\rho_1,..,\rho_i,..,\rho_j,..,\rho_L)$ to $(\rho_1,..,\rho_i + \delta_{ij},..,\rho_j - \delta_{ij},..,\rho_L)$ be given as:

$$W_{ij} = \alpha\cdot\exp(-\delta_{ij}^2/\Delta_{ij})\cdot\exp\left[-\frac{\beta}{2}\left\{V(..,\rho_i+\rho_{ij},..,\rho_j+\rho_{ji},..) - V(\rho)\right\}\right] \qquad (IV.23)$$

where Δ_{ij} is a positive, (i-j)-flow specific weighting factor ($\alpha > 0$). The total change δ_i in the population n_i of area i is the sum over all independent changes δ_{ij}, $j = 1,..,L$. So a total population change in area i is build up from (L-1) independent mass-flows between area i and area j, $j \neq i$.

Applying now again the procedure of calculating the mean value equation and/or most probable path equation on the system with $0.5(L^2 - L)$ independent changes δ_{ij}, results in the following deterministic equation:

$$\tau\dot{n}_i = -M_i\left[\sum_{j=1}^{L}\Psi(i,j)\left\{\frac{1}{A_i}\cdot\frac{\delta V}{\delta\rho_i} - \frac{1}{A_j}\cdot\frac{\delta V}{\delta\rho_j}\right\}\right],\quad i = 1,..,L \qquad (IV.24a)$$

where M_i is a positive scaling factor and $\Psi(i,j)$ is a positive symmetric weighting matrix with

$$\Psi(j,i) = \Psi(i,j) = \sqrt{\Delta_{ij}} \quad \text{for } i < j. \qquad (IV.24b)$$

Equation (IV.24a-b) will be called the general migration equation. Note that it is assumed that the functional V is still written in the density ρ rather than in the population number n.

For equal spacing with area A (IV.24a) reduces to

$$\tau\dot{\rho}_i = -M\left[\sum_{j=1}^{L}\Psi(i,j)\left\{\frac{\delta V}{\delta\rho_i} - \frac{\delta V}{\delta\rho_j}\right\}\right],\quad i = 1,..,L \qquad (IV.24c)$$

with $M = M_i/A^2$. In the following chapter it will be shown that the evolution equations (IV.24c) are a particular form of the equations (IV.22); however the stochastic formulation is different and defines consequently a different error structure.

IV.7 Specific most probable path equations

In the discrete case the matrix K with

$$K = \begin{cases} K(i,i) = 2, \ i = 2,..,N-1 \\ K(1,1) = 1; \ K(N,N) = 1 \\ K(i,j) = -1 \ \text{if} \ |i - j| = 1 \\ K(i,j) = 0 \ \ \text{if} \ |i - j| > 1 \end{cases} \qquad \text{(IV.25)}$$

defines the anti-diffusion equation where the condition $K(1,1) = K(N,N) = 1$ gives the no-flux boundary conditions. The Laplacian $\frac{\partial^2 \rho}{\partial x^2}$ is approximated by $(\rho_{n+1} - 2\rho_n + \rho_{n-1})/h^2$ where $\rho(x) = \rho(nh) = \rho_n$ with h the grid spacing (see chapter VIII). The matrix K defined in (IV.25) shall be denoted as D^2. The discrete Laplace operator is given as $-D^2$.

Define the NxN matrix Ψ such that $\Psi(i,j) = \delta(i,j) - K(i,j)$. Then the equation (IV.22) can be written as

$$\tau\dot{\rho}_n = -M\left\{\frac{\delta V}{\delta \rho_n} - \sum_{i=1}^{N} \Psi(n,i)\frac{\delta V}{\delta \rho_i}\right\} \qquad \text{(IV.26)}$$

Use $\sum_{i=1}^{N}\Psi(n,i) = 1$ and $\Psi(n,i) = \Psi(i,n)$ to find that

$$\tau\dot{\rho}_n = -M\left[\sum_{i=1}^{N} \Psi(n,i)\left\{\frac{\delta V}{\delta \rho_n} - \frac{\delta V}{\delta \rho_i}\right\}\right] \qquad \text{(IV.27)}$$

which is of the same form as the migration equation (IV.24c).
The change in ρ_n is build up from fluxes generated by the weighted potential differences $\left\{\frac{\delta V}{\delta \rho_n} - \frac{\delta V}{\delta \rho_i}\right\}$ between grid point n and each other grid point i.
The condition of positivity of K gives the condition that all eigenvalues of Ψ must be less than or equal to 1. This condition is met if Ψ is symmetric with all elements $\Psi(i,j)$ non-negative and the row elements adding up to 1: the eigenvalues are real and by Gerschgorin's theorem (Dahlquist et al., 1974), each eigenvalue λ_i lies in the union of the circles: $|z - \psi(n,n,)| \leq r_n$ with $r_n = \sum_{\substack{m=1 \\ m \neq n}}^{N} |\psi(n,m)|$. Hence $\lambda_i \leq \max_n (r_n + \psi(n,n)) = 1$.

Above Ψ is given as $\Psi(i,j) = \delta(i,j) - K(i,j)$, but in general Ψ can be defined as: $\Psi(i,j) = \Delta(i)\cdot\delta(i,j) - K(i,j)$ with $\Delta(i)$ a positive constant; hence the only restrictions on the matrix Ψ are symmetry and $\Psi(i,j) \geq 0$.

Example 1: $\Psi(i,j) = 1/N$ for all i, j.
Example 2: $\Psi(i,j)$ can be constructed from a distance matrix with elements $\exp(-\beta D(i,j))$ with $D(i,j) = D(j,i) \geq 0$ and β positive, see chapter X.

In the continuous case the anti-diffusion equation is found by setting $K(x,y) = \delta(x,y) - \Psi(x,y)$ with

$$\Psi(x,y) = 0 \quad \text{if } |x - y| > \lambda$$

$$\Psi(x,y) = \frac{1}{2\lambda} \text{ if } |x - y| \leq \lambda$$

Then, for small λ, the integral $\int_0^L \Psi(x,y)\frac{\delta V}{\delta \rho}(y)dy$ can be approximated by

$$\phi(\rho(x)) - \gamma\frac{\partial^2\rho}{\partial x^2} - \left(\phi(\rho(x+\lambda)) - \gamma\frac{\partial^2\rho(x+\lambda)}{\partial x^2} + \phi(\rho(x-\lambda)) - \gamma\frac{\partial^2\rho(x-\lambda)}{\partial x^2}\right)/2 \tag{IV.28}$$

Using the approximation:

$$f(\rho(x+\lambda)) = f(\rho(x)) + \lambda\frac{\partial}{\partial x}f(\rho(x)) + \frac{1}{2}\lambda^2\frac{\partial^2}{\partial x^2}f(\rho(x))$$

in (IV.28) one finds for (IV.18b)

$$\tau\frac{\partial\rho}{\partial t} = \frac{1}{2}M\lambda^2\frac{\partial^2}{\partial x^2}\left(\phi(\rho(x)) - \gamma\frac{\partial^2\rho}{\partial x^2}\right) \tag{IV.29}$$

Note that λ^2/τ has the right dimensions to be able to identify $M\lambda^2/2\tau$ as a diffusion coefficient. The operator $-\frac{\partial^2}{\partial x^2}$ satisfies the positivity condition.
The exact anti-diffusion operator $K(x,y)$ is defined as:

$$K(x,y) := -\int t^2\exp(-i(y - x)t)dt \tag{IV.30}$$

If K is the identity transformation ($K(x,y) = \delta(x - y)$, the Dirac δ-function) then equation (IV.18b) is reduced to the standard reaction diffusion equation: $\tau\frac{\partial\rho}{\partial t} = M\left\{-\phi(\rho) + \gamma\frac{\partial^2\rho}{\partial x^2}\right\}$.

IV.8 Deviations from the most probable path

The most probable path equations are not sufficient in describing the full characteristics of the system. If the probability density $P(\rho,t)$ has two or more maxima (multimodal), the most probable evolution becomes meaningless, since two different density profiles may have nearly equal weights but the most probable evolution takes into account only the one whose weight is slightly larger. Furthermore, jumps to other solutions branches will not occur. The initial state defines completely the evolution.

Deviations can be incorporated by adding a random variable to the deterministic equations (IV.22) or (IV.24). The result is the so-called Langevin equation. The standard Langevin equation was proposed by Langevin in 1908 as a generalization of Einstein's theory of Brownian motion. It describes the motion of a particle in viscous fluid. Langevin's equation was the first mathematical equation describing non-equilibrium thermodynamics (Haken, 1978). The standard form is

$$d\rho(t) = \sqrt{2T}\, dw(t) - \frac{\delta V}{\delta \rho} dt \qquad \text{(IV.31)}$$

where $\sqrt{2T}\, dw(t)$ corresponds to microscopic fluctuations caused by Brownian force (T is temperature). The second term $-\frac{\delta V}{\delta \rho} dt$, called the "drag" force is generated by the viscosity of the fluid. On the short time scale the Brownian fluctuations are dominant; at the long time scale the drag force dominates (Powles, 1968; Haken, 1978).

For equation (IV.22) the Langevin equation may be written as:

$$\tau \dot{\rho}_n = -M \left[K \left(\frac{\delta V}{\delta \rho} + R(t) \right) \right]_n , \quad n = 1,..N \qquad \text{(IV.32a)}$$

where R is an N array of random variables with

$$\langle R(t) \rangle = 0 \qquad \text{(IV.32b)}$$

$$\langle R_i(t) R_j(t^1) \rangle = Q(i,j) \cdot \delta(t - t^1) \qquad \text{(IV.32c)}$$

and for equation (IV.24c) with L equidistant cells

$$\tau \dot{\rho}_i = -M \left[\sum_{j=1}^{L} \Psi(i,j) \left\{ \frac{\delta V}{\delta \rho_i} - \frac{\delta V}{\delta \rho_j} + S_{ij}(t) \right\} \right] \qquad \text{(IV.32d)}$$

where $S_{ji} = -S_{ij}$ and $S_{ij} = R_n$ with $n = j-i + (i-1)L$ for $1 \leq i < j$,

$i = 1,2,..,L-1$ and R is a $0.5(L^2 - L)$ array of random variables with

$$\langle R(t)\rangle = 0 \qquad \text{(IV.32e)}$$

$$\langle R_i(t)R_j(t^1)\rangle = Q(i,j)\cdot\delta(t - t^1) \qquad \text{(IV.32f)}$$

The structure of the stochastic term is a direct consequence of the definition of the transition probability W as formulated in paragraph IV.3, respectively paragraph IV.5. In both cases the mass conservation properties are retained. In the following only equation (IV.32a) with (IV.32b) and (IV.32c) is considered only.

Defining $P(\rho,t)$ as the probability density function for the system (IV.32a-c), the time evolution of P is given approximately by the so-called Fokker-Planck equation. (The Fokker-Planck equation is exact in the case of Gaussian random variables (Haken, 1978).)

$$\tau\frac{\partial P}{\partial t} = \sum_{n=1}^{N}\frac{\partial}{\partial\rho_n}\left[\sum_{l=1}^{N}K(n,l)\left\{M\frac{\delta V}{\delta\rho_l} + \frac{1}{2}\sum_{m=1}^{N}Q(l,m)\frac{\partial}{\partial\rho_m}\right\}P\right] \qquad \text{(IV.33)}$$

The term between the square brackets is called the probability current j with $j_n = \sum_{l=1}^{N}K(n,l)\left\{M\frac{\delta V}{\delta\rho_l} + \frac{1}{2}\sum_{m=1}^{N}Q(l,m)\frac{\partial}{\partial\rho_m}\right\}P$ and hence

$$\frac{\partial P}{\partial t} = 0 \Leftrightarrow \left(\langle\nabla_\rho, j\rangle = 0 \text{ with } \nabla_\rho = \left(\frac{\partial}{\partial\rho_1},\ldots,\frac{\partial}{\partial\rho_N}\right).\right) \qquad \text{(IV.34)}$$

If $Q(l,m) = Q\cdot\delta(n - m)$ then (IV.34) implies that the stationary solutions of P are given for $j = 0$ only (Haken, 1978).

Let K such that the null space $\mathcal{N}_K = [\iota]$, with $\iota^T = (1,..,1)$. Hence the Langevin equation (IV.31a) is mass conserving and the solution space of ρ is restricted to the subspace $\sum_{n=1}^{N}\rho_n = M_\rho$. Writing a stationary solution $P(\rho)$ of the Fokker-Planck equation in the form

$$P(\rho) = \mathcal{N}\cdot\exp\left[-2M\,\Psi(\rho)/Q\right] \qquad \text{(IV.35)}$$

where $\mathcal{N}$ is a scaling constant, then $\Psi(\rho) = V(\rho) - \beta\langle\iota,\rho\rangle$, with β constant.

Critical (stationary) points of $P(\rho)$ (IV.35) are given for ρ satisfying

$$\frac{\delta V}{\delta\rho} = \beta\iota \qquad \text{(IV.36a)}$$

or equivalently:

$$K\frac{\delta V}{\delta\rho} = 0 \qquad \text{(IV.36b)}$$

The same characterization was found for the stationary solutions of the anti-diffusion equation (see chapter II). A stationary point defined by (IV.36b) will be a strict local maximum of $P(\rho)$ if

$$\langle \rho, \frac{\delta^2 V}{\delta \rho^2} \cdot \rho \rangle > 0 \text{ on the subspace } \sum_{n=1}^{N} \rho_n = M_\rho . \qquad \text{(IV.37)}$$

This is just the condition that the stationary point (IV.35) is a strict minimum of V.

So multiple strict minima of V will give multiple maxima of P. At the change of one minimum to two or more minima of V, the distribution becomes multimodal giving rise to large variances. For example, with a bimodal symmetric distribution, the system will be mostly in one of the peaks. The deviations of the mean value will be large. By observation it may be possible to determine in which peak the system is in fact (and assume wrongly that the distribution is unimodal). However, a fluctuation can carry the system spontaneously to another peak. This behavior can not be simulated neither by the mean value equation which is based on unimodality, nor by the most probable path equation which restricts the evolution to the most probable branch.

CHAPTER V

EXISTENCE AND STABILITY OF STATIONARY SOLUTIONS

V.1 Introduction

In chapter IV, the most probable path equations are derived in the form:

$$\tau\dot{\rho}_n = -M\left(K\,\frac{\delta V}{\delta \rho}\right)_n \,, \quad n = 1,..N \tag{V.1a}$$

where K is a symmetric and positive N×N matrix, i.e. $\langle x,Kx\rangle \geq 0$ all $x \in \mathbb{R}^N$, with null space $\mathcal{N}_K = [\iota]$, $\iota^T = (1,1,\ldots,1)$; ρ_n is an element of an N dimensional vector ρ; M and τ are positive constants.
In continuous form the equation is written as

$$\tau\frac{\partial \rho}{\partial t} = -M\int K(x,y)\frac{\delta V}{\delta \rho}(y)dy \tag{V.1b}$$

where

$$\frac{\delta V}{\delta \rho} = \phi(\rho) - \gamma\frac{\partial^2 \rho}{\partial x^2}, \quad \gamma > 0 \tag{V.2}$$

with ϕ cubic in ρ.
In this chapter some concepts of linear stability analysis in relation to asymptotic stability are introduced in section V.2. In the next two sections it is shown that systems (V.1a) have the same stationary solutions with the same stability properties independently of K. The same statements holds for system (V.1b) for varying K. Moreover, it is proven that both systems have stable, non-constant solutions if the null solution is unstable.

V.2 Linear stability analysis

Let the general evolution equation be given as:

$$\frac{\partial u}{\partial t}(x,t) = G(u;\gamma) \qquad (V.3a)$$

(γ is the parameter (vector) controlling the structure of G) defined on $D \subset \mathbb{R}^q$, with initial conditions

$$\forall x \in D : u(x,t_o) = u_o(x) \qquad (V.3b)$$

and boundary conditions of

Dirichlet type: $\forall x \in \partial D \;\&\; \forall t \in \mathbb{R} : u(x,t) = c_o$ (V.3c)

or of

Neumann type: $\forall x \in \partial D \;\&\; \forall t \in \mathbb{R} : \nabla_n u(x,t) > = c_o$ (V.3d)

where ∇_n is the spatial derivative in the direction of n, the normal to the boundary ∂D of D, and c_o is some constant. With the boundary conditions, the system may not always be solvable.

The basic concepts of stability are due to Lyapunov (Sattinger, 1973). This Lyapunov stability means that solutions belonging to neighbouring conditions evolve in a neighbourhood of each other. For partial differential equations stability analysis involves the structure of the equations (system), boundary and initial conditions of the solutions. To be more precise, stability definitions will be given for the general evolution system (V.3).

With $\|\cdot\|$ is denoted the norm on some function space; for finite dimensional systems defined on $\mathbb{R}^N$, the norm can be the standard euclidean norm. To discriminate between solutions belonging to different initial conditions we shall write $u(x,t,u_o)$ instead of $u(x,t)$ for solutions of (V.3a-d).

Definition V.1

A solution u of system (V.3a-c,d) is called *stable* if $\forall\, \varepsilon > 0$, $\forall\, t_o \in \mathbb{R}$, $\exists\, \eta > 0$: $\|u - u_{o1}\| < \eta \Rightarrow \forall\, t > t_o : \|u - u_1\| < \varepsilon$ where $u_1(x,t,u_{o1})$ is a solution of (V.3a-c,d) with initial condition u_{o1}. (V.4)

Definition V.2

A solution u of system (V.3) is called *attractive* if

$$\exists\, \eta > 0 : \|u - u_{o1}\| < \eta \;\Rightarrow\; \lim_{t\to\infty} \|u - u_1\| = 0$$

with the same notations as in (V.4) (V.5)

Definition V.3

A solution u is called *asymptotically stable* if u is both stable and attractive. (V.6)

Definition V.4

A solution is called *unstable* if u is not stable. (V.7)

Global stability of a solution u does not involve any condition on the initial values. This is a rare case, at least for nonlinear systems, since it means that all solutions are attracted to a single stable solution. Note that stability does not imply asymptotic stability.

Definition V.5 (Nicolis, 1981)

The system (V.3) is *structurally* stable (in norm, within the family of evolution equations parameterized by γ) if

$\forall\, \varepsilon > 0,\ \forall\, t_o \in \mathbb{R},\ \exists\, \eta > 0$:

$\|\gamma - \gamma_1\| < \eta \;\Rightarrow\; \forall\, t > t_o : \|u - u_1\| < \varepsilon$ where u and u_1 are solutions with respectively parameter γ and γ_1 and $\|\gamma\|$ denotes a norm in parameter space. (V.8)

This is called by Nicolis structurally stable and so shall we do in the following.

The first four definitions are related to the initial conditions whereas the fifth condition involves the structure of the equations and the boundary conditions as well, since both can depend on a parameter (vector) γ.

Stability analysis requires a general solution of the system which is often impossible to obtain. A first step is to restrict oneself to infinitesimal perturbations only around the asymptotic solution; after linearization the global analysis becomes a local linear problem.

Lyapunov's theorem states the equivalence of both analyses for general systems (Iooss et al., 1980).

Let us first describe the linearization procedure.

Consider system (V.3) having a reference solution u_s such that:

$$\frac{\partial}{\partial t}u_s = G(u_s,\gamma) \tag{V.9}$$

Let the evolution operator G act on the function space X. Let G be Fréchet-differentiable at (u_s,γ) in u. The derivative with respect to u is denoted as:

$$d_u G(u_s,\gamma) = G'(u_s,\gamma). \tag{V.10}$$

The Fréchet-derivative of an operator is the natural generalization of the concept of a derivative of functions defined on finite dimensional spaces to operators on infinite dimensional normed linear spaces (see Appendix E and references there). This means, among other things, that $d_u G(u_s,\gamma)$ is a linear operator acting on the function space X. Furthermore, an analogon of the Taylor expansion exists provided higher derivatives exist.

Assume that u_s is a solution of (V.3a-d) for all γ. Then by replacing u with $u - u_s$, and assuming a bit of analyticity, the right hand side $G(u;\gamma)$ of (V.3a) can be arranged to get

$$G(u;\gamma) = Bu - \gamma Au + N(u;\gamma) \tag{V.11}$$

where B and A are linear transformations defined on M, and N is the nonlinear part in u such that $N(0;\gamma) = 0$ and $d_u N(0;\gamma) = 0$; So $d_u G(0;\gamma) = B - \gamma A$. (The anti-diffusion equation is easily written in the form (V.11)). The boundary conditions are of the same type as those of the original equation except that $c_o = 0$ (homogeneous case). The null solution $u \equiv 0$ represents the reference state $u = u_s$ and the evolution equation of u is:

$$\frac{\partial u}{\partial t} = L\cdot u + N(u;\gamma) \tag{V.12}$$

The first, linear, approximation to (V.12) is:

$$\frac{\partial u}{\partial t} = L\cdot u \tag{V.13}$$

where $L = L(\gamma) = d_u G(0,\gamma) = B - \gamma A$.

The relationship between the linear problem (V.13) and the nonlinear one (V.12) is given by the following Lyapunov theorem (Nicolis, 1980):

Theorem V.6

If the null solution of (V.12) is asymptotically stable, then u_s is an asymptotically stable solution of (V.3). If the null solution of (V.12) is unstable then u_s is an unstable solution of (V.3).

This theorem is an analog of the Poincaré-Lyapunov theorem for finite dimensional vector spaces. For infinite dimensional function spaces it is only proven for systems with one component (Grasman, 1982).

Let M be the set of u for which the evolution problem (V.11) is well defined. (M may be infinite dimensional, i.e. a Hilbert space.) The spectral problem associated with the linear operator L (V.13) is

$$L \cdot v = \lambda v$$

which defines the eigenvalues λ and eigenvectors v of L in M. As long as each solution u of (V.13) can be expressed as a linear combination (maybe infinite) of terms proportional to $\exp(\lambda_n t)v_n$ with λ_n eigenvalue and v_n eigenvector of L in M, the (linear) stability properties of the reference state u_s are given by the (real part of) the eigenvalues λ_n of L. The problem is that it may not be possible to write u as such a linear combination.

However, in the case of anti-diffusion system (V.1b), with $\frac{\delta V}{\delta \rho} = \phi(\rho) - \gamma\frac{\partial^2 \rho}{\partial x^2}$, the linear operator L can be written as -KH with H the second derivative of V evaluated at the reference state $\rho = u_s$ ($Hv = \phi'(u_s)v - \gamma\frac{\partial^2}{\partial x^2}v$); now it is possible to use the property that the operator H has a complete orthonormal set of eigenvectors which form a basis in L^2 (Coddington and Levinson, 1955; Gohberg and Goldberg, 1981). With K positive and even strictly positive on the specific solution space we will use, it is possible to show that the stability of the reference state u_s depends only on the eigenvalues of H.

V.3 Stationary solutions (finite dimensional)

If $\rho_n = \rho_o$, $n = 1,\ldots,N$ with ρ_o constant is a stationary solution of (V.1) then the equations can be written in terms of $u_n = \rho_n - \rho_o$ as

$$\tau \dot{u}_n = -M\left(K \frac{\delta V}{\delta u}\right)_n , \quad n = 1,..N \tag{V.14}$$

with initial condition such that $\langle u, \iota \rangle = 0$ where $\langle \cdot, \cdot \rangle$ denotes the standard Euclidean inner product and $\iota^T = (1,1,..,1) \in \mathbb{R}^N$.
Define the linear subspace $\mathbb{R}^N_*$ of $\mathbb{R}^N$ by

$$\mathbb{R}^N_* = \left\{ u \in \mathbb{R}^N \mid \langle u, \iota \rangle = 0 \right\} \tag{V.15}$$

Since the equations (V.14) are mass conserving, all solutions of (V.1) must belong to $\mathbb{R}^N_*$. The positive constants τ and M in the system equations (V.1) are taken such that $\tau/M = 1$.

We want to show that existence and stability properties of stationary solutions of (V.14) are independent of K (as long as K belongs to the same type of symmetric, positive matrices as defined in Chapter IV, section 3). A stationary solution of (V.14) is given by

$$\langle K\frac{\delta V}{\delta u}, v \rangle = 0 \text{ for all } v \in \mathbb{R}^N \tag{V.16a}$$

Denote the null space of K as $\mathcal{N}_K$. If $\mathcal{N}_K \supseteq [\iota]$ then some stationary solutions of (V.1) are given by

$$\frac{\delta V}{\delta u} = \beta \iota, \text{ for some } \beta \in \mathbb{R} \tag{V.16b}$$

If $\mathcal{N}_k = [\iota]$ then (V.16b) defines the only stationary solutions.
Condition (V.16b) is independent of K, so all systems with $\mathcal{N}_K = [\iota]$ have the same stationary solutions.
In what follows K is taken such that the null space of K is $[\iota]$.

The second observation is that all systems (V.1) have the same Lyapunov function V(u) as well, since

$$\frac{dV}{dt} = \langle \frac{\delta V}{\delta u}, \dot{u} \rangle = -\langle \frac{\delta V}{\delta u}, K\frac{\delta V}{\delta u} \rangle \leq 0 \tag{V.17a}$$

$$\frac{dV}{dt} = 0 \iff \frac{\delta V}{\delta u} = \beta\iota, \ \beta \in \mathbb{R} \tag{V.17b}$$

since K is positive with null space $\mathcal{N}_K = [\iota]$.
Let the discrete V(u) be defined as:

$$V(u) = V(u_1, \ldots, u_N) = \sum_{n=1}^{N} \left\{ f(u_n) + \frac{1}{2}(\gamma/h^2) u_n \left(D^2 u\right)_n \right\} \tag{V.18a}$$

where D^2 is defined by (IV.25) ($-D^2$ is the discrete Laplace operator, subject to no-flux boundary conditions, see chapter IV, section 7) and h is the spatial gridspacing (see also chapter VIII). As before we set $\frac{df(u)}{du} = \phi(u)$, with f(0) = 0 and

$$\phi(u) = -u + r_1 u^2 + r_2 u^3 \tag{V.18b}$$

It follows, by a Taylor expansion of (V.18a), that for fixed $u \in \mathbb{R}^N$

$$V(u + v) = V(u) + d_u V(v) + \frac{1}{2} d_u^2 V(v, v) + o(\langle v, v \rangle) \tag{V.19a}$$

for $v \in \mathbb{R}^N$, $\langle v, v \rangle \to 0$, where

$$d_u V(v) = \sum_{n=1}^{N} \left\{ \phi(u_n) v_n + (\gamma/h^2) \left(D^2 u\right)_n v_n \right\} = \langle \frac{\delta V}{\delta u}, v \rangle \tag{V.19b}$$

and

$$d_u^2 V(v, v) = \sum_{n=1}^{N} \left\{ \phi'(u_n) v_n^2 + (\gamma/h^2) \left(D^2 v\right)_n v_n \right\} = \langle v, Hv \rangle \tag{V.19c}$$

where $\phi'(u_n)$ denotes the derivative of ϕ evaluated at u_n and H is the Hessian of V, i.e. $\left(\frac{\delta^2 V}{\delta u^2}\right)$, evaluated at u. It is possible to write $d_u V(v)$ and $d_u^2 V(v, v)$ as in (V.19b) and (V.19c), because of the definition of D^2 which includes already the no-flux boundary conditions: see chapter IV, section 7 and chapter VIII. The critical points of V on $\mathbb{R}^N_*$ are the critical points of V subject to the condition $\langle u, \iota \rangle = 0$:

$$\langle \frac{\delta V}{\delta u}, v \rangle = \beta \langle \iota, v \rangle \text{ for some } \beta \in \mathbb{R} \tag{V.20a}$$

Condition (V.20a) is equivalent with

$$\langle K \frac{\delta V}{\delta u}, v \rangle = 0 \tag{V.20b}$$

Hence critical points of V on $\mathbb{R}^N_*$ are stationary solutions of (V.1) and vice versa.

The equivalence of stability properties of stationary solutions of mass conserving evolution equations (V.1) can now be established.

Let $u_o = (u_{o1},\ldots,u_{oN})$ be a stationary solution of (V.14). Taking $u = u_o + v$ with $\sum_{n=1}^{N} v_n = 0$ and substituting this in (V.14), gives to the first order in u:

$$\dot{v}_n = -\left(KHv\right)_n, \quad n = 1,\ldots,N \tag{V.21}$$

where H is the Hessian of V evaluated at $u = u_o$.

Two cases are now distinguished:

a) The Hessian H has a negative eigenvalue λ with corresponding eigenvector v, then

$$\frac{d<v,v>}{dt} = -<v,KHv> - <KHv,v>= -2\lambda<v,Kv>, \quad \lambda < 0 \tag{V.22a}$$

Since K is strictly positive on $\mathbb{R}^N_*$, $<v,Kv> \geq \mu_k<v,v>$ where μ_k is the smallest eigenvalue of K. Hence

$$\frac{d<v,v>}{dt} \geq -2\lambda\mu_k<v,v> > 0 \tag{V.22b}$$

So $<v,v> = \|v\|^2$ is a monotone increasing function of t hence the null solution of (V.21) is unstable, and by theorem V.6, the stationary solution $u = u_o$ of (V.14) is unstable.

b) The Hessian H is strictly positive. Let the smallest eigenvalue of H be given by λ_1, then

$$\|\sqrt{H}v\|^2 = <v,Hv> \geq \lambda_1<v,v> = \lambda_1\|v\|^2 \text{ all } v \in \mathbb{R}^N_* \tag{V.23a}$$

where $\sqrt{H}$ is the positive square root of H.

$$\frac{d<v,Hv>}{dt} = -2<v,HKHv> \tag{V.23b}$$

Let again μ_k be the smallest eigenvalue of K ($\mu_k > 0$) then $<v,HKHv> \geq \mu_k<v,HHv>$. $\sqrt{H}H\sqrt{H}$ and HH have the same eigenvectors as H, hence $<v,HHv> \geq \lambda_1<v,Hv>$ all $v \in \mathbb{R}^N_*$. So we find that

$$\frac{d<v,Hv>}{dt} \leq -2\lambda_1\mu_k<v,Hv> < 0 \text{ if } v \neq 0. \tag{V.23c}$$

Which means that $<v,Hv> = \|\sqrt{H}v\|^2$ is monotone decreasing in t. Suppose $\lim_{t\to\infty} \|\sqrt{H}v\|^2 = \alpha > 0$, then follows from (V.23c) that

$$\frac{d}{dt}\|\sqrt{H}v\|^2 \leq -2\lambda_1\mu_k\alpha < 0 \tag{V.23d}$$

and there will be a t such that $\|\sqrt{H}v\|^2$ is negative. So α must be zero and $\lim_{t\to\infty} \|\sqrt{H}v\|^2 = 0$. Hence by (V.23a) the null solution of (V.21) is asymptotically stable and by theorem V.6 the stationary solution $u = u_o$ of (V.14) is stable.

The case that H has a zero eigenvalue will give the possibility of bifurcating solutions and is treated in appendix A.

As a summary the following theorem is formulated:

Theorem V.7

All systems with the evolution equations

$$\tau \dot{u}_n = -M\left(K\frac{\delta V}{\delta u}\right)_n \quad , \; n = 1,..N; \; \tau \text{ and } M \text{ positive constants}$$

with K symmetric, positive and $N_K = [\iota]$, and with the same initial condition $\int u(x,0)dx = 0$, are identical with respect to stationary solutions and the stability properties of these solutions.

The existence of a stable non-trivial solution can be established as follows. Assume that the null-solution ($u_n = 0$, $n = 1,..,N$) is not a minimum of V and let ϕ be given by (V.18b). Using the definition of V in (V.18a) where D^2 is a positive operator, one finds that

$$V(u) \geq \sum_{n=1}^{N} f(u_n) = \sum_{n=1}^{N} \left\{ -\frac{1}{2}u_n^2 + \frac{1}{3}r_1 u_n^3 + \frac{1}{4}r_2 u_n^4 \right\}$$

Hence, if $r_2 > 0$, there exists a constant R such that $V(u) \geq 0$ for u with $\langle u,u\rangle > R$. Since V is continuous and the domain $\left\{u \in \mathbb{R}^{N*} \,|\, \langle u,u\rangle \leq R\right\}$ is compact, V attains its minimum on this domain. This minimum is not at the null solution and not on the boundary $\langle u,u\rangle = R$; so there exists a point u with not all u_n equal to zero where V attains its minimum. Since $\frac{dV(u)}{dt} < 0$ if u is not a stationary point (see V.17a and V.17b), it follows that there must exist a minimum of V which is a non-trivial stable solution of (V.14). This conclusion can be formulated as the following theorem:

Theorem V.8

All systems with evolution equation

$$\tau\dot{u}_n = -M\left(K\frac{\delta V}{\delta u}\right)_n \quad , \; n = 1,..N, \; M \text{ and } \tau \text{ positive constants}$$

with K symmetric, positive and $\mathcal{N}_K = [\iota]$, and with $V(u) = V(u_1,\ldots,u_N) = \sum_{n=1}^{N}\left\{f(u_n) + \frac{1}{2}(\gamma/h^2)\left(u^T D^2 u\right)_n\right\}$ and $f(u) = -\frac{1}{2}u_n^2 + \frac{1}{3}r_1 u_n^3 + \frac{1}{4}r_2 u_n^4$ with $r_2 > 0$ where D^2 a positive mapping from $\mathbb{R}^N$ to $\mathbb{R}^N$ (V is C^2), have a non-trivial stable stationary solution if the trivial solution is not a minimum of V.

V.4 Stationary solutions (infinite dimensional)

For the discrete system theorems V.8 and V.9 are proven under the condition that V is C^2 and bounded from below and that the matrix K is positive and symmetric. The main object of this section is to show under which conditions the results for the discrete model hold also for the continuous model. Written in terms of $u = \rho - \rho_o$ with $\rho_o(x) = \rho_o$ constant, the model equation is

$$\tau\frac{\partial u}{\partial t} = -M\int_0^L K(x,y)\frac{\delta V}{\delta u}(y)dy, \; \tau \text{ and } M \text{ positive constants} \qquad (V.24a)$$

$$\frac{\delta V}{\delta u} = \phi(u) - \gamma\frac{\partial^2 u}{\partial x^2}, \; \gamma > 0 \qquad (V.24b)$$

and

$$\phi(u) = -u + r_1 u^2 + r_2 u^2 \qquad (V.24c)$$

no-flux boundary conditions being assumed. In the following we take the positive constants τ and M such that $\tau/M = 1$. The equation (V.24a) is called an integro-differential equation with kernel K(x,y).

Definition V.9

A mapping $f: (0,T) \to E$, where E is a Banach space, defined by $t \mapsto f[t]$, $f[t] \in E$, is called a E-valued function.

Since E is a normed space, the definition of continuity of f is

straightforward; the derivative $\frac{df}{dt}$ of f is defined as the Fréchet derivative which is the natural extension of the notion of derivative from finite dimensional spaces to infinite dimensional ones (see also appendix E).

It is now possible to write the evolution equation (V.23) as

$$\frac{d}{dt}u[t] = -K\frac{\delta V}{\delta u} \tag{V.25a}$$

with

$$Ku = \int_0^L K(x,y)u(y)dy \tag{V.25b}$$

The advantage of this approach is that in a certain sense separation of variables is achieved. Furthermore, in Sobolev theory, the required boundary conditions are expressed by the fact that a function must belong to a specific Sobolev space.

If u satisfies (V.25) then

$$<\frac{d}{dt}u[t], v>_0 = -<K\frac{\delta V}{\delta u}, v>_0 \quad \text{for all v belonging to the solution space.} \tag{V.26a}$$

Definition V.10

A *weak* solution on (0,T) of the evolution equation (V.24a) is defined as a function u which satisfies (V.26a) (and the initial conditions.)

A function u is a weak stationary solution if

$$<K\frac{\delta V}{\delta u}, v>_0 = 0 \text{ for all v} \tag{V.26b}$$

hence

$$K\frac{\delta V}{\delta u} = 0 \text{ a.e.} \tag{V.26c}$$

To proceed, a solution space must be chosen. In Appendix E, definitions of Hilbert spaces L^2 of square integrable functions, and H^m, the Sobolev space of functions with square integrable (generalized) derivatives to the order m, are given.

Since the operator $\frac{\delta V}{\delta u}$ involves the Laplace operator (see (V.2)), the functions must be differentiable to the fourth order if K self is also the Laplace operator. However this is not needed for weak solutions. Note that $<\Delta^2 u, v>_0 = <\Delta u, \Delta v>_0$ is correct and well defined for functions

u and v belonging to the Sobolev space H^2. So for weak solutions the function space will be $H^2(\Omega)$ which gives also the desired no-flux boundary conditions.

Let $\Omega = (0,L) \subset \mathbb{R}$. With the mass conservation property of the system, the solution space is taken as:

$$H^2_*(0,L) = \left\{ u \in H^2(0,L) \mid \langle u,1\rangle_2 = \langle u,1\rangle_0 = 0 \right\} \qquad (V.27a)$$

where the symbol 1 denotes the function $v(x) = 1$ all x.

If K is not the Laplace operator but for instance given by $K(u) = u - \frac{1}{L}\int_0^L u\,dx$, then the solution space is H^1_* which is defined as:

$$H^1_*(0,L) = \left\{ u \in H^1(0,L) \mid \langle u,1\rangle_1 = \langle u,1\rangle_0 = 0 \right\} \qquad (V.27b)$$

The following assumptions are made with respect to K:

i) $K(x,y) = K(y,x)$; K is symmetric.

ii) K is positive.

iii) $\langle u,Ku\rangle_0 = 0 \Leftrightarrow u(\cdot) =$ constant a.e.. On a reduced space (e.g. H^2_*) the operator K is strictly positive: $\langle u,Ku\rangle_0 > 0$.

(V.28)

The negative diffusion operator $K(u)(x) = -\frac{\partial^2 u}{\partial x^2}$ satisfies all conditions (V.28). The same holds for $K(u)(x) = u(x) - \frac{1}{L}\int_0^L u(y)dy$.

A stationary solution defined by (V.26b) is an element $u \in H^2_*$ with

$$\frac{\delta V}{\delta u} = \beta, \ \beta \text{ is constant} \qquad (V.29)$$

which identifies all stationary solutions independently of K.

The functional V is given by:

$$V(u) = \int_0^L f(u(x)) + \tfrac{1}{2}\gamma\left|u_x(x)\right|^2 dx \qquad (V.30a)$$

with

$$f(u(x)) = -\tfrac{1}{2}u^2(x) + \tfrac{1}{3}r_1u^3(x) + \tfrac{1}{4}r_2u^4(x) \qquad (V.30b)$$

Since $\frac{dV(u)}{dt} = \int \frac{\delta V}{\delta u}\cdot\frac{du[t]}{dt}dx$, it follows directly from (V.26a) (and condition iii of V.28) that

$$\frac{dV(u)}{dt} \leq 0 \tag{V.31a}$$

$$\frac{dV(u)}{dt} = 0 \Leftrightarrow \frac{\delta V}{\delta u} = \beta, \ \beta \text{ is constant} \tag{V.31b}$$

So V is a Lyapunov functional. We now show that critical points of V on H^2_* are stationary solutions of (V.26a) and vice versa.
Writing $df(u) = \phi(u)$, the Taylor expansion of V for fixed $u \in H^2_*$ is

$$V(u + v) - V(u) = d_u V(v) + \tfrac{1}{2} d^2_u V(v,v) + o(\|v\|^2_0) \tag{V.32}$$

for $v \in H^2_*$, $\|v\|_0 \to 0$, where

$$d_u V(v) = \int \left(\phi(u(x))v(x) + \gamma u_x(x)v_x(x)\right)dx \tag{V.33a}$$

and

$$d^2_u V(v,v) = \int \left(\phi'(u)v^2(x) + \gamma|v_x(x)|^2\right)dx \tag{V.33b}$$

The critical points of V on H^2_* are critical points subject to the condition $\langle u,1\rangle_2 = \langle u,1\rangle_0 = 0$. Then by Ljusternik's theorem (Groesen, 1976), the critical points are given by

$$d_u V(v) = \beta\langle 1,v\rangle_2 = \beta\langle 1,v\rangle_0 \text{ for some } \beta \in \mathbb{R}, \text{ all } v \in H^2_* \tag{V.34}$$

Suppose $u \in H^2_*$ is a critical point, then it is possible to prove that u satisfies the no-flux boundaries conditions. We follow the procedure given in Diekmann (1982). Let q(x) be the solution of

$$\gamma\frac{\partial^2}{\partial x^2}q = \phi(u) - \beta, \ q(0) = q_x(0) = 0 \ (\gamma > 0) \tag{V.35a}$$

Let $v \in C^2$ with $v_x(0) = v_x(L) = 0$ and $v(L) = 0$ then by partial integration of the right hand side of (V.33a), one finds:

$$\int q(x) + u(x))v_{xx}dx = 0, \tag{V.35b}$$

hence

$$q(x) + u(x) = c_1 + c_2 x. \tag{V.35c}$$

So u is at least twice differentiable and $\gamma u_{xx} = \phi(u) - \beta$ and now partial integration of $d_u V(v)$ yields:

$$u_x(0)v(0) - u_x(L)v(L) = 0 \text{ for all } v \in H^2_*, \tag{V.35d}$$

and thus $u_x(0) = u_x(L) = 0$. Since u is twice differentiable, q in (V.35a) is four times differentiable and by (V.35c) the same holds for u. Since $\gamma u_{xx} = \phi(u) - \beta$

$$\int(\phi(u) - \gamma u_{xx})_x v_x dx = 0 \quad \text{all } v \in H^2_* \tag{V.36a}$$

Then again by partial integration one finds:

$$u_{xxx}(0)v(0) - u_{xxx}(L)v(L) = 0 \quad \text{all } v \in H^2_* \tag{V.36b}$$

and so $u_{xxx}(0) = u_{xxx}(L) = 0$. So if u is critical point then u satisfies the no-flux boundary conditions and we can write in (V.34)

$$d_u V(v) = <\frac{\delta V}{\delta u}, v>_0,$$

hence a critical point is given by:

$$<\frac{\delta V}{\delta u}, v>_0 = \beta<1, v>_0 \tag{V.37}$$

If K satisfies condition iii) in (V.28) then (V.37) is equivalent with

$$<K\frac{\delta V}{\delta u}, v>_0 = 0 \text{ for all } v \in H^2_* \tag{V.38}$$

Hence critical points of V on H^2_* are stationary solutions of (V.26a) and vice versa.

Corollary V.11:

If $u \in H^1_*(0,L)$ is a critical point of V then $u \in H^2_*(0,L)$.

Proof:

Let $u \in H^1_*$ be a critical point of V. By the Sobolev lemma (see appendix E) there exists a constant C such that $|u|_0 \leq C\|u\|_1$ where $|u|_0$ is a supremum of $|u(x)|$ on [0,L]. For $u \in H^1_*$ we can apply the same reasoning of (V.35a-d), so $\gamma u_{xx} = \phi(u) - \beta$ with $\phi(u)$ given by (V.24c). The integral $\int_0^L (\phi(u) - \beta)^2 dx$ is bounded because $|u|_0$ is bounded, hence $\int u_{xx}^2 dx$ is bounded and so $u \in H^2_*$. □

Since K is symmetric and strictly positive on H^2_*, the time evolution is characterized by minimization of V on H^2_*, see (V.30a) and (V.30b). This

implies that we can link the stability properties of a stationary solution u with the properties of u as a critical point of V. Let u be a stationary solution then

if there exists $v \in H^2_*$ such that $d^2_u V(v,v) < 0$, then u is not a minimum of V (see theorem 8.1 in Diekmann (1982));

if V is minimal at u, then $d^2_u V(v,v) \geq 0$ for all $v \in H^2_*$ (see corollary 8.2 in Diekmann (1982)).

Theorem 5.3 of Koornwinder (1982) gives a sufficient condition for u being stable. This theorem is formulated for $u \in H^1(0,L)$:

Theorem V.12:

If there exists an $a > 0$ such that $d^2_u V(v,v) \geq a(|v|_o)^2$ for all $v \in H^1(0,L)$ where sup-norm $|v|_o$ denotes the supremum of $|v(x)|$ on $[0,L]$, then u is stable.

The proof in Koornwinder (1982) is as follows: the condition $d^2_u V(v,v) \geq a(|v|_o)^2$ means that V attains a strict local minimum in u with respect to the C^0 topology; as $H^1(0,L)$ is compactly embedded in $C^0([0,L])$, V attains also a strict local minimum at u in $H^1(0,L)$.
In this case, the stability of a stationary solution is related to the sign of

$$\inf\{d^2_u V(v,v) \mid v \in H^1,\ |v|_o = 1\} \tag{V.39}$$

Since $H^2(0,L)$ is compactly embedded in $H^1(0,L)$ (see Wloka, 1969) the same reasoning can be applied to solutions in H^2. And the same holds if we restrict the solution spaces to functions u with $\int u dx = 0$. Hence we get:

Corollary V.13:

If u is a stationary solution with $d^2_u V(v,v) \geq a(|v|_o)^2$ for all $v \in H^2_*(0,L)$ then V attains a strict local minimum on $H^2_*(0,L)$ in u and u is stable. (V.40)

The stability of a stationary solution is now related to the sign of

$$\inf\{d^2_u V(v,v) \mid v \in H^2_*,\ |v|_o = 1\} \tag{V.41}$$

The number defined by (V.39) has the same sign as the smallest eigenvalue λ of the Sturm-Liouville problem

$$\gamma v_{xx} + (\lambda - \phi'(u))v(x) = 0, \quad v \in C^2([0,L]) \cap H^1(0,L) \tag{V.42}$$

see Koornwinder (1982), page 150-153. Since $H^2_* \subset H^1$ the same reasoning can be applied with respect to the number defined in (V.41); hence the sign of this number is the same as the smallest eigenvalue λ of the Sturm-Liouville problem defined in (V.42), but now the eigenvectors must belong to H^2_* or rather to H^1_* since, if v is an eigenvector then

$$v_{xx} = -\frac{1}{\gamma}((\lambda - \phi'(u))v(x) \tag{V.43a}$$

and

$$\int (v_{xx})^2 dx \leq (1/\gamma)^2 (|\lambda - \phi'(u)|_o)^2 \int v^2(x)dx \tag{V.43b}$$

hence

$$\langle v,v\rangle_2 \leq \left\{1 + (1/\gamma)^2(|\lambda - \phi'(u)|_o)^2\right\}\int v^2(x)dx + \int v_x^2(x)dx \leq$$

$$\leq C_o \langle v,v\rangle_1 \text{ with } C_o = 1 + (1/\gamma)^2(|\lambda - \phi'(u)|_o)^2 \tag{V.43c}$$

Thus if $v \in H^1_*(0,L)$ is an eigenvector of (V.42), then also $v \in H^2_*(0,L)$.

The relation between the stability of a stationary solution and the eigenvalues of the Sturm-Liouville problem (V.42) can also be found by applying the principle of linearized stability (theorem V.6) to the model formulation (V.24a-24c). Let u_o be a stationary solution of (V.24a-24c); let $v = u - u_o$, then in first order approximation the time evolution of v is

$$\frac{\partial v}{\partial t} = -KHv \tag{V.44a}$$

where

$$Hv = \phi'(u_o)v - \gamma v_{xx} \tag{V.44b}$$

Since H is self-adjoint and has a complete set of orthonormal eigenvectors which is an basis in $L^2([0,L)$ (Coddington and Levinson, 1955; Gohberg and Goldberg, 1981, see also appendix E) we can apply the same procedure with respect to the relation between the eigenvalues of H and the stability of the null solution of (V.44a) as in (V.22a-b,

V23a-d). So again two cases are distinguished:

a) H has a negative eigenvalue λ with eigenvector v; then

$$\frac{d}{dt}\langle v,v\rangle_o = -\langle v,KHv\rangle_o - \langle KHv,v\rangle_o = -2\lambda\langle v,Kv\rangle_o \geq -2\lambda\mu_k\langle v,v\rangle_o > 0 \tag{V.45}$$

where μ_k is the smallest eigenvalue of K; since K is strictly positive $\mu_k > 0$. Hence $\|v\|_o^2 = \langle v,v\rangle_o$ is monotone increasing in t; so the null solution is unstable and by theorem V.6 the stationary solution $u = u_o$ of (V.24a-c) is unstable.

b) H is strictly positive. Let λ_1 be the smallest (positive) eigenvalue of H and $\sqrt{H}$ be the positive square root of H then for all v

$$\|\sqrt{H}v\|_o^2 = \langle v,Hv\rangle_o \geq \lambda_1\langle v,v\rangle_o = \lambda_1\|v\|_o^2 \tag{V.46a}$$

and

$$\frac{d}{dt}\langle v,Hv\rangle_o = -2\langle v,HKHv\rangle_o \leq -2\mu_k\langle v,HHv\rangle_o \leq -2\mu_k\lambda_1\langle v,Hv\rangle_o \tag{V.46b}$$

where μ_k is the smallest eigenvalue of K which is positive because K is strictly positive on H_*^2. So $\|\sqrt{H}v\|_o^2$ is a monotone decreasing function of t and by the same arguments as before, see (V.23c-d), $\lim_{t\to\infty}\|\sqrt{H}v\|_o^2 = 0$. Then by (V.46a) $\lim_{t\to\infty}\|v\|_o^2 = 0$ so the null solution of (V.44a) is asymptotically stable and the stationary solution $u = u_o$ of (V.24a-c) is stable (theorem V.6).

The case that H has a zero eigenvalue is treated in chapter VI and appendix A.

So we can formulate the following theorem:

Theorem V.14:

All systems with the evolution equations defined on $H_*^2(0,L)$ by $\tau\frac{\partial u}{\partial t} = -M\int_0^L K(x,y)\left\{\phi(u(y)) - \gamma u_{yy}\right\}dy$, τ, M and γ positive constants, with no-flux boundary conditions, and with K symmetric, positive and $N_K = [u]$, $u(x) = 1$ all x, and with the same initial condition $\int u(x,0)dx = 0$, are identical with respect to stationary solutions and the stability properties of these solutions.

The existence of a non-constant stable solution based on the existence of a minimum of V at a non-zero u was formulated for the discrete system in theorem V.8. Since $H_*^2(0,L) \subset H_*^1(0,L)$ and by corollary V.11 it

is sufficient to prove the existence of a minimum of V defined as a functional on H^1_*. The existence can be concluded from theorem 5.10 page 140 in Chow and Hale (1982):

Theorem V.15:

Let $f: X \to \mathbb{R}$, with X a Banach space, be C^1 and satisfy condition (C). If f is bounded above (below), then f attains its maximum (minimum).

Condition (C) is a compactness condition (Chow and Hale, page 130):

Definition V.16 (Condition C)

Let X be a Banach space and $f: X \to \mathbb{R}$ be C^1; f satisfies condition (C) if, for any sequence $\{v_n\} \subset X$ such that $|f(v_n)|$ is bounded and $|d_v f(v_n)| \to 0$ as $n \to \infty$, there exists a convergent subsequence of $\{v_n\}$.

Now it is to be shown that V defined in (V.31) satisfies the conditions of theorem V.15.
It is obvious that V is C^1 and bounded from below if $r_2 > 0$; since for $r_2 > 0$ there exists a constant $M_1 \geq 0$ such that

$$-\frac{1}{2}u^2 + \frac{1}{3}r_1u^3 + \frac{1}{4}r_2u^4 > -M_1 \text{ for all } u \in \mathbb{R}. \tag{V.47}$$

Hence $V(u) > -M_1 \cdot L$.
To prove condition (C) for V, assume $\{u_n\}$ is a sequence in $H^1_*(0,L)$ with $|V(u_n)|$ is bounded and $|d_u V(u_n)| \to 0$ if $n \to \infty$.
Let $M > 0$ such that $|V(u_n)| < M$, then one uses (V.47) again to find that

$$\int_0^L \frac{1}{2}\gamma |u_{nx}|^2 dx < M + M_1 \cdot L \tag{V.48}$$

where $u_{nx} := (\partial u_n / \partial x)$.
For functions $v \in H^1_o(0,L)$ Friedrich's inequality holds (Groesen, 1978):

$$\int_0^L u^2(x)dx \leq D\int_0^L \left|\frac{\partial u}{\partial x}\right|^2 dx \ , \ D > 0 \tag{V.49}$$

If $v \in H^1_o(0,L)$ then $v(0) = v(L) = 0$. Of course the inequality is true

if u is zero everywhere. A non-zero function $u \in H^1_*$ (with $\int_0^L u dx = 0$) must have a zero, say at $x = a$. Define a function v as an even extension of u in $x = 0$ and $x = L$ as follows: $v(x) = u(x)$ if $x \in [0,L]$, $v(x) = u(-x)$ if $x \in [-a,0]$ and $v(x) = u(2L-x)$ if $x \in [L,2L-a]$. Then the function v satisfies the condition of Friedrich's inequality and by the definition of v, Friedrich's inequality holds also for $u \in H^1_*$.

By equation (V.49) the norms generated by $\langle \cdot,\cdot \rangle_1$ and the inner product $\langle u,v \rangle_{x0} := \int u_x(x)v_x(x)dx$ are equivalent. So instead of $\langle \cdot,\cdot \rangle_1$ the inner product $\langle \cdot,\cdot \rangle_{x0}$ can be used on the function space H^1_*. Then by (V.48) the sequence $\{u_n\}$ is bounded in H^1_*.

Given the specific form of V, $\langle d_u V(u), v \rangle_{x0}$ can be written as:

$$\langle d_u V(u), v \rangle_{x0} = \gamma \langle u, v \rangle_{x0} - \langle Tu, v \rangle_{x0} \qquad \text{(V.50a)}$$

where T is a compact operator (see definition in Appendix E) defined by

$$\langle Tu, v \rangle_{x0} = \int u(x)v(x) - r_1 u^2(x)v(x) - r_2 u^3(x)v(x)\, dx \qquad \text{(V.50b)}$$

By the definition of a compact operator and since $\{u_n\}$ is bounded, the sequence $\{Tu_n\}$ contains a convergent subsequence (see Appendix E). Using in (V.50a) that $|d_u V(u_n)| \to 0$ if $n \to \infty$, implies that $\{u_n\}$ contains a convergent subsequence which proves condition (C) for V for $u \in H^1_*$.

Now theorem (V.15) is applicable; so V attains its minimum on $H^1_*(0,L)$ and hence on $H^2_*(0,L)$.

If the null solution is unstable then V(0) is not a minimum of V; so if $r_2 > 0$ then V attains its minimum for u not identical zero; since u belongs to $H^2_*(0,L)$ the function u can not be constant. Since $\frac{dV(u)}{dt} < 0$ if u is not a stationary solution (see V.34a and V.34b), the system (V.26a) must have a non-trivial stable stationary solution if V does not have a minimum at $u = 0$.

CHAPTER VI

BIFURCATION ANALYSIS

VI.1 Introduction

The object of this chapter is to introduce some general bifurcation analysis tools which are applicable to the anti-diffusion system. Let the general evolution equation be given as in chapter V

$$\frac{\partial u}{\partial t}(x,t) = G(u;\gamma) \qquad \text{(VI.1a)}$$

(γ is a parameter (vector) controlling the structure of G) defined on $D \subset \mathbb{R}^q$, with initial conditions

$$\forall x \in D : u(x,t_o) = u_o(x) \qquad \text{(VI.1b)}$$

and boundary conditions of

Dirichlet type: $\forall x \in \partial D \wedge \forall t \in \mathbb{R} : u(x,t) = c_o$ (VI.1c)

or of

Neumann type: $\forall x \in \partial D \wedge \forall t \in \mathbb{R} : \nabla_n u(x,t) = c_o$ (VI.1d)

where ∇_n is the spatial derivative in the direction of n, the normal to the boundary ∂D of D, and c_o is some constant.

In full generality bifurcation theory is concerned with the way the solutions of an equation (like VI.1a), involving a parameter, change in dependence of that parameter. One important topic is the way the set of equilibrium solutions, i.e. the solutions of $G(u;\gamma) = 0$, changes as γ varies, and which stability properties the various solutions have.

An evolution system such as (VI.1) can have many types of solutions: stationary (time independent) constant, space-periodic, time-periodic and so on. The set of solutions will as a rule depend on the parameter (vector) γ; the dependence on γ can involve (besides $G(u;\gamma)$) also the boundary conditions. In dependence on the parameter γ the nature of the set of equilibrium solutions can change, e.g. a stable one may become unstable, and new solutions may appear. In this section the main object is the study of stationary solutions of (VI.1) in dependence of the parameter γ. The basic references are Sattinger (1973) and Iooss et al. (1980).

An equilibrium solution is a pair (u,γ) satisfying (VI.1). Roughly speaking, *bifurcating solutions* are equilibrium solutions which form intersecting branches in a space $M\times\mathbb{R}$, where M is a suitable space of functions in which solutions lie. One equilibrium solution bifurcates from another at $\gamma = \gamma_c$ if there are two distinct branches of equilibrium solutions (u_1,γ) and (u_2,γ) of an evolution problem, continuous in γ and such that $(u_1,\gamma_c) = (u_2,\gamma_c)$. The point γ_c is called a bifurcation point. So bifurcation theory studies the relation between a (bifurcation) parameter and the equilibrium solutions, quantitatively and qualitatively.

Solutions will be real valued functions defined on a spatial domain $D \subset \mathbb{R}^q$, $q \in \mathbb{N}$. In general u will belong to a linear function space M supplemented with an appropriate norm $\|\cdot\|$. As a rule this space will be a Banach-space, see appendix E. As in chapter V, we will denote the derivative in u and γ by $d_u G$ respectively $d_\gamma G$.

The first question is to know under which conditions a solution (u_s,γ_s) is guaranteed not to be a bifurcation point, which means that (u_s,γ_s) lies on a unique simple curve (u,γ) of solutions for $\gamma_s - \delta < \gamma < \gamma_s + \delta$ with $\delta > 0$. The answer is given by a theorem based on the implicit function theorem.

Definition VI.1 (Iooss et al., 1980)

A *regular* point of $G(u;\gamma) = 0$ is one for which the implicit function theorem applies: $d_u G \neq 0$ or $d_\gamma G \neq 0$.

If (u_s,γ_s) is a regular point then we can find a unique curve $\gamma = \gamma(u)$ or $u = u(\gamma)$ through that point.

Definition VI.2 (Iooss et al., 1980)

A *singular* point of $G(u;\gamma) = 0$ is a point at which $d_u G = d_\gamma G = 0$.

Assuming branches of solutions bifurcate in a continuous way, the Lyapunov stability or instability of an equilibrium solution and bifurcation are strongly connected (however the instability of an equilibrium solution is not in all cases a necessary condition for bifurcation).

The following theorem relates the existence of bifurcating branches with the eigenvalues of the linearized system, i.e. the linear stability of an equilibrium solution. As in chapter V (see equation (V.11)) we assume that $u = u_s$ is a solution for all γ and replace u with $u - u_s$ to arrange the right hand side of (VI.1a) as

$$G(u;\gamma) = Bu - \gamma Au + N(u;\gamma) \tag{VI.2}$$

where B and A are linear maps from X to Z, with X, Z Banach spaces and N is nonlinear in u such that $N(0;\gamma) = 0$ and $d_u N(0;\gamma) = 0$. So $d_u G(0;\gamma) = B - \gamma A$.

The linear stability of the null solution is determined by the eigenvalues of $(B - \gamma A)$. If the null solution becomes unstable at $\gamma = \gamma_c$, then $\dim N(B - \gamma_c A) \geq 1$; γ_c is called an eigenvalue of (B,A) (Chow et al., 1982). ($N(C)$: null space of C; see appendix E). Suppose now this eigenvalue to be simple: $\dim N(B - \gamma_c A) = 1 = \operatorname{codim} R(B - \gamma_c A)$ ($\mathcal{R}$ is range) and $AN(B - \gamma_c A) \oplus R(B - \gamma_c A) = Z$ then the following theorem applies:

Theorem VI.3

Let X and Z be real (or complex) Banach spaces, Λ be an open set in $\mathbb{R}$ (or $\mathbb{C}$) and $G \in C^m(X \times \Lambda, Z)$, $m \geq 2$. Suppose that

$$G(u;\gamma) = Bu - \gamma Au + N(u;\gamma) \tag{VI.3a}$$

$$N(0,\gamma) = 0, \quad d_u N(0,\gamma) = 0. \tag{VI.3b}$$

If γ_c is a simple eigenvalue of (B,A) with eigenvector $u_o \neq 0$, then $(u,\gamma) = (0,\gamma_c)$ is a bifurcation point of $G(u;\gamma) = 0$.

Moreover, there exist C^{m-1} functions

$$\gamma(\varepsilon) = \gamma_c + O(|\varepsilon|) \tag{VI.4a}$$

$$u(\varepsilon) = \varepsilon u_o + O(\varepsilon^2) \tag{VI.4b}$$

for real ε near zero such that $G(u(\varepsilon);\gamma(\varepsilon)) \equiv 0$. All zeros of G near $(0,\gamma_c)$ are either the trivial solution $u = 0$ or given by (VI.4a-b). Finally, if G is an analytic function of u,γ near $(0,\gamma_c)$, then $u(\varepsilon),\gamma(\varepsilon)$ are analytic near zero.

Proof: see proof of Theorem 5.3, page 189 in Chow et al. (1982).

The branching solutions given by (VI.4a-b) can be constructed by expanding u and γ in powers of a small parameter ε, the so-called Poincaré-Lindstedt series (see Appendix A). This expansion gives information about the way the branches cross each other at the critical point which in turn defines the stability properties. These stability properties are summarized in the following definitions and theorems.

Definition VI.4 (Sattinger, 1973; Nicolis, 1981)

Consider two branches (u_s,γ) and (u_s^1,γ) depending on a scalar parameter γ, crossing each other at a critical point $\gamma = \gamma_c$ ($u_s = u_s^1$). Suppose that u_s is asymptotically stable for $\gamma > \gamma_c$. A solution $u(\gamma)$ is called :

- *subcritical* if it is branching for $\gamma > \gamma_c$
- *supercritical* if it is branching for $\gamma < \gamma_c$

and the branch (u_s^1,γ) is said to be a

- *subcritical branch* if all its elements (u_s^1,γ) are subcritical.
- *supercritical branch* if all its elements are supercritical.
- *transcritical branch* if some elements are sub- and other are supercritical.

As in most bifurcation studies and applications the crossing of the eigenvalue is (assumed to be) strict:

Definition VI.5

If the branch (u_s,γ) becomes unstable because of an eigenvalue $\omega_c(\gamma)$ crossing zero, this bifurcation is called *transverse* if

$$\mathrm{Re}\ \frac{d\omega_c}{d\gamma}(\gamma_c) \neq 0. \qquad \text{(VI.5)}$$

Condition (VI.5) is called the *transversality condition* and the eigenvalue *transverse*.

Definition VI.6

A *double* point of the curve $G(u;\gamma) = 0$ is a singular point through which pass two and only two branches of $G(u;\gamma) = 0$ possessing distinct tangents (Iooss et al., 1980).

Definition VI.7

A *regular turning* point is a point at which $d_u\gamma(u)$ changes sign and $d_\gamma G(u;\gamma) \neq 0$ (see figure VI.1b below where the branch bifurcating from the null solution has a regular turning point.) (Iooss et al., 1980.)

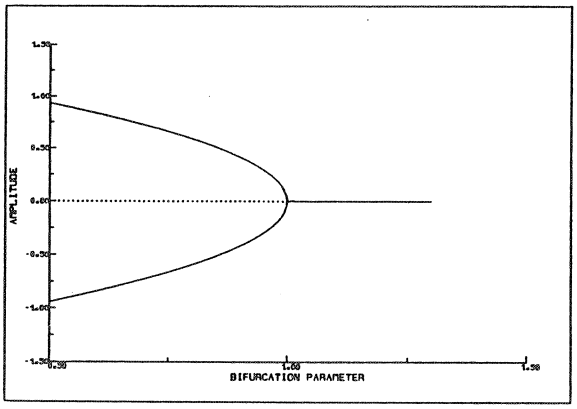


Figure VI.1a:
Supercritical branching from the null solution at a singular double point (0,1).

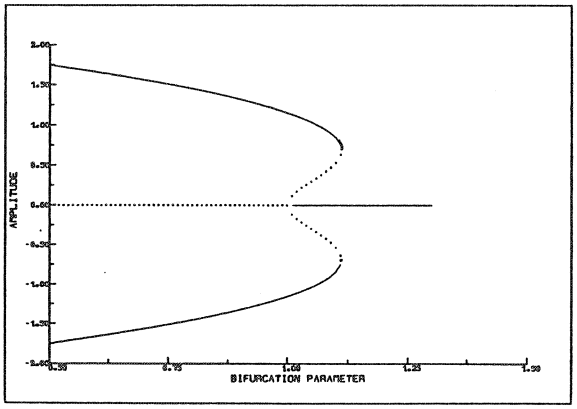


Figure VI.1b:
Subcritical branching from the null solution.
Also depicted are regular turning points where the unstable bifurcating branch becomes stable.

Definition VI.8

A *singular double* point of the curve $G(u;\gamma) = 0$ is a double point at which $d_u\gamma(u)$ changes sign on one branch (see figure VI.1a-b where the bifurcation from the null solution occurs at a singular double point.) (Iooss et al., 1980.)

The exchange of stability at a double point (where only two branches intersect) can now be formulated by the following theorem. See Sattinger (1973) and Iooss et al., (1980); see also appendix A where the exchange of stability is calculated for the anti-diffusion system.

Theorem VI.9

If a branch (u_s,γ) which is asymptotically stable for $\gamma < \gamma_c$, looses its stability at a simple critical point because of a transverse eigenvalue $\omega_c(\gamma)$ crossing the imaginary axis, then:

1) supercritical bifurcating branches are stable and subcritical are unstable.

2) bifurcating solutions from a stationary state will be stationary if $Im(\omega_c(\gamma_c)) = 0$ and time periodic if $Im(\omega_c(\gamma_c)) \neq 0$.

Figure VI.1 gives an illustration of these notions applied to the null solution of the anti-diffusion model.

VI.2 The anti-diffusion equation, stability and bifurcation from the null solution

The anti-diffusion system equations defined for $x \in [0,L] \subset \mathbb{R}$ are (see Chapter III, equation III.2)

$$\frac{\partial u}{\partial t} = \frac{\partial^2}{\partial x^2}\left[\phi(u) - \gamma\frac{\partial^2 u}{\partial x^2}\right], \quad \gamma > 0 \tag{VI.6a}$$

and

$$\phi(u) = -u + r_1u^2 + r_2u^3 \text{ with } r_2 > 0. \tag{VI.6b}$$

No-flux boundary conditions are assumed.

If at initial time $t = 0$, $\int u(x,0)\,dx = 0$, then the mass conserving property is expressed by:

$$\int u(x,t)dx = 0 \text{ for } \forall\ t \in \mathbb{R} \tag{VI.6c}$$

The solution space is a linear subspace L^2_* of L^2 which is defined by

$$L^2_* = \left\{ u \in L^2 \mid \langle 1,u\rangle_o = 0 \right\} \tag{VI.7}$$

and $\langle u,v\rangle_o = \int uv\,dx$. Suitable differentiation conditions define the specific solution space.

With initial condition (VI.6c) the null function $u(x) = 0$ is a stationary solution of system (VI.6a). Linearizing the right hand side of (VI.6a) in $u = 0$ gives:

$$\frac{\partial v}{\partial t} = \frac{\partial^2}{\partial x^2}\left[\phi'(0)v - \gamma\frac{\partial^2 v}{\partial x^2}\right] \tag{VI.8}$$

where $\phi'(0)$ is the derivative of ϕ in $u = 0$; so $\phi'(0) = -1$ in the case of (VI.6b). Define:

$$L(\gamma) = \frac{\partial^2}{\partial x^2}\left[\phi'(0) - \gamma\frac{\partial^2}{\partial x^2}\right] \tag{VI.9}$$

Note that $L = B - \gamma A$ with $Bv = \frac{\partial^2}{\partial x^2}\phi'(0)v$ and $Av = \frac{\partial^4}{\partial x^4}v$.

The eigenmodes (vectors) of the operator $\frac{\partial^2}{\partial x^2}$ form an orthonormal and complete set in L^2 (see appendix E (E.12)):

$$u_k(x) = \cos\left(\frac{k\pi x}{L}\right)/N_k \quad \text{for } k = 0,\ 1,\ 2.... \tag{VI.10a}$$

where N_k is given by some normalization.

For u with $\int u dx = 0$, $k = 0$ is excluded. Hence the eigenmodes of $L(\gamma)$ are also given by (VI.10a) with $k \neq 0$. And the eigenvalues of the operator $L(\gamma)$ are:

$$\omega_k(\gamma) = p_k^2\left[-\phi'(0) - \gamma\ p_k^2\right] \tag{VI.10b}$$

where

$$p_k^2 = \left(\frac{k\pi}{L}\right)^2,\ k = 1,2,..... \tag{VI.10c}$$

Applying the principle of linearized stability (see theorem V.6 in chapter V) the stability of the null solution depends on the sign of

the eigenvalues (see also theorem V.14, chapter V). Since the zero eigenvalue is simple, using (VI.10b) in relation to the theorems of the foregoing section, the linear stability properties of the null solution are easily established. The following theorem is a summary of the qualitative properties of the null solution and bifurcating branches.

Theorem VI.10

If $\phi'(0) = -1$ then the stability properties of the null solution of system (VI.6) are as follows:

a) if $\gamma \leq 0$ then all eigenvalues ω_k (VI.10b) are positive. The null solution is unstable in all eigenmodes. The eigenvalues are monotone increasing functions of k.

b) if $\gamma > \frac{L^2}{\pi^2}$ then all eigenvalues ω_k are negative. The null solution is stable.

c) if $0 < \gamma < \frac{L^2}{\pi^2}$ then

c1) there are a finite number R of positive eigenvalues ω_k with $1 \leq k \leq R$, $k \in \mathbb{N}$ and R the largest integer such that $\gamma\left(\frac{R\pi}{L}\right)^2 < 1$.

c2) there exist a maximal eigenvalue ω_m; the maximal eigenvalue is reached for a finite frequency (non-zero wave length). (VI.11)

Note that the maximal eigenvalue ω_m is not necessarily given for m = 1. This is specific for the anti-diffusion system. For the migration mass-conserving systems as formulated in chapter IV, we will find that this maximal eigenvalue is always given for m = 1 (see Appendix A).
A zero eigenvalue is simple and with (VI.8), theorem (VI.3) applies to the null solution of (VI.6): for each γ_c such that one of the eigenvalues (VI.10b) becomes zero, the point $(0,\gamma_c)$ is a bifurcation point. Furthermore this bifurcation is transverse:

$$\frac{d\omega_k}{d\gamma} = -p_k^4 = -\left(\frac{k\pi}{L}\right)^4, \quad k = 1,2,..$$

To apply theorem (VI.9) the direction of the bifurcating branch must be known. To this end the equations (VI.4a-b) are constructed by means of the Poincaré-Lindstedt series (Sattinger, 1973). These series are

described in terms of a decomposition consisting of the null-space of the linear operator $L(\gamma_c)$ defined in (VI.9) and a part perpendicular to the null space of the adjoint operator of $L(\gamma_c)$, which in this case is $L(\gamma_c)$ itself again. The method of finding the elements of the decomposition is the infinite dimensional analogy from the following finite dimensional problem: for which $y \in \mathbb{R}^N$ does equation $Ax = y$ with A a singular linear transformation from $\mathbb{R}^N$ to $\mathbb{R}^N$, have a solution?The condition is, of course, that $y \in R(A)$, the range of A and this condition is equivalent with the condition that y must be perpendicular to the null space $N(A^T)$ of A^T: if y has a solution x then $\langle Ax, z\rangle = \langle y, z\rangle$ for all $z \in \mathbb{R}^N$; if $z \in N(A^T)$, the null space of A^T, one must have $\langle x, 0\rangle = \langle x, A^T z\rangle = \langle y, z\rangle$, hence $\langle y, z\rangle = 0$. For infinite dimensional problems the solvability condition is given by a condition similar to the Fredholm alternative (see appendix E).
In Appendix A, section 2, the solutions for small ε, are calculated for the anti-diffusion system. The solutions are:

$$u(x) = \pm\beta\cos(p_k x) - \frac{r_1}{6}\beta^2\cos(2p_k x) + O(\varepsilon^2) \qquad \text{(VI.12a)}$$

where

$$\beta^2 = -p_k^4(\gamma - \gamma_c)/(\tfrac{1}{6}r_1^2 - \tfrac{3}{4}r_2) \qquad \text{(VI.12b)}$$

with

$$\gamma_c = \left(\frac{k\pi}{L}\right)^{-2} \qquad \text{(VI.12c)}$$

The sign of the denominator in (VI.12b) gives the bifurcation direction. For negative r_2 the bifurcation is always subcritical (the bifurcating solution is unstable); for r_2 positive both cases can occur: restricting to $r_2 = 1$, the bifurcation is supercritical if $r_1^2 < \frac{9}{2}$, and subcritical for $r_1^2 > \frac{9}{2}$. The stability properties of the bifurcating branch follow from Theorem VI.9 (see also section A.2 of Appendix A).

VI.3 Wave amplitude equations

As mentioned above, the eigenmodes (eigenvectors) of the linearized anti-diffusion system

$$d_u G(0;\gamma)v = \frac{\partial^2}{\partial x^2}\left[\phi'(0)v - \gamma\frac{\partial^2}{\partial x^2}v\right] \qquad (VI.13)$$

form an orthonormal basis of L^2. The eigenvectors are given by (VI.10a). This gives the possibility to perform some Fourier analysis. By restricting to only three modes k, 2k and 4k (and neglecting all other modes), a closed form for the evolution equations of the amplitudes of these three modes k, 2k and 4k is derived. This reduced system can still give important information about the behavior of the original complete system. (The well known Lorenz system was also derived as a truncation of a partial differential equation for fluid convection (Holden et al., (1986)).

For a two mode system (k,2k) the equilibrium points are calculated; as is the stability of these solutions. It is shown that bifurcation qualities are similar to those derived in appendix A for the whole system.

Let $\phi'(0) = -1$ and assume a deviation u(x,t) from the null solution in the following form:

$$u(x,t) = \sum_{n=-\infty}^{\infty} a_n(t)\cos(n\pi x/L) \qquad (VI.14a)$$

with $a_n(t) \in \mathbb{R}$, $a_0(t) = 0$ and $a_{-n}(t) = a_n(t)$ for all t. These conditions on a_n are compatible with the mass-conserving quality of the anti-diffusion system and with the no-flux boundary conditions. Inserting (VI.14a) in (VI.6a) with (VI.6b) gives the evolution equations for the amplitudes a_n:

$$\dot{a}_n = \left\{(1 - \gamma p_n^2)a_n + \tfrac{1}{2}r_1\left(\sum_{l+k=n} a_l a_k\right) + \tfrac{1}{4}r_2\left(\sum_{l+k+m=n} a_l a_k a_m\right)\right\}p_n^2 \qquad (VI.14b)$$

where $p_n = n\pi/L$. Define V: $(..,a_{-2},a_{-1},a_0,a_1,a_2,...) \to \mathbb{R}$ as follows:

$$V = \sum_{n=-\infty}^{\infty}\left\{-\tfrac{1}{2}(1 - \gamma p_n^2)a_n^2 + \tfrac{1}{6}r_1\left(\sum_{l+k=n} a_l a_k a_n\right) + \tfrac{1}{16}r_2\left(\sum_{l+k+m=n} a_l a_k a_m a_n\right)\right. \qquad (VI.15)$$

So we find that

$$\dot{a}_n(t) = -V_n p_n^2, \qquad n = ...,-2,-1,1,2,... \qquad (VI.16)$$

where V_n is the partial derivative of V with respect to a_n. Since

$$\frac{dV}{dt} = \sum_{n=-\infty}^{\infty} V_n \dot{a}_n = \sum_{n=-\infty}^{\infty} -V_n^2 p_n^2 \leq 0 \qquad \text{(VI.17a)}$$

and

$$\frac{dV}{dt} = 0 \iff V_n^2 = 0 \text{ for all } n, \qquad \text{(VI.17b)}$$

the functional V is a Lyapunov function.

In the following all modes except a_k, a_{-k}, a_{2k}, a_{-2k}, a_{4k} and a_{-4k}, are set to zero. Since $a_{-n} = a_n$ we need only to consider the modes k, 2k and 4k. Introduce the notations:

$$a_1(t) = a_k(t),\ a_2(t) = a_{2k}(t) \text{ and } a_4(t) = a_{4k}(t) \qquad \text{(VI.18a)}$$

$$\gamma_o = \gamma\, p_k^2 \qquad \text{(VI.18b)}$$

($\gamma_o = 1$ means that $d_u G$ has a (simple) eigenvalue with eigenvector $\cos(k\pi x/L)$.) Then we find the following evolution equations:

$$\dot{a}_1 = \Big\{a_1 - \gamma_o a_1 - a_1 a_2 r_1 - \tfrac{3}{4} a_1^3 r_2 - \tfrac{3}{2} a_1 a_2 a_4 r_2 - \tfrac{3}{2} a_1 a_2^2 r_2 + -\tfrac{3}{2} a_1 a_4^2 r_2\Big\} p_k^2 \qquad \text{(VI.19a)}$$

$$\dot{a}_2 = \Big\{4a_2 - 16\gamma_o a_2 - 2a_1^2 r_1 - 4a_2 a_4 r_1 - 6a_1^2 a_2 r_2 - 3a_2^3 r_2 + -3a_1^2 a_4 r_2 - 6a_2 a_4^2 r_2\Big\} p_k^2 \qquad \text{(VI.19b)}$$

$$\dot{a}_4 = \Big\{16a_4 - 256\gamma_o a_4 - 8a_2^2 r_1 - 12a_1^2 a_2 r_2 - 24a_1^2 a_4 r_2 + -24a_2^2 a_4 r_2 - 12a_4^3 r_2\Big\} p_k^2 \qquad \text{(VI.19c)}$$

Stationary solutions (a_1, a_2, a_4) are stable if (a_1, a_2, a_4) is a minimum of V (defined in (VI.15) with the first summation only over -k, k, -2k, -2k, -4k, 4k). In particular the null solution is unstable if $\gamma_o < 1$. Furthermore: if $r_2 > 0$ then V is bounded from below and $V \to \infty$ if $|a_1| + |a_2| + |a_3| \to \infty$; V is continuous, so V attains a (finite) absolute minimum which gives the global existence of a stable stationary solution of the system (VI.19a-c) and the following theorem:

Theorem VI.11

If $r_2 > 0$ and $\gamma_o < 1$ then the three wave amplitude equations system (VI.19a-c) has a non-trivial stable solution $(a_1, a_2, a_4) \neq (0,0,0)$.

If $r_2 < 0$ then V is unbounded from below.

Solutions sets with $(a_1, a_2, 0)$ and $(0, a_2, a_4)$ are qualitative the same: given $\gamma_o = \gamma_{o1} \in \mathbb{R}$ the number of solutions, stability and bifurcation direction of solutions $(a_1, a_2, 0)$ are the same as for solutions $(0, a_2, a_4)$ with $\gamma_o = \frac{1}{4}\gamma_{o1} \in \mathbb{R}$.

In the following the evolution of two modes is studied: $a_4(t)$ is set to zero for all $t \in \mathbb{R}$. Then stationary solutions (a_1, a_2) are given by:

$$a_1 - \gamma_o a_1 - a_1 a_2 r_1 - \tfrac{3}{4} a_1^3 r_2 - \tfrac{3}{2} a_1 a_2^2 r_2 = 0 \qquad \text{(VI.20a)}$$

and

$$4a_2 - 16\gamma_o a_2 - 2a_1^2 r_1 - 6a_1^2 a_2 r_2 - 3a_2^3 r_2 = 0 \qquad \text{(VI.20b)}$$

If $r_2 \neq 0$ then the solutions belong to sets S_1 with:

$$S_1 = \left\{ (a_1, a_2) \,\middle|\, (a_1, a_2) = (0,0) \right\} \qquad \text{(VI.21a)}$$

$$S_2 = \left\{ (a_1, a_2) \,\middle|\, (a_1, a_2^2) = (0, \tfrac{4}{3r_2}(1-4\gamma_o)) \right\} \qquad \text{(VI.21b)}$$

$$S_3 = \left\{ (a_1, a_2) \,\middle|\, a_1^2 = \tfrac{4}{3r_2}\left(1 - \gamma_o - a_2 r_1 - \tfrac{3}{2} a_2^2 r_2\right) \;\&\; 9r_2 a_2^3 + 12 r_1 a_2^2 + \left(-4 - 8\gamma_o + \tfrac{8r_1^2}{3r_2}\right) - \tfrac{8r_1}{3r_2}(1 - \gamma_o) = 0 \right\} \qquad \text{(VI.21c)}$$

For this two wave system the following theorems can be formulated. To illustrate the theorems we give a set of figures which display the relation between a_2 and γ_o. Also is displayed the relation between γ_o and a quantity called 'amplitude'; this last quantity is defined as $\pm\sqrt{(a_1^2 + a_2^2)}$ where the minus sign is chosen if $a_2 < 0$. Unstable branches are depicted as small dots, stable branches as continuous lines.

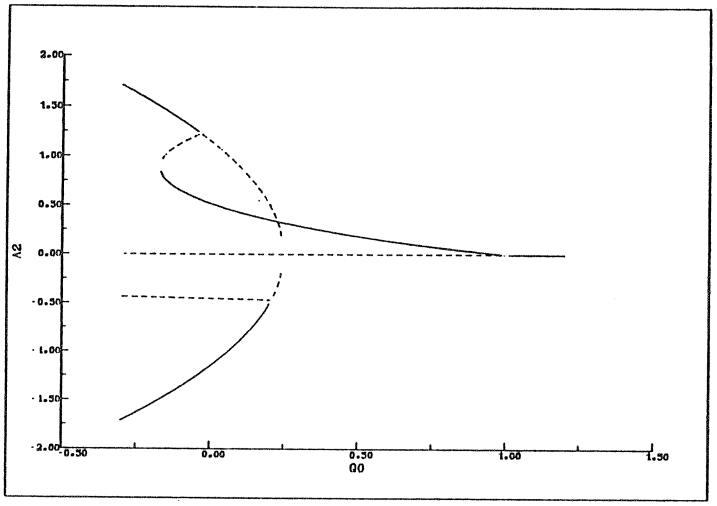


Figure VI.2a: parameters $r_1 = -1$, $r_2 = 1$. Relation between a_2 and γ_o.

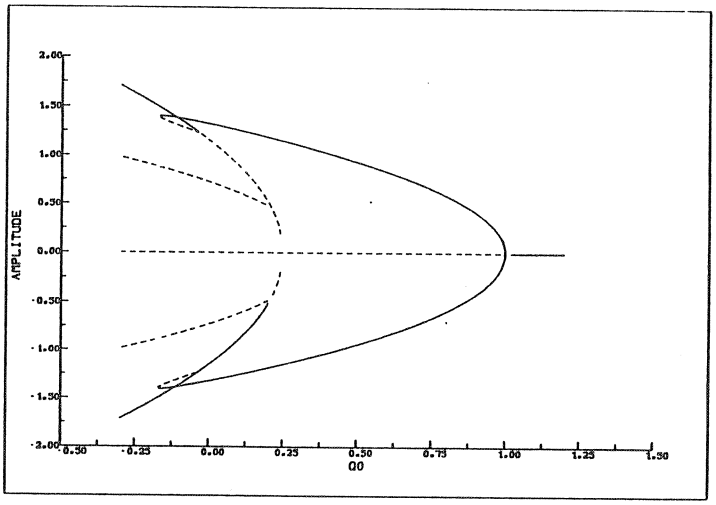


Figure VI.2b: parameters $r_1 = -1$, $r_2 = 1$. Relation between amplitude and γ_o.

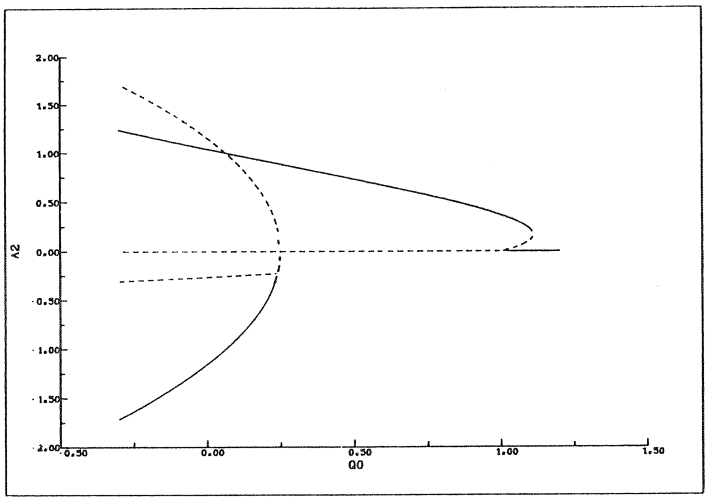


Figure VI.3a: parameters $r_1 = -3$, $r_2 = 1$. Relation between a_2 and γ_o.

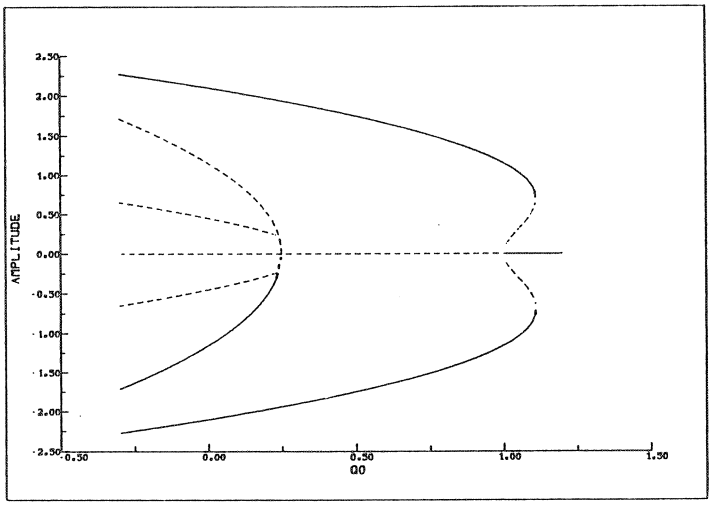


Figure VI.3b: parameters $r_1 = -3$, $r_2 = 1$. Relation between amplitude and γ_o.

Theorem VI.12

The bifurcation from the null solution at $\gamma_o = 1$ is subcritical if $r_1^2 \geq \frac{9}{2}r_2$; supercritical if $r_1^2 < \frac{9}{2}r_2$.

Proof: see appendix B, paragraph 1, Theorem B.1. (See figure VI.2a-b and VI.3a-b.)

Theorem VI.13

If $r_2 > 0$ and $r_1^2 \geq \frac{9}{2}r_2$ the branch, bifurcating subcritically from the null solution at $\gamma_o = 1$, has a turning point and becomes stable.

Proof: see appendix B, section 3, theorem B.2. (See figure VI.3a-b.)

Theorem VI.14

If $r_2 < 0$ then every non-trivial solution $(a_1, a_2) \neq (0,0)$ is unstable.

Proof: see appendix B, section 2. (See figure VI.4a-b.)

Theorem VI.14 means that for $r_2 < 0$, if the null solution becomes unstable, the solutions become unbounded. (The functional V is unbounded from below and $\frac{dV}{dt}(a_1, a_2) < 0$ if (a_1, a_2) is not a stationary solution, see (VI.18a-b).)

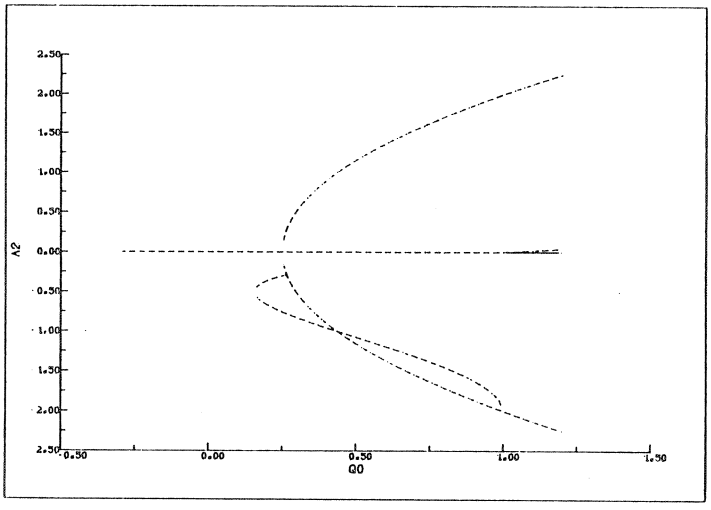


Figure VI.4a: parameters $r_1 = -3$, $r_2 = -1$. Relation between a_2 and γ_o.

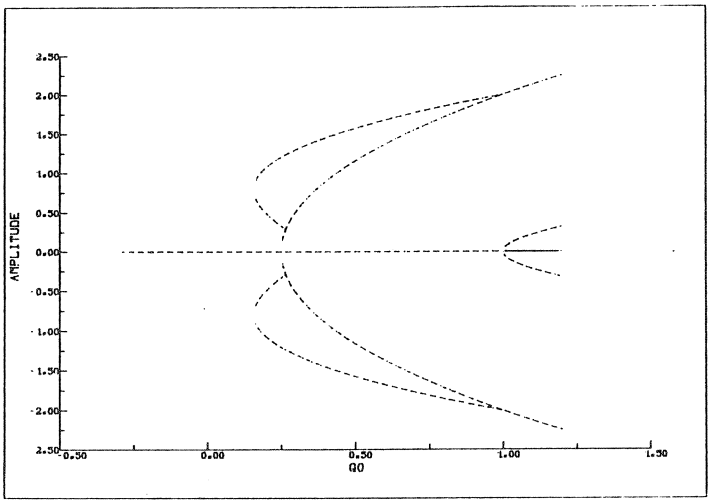


Figure VI.4b: parameters $r_1 = -3$, $r_2 = -1$. Relation between amplitude and γ_o.

CHAPTER VII

NON CONSTANT STATIONARY SOLUTIONS

VII.1 Introduction

In this chapter some analytic solutions of the anti-diffusion equation are introduced but none of the solutions satisfy completely the conditions of the system as formulated in Chapter II. Some solutions are only valid for an infinite spatial domain.
The second part deals with the stability of non-constant stationary solutions. In contrast with the standard reaction-diffusion equation, non-constant monotone solutions can be stable; however, these are also the only ones.
In the final section 5 the anti-diffusion equation is compared with the Swift-Hohenberg equation.

VII.2 Analytic stationary solutions of the anti-diffusion equation

For the evolution equations defined in Chapter II, equation (II.18), stationary solutions must satisfy:

$$\frac{\partial^2}{\partial x^2}\left[\phi(u) - \frac{\partial^2 u}{\partial x^2}\right] = 0 \qquad \text{(VII.1a)}$$

with the boundary conditions

$$\frac{\partial u}{\partial x}\Big|_{x=0,L} = \frac{\partial^3 u}{\partial x^3}\Big|_{x=0,L} = 0 \qquad \text{(VII.1b)}$$

and

$$\int_0^L u(x)dx = 0 \qquad \text{(VII.1c)}$$

where

$$\phi(u) = -u + r_1 u^2 + r_2 u^3 \qquad \text{(VII.1d)}$$

Hence, given the boundary conditions, a stationary solution must satisfy (VII.1c) and

$$\phi(u) - \gamma u_{xx} = \beta \qquad \text{(VII.1e)}$$

where $u_{xx} = \frac{\partial^2 u}{\partial x^2}$ and $\beta = \int_0^L \phi(u)dx$, see Chapter III, equation (III.3))
If v(x) is a solution of

$$c_1 v + c_2 v^2 + c_3 v^3 - \gamma v_{xx} = 0 \qquad \text{(VII.2a)}$$

with

$$\frac{\partial v}{\partial x}\Big|_{x=0,L} = 0 \qquad \text{(VII.2b)}$$

then $u = v + \delta$ with $\delta = -\frac{1}{L}\int v(x)dx$, is a solution of (VII.1) if

$$\beta = -\delta + r_1\delta^2 + r_2\delta^3 = \phi(\delta) \qquad \text{(VII.3a)}$$
$$c_1 = -1 + 2r_1\delta + 3r_2\delta^2 = \phi'(\delta) \qquad \text{(VII.3b)}$$
$$c_2 = r_1 + 3r_2\delta = \tfrac{1}{2}\phi''(\delta) \qquad \text{(VII.3c)}$$
$$c_3 = r_2 = \tfrac{1}{6}\phi'''(\delta) \qquad \text{(VII.3d)}$$

A first set of solutions of (VII.2) is of the form:

$$v(x) = \frac{1}{a + b\cos(p_k x)} \qquad \text{(VII.4a)}$$

with

$$p_k = k\pi/L \qquad \text{(VII.4b)}$$
$$c_1 = -\gamma p_k^2 \qquad \text{(VII.4c)}$$
$$c_2 = -3c_1 a \qquad \text{(VII.4d)}$$
$$c_3 = 2c_1(a^2 - b^2) \qquad \text{(VII.4e)}$$

This solution (VII.4) is bounded iff $a^2 > b^2$. However for $\gamma > 0$, c_1 must be negative. So the solutions are unbounded if $c_3 > 0$ which

coincides with $r_2 > 0$.

A second set of solutions is given by:

$$v(x) = \frac{1}{a + b\cosh(p_k x)} \qquad \text{(VII.5a)}$$

with

$$c_1 = \gamma p_k^2 \qquad \text{(VII.5b)}$$

$$c_2 = -3c_1 a \qquad \text{(VII.5c)}$$

$$c_3 = 2c_1(a^2 + b^2) \qquad \text{(VII.5d)}$$

Bounded solutions are possible for $c_3 > 0$. However in this case the boundary condition is not satisfied. The solution (VII.5) is valid for an infinite spatial domain.

For a, b > 0, by the translation $v \to v + \delta = u$,

$$u(0) = \frac{1}{a + b} + \delta \text{ and } u \to \delta \text{ if } |x| \to \infty.$$

Then, if a = 3b, the solution satisfies exactly the lower/upperbounds for stationary solution defined in chapter III, see (III.8c); thus $\phi'(u(0)) = \phi'(\delta)$ and $\phi(u(0)) = \phi(\delta)$. Note that also $\phi'(\delta) > 0$.

The same sort of incompatibility of analytic solutions is found in Tsakalakos and Dugan (1985): the solution is given as

$$v(x) = (1 - \mu^2)^{1/2}\mathrm{sn}[(1 + \mu^2)^{1/2}] \qquad \text{(VII.6a)}$$

where sn is the Jacobian elliptic function, periodic with wave length:

$$\lambda = 4(1 + \mu^2)^{-1/2}K(k^2) \qquad \text{(VII.6b)}$$

and $k^2 = (1 - \mu^2)/(1 + \mu^2)$ with K the complete elliptic integral of the first kind (Cayley, 1956).

Equation (VII.6a) does not satisfy the boundary condition; if in (VII.6a) sn(·) is replaced by cn(·) then the boundary condition is satisfied; however, at the same time c_3 (r_2) must be negative.

The function (VII.4) and (VII.5) are particular forms of (VII.6): if $k^2 = 1$, then sn(z) = tanh(z); if $k^2 = 0$ then sn(z) = sin(z).

VII.3 Eigenvalues of a linear anti-diffusion system

Let $u_o(x)$ be a stationary solution of the anti-diffusion equation (VII.1). Linearization of the anti-diffusion equation in $u = u_o$ gives:

$$\frac{\partial v}{\partial t} = \frac{\partial^2}{\partial x^2}\left(\phi'(u_o)v - \gamma \frac{\partial^2 v}{\partial x^2}\right) \qquad \text{(VII.7)}$$

with $\phi'(u_o) = \left.\frac{d\phi}{du}\right|_{u=u_o}$.

Defining the operator K by

$$Kv = -\frac{\partial^2}{\partial x^2}v \qquad \text{(VII.8a)}$$

and the operator H by

$$Hv = \phi'(u_o)v - \gamma \frac{\partial^2 v}{\partial x^2} \qquad \text{(VII.8b)}$$

we can write (VII.7) as

$$\frac{\partial v}{\partial t} = -KHv \qquad \text{(VII.8c)}$$

As shown in chapter V, section 4 the stability of the stationary solution u_o depends on the eigenvalues of the Sturm-Liouville problem:

$$\gamma \frac{\partial^2 v}{\partial x^2} + (\lambda - \phi'(u_o))v = 0, \quad v \in C^2([0,L]) \cap H^1_*(0,L) \qquad \text{(VII.9)}$$

with no-flux boundary conditions. The elements of H^1_* are functions which have square integrable generalized first derivatives and which are orthogonal to the constant function $u(x) = 1$ for all x, hence if $v \in H^1_*$ then $\int v(x)dx = 0$. Denoting the smallest eigenvalue by λ_1^* then the solution u_o is stable if λ_1^* is positive.

With respect to a standard reaction-diffusion system

$$\frac{\partial u}{\partial t} = -\phi(u) + \gamma \frac{\partial^2 u}{\partial x^2} \qquad \text{(VII.10)}$$

we note the following: assume $u = u_o$ is a stationary solution of (VII.10) then the stability of this solution depends on the sign of the minimal eigenvalue λ_o of the following eigenvalue problem:

$$\gamma \frac{\partial^2 v}{\partial x^2} + (\lambda - \phi'(u_o))v = 0, \quad v \in C^2([0,L]) \cap H^1(0,L) \qquad \text{(VII.11)}$$

where H^1 is the space of function which have square integrable generalized first derivatives (see chapter V, section 4). But in contrast to the eigenvalue problem (VII.9), eigenvectors with $\int v(x)dx \neq 0$ are allowed. In the variational formulation the smallest eigenvalue λ_o is given by:

$$\lambda_0 = \inf_{v \in H^1} \frac{\int \phi'(u_o)v^2 + \gamma v_x^2 \, dx}{\int v^2 \, dx} \qquad \text{(VII.12)}$$

where the infimum is taken over all $v \in H^1(0,L)$.
And the next eigenvalue λ_1 is given by:

$$\lambda_1 = \inf_{\substack{v \in H^1 \\ <v, v_0>_1 = 0}} \frac{\int \phi'(u_o)v^2 + \gamma v_x^2 \, dx}{\int v^2 \, dx}$$

where v_o is an eigenvector corresponding with λ_o. And so on. ($<\cdot,\cdot>_1$ is the inner product in H^1.) In this way a set of orthogonal eigenvectors is obtained such that $\lambda_o \leq \lambda_1 \leq \lambda_2 \leq \lambda_3 \ldots$ (Reid, 1980).
This construction procedure is based on the orthogonal decomposition of the domain X of an operator T with only isolated eigenvalues in subspaces M^i where $T_{M^i} \subset T$ has only one eigenvalue (see appendix E).

Similar the smallest eigenvalue λ_1^* of the eigenvalue problem (VII.9) is given by

$$\lambda_1^* = \inf_{v \in H_*^1} \frac{\int \phi'(u_o)v^2 + \gamma v_x^2 \, dx}{\int v^2 \, dx} \qquad \text{(VII.13)}$$

where the infimum is taken over all $v \in H_*^1$. And the next eigenvalue λ_2^* is given by:

$$\lambda_2^* = \inf_{\substack{v \in H_*^1 \\ <v, v_1>_1 = 0}} \frac{\int \phi'(u_o)v^2 + \gamma v_x^2 \, dx}{\int v^2 \, dx}$$

where v_1 is an eigenvector corresponding with λ_1^*. And so on. And similar as above a set of orthogonal eigenvectors can be obtained such that $\lambda_1^* \leq \lambda_2^* \leq \lambda_3^* \ldots$

The general form of a Sturm-Liouville problem is:

$$Lu = (p(x)u')' + g(x)u = 0 \qquad (a < x < b) \tag{VII.14}$$

where primes denote derivatives with respect to x; $p(x) > 0$ all x and p, p' and g are continuous on (a,b). (Coddington & Levinson, (1955)). Two theorems with respect to the Sturm-Liouville problem will be used. Therefore the following notations and notions are introduced. Let

$$p(x)u' = w \text{ and } w' = -g(x)u \tag{VII.15}$$

Let

$$u = r\sin(\theta) \text{ and } w = r\cos(\theta) \tag{VII.16}$$

Then the following differential equations are derived from (VII.14):

$$r' = \left(\frac{1}{p} - g\right) r \sin(\theta).\cos(\theta) \tag{VII.17}$$

$$\theta' = \frac{1}{p}\cos^2(\theta) + g\sin(\theta) \tag{VII.18}$$

Let ν a solution of (VII.14) then there is a solution $r = \rho(x)$ and $\theta = \omega(x)$ of (VII.17), (VII.18) with

$$\rho^2 = (p\nu')^2 + \nu^2 \text{ and } \omega = \tan^{-1}\left(\frac{\nu}{p\nu'}\right).$$

Since ν and ν' do not vanish simultaneously (ν is not trivial), it follows that $\rho^2(x) > 0$ on (a,b); it is assumed that $\rho(x) > 0$. Consequently $\nu(x) = \rho(x)\sin(\omega(x))$ can only vanish where $\omega(x)$ is an integer multiple of π.

Theorem VII.1 (Comparison Theorem.)

Let $L_1u = (p_1u')' + g_1u = 0$, $i = 1,2$.
Let p_1, g_1 piecewise continuous on [a,b], and let
$0 < p_2(x) \leq p_1(x)$, and $g_2(x) \geq g_1(x)$ on [a,b].
Let $L_1\nu_1 = 0$ and $L_2\nu_2 = 0$ with $\omega_2(a) \geq \omega_1(a)$.
Then $\omega_2(x) \geq \omega_1(x)$ on [a,b].
If $g_2 > g_1$ on (a,b) then $\omega_2(x) > \omega_1(x)$ on $a < x \leq b$.

Proof: see Theorem 1.2, Ch. 8 of Coddington e.a. (1955).

Let

$$Lu = (pu')' + (\lambda r - q)u = 0. \qquad \text{(VII.19)}$$

where $\lambda \in \mathbb{R}$, p', r and q are real and continuous over $[a,b]$ and $p > 0$, $r > 0$ over $[a,b]$.
Given $\alpha, \beta \in \mathbb{R}$, the values λ for which there is a solution u, not trivial, of (VII.19) satisfying :

$$u(a)\cos\alpha - p(a)u'(a)\sin\alpha = 0 \qquad \text{(VII.20)}$$

$$u(b)\cos\beta - p(b)u'(b)\sin\beta = 0 \qquad \text{(VII.21)}$$

are called eigenvalues.

Theorem VII.2 (Existence of eigenvalues.)
There are infinitely many eigenvalues $\lambda_0, \lambda_1, \ldots$ of (VII.19) forming a monotone increasing sequence with $\lambda_n \to \infty$ as $n \to \infty$. Moreover the eigenfunction corresponding to λ_n has exactly n zero's on (a,b).

Proof: see Theorem 2.1 Ch.8 of Coddington e.a. (1955).

Denote $(\lambda r(x)-q(x))$ by $g(x,\lambda)$ and the corresponding polar coordinates of the solution by $\rho(x,\lambda)$ and $\omega(x,\lambda)$.
Fixing the left boundary, $\omega(a,\lambda) = \omega_c$ for each λ, then holds:

i) $\theta = \omega(x,\lambda)$ is, for fixed x, a monotone increasing function of λ. (see theorem VII.1.)

ii) If $\omega = 0 (\text{mod } \pi)$ then $\omega' > 0$. (see (VII.18)).

VII.4 Instability of non-monotone, non-constant stationary solutions of an anti-diffusion equation

The no-flux boundary eigenvalue problem (VII.11) is a Sturm-Liouville problem with $p(x) = \gamma$ ($\gamma > 0$), $a = 0$ and $b = L$.
The principal observation is that if u_o is a non-constant stationary solution of the anti-diffusion equation (VII.1a-c) then

$v = u_{ox} = \partial u_o/\partial x$ is a solution of (VII.11) with $\lambda = 0$. However, $v = u_{ox}$ does not satisfy the no-flux boundary condition; u_{ox} is an eigenvector with eigenvalue 0 with Dirichlet boundary conditions. But the smallest eigenvalue of the no-flux boundary problem (VII.11) is smaller than the smallest eigenvalue of the corresponding Dirichlet problem (Coddington e.a., 1955). This gives directly the instability of non-constant solutions of a reaction-diffusion equation with constant diffusion coefficient.

Now suppose u_o is a non-constant, non-monotone solution of (VII.1a-c). Then u_{ox} must have at least one internal zero on [0,L]. Assume u_{ox} has exactly one zero on (0,L) and writing u_{ox} in polar coordinates gives: $u_{ox} = \rho_o(x)\sin \omega_o(x)$ with $\omega_o(0) = 0$ and $\omega_o(L) = 2\pi$.

Write also the no-flux boundary eigenvectors of the Sturm-Liouville problem (VII.11) corresponding to the two smallest eigenvalues λ_0 and λ_1 in polar coordinates with respectively $\omega(.,\lambda_0)$ and $\omega(.,\lambda_1)$.

Then $\omega(0,\lambda_0) = \omega(0,\lambda_1) = \pi/2$, $\omega(L,\lambda_0) = \pi/2$ and $\omega(L,\lambda_1) = 3\pi/2$ (Theorem VII.2.), and $\omega(.,\lambda_1)$ must have at least one intersection with ω_o on (0,L).

Corollary VII.3

If u_o is non-constant, non-monotone solution of (VII.1a-c), then the Sturm-Liouville eigenvalue problem (VII.11) has at least two negative eigenvalues.

Proof:

Suppose u_{ox} has one internal zero. Let $\omega_o(x_1) = \omega(x_1,\lambda_1)$. Apply theorem VII.1. with $a = x_1$, $b = L$, $p_1 = p_2 = \gamma$ and $g_1 = (\lambda_1 - \phi'(u_o))$, $g_2 = (0 - \phi'(u_o))$. Since $\omega_o > \omega(.,\lambda_1)$ on $(x_1,L]$, $\lambda_1 > 0$ would contradict theorem VII.1.. For $\lambda_1 = 0$, g_1 and g_2 are interchangeable ($p_1 = p_2$); so from theorem VII.1. it would follow that $\omega_o(x) = \omega(x,\lambda_1)$ on $[x_1,L]$. But $\omega(L,\lambda_1) = \frac{3}{2}\pi < 2\pi = \omega_o(L)$. Hence $\lambda_1 < 0$.

This can easily extended to the case where $u_{ox}(x)$ has more than one internal zero, since again $\omega(.,\lambda_1)$ will have at least one internal intersection with ω_o. □

Corollary VII.4

Every non-constant, non-monotone stationary solution of the anti-diffusion equation (VII.1a-c) is unstable.

Proof:

Let u_o be a non-constant, non-monotone solution of (VII.1a-c).

Let $v_0(x)$, respectively $v_1(x)$ be eigenvectors corresponding to the eigenvalues λ_0 and λ_1 of the eigenvalue problem (VII.11).

If v_1 is such that $\int v_1(x)\,dx = 0$ then u_o is unstable with respect to disturbances of the form $v(x,t) = \alpha(t)v_1(x)$: insert v in (VII.7) to find:

$$\dot{\alpha}(t)v_1(x) = \alpha(t)\left[\frac{\partial^2}{\partial x^2}\left\{\phi'(u_o)v_1 - \gamma\frac{\partial^2}{\partial x^2}v_1\right\}\right] \qquad \text{(VII.22)}$$

where $\dot{}$ means derivative with respect to time t.

Using that v_1 is an eigenvector with eigenvalue λ_1 of (VII.11) one finds

$$\dot{\alpha}(t)v_1(x) = \alpha(t)\left[\frac{\partial^2}{\partial x^2}\lambda_1 v_1\right] \qquad \text{(VII.23)}$$

Multiplying both sides of (VII.23) with $v_1(x)$ and taking the integral gives:

$$\dot{\alpha}(t)\int v_1(x)dx = \alpha\lambda_1\int\left\{\frac{\partial^2}{\partial x^2}v_1\right\}v_1 dx = -\alpha\lambda_1\int(v_{1x})^2dx \qquad \text{(VII.24)}$$

where $v_{1x} = dv_1/dx$.

Since λ_1 is negative as v_x has at least one internal zero this proves the instability with respect to v_1 if $\int v_1\,dx = 0$.

If v_1 is such that $\int v_1(x)dx \neq 0$ then since $\int v_0(x)dx \neq 0$ there is a $\mu \in \mathbb{R}$ such that $\int(v_1(x) + \mu v_0(x))dx = 0$. Since v_1 and v_0 are independent $v_1(x) + \mu v_0(x)$ is not identically zero on (0,L).

Now take a disturbance of the form:

$$v(x,t) = \alpha(t)\left(v_1(x) + \mu v_0(x)\right)$$

Apply (VII.22) to find:

$$\dot{\alpha}(t)\left\{v_1(x) + \mu v_0(x)\right\} = \alpha(t)\left[\frac{\partial^2}{\partial x^2}\left\{\phi'(v)(v_1(x) + \mu v_0(x)) +\right.\right.$$

$$-\gamma \frac{\partial^2}{\partial x^2}(v_1(x) + \mu v_0(x))\Big\}\Big] \qquad \text{(VII.25)}$$

Since v_0, v_1 are eigenvectors with eigenvalues λ_0, λ_1 respectively of (VII.11) one finds

$$\dot{\alpha}(t)\Big\{v_1(x) + \mu v_0(x)\Big\} = \alpha(t)\Big[\frac{\partial^2}{\partial x^2}\Big\{\lambda_1 v_1 + \mu\lambda_0 v_0\Big\}\Big] \qquad \text{(VII.26)}$$

Multiplying both sides of (VII.26) with $\lambda_1 v_1(x) + \lambda_0 \mu v_0(x)$, taking the integral, and using $\int v_0(x)v_1(x)dx = 0$, one finds:

$$\dot{\alpha}(t)\int(\lambda_1 v_1^2(x)+\lambda_0\mu^2 v_0^2(x))dx = \alpha(t)\Big[\int-(\lambda_1 v_{1x}(x) + \lambda_0\mu v_{0x}(x))^2 dx\Big] \qquad \text{(VII.27)}$$

Since λ_0 and λ_1 are negative the left hand integral is negative just as the right hand integral of (VII.27).
This proves the instability of a non-constant, non-monotone solution of (VII.1a-c). □

Since it has been shown before that the anti-diffusion equation has a stable non-constant stationary solution (if the trivial null solution is unstable) (see chapter V, section 4) it follows that the only possible non-constant stable stationary solutions are the monotone ones.

Remarks.
The proof depends on the observation that if u_o is a solution of (VII.1a-c) then $u_{ox}(x)$ is a solution of (VII.11) with $\lambda = 0$. This is not the case if instead of the continuous form of the anti-diffusion equation, the discrete spatial form is used. In the latter case, non-monotone, non-constant stationary solutions can be stable, see chapter VIII, section 2.a, corollary VIII.1. So with a large grain structure where the continuous form is a bad approximation of the intrinsic discrete structure of the system, non-monotone, non-constant stable stationary solutions can be found.

VII.5 The anti-diffusion equation and the Swift-Hohenberg equation

The anti-diffusion system

$$\frac{\partial u}{\partial t} = \frac{\partial^2}{\partial x^2}\left[\phi(u) - \gamma\frac{\partial^2 u}{\partial x^2}\right] \qquad \text{(VII.28)}$$

with $\phi(u)$ given by (VII.1d), $r_2 > 0$, is characterized by minimization of the functional

$$V(u) = \int_0^L f(u) + \tfrac{1}{2}\gamma|u_x|^2 dx \qquad \text{(VII.29)}$$

under the restriction $\int u(x)dx = 0$ with $f(u) = \int_0^u \phi(s)ds$ and $\gamma > 0$. Although the evolution from a randomly disturbed null solution will be initially dominated (more or less) by the fastest growing mode(s) corresponding with the largest eigenvalue(s) of the linearized system, the final pattern will be a monotone one.

In chapter II, section 4, equation (II.31), the Swift-Hohenberg equation was given in the following form:

$$\frac{\partial u}{\partial t} = -2\frac{\partial^2 u}{\partial x^2} - \gamma_1\frac{\partial^4 u}{\partial x^4} - (1 - \varepsilon)u - u^3 \qquad \text{(VII.30)}$$

with $\gamma_1 > 0$ and $0 < \varepsilon < 1$. (Swift and Hohenberg, 1977; Saarloos, 1987.) We shall the system equation (VII.30) denote by SH.

Equation VII.30 need not to be mass conserving but in the line of chapter IV a mass conserving variant can easily be constructed, e.g.:

$$\frac{\partial u}{\partial t} = \frac{\partial^2}{\partial x^2}\left[2\frac{\partial u^2}{\partial x^2} + \gamma_1\frac{\partial u^4}{\partial x^4} + (1 - \varepsilon)u + u^3\right] \qquad \text{(VII.31)}$$

Let the system be defined on $[0,L] \subset \mathbb{R}$ with no-flux boundary conditions. In linear approximation the SH-system (VII.30) is given by

$\frac{\partial u}{\partial t} = Lu$ with

$$Lu = -2\frac{\partial^2 u}{\partial x^2} - \gamma_1\frac{\partial^4 u}{\partial x^4} - (1 - \varepsilon)u$$

The eigenvalues of L are

$$\omega_k = 2p_k^2 - \gamma_1 p_k^4 - (1 - \varepsilon),\ p_k = k\pi/L \qquad \text{(VII.32a)}$$

For the linearized system (VII.31) the eigenvalues are

$$\omega_k = p_k^2\left[2p_k^2 - \gamma_1 p_k^4 - (1 - \varepsilon)\right] \qquad \text{(VII.32b)}$$

Hence the instability condition of the null solution are for both systems the same. We will assume that the null solution is unstable:

$$\exists k:\ 2p_k^2 - \gamma_1 p_k^4 \ > (1 - \varepsilon) > 0 \qquad \text{(VII.33)}$$

Without going in details we note the following. The Lyapunov functional V for the SH-system is

$$V(u) = \int_0^L \tfrac{1}{2}(1 - \varepsilon)u^2 + \tfrac{1}{4}u^4 - |u_x|^2 + \tfrac{1}{2}\gamma_1|u_{xx}|^2 dx \qquad \text{(VII.34)}$$

Just as the AD-system, the time evolution of the SH-system is characterized by minimization of the corresponding functional V. However, in the case of the AD-system the positive coefficient of the quadratic gradient term $|u_x|^2$directs the evolution to a solution with as less variation as possible whereas in the case of the SH-system, the negative coefficient of the same quadratic term indicates a tendency in the opposite direction, i.e. away from the constant solution. Secondly, the functional V (VII.34) is bounded from below. By Hölder's inequality we have:

$$\left\{\int_0^L u^2(x)dx\right\}^2 \le L\left\{\int_0^L u^4(x)dx\right\} \qquad \text{(VII.35)}$$

(Hardy et al., (1967)). Hence

$$V(u) \ge \int_0^L \tfrac{1}{2}(1-\varepsilon)u^2 - |u_x|^2 + \tfrac{1}{2}\gamma_1|u_{xx}|^2 dx + \frac{1}{4L}\left\{\int_0^L u^2(x)dx\right\}^2 \qquad \text{(VII.36)}$$

Since the eigenmodes of the Laplace operator form an orthonormal base in $L^2[0,L]$ we can write $u \in L^2[0,L]$, using the no-flux boundary conditions, as

$$u(x) = \sum_k \alpha_k \cos(k\pi x/L) \qquad \text{(VII.37)}$$

The right hand side of (VII.36) involves only integrals over quadratic terms hence we find

$$V(u) \ge \sum_k \tfrac{1}{2}L\alpha_k^2\left\{\tfrac{1}{2}(1 - \varepsilon) - p_k^2 + \tfrac{1}{2}\gamma_1 p_k^4 + \tfrac{1}{8}\alpha_k^2\right\} \qquad \text{(VII.38)}$$

The lowest value of the k-the term in (VII.38) is obtained either for $\alpha_k = 0$ or for $p_k^2 = 1/\gamma_1$ with $\alpha_k^2 = 2(\varepsilon - 1) + 2/\gamma_1$; in the latter case the minimum value is $-\frac{1}{4}L\left\{(1/\gamma_1) - (1 - \varepsilon)\right\}^2$. Since only a finite number of terms can be negative, the right hand side of (VII.38) is bounded from below and so is the functional V.

Now using the same arguments as in chapter V, section 4, one finds that the functional (VII.34) attains its minimum and consequently that the SH-system will have a non-constant stable solution if the null solution is unstable.

Moreover, the SH-system may have stable non-monotone, non-constant solutions since, given the eigenvalues (VII.32a or VII.32b) of the linearized system one can find system parameters ε, γ_1 and L such that only one eigenvalue ω_k with $k > 1$ is zero. Applying the bifurcation analysis of chapter VI, one gets a (stable) bifurcation branch with leading term $\cos(k\pi x/L)$. Note that for the anti-diffusion system this is only possible for $k = 1$.

Summarizing: the SH-system can be seen as an extension of the anti-diffusion system beyond $\gamma = 0$. We recall from chapter II, section 2, that the coefficients of the linear terms of the evolution equations based on Thom's river basin width model, will have the same sign. If $\gamma < 0$ in the AD-model then we have a 'negative' visco-elasticity effect (no cohesion between particles). This is compensated by the fourth order derivative term with a negative coefficient ($-\gamma_1$, $\gamma_1 > 0$) in the standard SH-model (VII.30) and with a positive coefficient (γ_1) in the mass-conserving variant (VII.31).

The anti-diffusion system and the Swift-Hohenberg system will have non-constant stable solutions if the null solution is unstable. In the case of the SH-equation, the effect of negative diffusion which drives the system away from constant solutions, is present at all stages of the evolution. For the anti-diffusion system the effectiveness of the negative diffusion depends on $\phi(u)$; if u reaches the stable branches of $\phi(u)$ the effect of negative diffusion diminishes and will be balanced by the smoothing effect of the viscosity term. An open question is how long it takes to reach the final monotone state. It is possible that the anti-diffusion system shows a time evolution with transient phases

which are very slowly changing and hardly distinguishable from stationary stable states. In physics and chemistry such slowly varying states are called metastable. In the numerical simulations of the discrete system we have found such a behavior, see the next chapter.

CHAPTER VIII

NUMERICAL SOLUTIONS

VIII.1 Finite difference schemes

The solution of partial differential equations by finite difference methods requires the definition of a grid on the spatial and time domains. The value of the derivative in each interval is approximated by a straight line connecting two grid points. For smooth curves, at least one point on the enclosed interval has a derivative parallel to that line. For slowly varying functions, this point is more or less in the centre of the interval. Taylor expansion about the central point provides the numerical expressions and estimates the errors.

Grid spacing along axes will be denoted by $\Delta\cdot$: spacing along the x-axes by Δx with N grid points (along the y-axes by Δy with M grid points). The grid spacing of the time domain is denoted Δt. In all directions constant spacing is assumed. The following notations are used. For a two dimensional spatial domain the value of some function u in say $x = (n-1)\Delta x$, $y = (m-1)\Delta y$ and $t = (j-1)\Delta t$ is denoted by $u^j_{n,m}$. In the one dimensional case the value in (x,t) is given as u^j_n.

Space derivatives are approximated by central difference schemes. The exact difference formula are obtained by Taylor expansion. Given some function $u(x,t)$: $\mathbb{R}\times\mathbb{R} \to \mathbb{R}$ the exact forward time difference formula is:

$$u(x,t+\Delta t) = \left(1 + \Delta t\frac{\partial}{\partial t} + \frac{1}{2}\Delta t^2 \frac{\partial^2}{\partial t^2} + \ldots\right)u(x,t) \qquad \text{(VIII.1)}$$

Hence a forward time difference scheme $\left[u_n^{j+1} - u_n^j\right]$, introduces a local truncation error of order $\frac{1}{2}\Delta t^2\left(\frac{\partial^2 u}{\partial t^2}\right)_n^j$, where the indices denote that the time derivative is evaluated at $x = (n-1)\Delta x$, $t = (j-1)\Delta t$.

Let δ_x be the central difference operator in the x-direction:

$$\delta_x u_n^j = u_{n+0.5}^j - u_{n-0.5}^j , \tag{VIII.2a}$$

$$\delta_x^2 u_n^j = u_{n+1}^j - 2u_n^j + u_{n-1}^j , \tag{VIII.2b}$$

$$\delta_x^4 u_n^j = u_{n+2}^j - 4u_{n+1}^j + 6u_n^j - 4u_{n-1}^j + u_{n-2}^j . \tag{VIII.2c}$$

The exact formula for connecting δ_x and the spatial (partial) derivative, is given by Taylor expansion:

$$\delta_x u_n^j = \Delta x\left(\frac{\partial u}{\partial x}\right)_n^j + \frac{1}{24}\Delta x^3\left(\frac{\partial^3 u}{\partial x^3}\right)_n^j + \ldots . \tag{VIII.3}$$

In a similar way exact formulas for δ_x^2, δ_x^4 and for instance δ_{xy}^2 can be obtained (Mitchell, 1969; Dahlquist et al., 1974).

$$\delta_x^2 u_n^j = \Delta x^2\left(\frac{\partial^2 u}{\partial x^2}\right)_n^j + \frac{1}{12}\Delta x^4\left(\frac{\partial^4 u}{\partial x^4}\right)_n^j + \ldots . \tag{VIII.4}$$

$$\delta_x^4 u_n^j = \Delta x^4\left(\frac{\partial^4 u}{\partial x^4}\right)_n^j + \frac{1}{6}\Delta x^6\left(\frac{\partial^6 u}{\partial x^6}\right)_n^j + \ldots . \tag{VIII.5}$$

For $\phi(u_k^j)$, with ϕ a function defined on the array $[u_1,\ldots,u_N]$, the second order central difference scheme $\delta_x^2\phi(u_k^j)$ is given as:

$$\delta_x^2\phi(u_k^j) = \phi(u_{k+1}^j) - 2\phi(u_k^j) + \phi(u_{k-1}^j) \tag{VIII.6}$$

And

$$\delta_x^2\phi(u_k^j) = \Delta x^2\left(\frac{\partial^2}{\partial x^2}\phi(u)\right)_n^j + \frac{1}{12}\Delta x^4\left(\frac{\partial^4}{\partial x^4}\phi(u)\right)_n^j + \ldots \tag{VIII.7}$$

Boundary conditions are approximated by introducing artificial grid points x_{-1}, x_0, x_{N+1} and x_{N+2}.

And then no-flux boundary condition are obtained by defining:

$$u_{-1}^j = u_2^j,\ u_0^j = u_1^j,\ u_{N+2}^j = u_{N-1}^j \text{ and } u_{N+1}^j = u_N^j. \quad \forall j \in \mathbb{N} \tag{VIII.8}$$

Assuming that one of these conditions holds, the operators δ_x^2 and δ_x^4 are mass-conserving: $\sum_{n=1}^N \delta_x^2 u_n^j = 0$ and $\sum_{n=1}^N \delta_x^4 u_n^j = 0$. (The same applies

to δ_x^2 and δ_x^4 acting on $\phi(u_k^j)$). Moreover, the following relations hold:

$$\sum_{n=1}^{N} \left(\delta_x^2 u_n^j\right)^2 = \sum_{n=1}^{N} u_n^j . \delta_x^4 u_n^j \qquad \text{(VIII.9)}$$

$$\sum_{n=1}^{N} \left(\delta_x u_n^j\right)^2 = -\sum_{n=1}^{N} u_n^j . \delta_x^2 u_n^j + O(\Delta x) \qquad \text{(VIII.10)}$$

(In equation (VIII.10) $u_{n+0.5}^j$ is to be interpreted as $0.5(u_{n+1}^j + u_n^j)$.)
And

$$\sum_{n=1}^{N} u_n^j . \delta_x^2 u_n^j \leq 0 \qquad \text{(VIII.11)}$$

(Since $\sum_{n=1}^{N} u_{n+1}^j (u_{n+1}^j - u_n^j) = \sum_{n=1}^{N} u_n^j (u_n^j - u_{n-1}^j)$ by virtue of one of the boundary conditions, the left hand of (VIII.11) can be written as: $\sum_{n=1}^{N} -(u_{n+1}^j - u_n^j)^2$.)
Using these discretizations, the one dimensional continuous anti-diffusion system (II.18) is reduced to a system of N ordinary difference equations :

$$u_n^{j+1} = u_n^j + r\, \delta_x^2 \left[\phi(u_n^j) - (\gamma/\Delta x^2)\delta_x^2 u_n^j\right] \qquad \text{(VIII.12)}$$

where $r = \Delta t/\Delta x^2$, and $n = 1,..,N$, $j = 1,...$ with the appropriate boundary conditions (VIII.8).
Given the mass-conservation properties of δ_x^2 and one of the boundary conditions (VIII.8), $\sum_{n=1}^{N} u_n^j$ = constant and independent of the time step variable j. So at least the important mass-conserving property is not lost by discretization.

VIII.1.1 Consistency, stability and convergence

From the equations as (VIII.4), (VIII.5) etc. it is clear that finite difference schemes introduce some errors with respect to the original continuous model equations. The numerical notions of consistency, stability and convergence deal with these deviations between the discrete and the continuous model.

Definition VIII.1 (Mitchell, 1969; Dahlquist et al., 1974):

A difference approximation is called *consistent* if:

$$\frac{\text{truncation error}}{\Delta t} \to 0 \text{ as } \Delta x, \Delta t \to 0.$$

Definition VIII.2 (Mitchell, 1969; Dahlquist et al., 1974):

Let $Z_n^j = u_n^j - U_n^j$ be the difference between the theoretical solution u and the numerical solution U of the difference equation. Let Δt be fixed. If Z_n^j remains bounded as j increases for all n, then the difference equation is called *stable*.

Definition VIII.3 (Mitchell, 1969; Dahlquist et al., 1974):

Let $Z(x,t) = u(x,t) - U(x,t)$ be the difference between the theoretical solutions of the differential and difference equations at a *fixed* point (x,t). The finite difference scheme is *convergent* if Z(x,t) tends to zero uniformly as the net is refined such that $\Delta x, \Delta t \to 0$ with $x = (n-1)\Delta x$ and $t = (j-1)\Delta t$ remaining fixed. The fixed point (x,t) is anywhere within the region under consideration.

In most cases convergency analysis is applied under an assumption of some relationship between Δx and Δt.
Here these notions shall be examined with respect to the one dimensional space difference equations (VIII.12).

Consistency

Using (VIII.1), (VIII.5) and (VIII.7) one finds for (VIII.12) a truncation error of order:

$$\Delta t\left[\frac{1}{2}\Delta t^2\left(\frac{\partial^2 u}{\partial t^2}\right)_n^j - \frac{1}{12}\Delta x^2\left(\frac{\partial^4}{\partial x^4}\phi(u)\right)_n^j + \frac{\gamma}{6}\Delta x^2\left(\frac{\partial^6 u}{\partial x^6}\right)_n^j\right] \qquad \text{(VIII.13)}$$

From (VIII.13) it follows that the discretization (VIII.12) is consistent with the continuous anti-diffusion model.

Stability

There are two methods which are commonly used for examining the

stability of a difference scheme. Both methods are essential linear. Let $Z_n^j = u_n^j - U_n^j$ be the difference between the theoretical solution u and the numerical solution U of the difference equation.

The von Neumann analysis assumes slowly varying coefficients of the linear difference equations; consequently these coefficients are considered constant in space and time. In this case an harmonic decomposition of the error Z at grid points at given time level (say t=0) can be made. To study the error propagation as t increases, it is sufficient to consider these independent solutions or eigenmodes of the linear difference equations. The eigenmodes are all of the form (restricting to the one dimensional space case):

$$Z_n^j = \xi^j e^{(1 l n \Delta x)} \qquad \text{(VIII.14)}$$

where l is a real spatial wave number and $\xi = \xi(l)$ is a complex number depending on l. The original error component $e^{(1 l n \Delta x)}$ will not grow with time if the amplification factor ξ satisfies:

$$|\xi| \leq 1 \qquad \text{(VIII.15)}$$

for all wave numbers l. This is von Neumann's stability criterion. (Mitchell, 1969; Press et al., 1986). The von Neumann method is of local character by the assumption of constant coefficients. Boundary conditions are neglected. However, numerical evidence supports the contention that if the von Neumann condition is satisfied locally, the difference scheme is stable (Mitchell, 1969).

The second method, called the matrix method, assumes again linear equations. Let $u^j = [u_1^j, \ldots\ldots, u_N^j]^T$. The difference equations with the boundary conditions included, are written in matrix form as:

$$u^{j+1} = B_j u^j \qquad \text{(VIII.16)}$$

where B_j is a square matrix eventually j (time) dependent. Let Z^j be the error vector $u^j - U^j$ with U^j the numerical solution vector; this gives:

$$Z^{j+1} = B_j Z^j \qquad \text{(VIII.17)}$$

Let $\|.\|$ denotes a suitable norm then from (VIII.17) it follows that:

$$\|Z^{j+1}\| \leq \|B_j\| . \|Z^j\| \qquad \text{(VIII.18)}$$

The necessary and sufficient condition for stability based on a constant time step and proceeding indefinitely in time is:

$$\|B_j\| \leq 1 \qquad \text{(VIII.19)}$$

As said before, both methods assumes linear equations. For a non-linear model as (VIII.12) the right-hand side is linearized by taken $u^j_n = u^j_{on} + z^j_n$ and expanding to the first order in z^j. The vector u^j_o is to be assumed an exact solution of the nonlinear difference equations. So the von Neumann analysis is nothing more than a discrete form of a linear stability analysis of an exact solution.

The null vector is a solution of (VIII.12). Since the object of this discretization is to follow the time evolution from the unstable null solution to any, if present, stable (stationary) solution, the von Neumann stability criterion can never be met. The same holds for criterion (VIII.19).

However, in this case it is possible to suppress the numerical instabilities corresponding to eigenvalues < -1 which are caused by discretization and which are not present in the continuous system. For this case the full matrix stability analysis will be applied to the model equations (VIII.12).

Let u^j_o again be a solution vector of (VIII.19). Let the boundary condition be of the no-flux type (VIII.8). Linearizing (VIII.12) in u^j_o gives the matrix B_j:

$$B_j = I + r\left[A_j - (\gamma/\Delta x^2)D^4\right] \qquad \text{(VIII.20a)}$$

where $A_j = -D^2.\Phi$ with $-D^2$ the discrete Laplace operator which is defined as

$$D^2 = \begin{cases} D^2(i,j) = 2 & \text{if } |i-j| = 0 \\ D^2(i,j) = -1 & \text{if } |i-j| = 1 \\ D^2(i,j) = 0 & \text{if } |i-j| > 1 \end{cases} \qquad \text{(VIII.20b)}$$

and the boundary condition $D(1,1) = 1$ and $D(N,N) = 1$ (see chapter IV, section 7); $D^4 = D^2.D^2$, I = identity matrix and the matrix Φ is a diagonal matrix with

$\Phi(i,i) = \phi'(u^j_{oi})$, $i = 1,..,N$ and ϕ' is the derivative of ϕ.

$\Phi(i,j) = 0$ if $i \neq j$ (VIII.20c)

Note that

$$\delta_x^2 u_n = -\left(D^2 u\right)_n \qquad \text{(VIII.20d)}$$

All matrices are of order N. The eigenvalues of D^2 are all non-negative by Gerschgorin's theorem (Dahlquist et al., 1974; see chapter V, section 7) and D^2 is the square of a symmetric matrix D. Since for any two matrices P and Q the eigenvalues of PQ and QP are the same, the same holds for the matrices D and $\left(-D\Phi - (\gamma/\Delta x^2)D^3\right)$. Since $-D\Phi D - (\gamma/\Delta x^2)D^4$ is symmetric, all eigenvalues are real and the same holds for the eigenvalues of $-D^2\Phi - (\gamma/\Delta x^2)D^4$ (see appendix E).

In what follows the subindex o is omitted.

Denoting the eigenvalues of B_j with λ_n, the system (VIII.17) will be stable if the spectral radius $\rho(B_j) = \max_{1\le n\le N} |\lambda_n| \le 1$. The matrix elements B(n,m) of the matrix B_j are given by

$$\text{if } |m-n| \ge 3 \text{ then } B(n,m) = 0$$

$$\text{if } |m-n| = 2 \text{ then } B(n,m) = -r(\gamma/\Delta x^2)$$

$$\text{if } |m-n| = 1 \text{ then } B(n,m) = r\left[\phi'(u_m^j) + 4(\gamma/\Delta x^2)\right]$$

$$\text{if } |m-n| = 0 \text{ then } B(n,m) = 1 + r\left[-2\phi'(u_m^j) - 6(\gamma/\Delta x^2)\right] \qquad \text{(VIII.21a)}$$

with for no-flux boundary conditions the following additional definitions:

$$B(m,m) = 1 + r\left[-\phi'(u_m^j) - 2(\gamma/\Delta x^2)\right] \text{ if } m = 1 \text{ or } m = N$$

$$B(1,2) = r\left[\phi'(u_2^j) + 3(\gamma/\Delta x^2)\right];\ B(N,N-1) = r\left[\phi'(u_{N-1}^j) + 3(\gamma/\Delta x^2)\right]$$

$$B(1,3) = B(N,N-2) = -r(\gamma/\Delta x^2)$$

$$B(2,1) = r\left[\phi'(u_1^j) + 3(\gamma/\Delta x^2)\right];\ B(N-1,N) = r\left[\phi'(u_N^j) + 3(\gamma/\Delta x^2)\right] \qquad \text{(VIII.21b)}$$

Bounds on the eigenvalues λ_n of B_j can be found by applying Gerschgorin's theorem which applied to B_j states that each eigenvalue of the NxN matrix B_j lies in the union of the circles:

$$|z - B(n,n)| \leq \left(\sum_{\substack{m=1 \\ m \neq n}}^{N} |B(n,m)| \right) \qquad \text{(VIII.22)}$$

Combining (VIII.21a) with (VIII.22) gives for $3 \leq n \leq N-2$

$$-1 \leq B(n,n) - |B(n,n-1)| - |B(n,n+1)| - 2r\gamma/\Delta x^2$$

&

$$B(n,n) + |B(n,n-1)| + |B(n,n+1)| + 2r\gamma/\Delta x^2 \leq 1 \qquad \text{(VIII.23)}$$

The second part of (VIII.23) is equivalent with:

$$r\left[-2\phi'(u_n^j) - 6\frac{\gamma}{\Delta x^2} + |\phi'(u_{n-1}^j) + 4\frac{\gamma}{\Delta x^2}| + |\phi'(u_{n+1}^j) + 4\frac{\gamma}{\Delta x^2}| + 2\frac{\gamma}{\Delta x^2}\right] \leq 0$$

Now supposing that $B(n,n+1)$ and $B(n,n-1)$ are positive the condition becomes:

$$\left[-2\phi'(u_n^j) + \phi'(u_{n-1}^j) + \phi'(u_{n+1}^j) + 4(\gamma/\Delta x^2)\right] \leq 0$$

and there seems to be no way to meet this condition under all circumstances. This must be seen in respect to the instability of the system, wanted at least for some u_o solution.

The first part of (VIII.23) is equivalent with:

$$r\left[2\phi'(u_n^j) + 6\frac{\gamma}{\Delta x^2} + |\phi'(u_{n-1}^j) + 4\frac{\gamma}{\Delta x^2}| + |\phi'(u_{n+1}^j) + 4\frac{\gamma}{\Delta x^2}| + 2\frac{\gamma}{\Delta x^2}\right] \leq 2 \qquad \text{(VIII.24)}$$

Violating this condition will cause an instability which is intrinsic to time discretization and not present in the continuous time model.

Now, in the continuous case for an appropriate form of ϕ, a priori bounds for stationary bounded solutions were found in Chapter III, section 2 (III.8). Assume the bounds are u_o and u_1, and define M_ϕ by

$$M_\phi = \max_{u_o \leq u \leq u_1} |\phi'(u)| \qquad \text{(VIII.25a)}$$

Then the left hand of (VIII.24) is bounded by $4M + 16(\gamma/\Delta x^2)$ and the following upperbound r_b for $r = \Delta t/\Delta x^2$ is obtained:

$$r_b = \frac{2}{4M_\phi + 16(\gamma/\Delta x^2)} \qquad \text{(VIII.25b)}$$

Note that the coefficients in the denominator of (VIII.25b) are the sum of the absolute values of the coefficients in δ_x^2 and δ_x^4 respectively

and consequently, the bound on r is also sufficient for the matrix boundary rows given by the additional definitions (VIII.21b).
In all simulations this upperbound on r was sufficient to achieve convergence. (The same bound can also be found by applying von Neumann linear stability analysis with the condition that all eigenvalues are greater or equal to -1.)

The third notion of convergence need no further investigation since consistency, stability and convergence are related as follows (Dahlquist et al., 1974):

consistent & stable $\Leftrightarrow$ convergent

(Since essentially a procedure of linearization around some exact solution u, with errors expressed in the truncation error as found in the consistency condition, has been applied, no stricter bounds on r can be found this way.)

For the two dimensional model

$$\frac{\partial u}{\partial t} = \Delta\left[\phi(u) - \gamma\Delta u\right]$$

the discretization with equal grid spacing h and equal grid points N in x- and y-direction, is based on

$$\Delta u \approx \frac{1}{h^2}(\delta_x^2 + \delta_y^2)u_{n,m} \qquad \text{(VIII.26)}$$

where $u_{n,m} = u(x,y)$ with $x = (n-1)h$, $y = (m-1)h$. ($h = \Delta x = \Delta y$.)
With M_ϕ as defined in (VIII.25a), the upperbound r_b on $r = \Delta t/h^2$ is

$$r_b = \frac{2}{8M_\phi + 64(\gamma/h^2)} \qquad \text{(VIII.27)}$$

VIII.2 The discrete anti-diffusion model

In this paragraph the discretizations obtained above are applied to the anti-diffusion and migration model. Computational results are reported for the one dimensional spatial case as well for the two dimensional spatial domain.

VIII.2.1 One dimensional spatial domain

We consider the following discrete model:

$$u_n^{j+1} = u_n^j + r\delta_x^2\left[\phi(u_n^j) - (\gamma/\Delta x^2)\delta_x^2 u_n^j\right] \qquad \text{(VIII.28)}$$

where $r = \Delta t/\Delta x^2$, and $n = 1,..,N$, $j = 1,...$ with the no-flux boundary condition (VIII.8). The basic form of ϕ is

$$\phi(u) = -u + r_1u^2 + r_2u^3, \quad r_2 > 0 \qquad \text{(VIII.29)}$$

Some qualitative aspects of the discrete model are equivalent to those of the continuous model.

The stability of the null solution $u_n = 0$, $n = 1,..,N$, depends on the stability of the independent (and orthogonal) eigenmodes:

$$u_k(n) = a_k\cos(k\pi(n-0.5)/N) \qquad \text{(VIII.30)}$$

Setting $p_k = k\pi/N$ and denoting the eigenvalues by $1+r\omega_k$, the (linear) stability condition becomes:

$$-1 < 1 + r\omega_k < 1 \qquad \text{(VIII.31a)}$$

with

$$\omega_k = 4\sin^2(\tfrac{1}{2}p_k)\left\{1 - (\gamma/\Delta x^2)4\sin^2(\tfrac{1}{2}p_k)\right\} \qquad \text{(VIII.31b)}$$

In the following it is assumed that r satisfies the constraint (VIII.25) such that $1 + r\omega_k > -1$ all k. The right hand inequality of (VIII.31a) is equivalent to:

$$1 - (\gamma/\Delta x^2)4\sin^2(\tfrac{1}{2}p_k) < 0 \qquad \text{(VIII.32a)}$$

which is consistent with the stability condition in the continuous case (see also appendix D). Let γ_o be defined as

$$\gamma_o = \gamma\frac{1}{\Delta x^2}4\sin^2(\tfrac{1}{2}p_1) \qquad \text{(VIII.32b)}$$

then the null solution is unstable if $\gamma_o < 1$.

The fastest growing mode(s) are the mode(s) with ω_k maximal where k is given by

$$|1 - 2(\gamma/\Delta x^2)4\sin^2(\tfrac{1}{2}p_k)| \text{ is minimal.} \qquad \text{(VIII.33)}$$

For N = 96 table VIII.1 gives the unstable modes for different γ (γ_o) and table VIII.2 gives the fastest growing mode. In the tables VIII.1 and VIII.2, #G denotes the wave length expressed in the number of grid points; the column 'length' gives the wave length as #G·Δx, where Δx is the grid spacing (for N = 96, $\Delta x = \frac{3\pi}{128}$).

γ	γ_o	unstable modes		
			periods	
		modes	#G	length l
0.0024	0.0043	$1 \le k \le 15.47$	≥ 6.7	$0.164 \le l \le 2.35$
0.0041	0.0073	$1 \le k \le 11.79$	≥ 16.8	$0.412 \le l \le 2.35$

Table VIII.1: Unstable modes (N=96).

γ	γ_o	fastest growing modes		
			periods	
		modes	#G	length l
0.0024	0.0043	k=11	18	0.444
0.0041	0.0073	k= 8	23	0.579

Table VIII.2: Fastest growing modes (N=96).

The time evolution of the discrete system is characterized by minimizing the following functional V:

$$V^j = \sum_{n=1}^{N} \left\{ f(u_n^j) + \frac{1}{2} \frac{\gamma}{\Delta x^2} u_n^j \left(D^2 u^j \right)_n \right\} \qquad \text{(VIII.34)}$$

where $f(u) = \int_0^u \phi(s)ds$ and D^2 is defined in (VIII.20b). The second term $u_n^j \left(D^2 u^j \right)_n = -u_n^j \delta_x^2 u_n^j$ is the approximation of the $-(\delta_x u_n)^2$ (see (VIII.10), see also chapter V for the continuous time case). Using:

$$f(u_n^{j+1}) - f(u_n^j) = \phi(u_n^j) r \delta_x^2 \left[\phi(u_n^j) - (\gamma/\Delta x^2) \delta_x^2 u_n^j \right] + O(r^2)$$

and inequality (VIII.11) one finds

$$V^{j+1} \le V^j \quad \text{for r sufficiently small}$$

and

$$V^{j+1} = V^j \iff \phi(u_n^j) - (\gamma/\Delta x^2) \delta_x^2 u_n^j = \beta, \ \beta \text{ constant}, \ \forall n, \ n = 1, .., N. \qquad \text{(VIII.35)}$$

The last condition is equivalent with the condition that $u^J = [u_1^J, \ldots\ldots, u_N^J]^T$ is a stationary solution of (VIII.28). Hence V is a Lyapunov functional for system (VIII.28).
Above all, the right hand side of the equivalence relation (VIII.35) gives a very useful stop-criterion for numerical solutions. Since under the no-flux boundary conditions (VIII.8) $\sum_{n=1}^{N} \delta_x^2 u_n^J = 0$, and β is equal to $\frac{1}{N}\sum_{n=1}^{N} \phi(u_n)$ for a stationary solution.
Furthermore, the conclusions with respect to the type of bifurcation from the null solutions based on Poincaré-Lindstedt expansions are analogous with those for the continuous model (see appendix D).

In the numerical simulations spatial grid spacing was $\Delta x = 3\pi/4N$, with $N = 48$, $N = 96$. (Simulations with $N = 192$ differ not essentially from those with $N = 96$). The maximal time step Δt is derived from $r_b = \Delta t/\Delta x^2$, with r_b given by (VIII.25). The initial condition was the null solution randomly disturbed such that $\sum_{n=1}^{N} u_n = 0$.

For the numerical simulation two different forms for the anti-diffusion driving function ϕ (VIII.29) are chosen; table VIII.3 gives in the third and fourth columns the bounds of the non-constant stationary solutions as derived in chapter III.

r_1	r_2	lower bound u_o	upper bound u_1
-1.0	1.0	-0.821	1.488
-3.0	1.0	-1.000	3.000

Table VIII.3: Boundaries of non-constant solutions.

For the continuous model it is proven in chapter VII that the only stable solution is a monotone function, where was mentioned also that the prove was not valid for the discrete case.

Corollary VIII.1

If the discrete system (VIII.28) has a stationary solution $u^s = (u_1^s, u_2^s, \ldots, u_N^s)$ with $\phi'(u_n^s) > 0$ for all $n = 1, .., N$, then this solution is linearly stable if r satisfies condition (VIII.25).

Proof:

Let $v^j = (v_1^j, .., v_N^j)$ be a small disturbance of the stationary solution u^s. Then in linear approximation the time evolution of v is given as

$$v^{j+1} = \left\{ I + r \left[A^s - (\gamma/\Delta x^2) D^4 \right] \right\} v^j \qquad \text{(VIII.36)}$$

where A^s is defined by

$$A^s = -D^2 \Phi \qquad \text{(VIII.37)}$$

with Φ a NxN diagonal matrix: $\Phi(n,m) = \phi'(u_n^s)\delta(n-m)$, and $-D^2$ is the discrete Laplacian operator, see definition (VIII.20b).

With all $\phi'(u_n^s)$ positive, the positive square $\sqrt{\Phi}$ of Φ exists. Since the eigenvalues of $-D^2\Phi$ and $-\sqrt{\Phi}D^2\sqrt{\Phi}$ are the same, $\langle v, -D^2\Phi v \rangle \leq 0$. Hence the operator between the square brackets in (VIII.36) is strictly negative on $\mathbb{R}^{N*}$ with $\mathbb{R}^{N*} = \left\{ u \in \mathbb{R}^N \mid \sum_{n=1}^N u_n = 0 \right\}$. If r satisfies condition (VIII.25), the operator between the curly brackets in (VIII.36) has (only real) eigenvalues lying between 1 and -1. ∎

If $r_2 > 0$ then for $\gamma = 0$ a solution u^s with all $\phi'(u_n^s)$ positive can be constructed and every spatial reordering of the solution is again a solution (see chapter II, section 3). Such a solution can be found as a pair (u_0, u_1) with $u_0 < 0 < u_1$ and $\phi(u_o) = \phi(u_1)$ subject to the condition that the total sum of u-values be zero. Then for γ small positive, it is possible to find a non-constant non-monotone solution u^s with all $\phi'(u_n^s)$ positive: take for simplicity $r_1 = 0$ and let u^s consists of a repeated sequence of four points (u_o, u_1, u_1, u_o) then the zero mass condition gives $u_o = -u_1$ (N is taken even) and u^s is a stationary solution if $u_o = \pm\sqrt{(1 - 2\gamma/\Delta x^2)}$. For γ sufficiently small $\phi'(u_o)$ and $\phi'(u_1)$ will be positive.

Since γ is scaled by Δx^2, the possibility to form stable patterns with all $\phi'(u_n)$ positive causes also the qualitative differences between patterns generated with a coarse-grain grid (e.g. N = 48, figure VIII.1) and those generated with a finer grid (N = 96, see figure VIII.2 ($r_1 = -3$)). With a small number of grid points, the system becomes easily locked in a profile with all $\phi'(u_n)$ positive. (The reported V-values are the functional values V(u) defined in (VIII.34).)

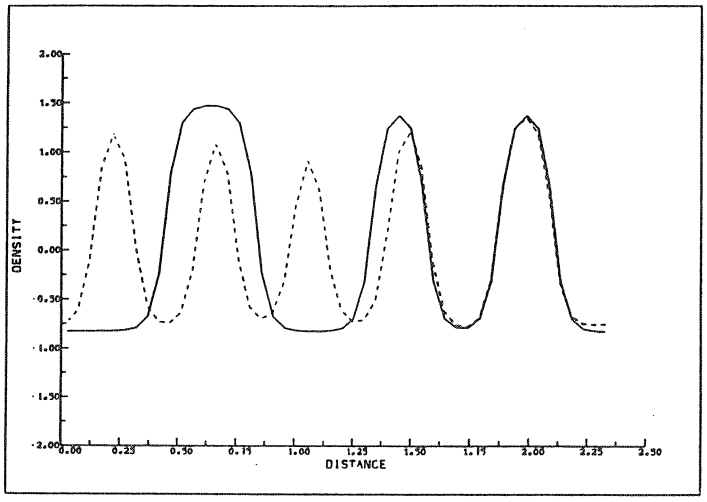


Figure VIII.1: Pattern evolution for N = 48.

γ = 0.0024; r_1 = -1; Time = 0.25: ---- (V = -0.72).

Final pattern: ———— (V = -1.58).

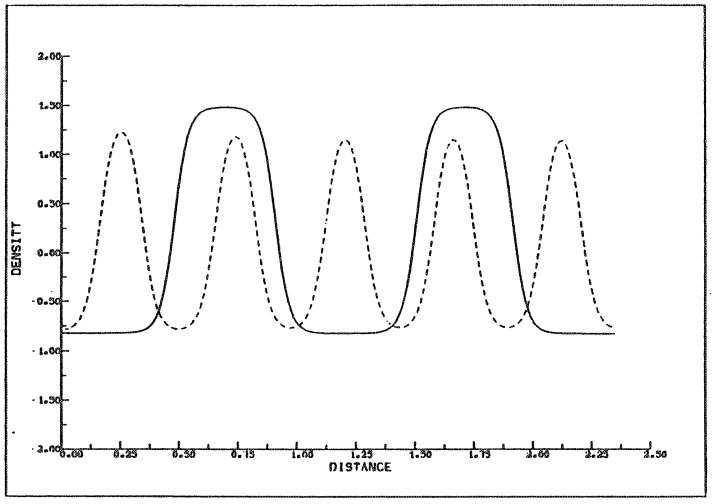


Figure VIII.2: Pattern evolution for N = 96.

Parameters as in Figure VIII.1. Time = 0.25: ---- (V = -0.85)

Final pattern: ——— (V = -2.03)

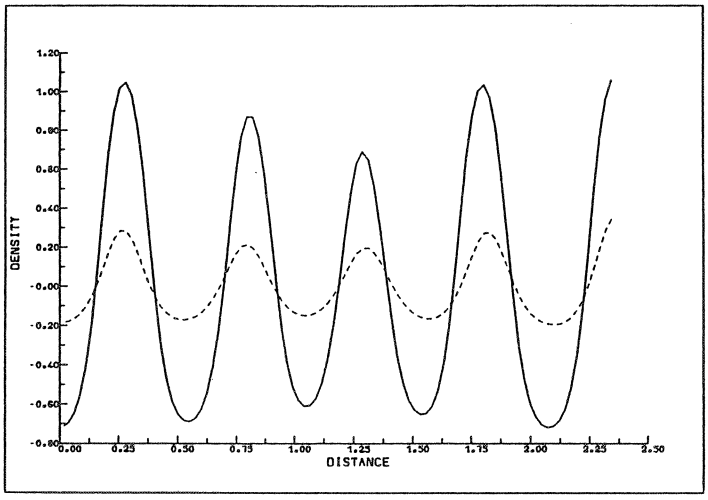


Figure VIII.3: Initial pattern evolution (time = 0.2):
r_1 = -1: profile ———; r_1 = -3: profile -----.

A second aspect is that one can have a different type of bifurcation (sub- or supercritical, see appendix D) from the null solution for the different values of r_1. However, if more than one mode is unstable, the initial evolution is not determined by the type of bifurcation but by the fastest growing mode, see table (VIII.2). Figure VIII.3 shows that (for γ = 0.0041) the initial evolution is the same for both type of functions (r_1 = -1 and r_1 = -3). But the similarity is lost after those initial stages, see figure VIII.4a and figure VIII.5.

Although the initial evolution was always according to the fastest growing mode, the further evolution is characterized by a tendency to a less profiled pattern. The discrimination between the sometimes slowly varying transient phases and the final stable phases was possible by checking the condition for stationary solutions, i.e. that $\phi(u_n^j) - (\gamma/\Delta x^2)\delta_x^2 u_n^j$ must be equal in all grid points (VIII.35). At some iteration stages changes in V were hardly recognizable whereas the above criterion was clearly not met. In Figure VIII.4b the time evolution of V is depicted for γ = 0.0042, r_1 = -1.

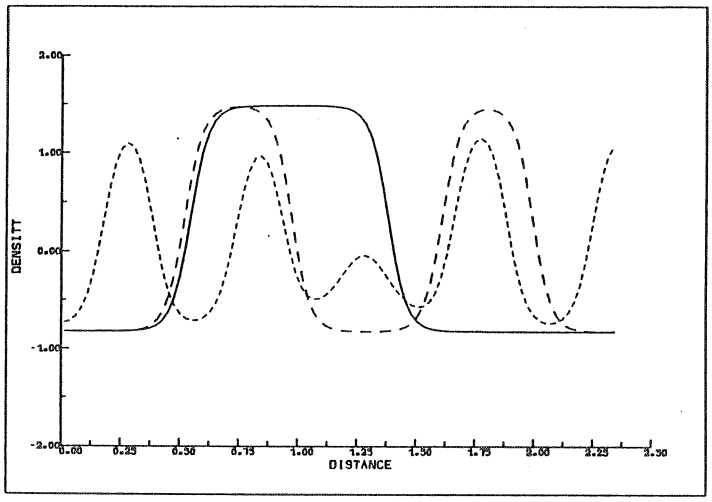


Figure VIII.4a: Pattern evolution with γ = 0.0042, r_1 = -1.
Time = 0.4: .....(V = -0.48); Time = 12.4: ----- (V = -1.71)
Time = 71.5: ——— (V = -2.35).

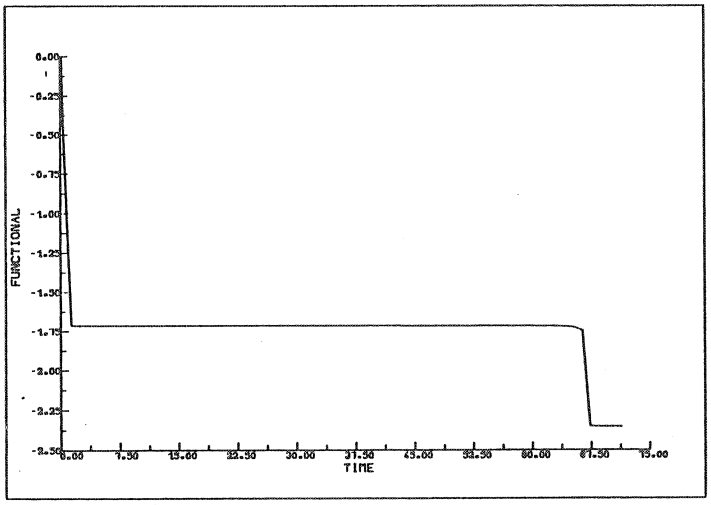


Figure VIII.4b: Time evolution of functional V(u), see VIII.34.
Parameters as in figure VIII.4a.

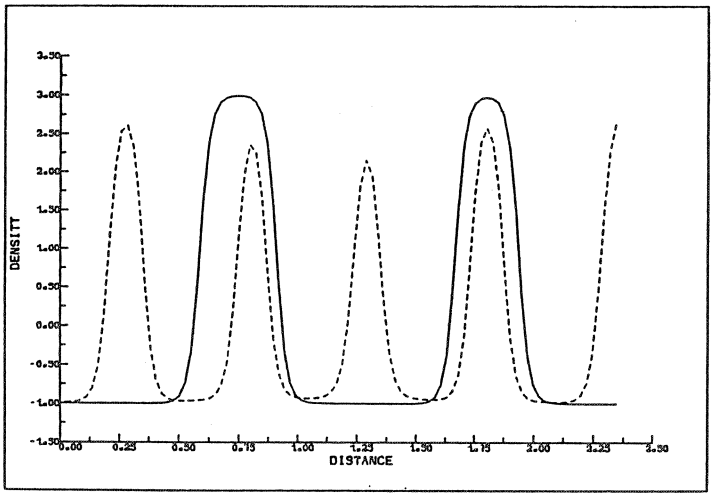


Figure VIII.5: Pattern evolution for γ = 0.0042, r_1 = -3.
Time = 0.3: ---- (V = -3.6); Final pattern: ——— (V = -11.43)

Finally, stability of the final patterns was confirmed by calculating numerically the signs of the eigenvalues of the linearized system. In all figures, the patterns formed by the continuous curve are numerically stable.

A solution may be classified by the lap-number z(u) defined by:

$$z(u) = z(u_1,..,u_N) = \#\left\{k \in \{1,..,N\} \mid u_{k+1}\cdot u_k < 0 \text{ or } u_k = 0\right\} \qquad \text{(VIII.38)}$$

Table VIII.4 summarizes the results for γ = 0.0024 and γ = 0.0041 (N = 96).

γ	γ_o	r_1	functional V(u)	lap-number z(u)
0.0024	0.0043	-1	-2.03	4
0.0041	0.0073	-1	-2.35	2
0.0024	0.0043	-3	-10.62	6
0.0041	0.0073	-3	-11.43	4

Table VIII.4: Classification of final patterns.

Simulations with larger γ values show an initial phase with hardly any profilation: the random disturbances just have to reorder themselves to fit (more or less) the pattern of the fastest growing mode. For $\gamma = 0.1$ with only two unstable modes k = 1, 2, the final pattern was a monotone one.
With respect to the reported patterns it is to be noted that none of the shown "final" patterns consists entirely of points with $\phi'(u) > 0$.

The numerical simulations show:

i) initial evolution corresponding to the fastest growing mode defined by (VIII.33);
ii) transient behavior to a less profiled pattern;
iii) the transient phases can have a very slowly varying time evolution, looking almost stable;
iv) the final stable pattern is not necessary a monotone pattern.

In physics and engineering, a state which seems to be 'stable' in the sense that it is showing only very small variation over a long time period is called *metastable*. In practice, such a metastable state can be of more interest than the final state: either the (environmental) parameters of the system are changed before the final state is ever reached (for example in socio-economical systems) or the metastable state becomes solidified as, for instance, can be the case in precipitation patterns, see Chapter IX. In a chemico-physical context a metastable state is called a state which is at a local, not global, minimum of the free energy functional. With fluctuations inherent in such a system, one can expect a (maybe slow) transition from a local minimum phase to a global minimum phase.

VIII.2.2 Two dimensional spatial domain

The spatial domain is $[0,L]\times[0,L] \subset \mathbb{R}^2$. Grid spacing in both space directions is taken equal to h with N grid points. ($h = \Delta x = \Delta y$.) The discrete model is:

$$u^{j+1}_{n,m} = u^{j}_{n,m} + r.(\delta_x^2 + \delta_y^2)\left[\phi(u^{j}_{n,m}) - (\gamma/h^2)(\delta_x^2 + \delta_y^2)u^{j}_{n,m}\right] \qquad \text{(VIII.39)}$$

Just as in the one dimensional case a Lyapunov functional V can be defined:

$$V^j = \sum_{m=1}^{N}\sum_{n=1}^{N}\left\{f(u^{j}_{n,m}) - \frac{1}{2}(\gamma/h^2)u^{j}_{n,m}(\delta_x^2 + \delta_y^2)u^{j}_{n,m}\right\} \qquad \text{(VIII.40a)}$$

with the properties

$$V^{j+1} \leq V^j \qquad \text{(VIII.40b)}$$

$$V^{j+1} = V^j \Leftrightarrow \phi(u^{j}_{n,m}) - (\gamma/h^2)u^{j}_{n,m} = \beta, \ \beta \text{ is constant for } \forall n,m. \qquad \text{(VIII.40c)}$$

The linear stability of the null solution is given by the time evolution of a disturbance in the form

$$v(x,y,t) = \sum_k \sum_l a_{kl}\cos(k\pi x/L)\cos(l\pi y/L) \qquad \text{(VIII.41)}$$

where the summation is over all non-negative k and l with $k + l \geq 1$, since the constant disturbance is not allowed.

Using orthogonality of the eigenvectors $\cos(k\pi x/L)\cos(l\pi y/L)$ gives the condition for instability:

$$\{k^2 + l^2\}\{1 - \gamma(k^2 + l^2)\pi^2/L^2\} > 0 \qquad \text{(VIII.42)}$$

The simulations are restricted to N = 24 with equal grid spacing h in x- and y-direction ($h = \pi/32$); this coarse grid introduces substantial deviations from the continuous model. In all simulations r is taken equal to r_b defined in (VIII.27). Table VIII.5 summarizes some simulations results with respect to the functional value V (VIII.40a).

γ	γ_o	r_1	functional V(u)
0.0024	0.0043	-1	-163.32
0.0041	0.0073	-1	-150.76
0.0024	0.0043	-3	-710.94
0.0041	0.0073	-3	-685.95

Table VIII.5: Results two dimensional simulations.

Figure VIII.6 shows the time evolution for $r_1 = -1$, $\gamma = 0.0041$. The U-values reported below the contour patterns are the five u levels on which the contours are based. The time is given by $\Delta t = r_b h^2$.

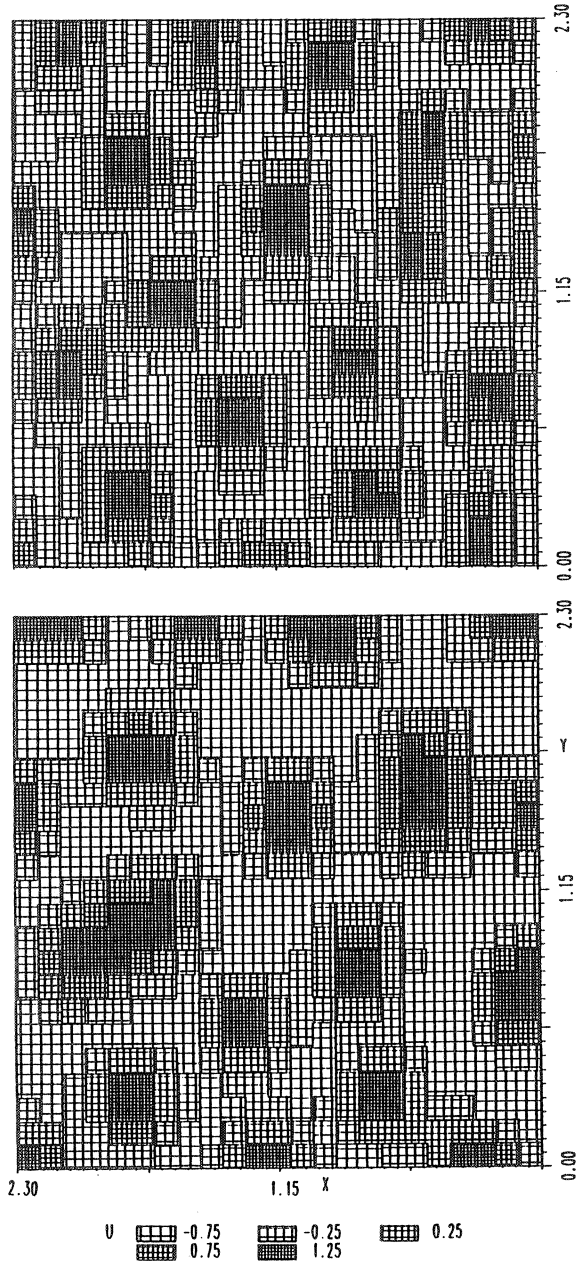


Figure VIII.6: Pattern evolution anti-diffusion equation.
γ = 0.0041; r_1 = -1.
Upper figure: time = 0.32; V = -33.12;
Lower figure: time = 0.68; V = -76.10.

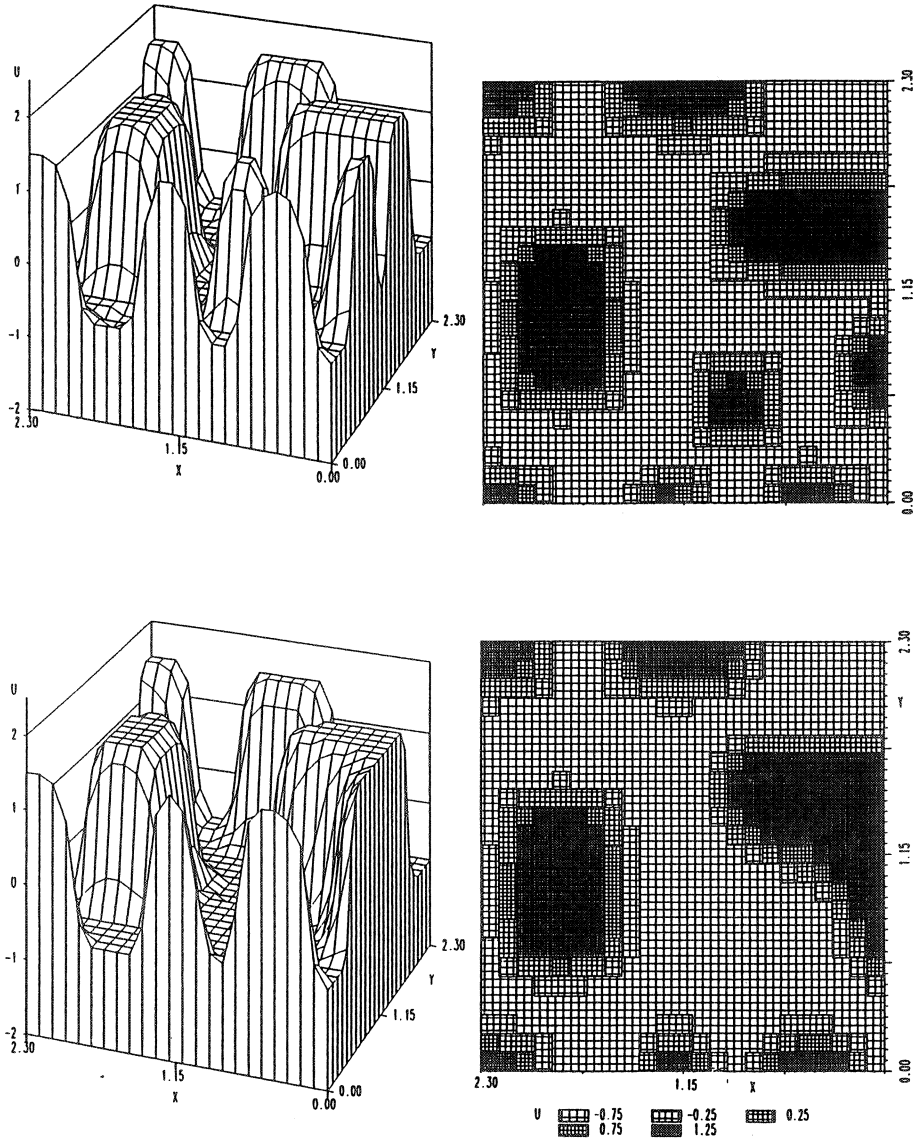


Figure VIII.6 (continued): left profile, right contour.
Upper figures: time=1.11; V = -111.94;
Lower figures: time=2.71; v = -134.04.

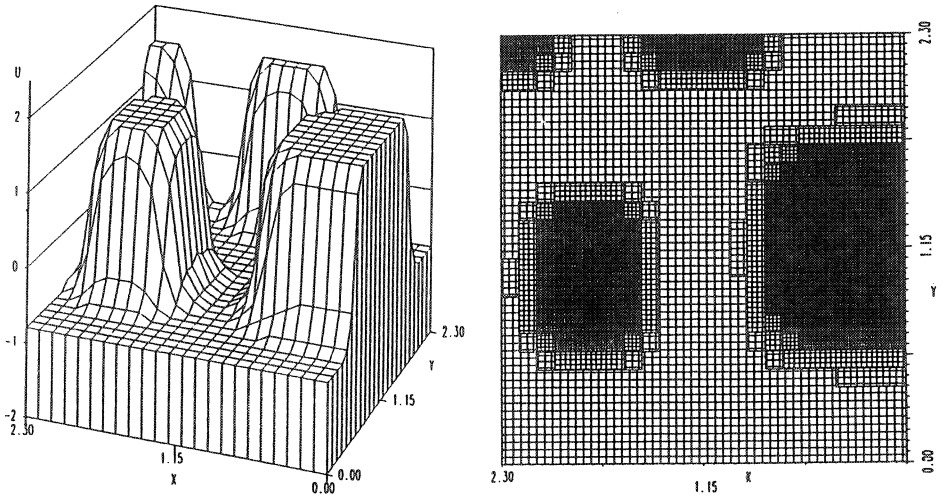


Figure VIII.6 (continued): Final pattern. Time = 7.5; V = -150.77.

VIII.3 The discrete migration model

The homogeneous migration model was defined in Chapter IV, equation (IV.23c) as

$$\tau \dot{u}_n = -M\left[\sum_{i=1}^{N} \Psi(n,i)\left\{\frac{\delta V}{\delta u_n} - \frac{\delta V}{\delta u_i}\right\}\right] \qquad \text{(VIII.43a)}$$

We use the same definition of V and the same time discretization as above to find the discrete time equations. If furthermore $\Psi(n,i)$ is set equal to 1/N, one finds after a time rescaling:

$$u_n^{j+1} = u_n^j + r\left[-\phi(u_n^j) + \frac{\gamma}{\Delta x^2}\cdot\delta_x^2 u_n^j - \frac{1}{N}\sum_{k=1}^{N} -\phi(u_k^j)\right] \qquad \text{(VIII.43b)}$$

No-flux boundary conditions (VIII.8) are added.

The upper bound r_b of r is calculated following the derivation of the upper bound in the case of the discrete anti-diffusion equation:

$$r_b = \frac{1}{M_\Phi + 2(\gamma/\Delta x^2)} \qquad \text{(VIII.44a)}$$

$$M_\Phi = \max_{u_o \le u \le u_1} |\phi'(u)| \qquad \text{(VIII.44b)}$$

(u_o, u_1: bounds on stationary bounded solutions (Chapter III)).
With respect to the discrete anti-diffusion model, the migration model differs only in one aspect: at an unstable null-solution the fastest growing mode is always given by the mode with the longest possible wave length, mode k = 1, see appendix D.

In numerical simulations with as initial condition a small random perturbation of the null solution, the evolution was (again) along the fastest growing mode: till the random deviations were reordered more or less as a mode with wave length $\frac{1}{2}L$, the amplitude of the perturbation was hardly changing. Then occurs a fast transformation to the final monotone (non-constant) stationary solution. The resulting pattern was completely determined by the bounds u_o and u_1 as given in (VIII.37).
Only by taking a strongly profiled initial condition, the migration system evolves to a non-monotone pattern.

VIII.4 Following a solution curve by continuation techniques

In the foregoing paragraphs the time evolution was followed for some fixed γ. The final pattern is a solution of

$$G(u;\gamma) = 0 \qquad \text{(VIII.45)}$$

for the chosen value of γ with G defined e.g. by the second term of the right hand of (VIII.28) or (VIII.39).
The continuation method is a technique to follow the solution branches of (VIII.45) for γ in some interval Γ of $\mathbb{R}$. Since a detailed description of the continuation algorithm with Fortran code can be found in Kubicek and Marek (1983), here only the outlines of the

algorithm are given.

Assume that G is twice continuously differentiable in both u and γ. Along a solution branch u and γ are parameterized by the arc length s. The unit tangent vector $(\dot{u},\dot{\gamma})$ satisfies the condition

$$G_u\cdot\dot{u} + G_\gamma\cdot\dot{\gamma} = 0 \qquad \text{(VIII.46a)}$$

$$\|\dot{u}\|^2 + \dot{\gamma}^2 = 1 \qquad \text{(VIII.46b)}$$

If (u_o,γ_o) is some starting point on a solution branch corresponding to arclength s_o, then solving (VIII.45) is equivalent with solving:

$$\dot{u} = \dot{u}(s),\ u(s_o) = u_o \qquad \text{(VIII.47a)}$$

$$\dot{\gamma} = \dot{\gamma}(s),\ \gamma(s_o) = \gamma_o \qquad \text{(VIII.47b)}$$

where $\dot{u}(s)$ and $\dot{\gamma}(s)$ satisfy (VIII.46).

Suppose $(u(s_o),\gamma(s_o))$ is a regular point then $G_u^{-1}(u(s);\gamma(s))$ will exist in a small neighborhood of s_o. Let y be the solution of

$$G_u(u(s),\gamma(s))\cdot y + G_\gamma(u(s),\gamma(s)) = 0$$

then

$$\dot{u}(s) = \dot{\gamma}(s)y$$

and $\dot{\gamma}(s)$ can be found by solving (VIII.46b). This gives two solutions; choosing an initial direction in which the branch is to be followed, the solution is unique.

When G_u becomes ill-conditioned in the neighborhood of a singular point the procedure is to be repeated with an other independent variable instead of γ. For the numerical application of the procedure, G is approximated by a suitable $\tilde{G}$: $\mathbb{R}^n\times\mathbb{R} \to \mathbb{R}^n$. This allows for the possibility to take as independent variable one of the components of u. The algorithm applies a full pivoting strategy to the weighted $N\times(N+1)$ matrix $P\cdot[G_u\,|\,G_\gamma]$ at each iteration step where P is some weighting matrix.

Having obtained say $\dot{\gamma}(s)$, equations (VIII.47) are numerically integrated using Adams-Bashforth formulas of maximal order 4. At each stage when the independent variable is changed, the integration formula is reduced to the order 1.

The numerical integration provides an estimate $(\hat{u}(s),\hat{\gamma}(s))$ of the next

point on the branch. This estimate is taken as starting point for a Newton iteration which refines the estimate up to some error tolerance. Stability of branches is determined by counting the positive eigenvalues where changes in this number indicate the neighborhood of turning- or bifurcation points.
Apart from the initial direction in which the branch is to be followed and the weighting matrix P, estimates for the starting points must be provided.
In the case of the anti-diffusion model $\tilde{G}$ is defined as:

$$\tilde{G}_k(u;\gamma) = \delta_x^2\left[\phi(u_k^j) - (\gamma/\Delta x^2)\delta_x^2 u_k^j\right] \qquad \text{(VIII.48)}$$

using the same defined notations as above.
Starting points, i.e. initial solutions u_o, can be found as follows:

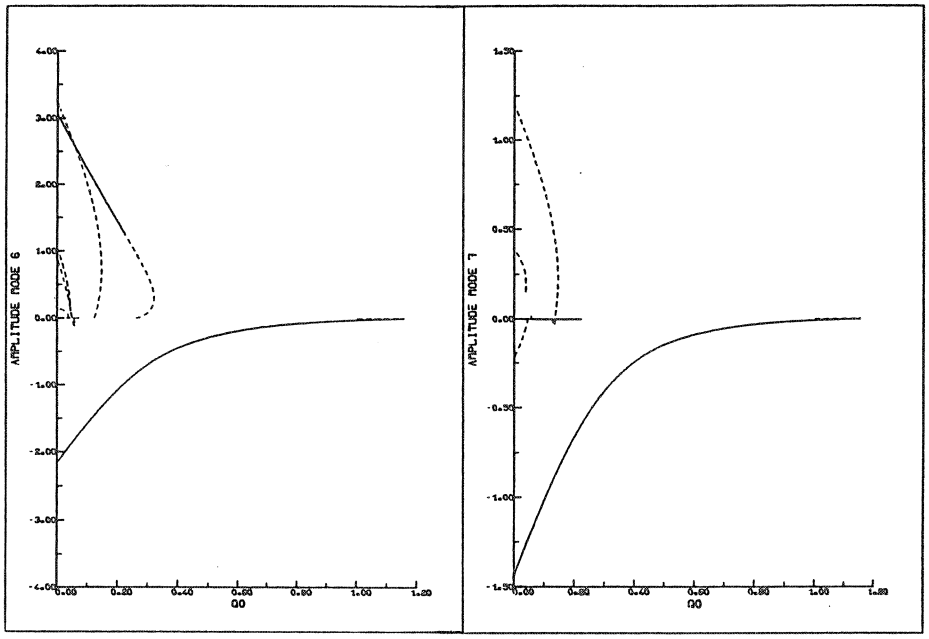
i) stationary solutions obtained by numerically time evolution of the full discrete system.

ii) for $\gamma = 0$, solutions are given by $\phi(u_i) = \phi(u_j)$ with $\sum_{n=1}^{N} u_n = 0$.

iii) approximations of bifurcating branches from the null solution $u_n = 0$ as given by the Poincaré-Lindstedt series. In appendix D the basic equations are calculated.

The algorithm is applied for a system with N = 8. To visualize the solutions, three relations are presented: the first one gives the relation between the functional V as defined in (VIII.34) and γ_o (VIII.32b) the second one depicts the projection on the mode $\cos(7\pi/N)$, denoted as amplitude mode 7 whereas the third one gives the projection on mode $\cos(6\pi/N)$.

Figure VIII.7 gives the bifurcation diagram obtained by starting with the Poincaré-Lindstedt expansions at bifurcation points of the null solution. The diagram is far from complete, only the direct continuation from the start branches is shown. At the transition from an unstable branch in a stable branch the corresponding unstable branches are not shown.



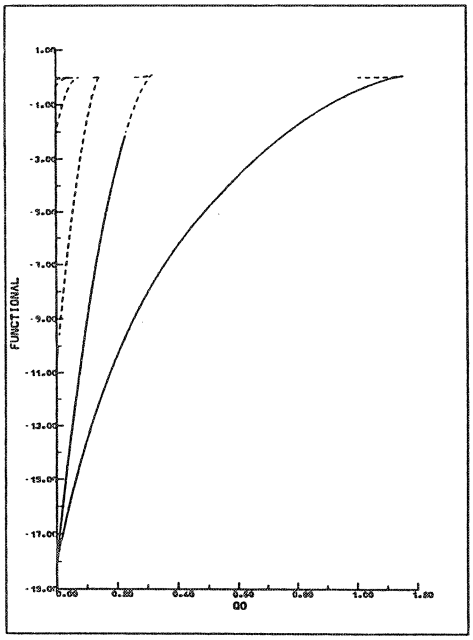


Figure VIII.7: Bifurcation diagram (N = 8).
Upper right: amplitude cos(7π/N)
Upper left: amplitude cos(6π/N)
Left: functional V value;
solutions on the most right branch have one zero, the following branch two and so on.
dotted curve .....: unstable;
continuous curve —— : stable;
zero solution not depicted.

Figure VIII.8 gives a far more complete picture: turning points and bifurcation points are all present. For the branch depicted with a turning point at $\gamma \sim 0.31$ no continuation in the direction of lower γ values was found; this solution with a functional value of -0.05 at the turning point has one maximum (z(u) = 2: the solution has two zeros) but the solution is asymmetric in this maximum. This is in contrast with other one maximum solutions lying on the branch bifurcating at $\gamma_o = 0.2599$ where the k = 2 mode becomes unstable.

The complexity of diagram increases with decreasing γ_o which reflects the observation that for $\gamma_o = 0$ every redistribution of a piecewise constant solution is again a solution (see figure VIII.8). Figure VIII.8 is obtained by starting with a solution for $\gamma = 0$ and applying the continuation method. Again the zero solution is not depicted.

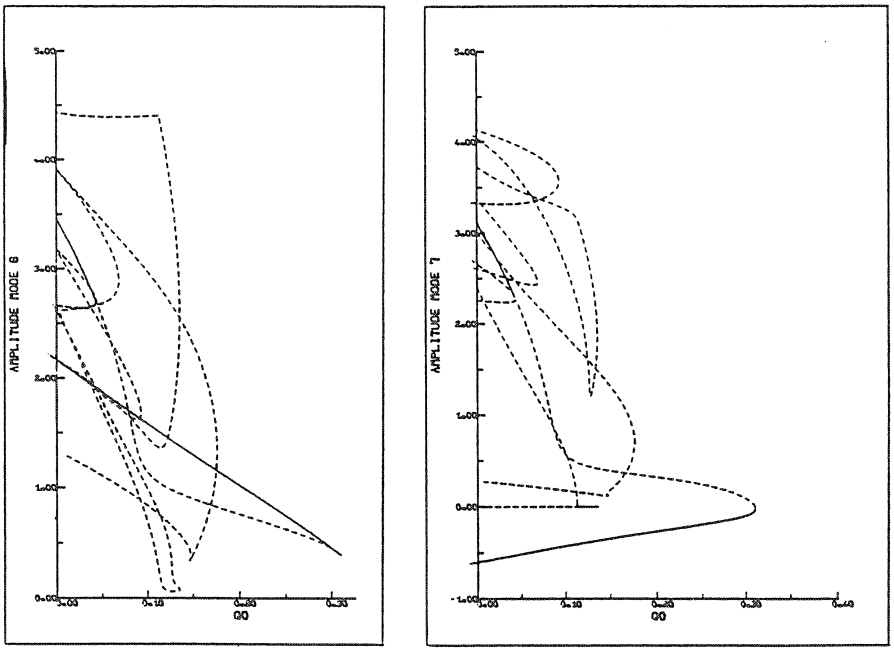


Figure VIII.8: Bifurcation diagram N = 8.

Left: amplitude cos(6π/N); right: amplitude cos(7π/N).

dotted curve ....: unstable; continuous curve ——— : stable;

VIII.5 Simulated annealing

The anti-diffusion evolution is characterized by minimization of the functional V, defined in equation (V.22) or (V.33), under the restrictions $\int u dx = 0$ and the boundary conditions. Stationary solutions coincide with stationary points of the functional; stable solutions with minima of V. Hence the evolution can be conceived as minimization of V by a gradient method:

$$\frac{du}{dt} = \Delta\left[\frac{\delta V}{\delta u}\right] \qquad \text{(VIII.49)}$$

where Δ is the Laplace operator.

Simulations with the discrete model show final states which are, in most cases, not monotone solutions and as such not given by the global minimum of V. The deterministic equation orders the states in a sequence of decreasing V values. To get on the branch which final state will coincide with a global minimum of V, some up-hill climbing must occur.

One way of introducing hill climbing, while preserving the tendency to descend along gradients, is to introduce random fluctuations into the path of u:

$$du = \Delta\left[\frac{\delta V}{\delta u}dt + \sqrt{2T}\, dw(t)\right] \qquad \text{(VIII.50)}$$

where w is a standard Brownian motion and T, "the temperature", controls the magnitude of the random fluctuations. Equation (VIII.50) is a Langevin equation for the anti-diffusion system (see Chapter IV, section 8).

Under suitable conditions on V (twice continuously differentiable) u approaches an equilibrium with density:

$$P_T(u) = \frac{1}{Z_T}\exp(-V(u)/T) \qquad \text{(VIII.51a)}$$

where

$$Z_T = \int_u \exp(-V/T)du \qquad \text{(VIII.51b)}$$

defined on the space of functions with $\int u dx = 0$.

The density P_T is called the Boltzmann distribution, see also Chapter IV, section 8, equation (IV.34).

As $T \to 0$, P_T concentrates on the global minima of V. Hence at low

temperature, one can expect to find u near a global minimum.

At thermal equilibrium, the probability of being in a state with energy ε was given by the Boltzmann distribution:

$$P(\varepsilon) = \frac{1}{Z_T}\exp(-\frac{\varepsilon}{k_b T}) \qquad \text{(VIII.52)}$$

where k_b is the Boltzmann constant (Powles, 1968).
In condensed matter physics, annealing is the process of heating a solid and cooling it slowly so as to remove strain and crystal imperfections. During this process the free energy of the solid is minimized. The initial heating is necessary to avoid becoming trapped in a local minimum. First a solid is brought into a state at which all particles have randomly arranged themselves in the liquid phase. Next it is cooled down such that at each phase of the cooling procedure, the solid is allowed to reach thermal equilibrium as defined by (VIII.52). As the temperature decreases, the Boltzmann distribution becomes more and more peaked around the states with lowest energy with finally, at zero temperature only states with minimal energy having a non-zero occurrence probability. The problem is that if the cooling is too fast, the system may be locked in a state with the free energy functional at a local minimum, not necessarily global. (Creutz et al., 1983; Laarhoven et al., 1987.)
This physical process of reaching a minimal energy level is transferred to a general minimization problem (VIII.49). Here the evolution to thermal equilibrium (at constant T) is simulated by Monte Carlo (MC) methods: the basic idea is to sample a set of states such that the probability of encountering any definite state with energy E is proportional to the measure factor $\exp(-\frac{\varepsilon}{k_b T})$ (Creutz et al., 1983). And instead of the energy ε and temperature T, a general costfunction (functional) V and control parameter c are considered.
The dynamic variables are denoted by $u_{n,m}$ (or u_n for a one dimensional spatial domain); let a configuration of the $u_{n,m}$ be denoted by C. The passage from one configuration C_i to the next one C_{i+1} is determined by a transition matrix $P(C \rightarrow C')$. In customary implementation of the MC algorithm, the transition involves the change of just one dynamic variable at a time: $u_{n,m} \rightarrow u'_{n,m}$. The variable can be picked at random

but it is computationally more convenient to proceed through the grid in an orderly fashion. Hence one does not define a single transition matrix $P(C \to C')$ but a collection $P_{n,m}(C \to C')$ where $P_{n,m}$ is the transition probability $P(u_{n,m} \to u'_{n,m})$ with all other variables kept fixed.

A Markovian chain is defined by $P_{tot} = \ldots P_{l,k}(C' \to C'')P_{n,m}(C \to C')$. The product is over all individual transition probabilities in the order in which one proceeds through the grid; P_{tot} determines the change at the end of one full Monte Carlo iteration.

The goal was to find a stochastic sequence with the property that the probability of finding any configuration C in the sequence becomes proportional to $\exp\{-V(C)\}$. A sufficient condition is that each step of the transition matrix obeys a detailed balance requirement (Creutz et al., 1983):

$$\exp\{-V(C)\}P_{n,m}(C \to C') = \exp\{-V(C')\}P_{n,m}(C' \to C) \qquad \text{(VIII.53)}$$

The detailed balance condition does not specify completely the transition probabilities $P_{n,m}(C \to C')$. Here the method of Metropolis et al. (see Metropolis et al., 1953) and a slight modification of this method is exposed:

a) *Metropolis algorithm.*

The transition from $u_{n,m}$ to $u'_{n,m}$ is a two step procedure.

A new possible value $\hat{u}_{n,m}$ is selected with an (arbitrary) probability distribution P_o obeying:

$$P_o(u_{n,m} \to \hat{u}_{n,m}) = P_o(\hat{u}_{n,m} \to u_{n,m}). \qquad \text{(VIII.54)}$$

Subsequently the change $\Delta V = V(\hat{C}) - V(C)$ is calculated. The perturbed configuration $\hat{C}$ differs from the current configuration C in only one variable $u_{n,m}$.

If $\Delta V \leq 0$ then the change is accepted and $u'_{n,m} = \hat{u}_{n,m}$; if not, then a pseudo random number r, uniformly distributed in the interval between 0 and 1, is generated.

if $r \leq \exp\{-\Delta V\}$ then the change is accepted: $u'_{n,m} = \hat{u}_{n,m}$;

if $r > \exp\{-\Delta V\}$ then the change is rejected: $u'_{n,m} = u_{n,m}$.

This rule is known as the Metropolis criterion.

b) *Modified Metropolis algorithm.*

The method is basically the same except that after the move from $u_{n,m}$ to $u'_{n,m}$ has been completed, the whole procedure is repeated one or more times on the same grid point (n,m) (Creutz et al., 1983).

The condition of detailed balance is fulfilled: suppose $\Delta V \geq 0$ then

$$P_{n,m}(C \to C') = P_o(u_{n,m} \to \hat{u}_{n,m})\cdot\exp\{-\Delta V\} =$$
$$= P_o(\hat{u}_{n,m} \to u_{n,m})\cdot\exp\{-\Delta V\} = P_{n,m}(C' \to C)\cdot\exp\{-V(C')\}/\exp\{-V(C)\}.$$

The formulation so far is at constant temperature (control parameter) (the homogeneous algorithm). For the nonhomogeneous algorithm, the temperature is decreased in between subsequent full Monte Carlo steps, i.e. after reaching equilibrium. As noted, too fast cooling may lock the system in a local minimum. In the application of the simulated annealing procedure to the anti-diffusion system, the problem is that the dynamic variables are continuous ones. Explicit non-homogeneous algorithm are formulated only for discrete variables (Hajek, 1985; Laarhoven et al., 1987). (For a pure diffusion process $du = -\nabla V(u)dt + \sqrt{2T}\, dw(t)$ with T a function of time t, Geman et al. (1986) give that for $T(t) = c/\log(2 + t)$ with c sufficiently high, the solution u converges weakly to a distribution concentrated at the global minima of V. They noted also that for most problems c will be most likely too large to be practical.)

VIII.5.1 Solutions of the anti-diffusion model by simulated annealing

The formulation of the stochastic version of the discrete anti-diffusion model in chapter IV, makes the application of simulated annealing rather straightforward with the exception of mass-conservation. The following implementation is chosen:

i) The initial configuration is given by the null solution: $u_n = 0$ for each $n = 1,..,N$ with N is grid length. ($u_{n,m} = 0$ for a two dimensional domain.)

ii) For one Monte Carlo step, the current configuration C is disturbed in two neighboring grid points n and n + nx with nx = 1, by selecting a random number $\hat{u}$ with probability distribution P_o equal to (truncated) $N(0,\sigma^2)$. The new candidate values are $\hat{u}_n = u_n + \hat{u}$ and $\hat{u}_{n+nx} = u_{n+nx} - \hat{u}$. Subsequently $\Delta V = V(\hat{C}) - V(C)$ with V the Lyapunov functional, is calculated and the Metropolis criterion is applied.

iii) Step ii) is repeated with nx = -1. (If necessary the boundary-conditions $u_0 = u_1$ and $u_{N+1} = u_N$ are applied in step i and step ii).

iv) Step ii) and step iii) is repeated for the grid point n + 2 till a full round is completed and the procedure is restarted at n = 1.

As a control parameter one takes T and the Metropolis criterion is applied to

$$\exp\left\{-\{V(\hat{C}) - V(C)\}/T\right\} \qquad \text{(VIII.55)}$$

where $\hat{C}$ is the perturbed configuration and C is the current configuration. In the specification of the transition probability W given in (IV.2), parameter β is equal to 2/T.

The acceptance rate (the fraction of iterations with accepted changes) depends not only on T, the control parameter, but also on σ, the standard deviation which defines the neighborhood structure of the current configuration (Laarhoven et al., 1987). In Creutz et al. (1983) an initial acceptance rate of 80% is recommended. However, this rate defines neither T nor σ initially.

In both cases $\hat{u}$ was drawn from a truncated normal distribution with zero mean and truncation points at $\hat{u} = 0.5$ and $\hat{u} = -0.5$. This truncated distribution satisfies the detailed balance condition. (Truncation was needed to prohibit the transition to unbounded solutions.) The best results were obtained for $\sigma = 1.0$ with initial T = 1.0 and $\sigma = 0.1$ with initial T = 0.1. In both cases the initial acceptance rate was about 80% percent.

Even with initially large fluctuations the system evolves to recognizable patterns with trough time an observable reduction in the lap-number z(u). If at a given temperature escapes from local minima are possible, then repeated escapes from global minima are also

guaranteed however with smaller probability. Accordingly, parameter T was lowered if for some iteration periods, a pattern was not changing essentially in the sense that the lap-number z(u) was 'stable'.
Finally, at a "low temperature" the simulated annealing procedure was concluded by a deterministic time evolution (T = 0). In all cases the pattern was not changed essentially by the deterministic evolution.
The best results are listed in Table VIII.6 for a one dimensional spatial domain with 96 grid points (with the same grid spacing as in paragraph VIII.2.1)

γ	γ_o	r_1	functional V(u)	lap-number z(u)
0.0024	0.0043	-1	-2.51	2
0.0041	0.0073	-1	-2.35	2
0.0024	0.0043	-3	-13.74	3
0.0041	0.0073	-3	-15.40	1

Table VIII.6: One dimensional simulated annealing results.

The results are better than those obtained by a pure deterministic evolution (see Table VIII.4).

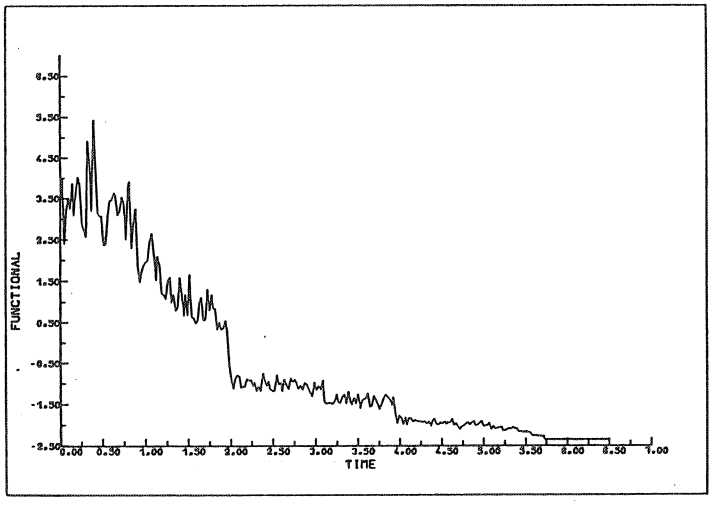


Figure VIII.9: Simulated annealing. Time evolution of the functional values V of the one dimensional anti-diffusion equation.
$r_1 = -1$; $\gamma = 0.0042$; (Final V-value: -2.35)

Figure VIII.9 gives the time evolution of V(u) in the case $\gamma = 0.0041$ and $r_1 = -1$ with an initial temperature T of 0.1. The time spacing was defined as follows: the time of one complete iteration is equal to $\Delta t = r_b \cdot \Delta x^2$ with r_b given by (VIII.25). The temperature T was lowered at time 0.75 (T=0.08), time 1.5 (T=0.05), time 2.0 (T=0.02), time 3.75 (T=0.01). Finally after time 5.75 the temperature was set at zero. Between time 1.5 and 2.0 the lap-number of the profile was already 2.

For a two dimensional spatial domain with 24 grid points in each of the two directions the results are given in Table VIII.7 with initial temperature parameter T equal to 1.0 and $\hat{u}$ are drawn from a truncated normal distribution with $\sigma = 1.0$ and truncation points -0.5 and 0.5.

γ	γ_o	r_1	functional V(u)
0.0024	0.0043	-1	-191.67
0.0041	0.0073	-1	-193.69
0.0024	0.0043	-3	-1200.06
0.0041	0.0073	-3	-1143.85

Table VIII.7: Two dimensional simulated annealing results.

The functional values in table VIII.7 are again better than those obtained by the deterministic procedure, even for $r_1 = -1$ (see table VIII.5). The reason is that this small number of grid points defines a rather coarse grid; the deterministic system becomes easily locked in a local minimum with all u such that $\phi'(u) > 0$. The stochastic procedure allows the system to escape from such a state. This effect is the more clear if the branches are far apart.

Figure VIII.10 gives at different time intervals the contours and profiles of the pattern for $\gamma = 0.0042$ and $r_1 = -1$. The in the figures reported U-values gives the u-levels which define the contour levels. The time scale is given by $\Delta t = r_b h$ with h the grid spacing in x- and y-direction and r_b defined in (VIII.27). The number of grid points is 24, grid spacing $h = \pi/32$.

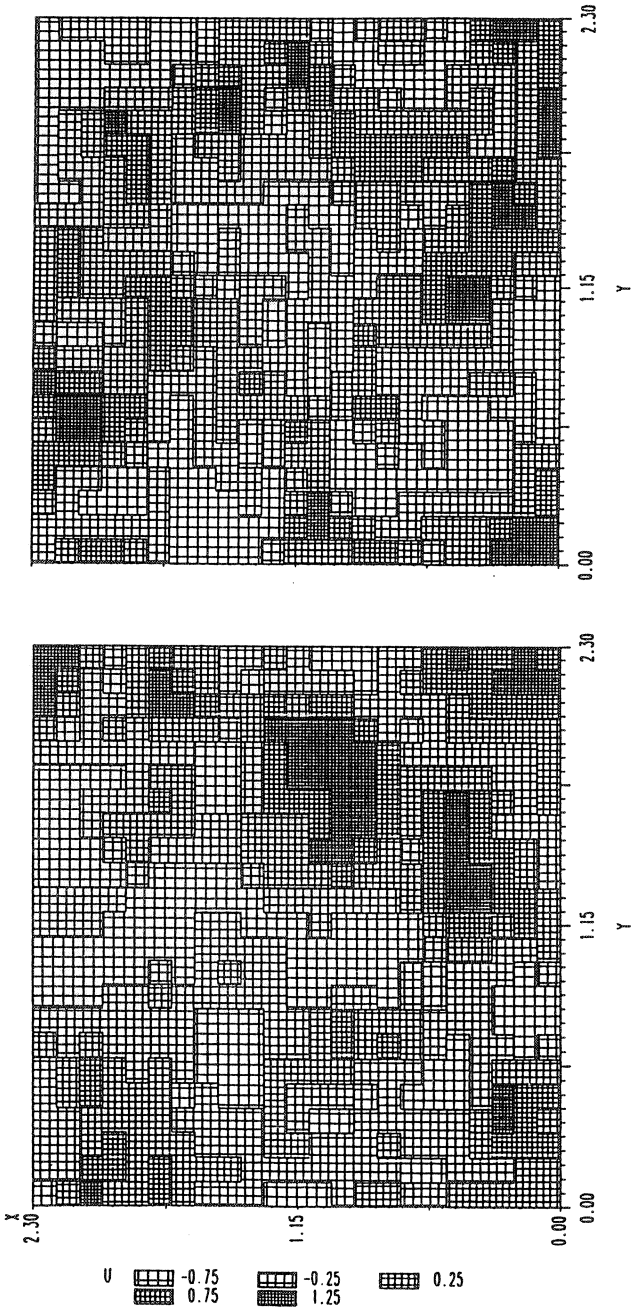


Figure VIII.10: Simulated annealing: γ = 0.0041, r_1 = -1.
Upper figure: T = 1.0; V = +57.0; Time = 2.69.
Lower figure: T = 0.6; V = -2.87; Time = 4.67.

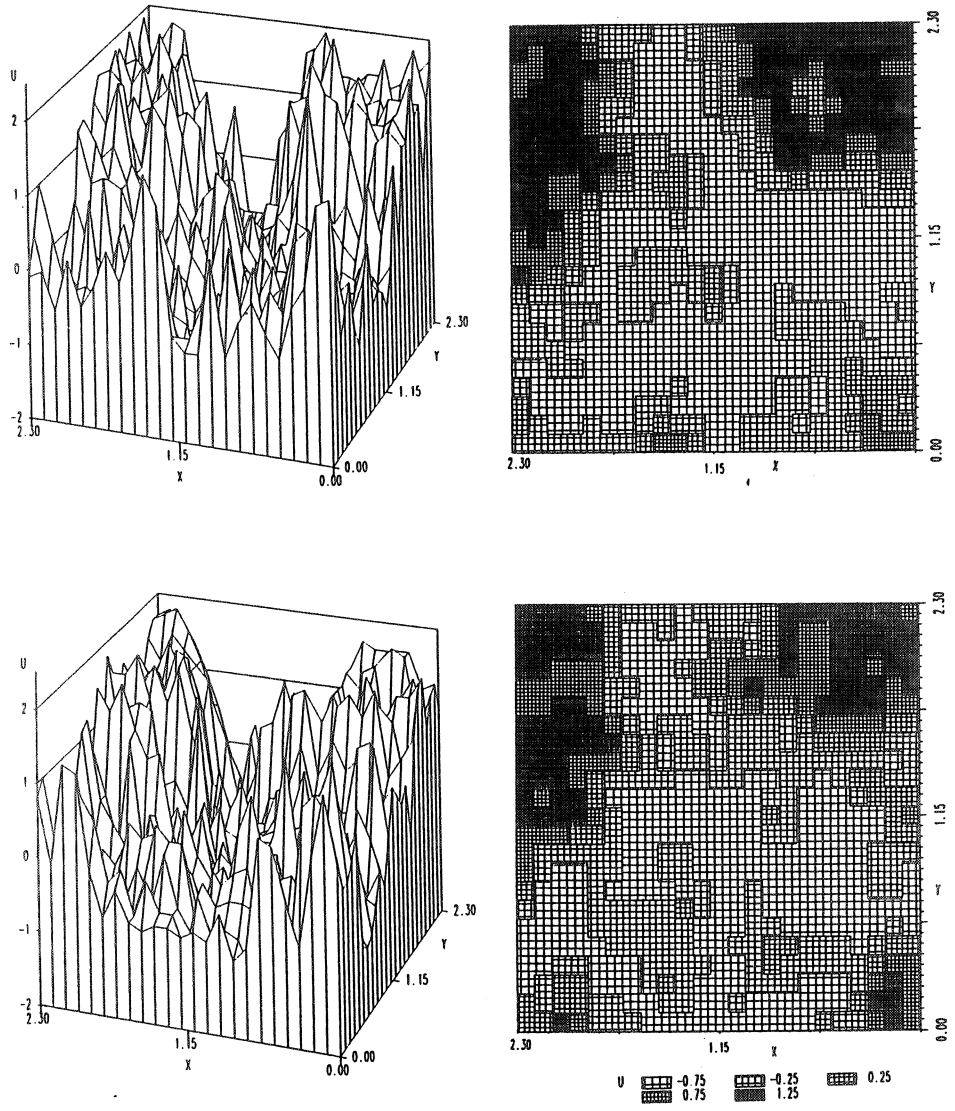


Figure VIII.10 (continued) Two dimensional simulated annealing.

Upper figure: T = 0.4; V = -15.86; Time = 5.06.

Lower figure: T = 0.4; V = -33.54; Time = 5.49.

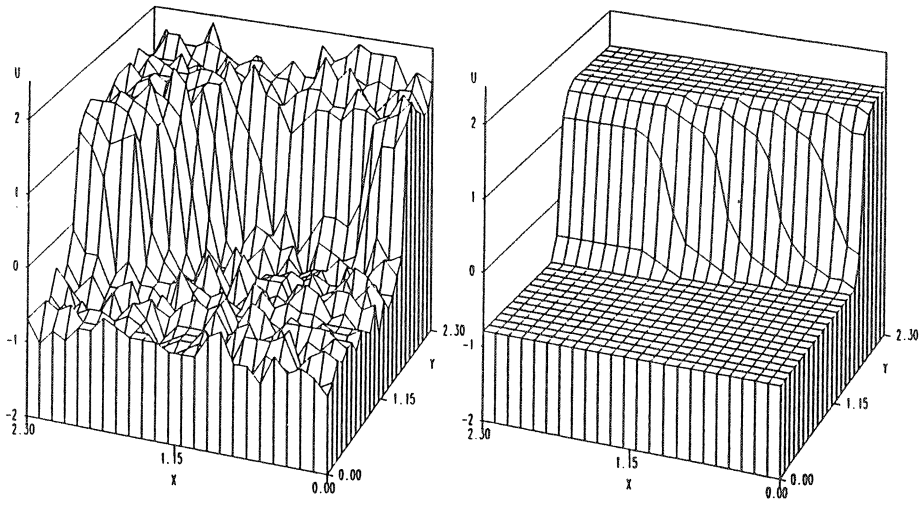


Figure VIII.10 (continued) Two dimensional simulated annealing.

Left: T = 0.1; V = -157.58; Time = 10.0.

Right: T = 0.0 (deterministic); V = -193.55; Time = 25.0.

The physical background of the simulated annealing procedure fits pretty well with the anti-diffusion system, and in general with all systems based on minimizing the Ginzburg-Landau free energy functional. But it is to be noted that during the simulations the functional form of V is not changed. In these simulations, V has at least two minima: the two symmetric monotone solutions. At any temperature the anti-diffusion clustering mechanism was active. In the general formulation of chapter III, the Ginzburg-Landau functional itself depends on the temperature. So the simulations are, with respect to low temperature pattern formation, only partial.

All simulated annealing results show a final pattern which has less or equal zeros (lap-number) than any of the patterns obtained by simulations of the deterministic evolution equation. The system tends

to form a monotone pattern. Secondly, with respect to minimizing the functional V, the results of the the simulated annealing procedure are better then the results obtained by the deterministic time evolution. The reported results are in both cases the best found but with sufficient large variations at the initial stages, the simulated annealing procedure gives results which are always better than any of the deterministic time evolution results, whatever the initial random perturbation (= starting point) of the deterministic system.

CHAPTER IX

PATTERN FORMATION IN PHYSICO-CHEMICAL SYSTEMS

IX.1 Introduction

Spatio-temporal structures are found in many physical systems. In chapter I, section 2, some examples are already give. As a fine example of periodic precipitation patterns in chemico-physical systems the so called Liesegang Rings will be introduced here. The experimental setup and assumptions are rather simple; however, many of the factors involved in pattern formation are present: multiple stationary solutions, phase separation, dependence on temperature and other system parameters, different time scales, sustainment of the non-equilibrium state by diffusion. Related phenomena can be found in geological systems: magmatic crystallization bands are mentioned in McBirney et al. (1979) and Ortoleva (1979).

The general context of the Liesegang Rings is that of binary mixtures which show phase separation and consequently have spatially differentiated properties. In this way, the onset of superconductivity is treated in Berggren et al. (1978). Memory properties of some alloys are explained as a phase transition initiated by external factors. In this context, memory is the exchange of properties belonging to different phases (Achenbach et al., 1983; Falk, 1983,1984).

After an overview of the results of some Liesegang experiments, two mathematical models will be reviewed.

The first model, called the competitive particle growth model

(CPG-model), models cluster size growth as an autocatalytic ripening process; the model equations are taken from Feeney et al. (1983): see also Ortoleva (1984).
The second model is based on the anti-diffusion equation, in this context better called the Cahn-Hilliard (CH) equation (Cahn and Hilliard, 1958; Cahn, 1966, 1968). However so far, the CH equation has always occurred on its own and not as part of a system of equations. In paragraph IX.3.2, the CH equation is part of a three variable component system.

IX.2 Liesegang rings: periodic pattern formation

In 1896 Liesegang published an article on the phenomena of periodic precipitation now named after him (Liesegang, 1896). Many compounds are capable of producing Liesegang rings or bands. In the experiments described below, an OH-component is diffusing into a gel containing cobalt chloride. Instead of a homogeneous precipitate, one gets under the proper conditions a precipitation pattern of successive rings. After some hours the first precipitation appears. The ring consists of microscopically small $Co[OH]_2$ crystals which shows up sharply against its neighborhood where the Co concentration is very low. Only at some distance of the first ring a second ring can form. Again the neighborhood becomes depleted of Co and eventually a third ring forms still further away and so on. The final pattern consists of consecutive rings surrounded by depleted areas.

IX.2.1 Liesegang ring experiments

The experimental results here reported are taken from the work of L. Zwang, Dept. Chem. Path. Erasmus Univ. Rotterdam. The experimental setup is as follows: a tube is divided in three successive zones: one with an initial cobalt concentration of 50 mmol/l (Co-zone), one

neutral zone without Co and OH (NZ-zone), and one with an initial OH concentration between 0.1 and 1.0 mol/l (OH-zone).

Figure IX.1 Liesegang experiment setup.

This configuration is denoted as (OH-NZ-Co, a-b-c) where a,b and c are respectively the length of the zones in mm. The overall medium is an Agar-Agar 1% concentrate.

The specific characteristics of the transient behavior in a Liesegang experiment are most clearly seen by contrasting experiments with and without NH_4CL. For an (OH-NZ-Co, 10-15-25) configuration, table IX.1 gives the results of an experiment with NH_4Cl (overall initial concentration 0.15 mol/l) and table IX.2 gives the results without NH_4Cl. The Co concentrations reported are measured by taking slices k, k = 1,2,3.. at different locations x_k ,k = 1,2,3.., always ordered in such a way that x_i is closer to the OH-zone then x_j iff i < j.

no. intersection	$[Co^{++}]$ (mmol/l)
1	0
2	0
3	0
4	0
5	1
6	2
7	1
8	34
9	49
10	54
11	35
12	33
13	45
14	55
15	58

table IX.1. Experiment with NH_4Cl.

no. intersection	$[Co^{++}]$ (mmol/l)
1	0
2	0
3	0
4	3
5	5
6	9
7	14
8	14
9	55
10	38
11	35
12	45
13	52
14	55
15	58

table IX.2. Experiment without NH_4Cl.

In both experiments it is found that in the neighborhood of the Co-NZ boundary (table IX.1, intersection 9; table IX.2, intersection 10), the germ of a ring is formed. At the intersections 9, resp. 10, Co becomes more concentrated then in neighboring locations by attracting Co ions.
In all these experiments a pH of approximately 8.5 was a necessary condition of germ-formation. But the NH_4Cl-and the non-NH_4Cl experiment differ completely in their subsequent evolution.
Whereas in the NH_4Cl experiment precipitation of $Co[OH]_2$ occurs only after some 190 minutes, in the non-NH_4Cl experiment precipitation starts already after 40 minutes. This means that in the first case the depletion of the neighborhood of a germ location takes far more time than in the second case.
At some distance of the germ the depletion will be less severe and a second germ can arise. In figure IX.2 a time evolution of a NH_4Cl experiment is depicted. At time t = 100 minutes a first ring is already clearly visible. The second ring at location 7.5 began to form at time t = 180 minutes. One observed that ring one was still growing further when ring two began to form. This observation contradicts the Ostwald theory which states that subsequent rings can only arise if the foregoing ring is completely formed and is not growing anymore (Ostwald, 1925).
In figure IX.3 a more evolved Co pattern is shown. Note that the concentration in a ring becomes far more higher then the initial concentration of 50 mmol/l. Precipitation solidifies the pattern.
In the non-NH_4Cl experiment sufficient depletion can not occur because of the fast precipitation. Consequently a continuous precipitate is formed. The time delay of precipitation caused by NH_4Cl is similar to the effect of some electrolytes on delaying or suppressing flocculation (Kruyt et al., 1977; Maron et al., 1974). By adding an electrolyte to the system the electric double layer of a $Co[OH]_2$ complex becomes more extended so that the probability that particles will lump together decreases.

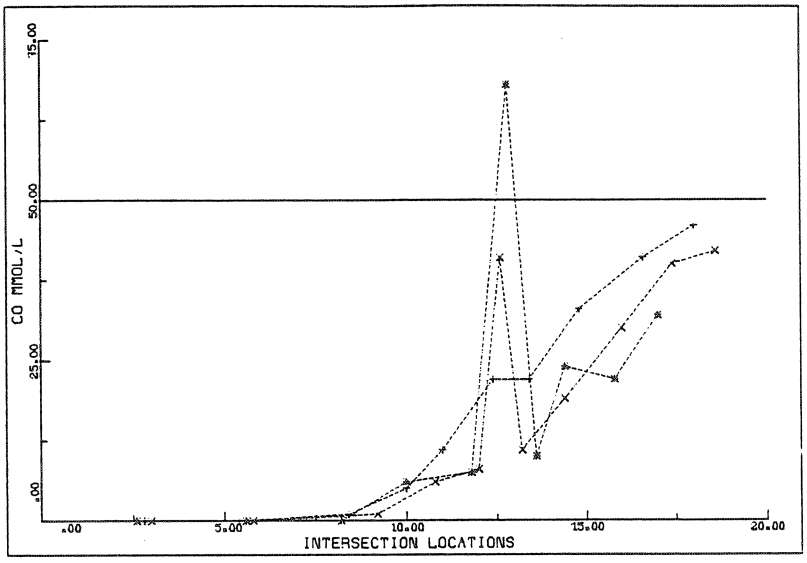


Figure IX.2: Co^{++} concentration time evolution in a NH_4CL experiment. +: 20 min., x: 100 min., *: 230 min..

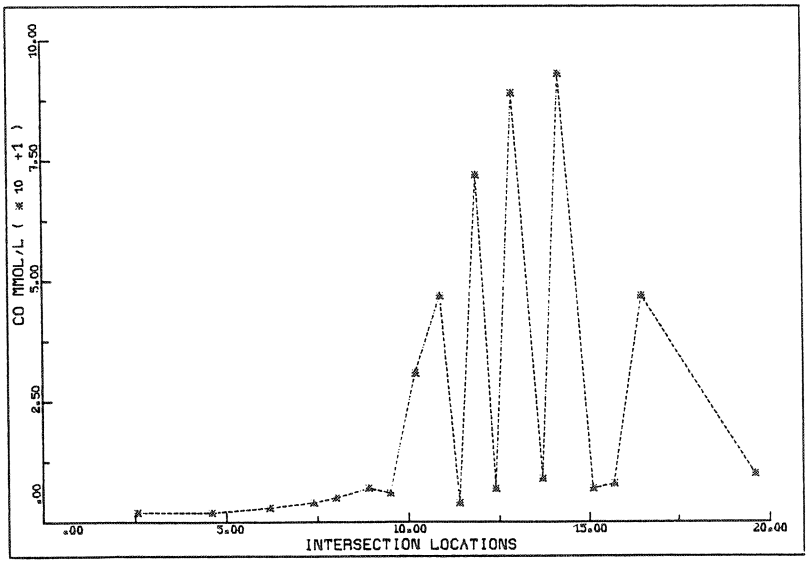


Figure IX.3: Co^{++} concentration pattern in a NH_4Cl experiment.

This competition between depletion and precipitation is also observed in the following experiments: as mentioned above, a pH - environment of 8.5 seems a necessary condition for ring forming. The time to get from a pH of 8.4 to a pH of 8.6 depends on the NH_4Cl concentration present in the system. Table IX.3 gives the results for different NH_4Cl concentrations with an Agar-Agar gel and with an AgaroseEF gel. Since Agar-Agar is more impure than AgaroseEF, clustering is easier in the former case (presence of nucleation kernels) than in the latter one.

	[NH_4Cl] (mmol/l)	time (minutes)	observed pattern
Agar-Agar	0	5	continuous precipitate
	150	11	ring formation
	400	20	no precipitate at all
AgaroseEF	0	8	continuous precipitate
	150	13	continuous precipitate
	400	17	ring formation
	800	30	no precipitate at all

Table IX.3. Time to get from pH 8.4 to 8.6 at different NH_4Cl concentrations and the relation to precipitation.

The reported effects on ring formation are consistent. A low NH_4Cl concentration has two consequences: fast precipitation of $Co[OH]_2$ and the fast adjustment rates for the OH^-- concentration between neighboring locations. Hence depletion will last a short time and be less effective. A high NH_4Cl concentrate will prohibit precipitation at all.

The same effects are observed by varying the OH gradient. If too strong, the growth in pH is fast and only continuous precipitation occurs. If too low, even if a pH of 8.5 can be reached, the final state is a homogeneous one with no precipitation at all.

IX.2.2 Reverse spacing and temperature

In the above reported experiments a relative strong OH gradient was imposed. This introduces a predominant direction in the system with as a consequence the observed spacing of the rings. (In this case a Co gradient is not even necessary, see below.) By making the Co gradient relative strong with respect to the OH gradient, reverse spacing was observed.

Temperature dependence: in a (OH-NZ-Co, 15-0-45) experiment with [Co^{++}] 16 mmol/l and 5% NH_4OH and a temperature of 23°C ring formation takes at least 30 hours. Inserting the same system in a water bath of 37°C ring formation occurs after a few minutes. Table IX.4 gives the distance of the first ring to the OH-Co boundary in relation to the time at which the system is heated up to 37°C.

no.	time T (minutes)	distance OH/Co (mm)
1	14	2.90
2	31	4.80
3	54	6.20
4	87	8.05
5	129	10.05
6	157	11.24
7	184	12.00
8	207	12.79
9	241	13.65
10	275	14.34
11	308	14.80

Table IX.4. Ringformation and temperature. Initial temp. 23°C, after time T (see col. 2) temp. is 37°C; location of first ring is given in col. 3.

The observations mentioned above are combined in the following experiment. At low temperature, Co is homogeneously distributed and an OH concentrate is injected in the centre of the system. After some time which allows OH to diffuse, the system is heated up and a three dimensional spherical precipitation pattern is observed (Leynse Spheres). In this process no initial Co gradient is involved.

IX.2.3 Interpretation

The Liesegang experiment is a system with multiple stationary states: homogeneous, continuous precipitate, periodic precipitate, no precipitate at all. The stability of a state is continuously tested by thermal fluctuations inherent to the system. Slight density differences will occur. If the homogeneous state is unstable such small deviations can be enhanced by a mass flow directed towards the local density maxima. Since in principle all local maxima want to grow, depletion of the neighborhood and competition between the growing centres determine the evolution to some final state. Which state will be reached will depend on the initial fluctuations (e.g. the imposed gradient(s)) and the strength of competition and depletion.

Particles are separated from each other by a potential barrier composed of an attraction force (van der Waals force) and a repulsing force (Powles, 1968; Widom, 1972). (Electric double layer effects.) In chapter I the Boltzmann's ordering principle was mentioned: the system tends to those states with lower free energy. We recall that the free energy F is defined by F = E -TS with E energy, T temperature and S entropy. At low temperature the dominant term is the energy E: in mixtures, as the result of the van der Waals interaction force, the most favored situation is that one where all molecules of the same type are clustered together. With the tendency to reduce the phase separation surface, larger clusters will grow at the cost of smaller ones thereby depleting the neighborhood. This provides a mechanism for autocatalytic growth.

Three aspects can be distinguished:

To get a cluster, the potential barrier must be taken. At high temperature, thermal fluctuations are stronger than at low temperature and consequently the probability to overcome this potential barrier is larger, but at the same time the possibility to escape is increased. Only if the clustered state has a lower free energy than the non-clustered one, germ (= local density maximum) growth will be sustained. In stability terms, the non-clustered state must be unstable or at least metastable, i.e. a state coinciding with a local minimum of the free energy functional, see IX.3.2.. Now it is known that the

stability of a mixture can depend on the pH (Maron et al. 1974; Metiu et al. 1975). From the experiments it seems clear that this is also the case of the Liesegang Rings. At a pH of approximately 8.5, the system becomes unstable which means that germs can form and be sustained.

A second aspect is that the addition of an electrolyte as NH_4Cl can make the potential barrier higher which reduces the possibility to form clusters (Kruyt et al., 1977).

Thirdly, the growth rate of a germ will depend on the local Co-concentration as one of the constituents of $Co[OH]_2$ complexes.

The Liesegang process is now interpreted as follows. (We refer to experiments with initially no Co^{++} gradient (see IX.2.2).) Initially, $Co[OH]_2$ clusters will be in equilibrium with the homogeneous Co^{++} background concentration. Since fluctuations are present in the system, some deviations from the equilibrium state will occur. It now depends on the pH-environment (i.e. the OH^--concentration) whether deviations are sustained and germ formation will occur or not. The OH^--flow may create locally a state which favors clustering. This state is characterized by a specific cluster size which is not in equilibrium with the Co^{++} background concentration. As a result of the van der Waals interaction force (reduction of the phase separation surface) a germ will grow causing at the same time a stronger deviation from the equilibrium cluster size defined by the Co^{++} background concentration.

The tendency to restore equilibrium with the background Co^{++} gives rise to dissolution of the germ as well as to a Co^{++} flux towards this germ. (The germ creates a sink in the Co^{++} concentration.) If clustering is favored, dissolution will be weak and the mean equilibrium restoring effect will be a Co^{++} flux towards the germ causing competition between the growing centres. However, the OH^- gradient provides a spatial differentiation. At the pH = 8.5 boundary a germ can grow easier by depletion as it is partly surrounded by an environment which does not favor clustering. With the autocatalytic growth mechanism mentioned above, we can reason that a precipitation ring can arise where the pH becomes 8.5. The pattern formation process now depends on the time scales of depletion and the moving boundary of the OH^- surplus. Since the electrolyte NH_4Cl influences the precipitation rate (and hence depletion), the process is tuned by the NH_4Cl concentration.

IX.3 Mathematical models

Already in 1897 Wi Ostwald sr. (1897) presented an explanation of the Liesegang phenomena in terms of supersaturation and diffusion. Ostwald's theory was of qualitative nature only. Mathematical treatments of Ostwald's supersaturation theory were put forward in former times by Prager (1952). Recently Keller and Rubinow (1981) presented a mathematical formulation of Wi Ostwald's supersaturation theory. Not only diffusion but also the chemical reaction and the precipitation of the product are considered. Similar models can be found in Flicker and Ross (1974). Both are examples of reaction-diffusion models with an autocatalytic growth term. Flicker and Ross criticized the Ostwald theory because it does not predict the other phenomena observed in the Liesegang experiment: reverse spacing (see section IX.2.2) and secondary structures (secondary banding: the initial structure breaks up in a finer structure). Moreover Ostwald's theory requires an imposed concentration gradient. In their opinion supersaturation is unnecessary for periodicity (see also Hazewinkel et al., 1986).

Strongly related to secondary banding are experiments where an uniform sol of the precipitate is allowed to age. Spatially inhomogeneous structures arise but, in contrast to the Liesegang experiment, this process is slow and it can take days for the larger particles to grow substantially at the cost of smaller ones. The model, called the competitive particle growth model (CPG model) following Ortoleva, has the formal structure of interaction between a diffusible substance and a non-diffusible variable representing the radius of large particles (Ortoleva, 1979,1984; Feeney et al., 1983). It is based on the principle discovered by Wi Ostwald (1925) and named for him: Ostwald's ripening (see IX.3.1).

The Liesegang ring phenomenon is a typical example of molecular aggregation and decomposition with a mass flux from low concentration areas to high concentration areas. The anti-diffusion equation with its physical background as an evolution equation minimizing the Ginzburg-Landau free energy functional, seems an appropriate candidate to model such a phenomenon. See IX.3.2..

IX.3.1 The competitive particle growth model

An extensive review of the competitive particle growth model can be found in Feeney et al. (1983). The model is based on interdependence of particle growth, diffusion and the precipitation particle depending on the equilibrium concentration. The basic assumptions are:

i) a particle growth-dissolution process is restricted to :

$$P_n + P_1 \overleftrightarrow{\longrightarrow} P_{n+1}$$

where P_n, $n = 1,2,..$ is an aggregate of n monomers.

ii) at each point in space, the concentration c_n of the polymers P_n is and stays narrowly peaked about some $n^*(x,t)$. So, assuming spherical particles, in any small spatial domain the (large) particles are represented by a particle with radius $R(x,t)$.

iii) surface free energy will cause any large particle to have an equilibrium monomer concentration C^{eq}. Assumed is that for large R, $C^{eq}(R)$ is monotonically decreasing in R. Then, for large R, a local maximum in R will grow and cause dissolution in its surroundings. In turn minima will induce secondary maxima in R.

The model is described in terms of the local monomer concentration $C(x,t)$ and the local average particle size $R(x,t)$. Changes in particle size are given by:

$$\frac{\partial R(x,t)}{\partial t} = \frac{K}{\rho}\left[C(x,t) - C^{eq}(R)\right] \qquad \text{(IX.1a)}$$

where ρ is molar density and K a reaction constant. Mass conservation leads to the following evolution equation for C:

$$\frac{\partial C(x,t)}{\partial t} = D\Delta C - n\rho\frac{\partial}{\partial t}(\tfrac{4}{3}\pi R^3) + \frac{qW}{\varepsilon} \qquad \text{(IX.1b)}$$

where n is number density of precipitation particles, assumed to be time independent, $D\Delta C$ is diffusion according to Fick's Law ($D > 0$, constant) and qW/ε is the source term of monomer production.

The equilibrium concentration $C^{eq}(R)$ is given by :

$$C^{eq}(R) = C^{eq}(\infty)\left[\, 1+ \frac{2\Gamma R^2}{2R^3 + R_c^3} \,\right] \qquad (IX.2)$$

with $C^{eq}(\infty)$ a scaling parameter, Γ a constant involving surface tension, crystal molar density, absolute temperature etc. and R_c the critical radius. Dimensionless variables are defined as follows :

$$C = C^{eq}(1 + s);\ R = \bar{R}\psi;\ x = \bar{L}\xi;\ t = \bar{t}\tau;\ n = \bar{n}\nu \text{ and } \sigma = \frac{\bar{R}}{\bar{\Gamma}}\cdot s,$$

where $^-$ denotes characteristic (averages) values. This gives the following model:

$$\frac{\partial \psi}{\partial \tau} = \sigma - g(\psi, \psi_c) \qquad (IX.3a)$$

$$\frac{1}{\beta}\frac{\partial \sigma}{\partial \tau} = \Delta\sigma - \psi^2\nu\frac{\partial \psi}{\partial \tau} + \frac{qW}{\varepsilon} \qquad (IX.3b)$$

where

$$g(\psi, \psi_c) = \frac{2\psi^2}{2\psi^3 + \psi_c^3} \qquad (IX.3c)$$

with no flux boundary conditions.

(β is a dimensionless combination of $C^{eq}(\infty)$, Γ, $\bar{n}$ and $\bar{R}$ or equivalently of D, $\bar{L}$ and $\bar{t}$; $\psi_c = R_c/\bar{R}$). In the following the source term qW/ε is neglected and ν is set to 1.

Any uniform distribution of ψ and σ defined by $\psi(\xi,.) = \psi_o$, $\sigma(\xi,.) = \sigma_o$ with $\sigma_o = g(\psi_o, \psi_c)$ is a solution of (IX.3)

Now consider the system on a closed interval $I = \{\, \xi \in \mathbb{R} \mid 0 \le \xi \le L\}$ then a linear stability analysis shows that every uniform solution with $\frac{dg}{d\psi}\big|_{\psi=\psi_o} < 0$ is unstable. The linear approximation of the right hand of (IX.3) defines a linear operator on the solution space $L^2[0,L]$, see appendix E. Then, given no flux boundary conditions, eigenvectors are proportional to $\cos(\frac{k\pi\xi}{L})$ and the eigenvalues $\mu(k)$ must satisfy :

$$\mu^2(k) + \mu(k)\left[g_1 + \beta p_k^2 + \beta\psi_o^2\right] + \beta g_1 p_k^2 = 0$$

where $g_1 = \frac{dg}{d\psi}\big|_{\psi=\psi_o}$, $p_k^2 = \frac{k^2\pi^2}{L^2}$. $\qquad (IX.4)$

If $g_1 < 0$ all eigenvalues $\mu(k)$ are real and the largest eigenvalue is positive. Moreover, this largest eigenvalue is monotone increasing in k. Therefore, linear stability analysis predicts the growth of a

spatial structure if $\psi_o > \psi_c$ but with an evolution according to the smallest possible wave length in the case of an initial homogeneous structure randomly disturbed.

IX.3.1.1 Numerical simulations

The partial differential equations (IX.3) with the boundary conditions are approximated by finite difference schemes; with 96 grid points, grid spacing h is L/95 with L = 10 or 20. The value of the parameter ψ_c is taken 0.25. The initial value ψ_o of ψ is 1.0.
In the first reported simulation, this initial value is randomly disturbed.

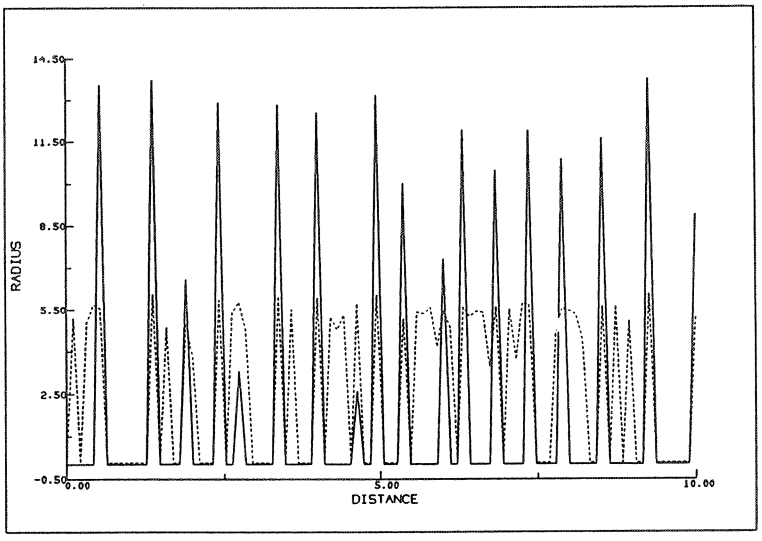


Figure IX.4 Competitive Particle Growth Model: β = 0.01, L = 10
Initial homogeneous state: randomly disturbed.
--- : time= $15h^2$; —— : time= $650h^2$, h = 10.0/95.

Initially the evolution takes the form of a (degenerate) pattern of alternating maxima and minima as the linear analysis predicts. Further growth leads to competition between the growing centres and gives the pattern as depicted in figure IX.4.

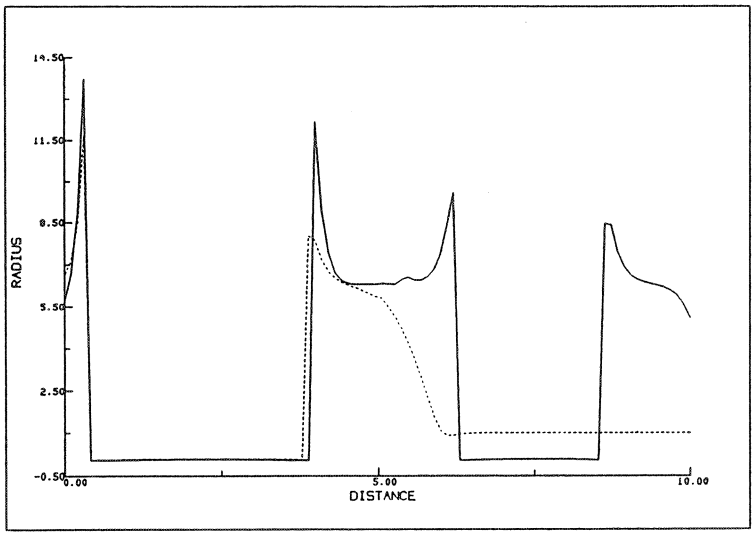


Figure IX.5 Competitive Particle Growth Model: β = 0.01, L = 10
Initial homogeneous state only locally disturbed in the four left grid points. --- : time=40h^2 ; —— : time=225h^2.

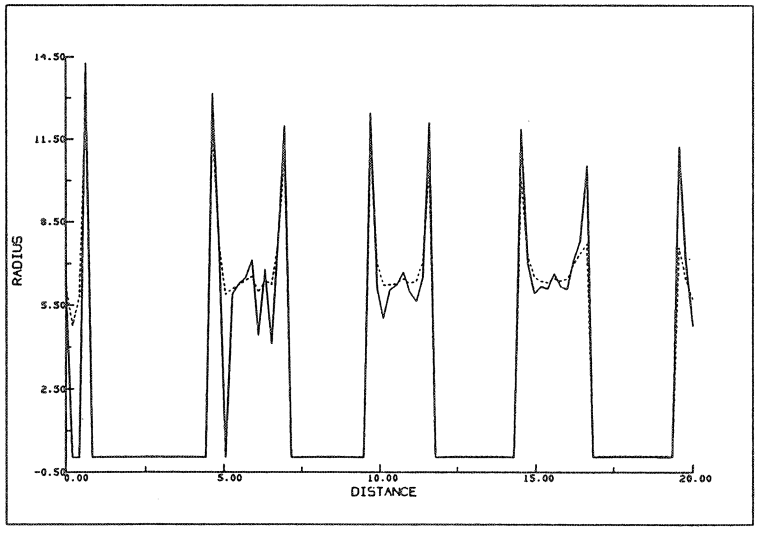


Figure IX.6 Competitive Particle Growth Model: β = 0.01, L = 20
Initial homogeneous state only locally disturbed in the four left grid points. --- : time=40h^2 ; —— : time=75h^2.

All maxima in the ψ-pattern go along with minima in the σ-pattern. It is to be noted that the peaks in figure IX.4 are at single grid points in the final stages of the evolution, so the final pattern has maximal frequency. This persists if finer spacings are taken.

The same sort of evolution is observed in the following simulations. Parameters and initial values are the same as above but now only the values of the four extreme left grid points are disturbed with the same positive value. As the initial bump grows, a depletion zone is formed. In figure IX.5 the dotted line gives the pattern at time $500h^2$. The patterns show a characteristic distance ξ_1 between successive bumps, except for the first and second one. Since β is the diffusion coefficient of σ, the degree of smoothing will be depend on β; this is indeed found in the simulations: for $\beta = 0.01$, $\xi_1 \approx 2.3$; $\beta = 0.1$, $\xi_1 \approx 3.0$, see figure IX.6 and IX.7).

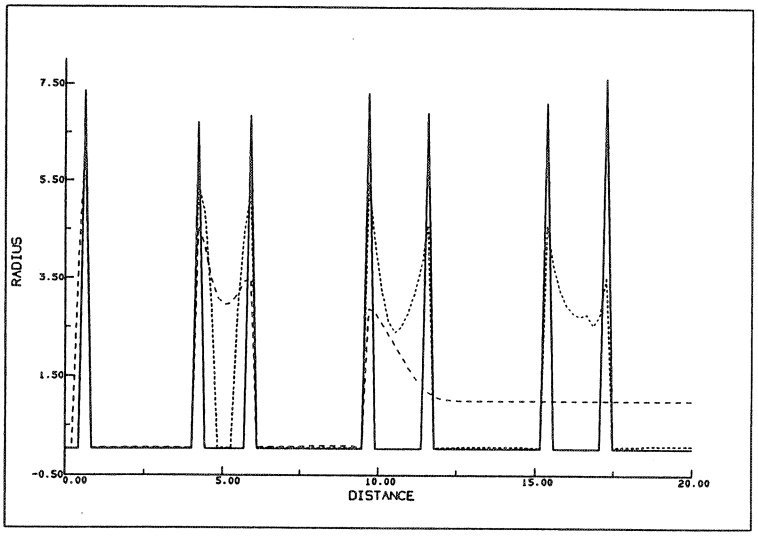


Figure IX.7 Competitive Particle Growth Model: $\beta = 0.1$, L = 20
Initial homogeneous state only locally disturbed in the four left grid points. ... : time=$40h^2$;--- : time=$75h^2$; —— : time=$225h^2$.

Since R is taken to be larger then R_c, the model describes the evolution after the particles have reached at least a considerable size R_c. In making the assumption on the peaked particle-size distribution plausible, Feeney et al. use the ripening process and state that such a distribution will be valid in the post nucleation regime. Accordingly, we interpret the equations rather as modeling phenomena such as secondary banding than as modeling the initial transient behavior in a Liesegang experiment. This means that the simulations reported here and in Feeney, are in themselves simulations of the secondary banding process and do not reflect the *final* breakup in finer peaks as stated by Feeney et al. (1983).

IX.3.2 An anti-diffusion model

The experiments (section IX.2.1 and IX.2.2) have shown that ring formation depends above all on two environmental parameters: temperature and pH. Thermal fluctuations will cause deviations in the distributions of the components; at sufficiently high temperature such deviations are strong enough to form the germs of ring formation. At some particular pH level these germs are sustained and enhanced by a mass flow directed towards local maxima in the Co^{++} density. This depletion effect is conceived as a mass redistribution process by nearest neighbor interaction with the change rate depending only on the gradient of the weighted mass density. In this way described, the clustering process is similar to the reverse of a Fickian, standard mass diffusion process, that is an anti-diffusion process. We recall from chapter II that this name is used only as a formal description of the observed mass redistribution process.

It is to be mentioned that such a diffusional clustering mechanism is also reported to be found in the so called spinodal alloys (e.g. Cahn, 1966, 1968; Coutsias et al., 1984). Phase separation by *spinodal decomposition* is characterized by the aspect that the whole solution appears to nucleate at once whereas phase separation by *nucleation* is a process in which sufficiently large nuclei appear randomly and grow.

The Landau theory of phase transitions provides a basis for a distinction between spinodal decomposition (second order phase transition) and nucleation (first order phase transition). In the case of spinodal decomposition the current state is not given by a minimum of the free energy functional; the state is unstable, every fluctuation will drive the system away from this state. At nucleation however the current state is linearly stable but there exists a state which has a lower free energy then the current one; the current state is called *metastable*: small fluctuations are damped out but as a consequence of large fluctuations, the onset of a new phase can occur. Restricting to one component u, given an initial density u, with increasing temperature the system will go from spinodal to nucleation and finally to a stable mixed regime. The spinodal decomposition phase comes before nucleation on the temperature scale. Gibbs called the spinodal the *limit of metastability* (Cahn, 1966).

For a one dimensional, one component system described by the density function u(x,t), the anti-diffusion equation gives a time evolution characterized by minimization of the functional V:

$$V(u) = \int f(u) + \frac{1}{2}\gamma u_x^2 dx \qquad \text{(IX.5a)}$$

where

$$f(u) = \int_0^u \phi(s)ds \qquad \text{(IX.5b)}$$

and γ a positive constant.

As mentioned in chapter III, section 5, the Ginzburg-Landau theory of phase transitions gives the free energy of a system in the form of equation (IX.5a). The gradient term accounts for non-homogeneities and is called the gradient-energy term (Widom, 1972). Since the properties of the system will depend on the temperature and, or the pH, a possible form of the function ϕ is

$$\phi(u) = r_o(\mu)u + r_1u^2 + r_2u^3, \quad r_2 > 0 \qquad \text{(IX.6)}$$

where $r_o(\mu)$ is a function of the environmental parameter μ, expressing temperature, and pH dependence.

The state of the system, given by $u \equiv 0$, is called spinodal if this state represents a maximum of V(u): every small fluctuation will be enhanced and the system will be driven to a state with lower free

energy (see also chapter III). The necessary condition is that $r_o(\mu)$ is negative; if γ is sufficiently small then the null state will be unstable.
For $r_o(\mu)$ positive and γ small, the system can still undergo phase separation by nucleation if in the u-f plane, the point with u = 0 on the double tangent to the graph of f lies below (0,0) which means that this point represents a state with a lower free energy than the uniform state $u \equiv 0$. In this case, the null solution is linearly stable but large fluctuations can drive the system to the lower free energy level.

At sufficiently high temperature Liesegang Rings are only formed if the pH is approximately 8.5. In the following we neglect the dependence on temperature and assume the system can be brought into the spinodal regime at a specific pH level; the coefficient r_o in (IX.6) depends only on the pH, i.e. the OH^- concentration. In terms of the free energy functional (IX.5a): for pH $\approx$ 8.5, the state u = 0, the mixed state, becomes a maximum of the functional which has in that case a minimum at $u^+ > 0$ (and $u^- < 0$) where u^+ denotes the clustered phase. The state (u^+, u^-) is reached by mass flow from low density into high density areas.
Note that here only the early stages of ring formation are considered: the $Co[OH]_2$ cluster size will be a monotonically *increasing* function of the cluster size. So in areas with a high background density, the clusters can grow whereas in the lower density areas the clusters dissolve. The equilibrium density defined by (IX.2) has the same property if $R < R_c$. But from the stability analysis applied to the CPG-model it is clear that for such small radii, fluctuations in the radii will be damped out if the time evolution of the background density is restricted to standard Fickian diffusion. One needs an unstable diffusion mechanism such as the anti-diffusion form to induce instabilities to the system.

The Liesegang process is formulated in terms of three variables.
Assumptions :

i) the formation of the $Co[OH]_2$ complex is approximated by the following scheme :

$$A + 2B \underset{k_1}{\overset{k_{-1}}{\rightleftarrows}} C \qquad \text{(IX.7)}$$

where A is positive ion (Co^{++}), B a negative ion (OH^-) and C is an aggregate of AB molecules ($Co[OH]_2$); k_{-1}, k_1 are positive reaction constants.

ii) For each cluster of $Co[OH]_2$ there exists an Co^{++} equilibrium concentration Co^{eq}, but now small clusters are assumed such that Co^{eq} is a monotone increasing function of the relevant cluster size.

iii) A flux of Co towards a local maximum of the Co concentration, which goes along with a local maximum in the cluster size by assumption ii), is only possible beyond some level B_c of the negative ion (OH^-) concentration. (Temperature effects are neglected.)

iv) Only standard, Fickian diffusion is assumed to be valid for the OH component since the experiments have not given any evidence that the OH-diffusion is affected by ring formation.

Essentially only the whole mechanism of cluster growth by competition and depletion by a flow of Co^{++} towards germs is modeled by the anti-diffusion equation included in the A-component evolution equation. The the linear coefficient in ϕ depends on that OH^- component such that for low values of the OH^- concentration, no clustering will occur. Only at high levels of [OH] the anti-diffusion term will induce instability in the system and becomes a real anti-diffusion.
Hence the aggregating process in A is governed by an anti-diffusion term:

$$\Delta\left[r_0 A - r_1 A^2 + r_2 A^3 - \gamma \Delta A\right], \qquad \text{(IX.8)}$$

with $r_o = r_o(B)$. $r_2 > 0$, $\gamma > 0$ and Δ is Laplace operator.
The reaction (IX.7) links the Co^{++} concentration with the growth of $Co[OH]_2$ and simulates precipitation effects.
A second stabilizing factor was the electrolyte NH_4Cl. The electrolyte influences the steepness of the van der Waals interaction potential.

Depending on the NH_4Cl concentration, the $Co[OH]_2$ clusters become more or less contracted. The coefficient γ of the gradient term in V (equation IX.6a), the wave length of the unstable modes (see chapter V and the numerical simulations, chapter VIII). So the role of NH_4Cl is simulated by γ as the bifurcation parameter.

Then the following model is derived , with $A = [Co^{++}]$, $B = [OH^-]$ and $C = [Co[OH]_2]$:

$$\frac{\partial A}{\partial t} = -k_1AB^2 + k_{-1}C + D_A \Delta \left[\psi(A,B) - E_A \Delta A\right] \qquad \text{(IX.9a)}$$

$$\frac{\partial B}{\partial t} = -2k_1AB^2 + 2k_{-1}C + D_B \Delta B \qquad \text{(IX.9b)}$$

$$\frac{\partial C}{\partial t} = -k_{-1}C + k_1AB^2 \qquad \text{(IX.9c)}$$

where D_A, D_B are positive diffusion constants,
$\psi(A,B) = (-B + B_c)A - r_1A^2 + r_2A^3$ with $r_2 > 0$ and B_c some positive constant reflecting pH-dependence of aggregation stability or instability of the Co-component; finally E_A is a positive constant corresponding to γ in the standard anti-diffusion model.

Let $A = A_o(1 + \alpha)$, $B = B_o(1 + \beta)$ and $C = C_o(1 + \gamma)$ such that $k_{-1}C_o = k_1A_oB_o^2$; let $t = \bar{t}\tau$ and $x = \bar{L}\xi$ with $\bar{t}$ and $\bar{L}$ time- and space scaling factors such that $D_A\bar{t}/\bar{L}^2 = 1$ then the equations (IX.9) are reduced for an one dimensional spatial domain $[\,0,\, L\,] \subset \mathbb{R}$ to:

$$\frac{\partial \alpha}{\partial \tau} = -k\left[(1 + \alpha)(1 + \beta)^2 - (1 + \gamma)\right] + \frac{\partial^2}{\partial \xi^2}\left[\phi(\alpha,\beta) - \varepsilon \frac{\partial^2 \alpha}{\partial \xi^2}\right] \qquad \text{(IX.10a)}$$

$$\frac{\partial \beta}{\partial \tau} = -2k\left[(1 + \alpha)(1 + \beta)^2 - (1 + \gamma)\right] + D_\beta \frac{\partial^2 \beta}{\partial \xi^2} \qquad \text{(IX.10b)}$$

$$\frac{\partial \gamma}{\partial \tau} = -k\left[(1 + \gamma) - (1 + \alpha)(1 + \beta)^2\right] \qquad \text{(IX.10c)}$$

where, for simplicity, one takes $A_o = B_o = C_o$, $k = k_1B_o^2$ and

$$\phi(\alpha,\beta) = (-\beta + \beta_c)\alpha - r_1'\alpha^2 + r_2'\alpha^3 \text{ with } r_2' > 0 \qquad \text{(IX.10d)}$$

No-flux boundary conditions are assumed.

For the homogeneous solution $(\alpha,\beta,\gamma) \equiv (0,0,0)$ the evolution equations for the disturbances u of $\alpha \equiv 0$, v of $\beta \equiv 0$ and w of $\gamma \equiv 0$ are given in linear approximation by :

$$\frac{\partial u}{\partial \tau} = -k(u+ 2v - w) + \beta_c \frac{\partial^2 u}{\partial \xi^2} - \varepsilon \frac{\partial^4 u}{\partial \xi^4} \qquad \text{(IX.11a)}$$

$$\frac{\partial v}{\partial \tau} = -2k(u + 2v - w) + D_\beta \frac{\partial^2 v}{\partial \xi^2} \qquad \text{(IX.11b)}$$

$$\frac{\partial w}{\partial \tau} = k(u + 2v - w) \qquad \text{(IX.11c)}$$

Given the no-flux boundary conditions the eigenvectors of this linear system are proportional to $\cos(\frac{l\pi\xi}{L})$, $l = 0,1,2,..$ and the eigenvalues $\mu(l)$ must satisfy :

$$\mu^3(l) + \mu^2(l)\left\{\varepsilon p_l^4 + D_\beta p_l^2 + \beta_c p_l^2 + 6k\right\} + \mu(l)\left\{\varepsilon D_\beta p_l^6 + \right.$$

$$\left. + (5\varepsilon k + D_\beta \beta_c) p_l^4 + (2kD_\beta + 5k\beta_c) p_l^2 \right\} + k(\varepsilon D_\beta p_l^6 + \beta_c D_\beta p_l^4) = 0$$

where $p_l^2 = \frac{l^2\pi^2}{L^2}$. (IX.12)

All eigenvalues are real because if we write (IX.11a-11c) in matrix form, e.g. $\frac{\partial z}{\partial \tau} = Lz$ with $z = (u,v,w)^T$ then L is symmetric.

For $\beta_c > 0$ all eigenvalues are negative and the state $(\alpha,\beta,\gamma) = (0,0,0)$ is stable.

For $\beta_c < 0$ the system can become unstable, see Table IX.5 below where for specific parameter values the unstable modes are given.

A non-homogeneous solution of (IX.10) can be constructed by using the existence of a non-constant bounded stable solution of the one dimensional anti-diffusion equation .

Let $\beta(\xi) = \beta_o$, constant such that $\alpha \equiv 0$ is an unstable solution of:

$$\frac{\partial \alpha}{\partial \tau} = \frac{\partial^2}{\partial \xi^2}\left[\phi(\alpha,\beta_o) - \varepsilon \frac{\partial^2 \alpha}{\partial \xi^2}\right] \qquad \text{(IX.13)}$$

with ϕ as defined in (IX.10d).

Then there exists a non-constant stable bounded solution $\alpha(\xi)$ of (IX.13). Take $\gamma(\xi)$ such that:

$$\gamma(\xi) = (1 + \beta_o)^2(1 + \alpha(\xi)) - 1 \quad , \forall\ \xi \in [0,L] \qquad \text{(IX.14)}$$

then $(\alpha(\xi),\beta_o,\gamma(\xi))$ is a stationary solution of (IX.10).
If the evolution of $\beta(\xi)$ is neglected, that is $\beta(\xi) = \beta_o$ for all ξ and all time t, the system is reduced to the equations (IX.10a) and (IX.10c). Then a solution $(\alpha(\xi),\gamma(\xi))$ will be a stable solution of the reduced system. Since $\alpha(\xi)$ is a stable solution of (IX.13) the equation obtained by linearizing (IX.13) in $\alpha(\xi)$ will have a complete set of eigenvectors $W_\alpha(\xi)$ with all eigenvalues equal or less than zero. The reaction terms in (IX.10a) and (IX.10c) are linear in α and γ, and stable, so the linear system obtained by linearizing (IX.10a) and (IX.10c) in $(\alpha(\xi),\gamma(\xi))$ is a stable system and all disturbances as expressed in terms of the eigenvectors $W_\alpha(\xi)$ will be damped.

IX.3.2.1 Numerical simulations

The numerical simulations can be divided in two sections. First: the initial homogeneous state $(\alpha,\beta,\gamma) \equiv (0,0,0)$ is randomly disturbed. If β_c is positive no pattern formation occurs (the null solution is stable).

ε	unstable modes	fastest growing
0.0042	$1 \le l \le 11$	$l = 8$
0.0024	$1 \le l \le 15$	$l = 11$

Table IX.5: unstable and fastest growing modes.
($\beta_c = -1$, $k = 1$, $D_\beta = 5$)

For $\beta_c = -1$, $k = 1$ and $D_\beta = 5$, table IX.5 gives the unstable modes for the two different ε values used in the numerical simulations. The fastest growing mode is the mode with the largest (positive) eigenvalue.
The simulations are performed on a grid with 96 points. In all simulations the coefficient r_2' in (IX.10d) is always equal to 1 with $D_\beta = 5.0$ and $k = 1$. The initial evolution is again according to the fastest growing mode. Final patterns however have a larger wavelength. See figure IX.8 with $r_1' = -1$ and $\varepsilon = 0.0024$; figure IX.9 with the same r_1' value and $\varepsilon = 0.0042$ and figure IX.10 with $r_1' = -3$ and $\varepsilon = 0.0042$.

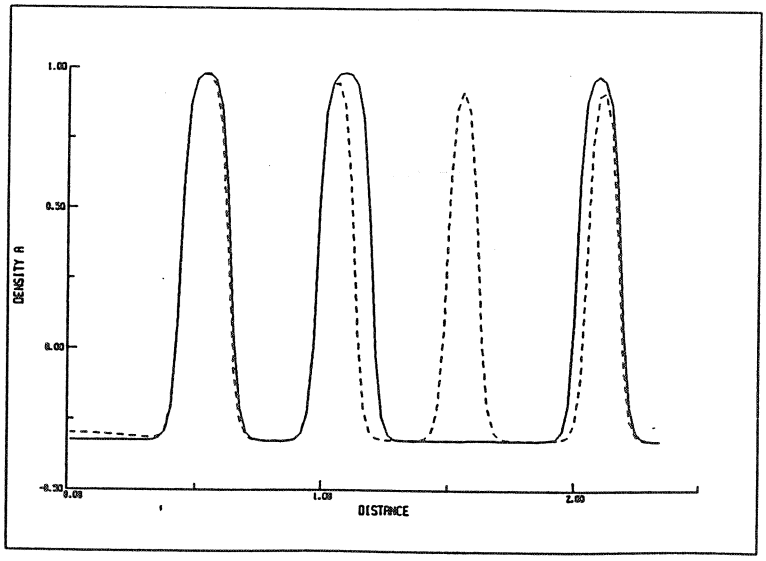


Figure IX.8 Anti-diffusion model: $\varepsilon = 0.0024$, $r_1' = -1$, $\beta_c = -1$
--- : time = $0.2h^2$; —— : time = $10.0h^2$.

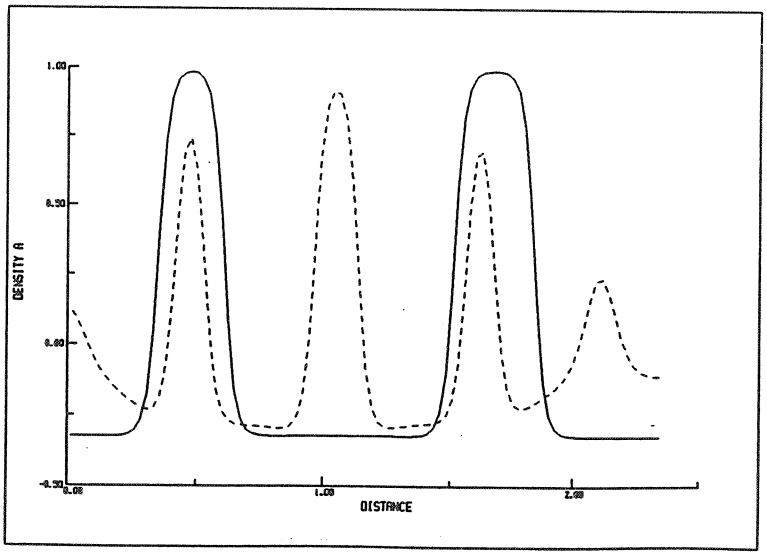


Figure IX.9 Anti-diffusion model: $\varepsilon = 0.0042$, $r_1' = -1$, $\beta_c = -1$
--- : time = $0.2h^2$; —— : time = $10.0h^2$.

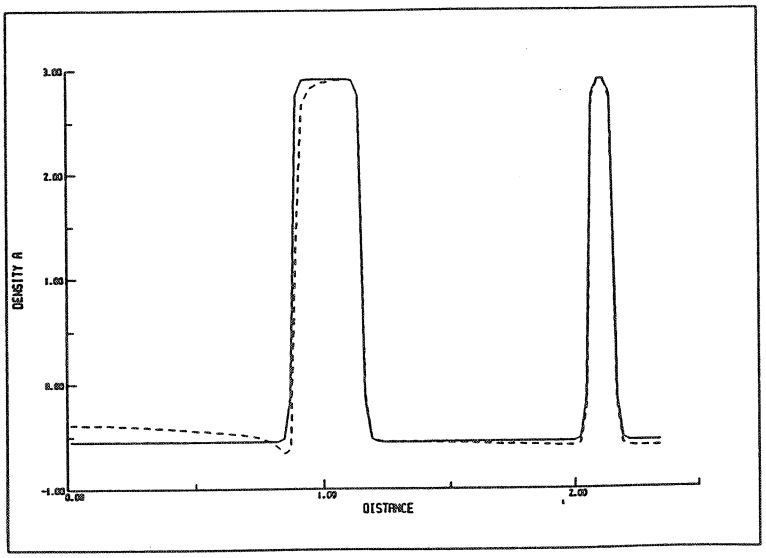


Figure IX.10 Anti-diffusion model: $\varepsilon = 0.0024$, $r_1' = -3$, $\beta_c = -1$
--- : time = $0.2h^2$; —— : time = $10h^2$.

The evolution of the γ-component is similar to that of the α-component; the final β-pattern is a homogeneous one such that $\beta_c - \beta$ is sufficiently negative to ensure that the null solution stays unstable. So the final pattern is indeed of the form as given in the paragraph (IX.3.1) of the foregoing section with $\alpha = \gamma$ and $\beta = \beta_o$ for all ξ.

In the second group of simulations the parameters are taken such that now the null solution $(\alpha,\beta,\gamma) \equiv (0,0,0)$ is stable. Now a pattern generating evolution is initiated by a large bump of the β-component on the left side of the grid. (This can be seen as an approximation of the experiments with homogeneous distributed $Co^{++}$and an OH^--injection in the centre of the system, see paragraph IX.2.2. For all reported simulations $\beta_c = 0.01$ with again $D_\beta = 5.0$ and $k = 1$.
The pattern depicted in figure IX.11 is generated for $r_1' = -1$ and $\varepsilon = 0.0024$ and that of figure IX.12 for $r_1' = -3$ and $\varepsilon = 0.0024$. In both cases the final pattern of β is an homogeneous one with a value sufficiently high to make the null solution unstable.

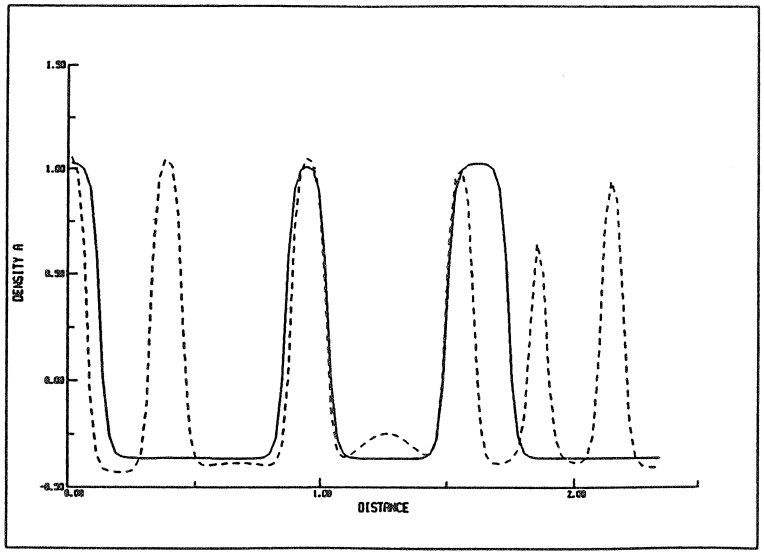


Figure IX.11 Anti-diffusion Model: $\varepsilon = 0.0024$, $r_1' = -1$, $\beta_c = 0.01$
Initial homogeneous state disturbed by a β-surplus at the left side only. --- : time $50h^2$; —— : time $1000h^2$; (h: grid spacing).

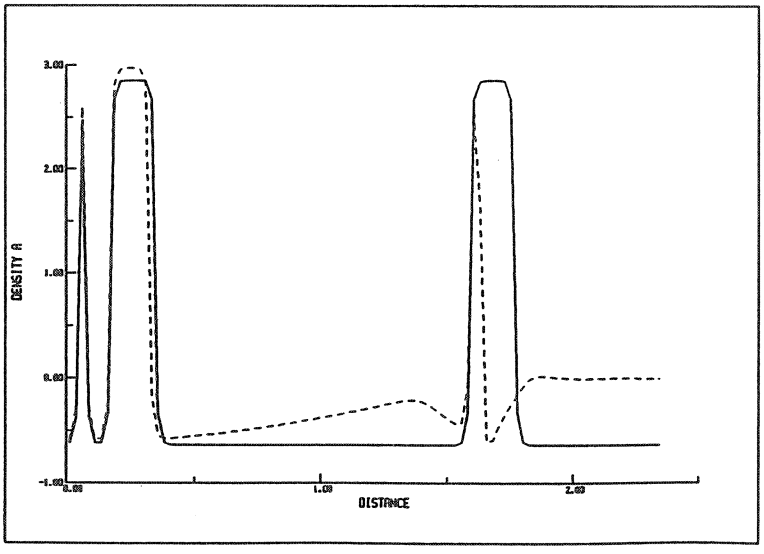


Figure IX.12 Anti-diffusion Model: $\varepsilon = 0.0024$, $r_1' = -3$, $\beta_c = 0.01$
Initial homogeneous state disturbed by a β-surplus at the left side only. --- : time $50h^2$; —— : time $1000h^2$; (h: grid spacing).

For fixed β_c the instability properties of a homogeneous solution depends on ε as well as on the final β-level reached after smoothing out of the initial β disturbance. With increasing ε the final pattern becomes less profiled, e.g. if $\varepsilon = 0.008$ with the same initial conditions as in figure IX.11 and IX.12 the final pattern is a monotone one; if the initial β disturbance is too low the final pattern shows no profile at all.

The anti-diffusion model has one major feature : aggregation instability depending on the β-component (OH^--concentration). Instabilities are enhanced by the Co^{++} flux as is observed in the experiments. Temperature dependence is not incorporated and the modeled phase separation is of the spinodal decomposition type (second order phase transition).
In the literature predictions about the final state with respect to spacing of the rings are based on linear analysis. In this case, the expected spacing would be given by the fastest growing mode as calculated for the linearized system (Metiu et al.,1979; Keller et al., 1970). However, the simulations with the anti-diffusion model show a tendency to solutions with a longer wave length than those given by the fastest growing mode. Moreover, all the calculations are based on an initial homogeneous state which is assumed to be unstable. This is not consistent with the reported experiments with an imposed OH^- gradient. So the linear analysis can only provide marginal evidence about the outcome of the process. Simulations with localized perturbations give a different pattern evolution than those with random perturbations, see figure IX.4 and figures IX.5 and IX.6 and also the simulations with the anti-diffusion model. In particularly the CPG model simulations with a localized perturbation show a dynamic pattern selection resulting in a characteristic spacing of approximately $\xi = 3.0$ which is not predicted by linear theory.

CHAPTER X

MIGRATION SYSTEMS

X.1 Introduction

In the recent era, the migration process within human population is characterized by the formation of new metropolitan areas. In 1860 the number of metropolises with more than one million inhabitants was only five, Berlin, London, Paris, Peking and Vienna; in 1960 the number was 109 and in 1975 191 (Papageorgiou et al., 1983). The cause for this steep increase in the number of large population centres can not be contributed only to the net surplus of births and the general increase of the total world population. The sudden urban growth is also due to the tendency of populations to agglomerate.

The reasons for this agglomeration process have been investigated in great detail (Forrester, 1970; Papageorgiou, 1979). Common to all explanations is the observation that people like and need to interact in various aspects, such as in the production and exchange of goods, services, information and education. Moreover, in all these aspects, scale factors are important, not only with respect to profitability of existing activities but also with respect to initiating new (branches of) activities. The support of a large home market, in both supply of labour and money, and demand for good and services, has an self-enhancing effect on the growth of population centres. These aspects become even more important with limited mobility (Allen, 1982). The concept of attractiveness is fundamental in the explanation of the

population flows. All the characteristics that make an area attractive, e.g. employment rates, economic mobility, housing, low-cost-housing programs, public services, schools, welfare budgets, legal restrictions, prejudice, racial and ethnic grouping, combine to influence migration (Forrester, 1970, 1974). An attractive area draws people. The influx of people can enhance the carrying capacity of a region through the appearance of better local infrastructure, transport facilities, formation of a skilled labor force; this represents an autocatalytic aspect (Allen, 1982). The differential growth of regions is supposed to be due to this self-sustaining mechanism of growth which can operate on initially small regional differences.

A second aspect is that, with limited carrying capacity, almost every component of attractiveness is driven down by overpopulation. If there is an excess of housing, the area is attractive but a rising population crowds housing. If there is an excess of jobs, the area is attractive, but the incoming flow of people fills those jobs. In other words, migration continues until the attractiveness of the area falls and becomes equal to that of all other places from which people might come. The condition of population equilibrium is defined as equal attractiveness of all areas for any given population class. If one component of attractiveness is increased in an area, other components must necessarily fall to establish a new equilibrium. If an area is more attractive, inward migration will occur until it is overloaded. Unable to cope with the influx, the area falls to the lowest attractiveness level with which it communicates (Forrester, 1970).

Regarding the migratory process as embedded in a dynamical system, two kinds of migrating dynamics can be distinguished:

a) The migration takes place under quasi-constant global social, economic and environmental (boundary) conditions, the control parameters of the system. If the migratory system starts from some unstable state, the system shall approach a stable state, if present, defined by the boundary conditions and will stay in that state.

b) In the course of the evolution, the global boundary conditions may change and the corresponding control parameters can cross a certain critical value which means by definition that the global dynamic

structure of the system is changed. If the system crosses a bifurcation point, the dynamic structure will change qualitatively and quantitatively: stability characteristics will change, new stable states can arise. Accordingly, a new migratory dynamics will evolve. Such a global change of the system's structure is called a phase transition in analogy to similar phenomena in physics and chemistry.
In Papageorgiou et al. (1983) the agglomeration process is regarded as the evolution of fluctuations from an unstable spatially uniform steady-state solution of the migration evolution equations. In this case, a structural change in the migration process, is given by a change in stability properties of the uniform solution of the system.
In this chapter, essentially two types of modeling migratory systems will be described. Both are based on the concept of attractiveness and use a statistical mechanical approach.
The first one stems from Haag and Weidlich (1983, 1984, 1986) and the second one is based on the migration form of the anti-diffusion equation as derived in chapter IV. Both models are 'phase transition' models. The attractiveness, formulated as a function of the population density, takes over the role of the Ginzburg-Landau free energy functional in physico-chemical systems. However as we shall see, the formulation of the migration dynamics in the two models is conceptually different.
In paragraph X.2 the model of Weidlich and Haag is introduced. In the following paragraph X.3.1, this model is compared with the general migration model derived in chapter IV.5. Using Dutch internal migration data, the parameters of the last model are estimated; the results are summarized in paragraph X.3.2. Surprisingly, indications of a structural change in the dynamic behavior are found.

X.2 Phase transition migration model (I)

The migration model as formulated by Haag and Weidlich (Weidlich and Haag, 1983; Haag and Weidlich, 1984, 1986) is based on two principles borrowed from statistical mechanics. The first one is the

description at the mezoscale level. The spatial domain is divided in subdomains (cells) where the specific individual behavior of the elements is assumed to be identical, see also chapter VI. Apart from the intrinsic stochastic behavior supposed to be present in the individual migration decision process, this coarsening introduces deviations from the observable migration process. Note that for instance the CPG model (chapter IX) is based on a similar assumption with respect to the particle size distribution in a cell.
The second one is the separation of the migration dynamics from the migration motivation factors as mentioned in the introduction of this chapter. The migration dynamics is fully determined by the evolution equations of the (probability distribution function of the) area population numbers n_1. The characteristics of the dynamics will depend on a parameter set $(\alpha_1,\ldots,\alpha_A)$. The parameters α_1 are called trend parameters. The individual decision to migrate is motivated by certain factors $(\mu_1,\ldots,\mu_M)$ describing the intensities of the different reasons 1,..,M. Hence the dynamics will depend through functional relationship of $(\alpha_1,..,\alpha_A)$ on $(\mu_1,..,\mu_M)$ on these specific economic, sociological, psychological reasons. The factors $(\mu_1,..,\mu_M)$ are comparable with physical quantities as temperature, pH etc.. The model is formulated purely in terms of the population numbers n_1 of an area and the trend parameters $(\alpha_1,..,\alpha_A)$. At a second level, the relation between specific motivation factors and the parameters $(\alpha_1,..\alpha_A)$ is made explicit by linking e.g. economic factors with the migration dynamics. Thus the approach is fully compatible with that described in chapter IV. In the Liesegang model, one of the physical "motivation factors" (pH) is an integral part of the system equations.

The migration model is derived in the following way. Let $n = (n_1,..,n_L)$ be the L-dimensional array of population numbers and let $P(n_1,..,n_L;t) = P(n;t)$ be the associated probability distribution function. The dynamics of the system is governed by the equation of motion of the probability distribution: the master equation. The process is assumed to be Markovian. In the approach of Haag and Weidlich the number of admissible transitions between states is reduced drastically. Let $E_1^{\pm k}$ be the translation operator defined by

$$E_1^{\pm k}\, f(n) := f(n_1,\ldots,n_1 \pm k,..,n_L),$$

where k is a positive integer and f is any function of $n = (n_1,..,n_L)$. This master equation is now defined as:

$$\frac{\partial P(n,t)}{\partial t} = \sum_{i,j=1}^{L} \left\{ W_{ij}(n^{ji})P(n^{ji},t) - W_{ji}(n)P(n,t) \right\} \qquad (X.1a)$$

where

$$n^{ji} = E_j^{+1}E_i^{-1}(n) \qquad (X.1b)$$

and

$W_{ji}(n)$ is the transition probability per unit time from n to n^{ji} by migration of any of the n_i individuals from area i into area j.

$$W_{ji}(n) = W(n^{ji};n) = \lim_{\Delta t \to 0} \frac{P(n^{ji}; t+\Delta t | n; t)}{\Delta t} \qquad (X.1c)$$

where $P(n^{ji}; t+\Delta t|n; t)$ is the probability that the system is in state n^{ji} at time $t + \Delta t$ if the system was in state n at time t.

In equation (X.1a) the transitions are restricted to the ones between adjacent states which supposes that only one individual will migrate per unit time. This is based on the assumption that individual decisions to migrate are independent (and identical). We give here the argumentation as found in Kanaroglou et al. (1986a).

Let $p_{ji}(t,\Delta t)$ denote the probability of migrating to region j from region i during time interval $[t,t+\Delta t]$ for a particular individual in region i. Then the corresponding instantaneous propensity of migrating to j from i is given by

$$q_{ji}(t) := \lim_{\Delta t \to 0} \frac{p_{ji}(t,\Delta t)}{\Delta t} \qquad (X.2a)$$

For infinitesimal time intervals, equation (X.2a) implies that

$$p_{ji}(t,\Delta t) = q_{ji}(t)\Delta t \qquad (X.2b)$$

Now using the assumption of independent individual decisions to migrate, the probability of h migrations from i to j during time Δt, given the population vector n at time t, is:

$$P(E_j^{+h}E_i^{-h}n, t + \Delta t | n, t) = \binom{n_i}{h} [q_{ji}\Delta t]^h [1 - q_{ji}\Delta t]^{n_i - h} \qquad (X.2c)$$

In consequence, as $\Delta t \to 0$, it is sufficient to concentrate on the probability of a single migration from i to j during time Δt.

Secondly, applying again the independence assumption, the probability of h migrations per individual during Δt is of the order Δt^h. Hence changes in the system are represented only by a sequence of adjacent states.

For a single migration from i to j during Δt, the probability is: $P(E_j^{+1}E_i^{-1}n, t + \Delta t|n, t) = q_{ji}n_i\Delta t[1 - q_{ji}\Delta t]^{n_i-1}$. Use (X1.c) to find for W_{ji}:

$$W_{ji} = n_i\, q_{ji}(t) \tag{X.2d}$$

Here the transition probability W_{ji} is given by the transition rate q_{ji} which describes mezo action. The macro dynamics are directly linked with mezoscopic behavior.

Now to specify the rates q_{ji}, it is assumed that the attractiveness of an area i for a member of the population is characterized by a utility function $f_i(n_i)$. This utility function is assumed to be polynomial in n_i with on area specific parameters.

$$f_i(n_i) = \delta_i + \kappa_i n_i + \mu_i n_i^2 \tag{X.3}$$

The trend parameters δ_i, κ_i and μ_i depend on all motivation factors. δ_i comprises all factors which are independent of the population: climate, landscape; κ_i contains the cooperative factors: employment, occupation, schools, and related factors such as distance between work and home. parameter μ_i contains all factors which have to do which saturation effects: rents, traffic congestion, housing (Haag and Weidlich, 1986). The attractiveness of an area influences the dynamics of the migration by the assumed effect on the individual migration decisions: the individuals are maximizing their utility. This assumption is formalized by taking q_{ji} as a function of the utility $f_j(n_j + 1)$ of the destination area j and the utility $f_i(n_i)$ leaving aside the utilities of all other areas $l \neq i, j$. As a specific functional form is chosen:

$$q_{ji} = \nu \cdot \exp[f_j(n_j + 1) - f_i(n_i)], \quad \nu > 0 \tag{X.4}$$

with ν a global mobility parameter determining the time scale of the migration process. A distance discounting factor is not included but can easily be incorporated. This formulation of q_{ji} is based on the

assumption that on the individual level, migration is motivated by differences in the attractiveness between origin and destination only (Weidlich and Haag, 1983). The individual decision process is based on individual preferences.

So the system description is given by the equations (X.1a-c) completed with the equations (X.2d), (X.3) and (X.4).

In Haag et al. (1986) the most probable stationary population numbers $\hat{n}_i$, i = 1,..L are calculated in the case that saturation parameter $\mu_i = 0$ for all i. The result is:

$$\hat{n}_i = N \cdot \exp[2\delta_i + 2\kappa_i(\hat{n}_i + 0.5)]/N, \quad i = 1,..,L. \tag{X.5a}$$

where $N = \sum_{i=1}^{L} n_i$, the total population number and

$$N = \sum_{i=1}^{L} \exp[2\delta_i + 2\kappa_i(\hat{n}_i + 0.5)] \tag{X.5b}$$

For $\delta_i = 0$ and $\kappa_i = 0$, i = 1,..,L, the only solution of (X.5a) is the equidistribution of the population, $\hat{n}_i = N/L$ for all i. In this case the stationary distribution P^{st} will be unimodal.

In general, at the crossing of some critical values of the parameters δ and κ, the set of L nonlinear transcendental equations (X.5a) will have several different solutions which define multiple maxima of the stationary probability distribution P^{st}. This change from unimodality to multimodality is denoted as a phase transition.

The full solution of the master equation is unknown. Therefore it is reasonable to seek the evolution of some particular states which characterize the probability distribution P(n,t). In particular the mean-value state $\bar{n}(t) = (\bar{n}_1(t),..,\bar{n}_L(t))$ is investigated.

The mean population size of j at time time t is defined by:

$$\bar{n}_j(t) = \sum n_j P(n,t)$$

where the summation is over all configuration $(n_1,..,n_L)$.

Our main interest is to compare the migration kinetics of the Haag-Weidlich model with those of the anti-diffusion approach. So for the derivation of the mean value evolution equations we refer to Haag and Weidlich (1984) and also to Kanaroglou et al. (1986a-b). The final

form is

$$\frac{d}{dt}\bar{n}_j(t) = \sum_{i=1}^{L} \nu\bar{n}_i \exp[f_j(\bar{n}_j) - f_i(\bar{n}_i)] - \sum_{i=1}^{L} \nu\bar{n}_j \exp[f_i(\bar{n}_i) - f_j(\bar{n}_j)] \tag{X.6}$$

The upper bar denotes mean values.

The equations are derived under the assumption that the probability distribution P(n,t) is unimodal and strongly peaked which allows for the approximation of $\overline{W_{ji}(n)}$ by $W_{ji}(\bar{n}) = \bar{n}_i q_{ji}(\bar{n})$, see also chapter VI.

We shall denote the Haag and Weidlich model (X.6) by HW model.

X.3 Phase transition migration model (II)

In chapter IV, the following migration model was formulated:

$$\tau\dot{n}_l = -M\cdot\left[\sum_{j=1}^{L} \Psi(l,j)\left\{\frac{1}{A_l}\cdot\frac{\delta V}{\delta\rho_l} - \frac{1}{A_j}\cdot\frac{\delta V}{\delta\rho_j}\right\}\right] \quad l = 1,..,L \tag{X.7a}$$

where M is a positive constant, ρ_l the population density in domain l, A_l the area of domain l, l = 1,..,L and Ψ a non-negative symmetric LxL matrix of weighting coefficients.

The dynamics is characterized by minimizing the functional V under the restriction of constant total population $N = \sum_{l=1}^{L} n_l$ where the functional V was defined by

$$V(\rho) = \int f(\rho) + \frac{1}{2}\gamma(\nabla\rho)^2 \, dx \tag{X.7b}$$

The gradient term $(\nabla\rho)^2$ takes in account the (possible) non-homogeneous environment of a point of the system (see chapter III).

For a discrete space with L subdomains l of area A_l the contribution of f to V can be written as $\sum_{l=1}^{L} f(\rho_l)A_l$. Denoting the boundary of domain l by Γ and the exterior normal derivative to Γ by $\frac{\partial}{\partial\nu}$, to find

$$\frac{1}{A_l}\cdot\frac{\delta V}{\delta\rho_l} = \phi(\rho_l) - \gamma\cdot\frac{1}{A_l}\cdot\int_{\Gamma} \frac{\partial}{\partial\nu}\rho_l \, d\Gamma \tag{X.8}$$

with $f(\rho) = \int\phi(\sigma)d\sigma$ and the integral term is obtained by applying Green's identity for a spatial domain (John, 1982).

This integral term gives the amount of mass flowing per unit time through the boundary Γ of domain l caused by density differences

denoted as flux. The flow is opposed to the gradient of ρ ($\frac{\partial \rho}{\partial x}$); in the limit case of a small domain, the term just gives the standard Fickian diffusion term.

Applying the separation between migration dynamics and motivation factors, as expressed above, the attractiveness F of domain l is given as a function of ρ only. In contrast to the formulation in paragraph X.2, F is not taken domain-specific. The relation between migration dynamics and density are assumed to be identical for all domains. Hence in this case the attractiveness must taken as a function of the density and not of the population number. (The non-homogeneity assumption is not excluded by the model formulation but will increase the number of parameters of the model significantly.)

The basic assumption is that the evolution of the system can be characterized by maximizing the total (global) attractiveness of the state given by minus $V(\rho)$; each domain l has as an attribute an attractiveness essentially given by $-f(\rho_l)A_l$ adjusted with the divergence term which models cohesion between neighboring domains. In this way equations (X.7a) with (X.8) are assumed to be modeling a migration process and denoted by AD model.

This model formulation differs essentially of that used by Haag and Weidlich, a fact which becomes clear by comparing the transition probabilities which form the kernel of both systems.

The time scale is always such that typical individual behavior can be neglected: all individuals in a particular domain act according to a similar pattern. In the case of the HW model the migration process is seen as a sequence of single transitions per unit time. And the migration dynamics is based on an individual (mezoscopic) decision process which depends on local attractiveness differences only. On the time scale of the AD model however, a net migration flux δ_{kj} depends on the attractiveness $f_k(\rho_k + \delta_{kj}/A_k)A_k + f_j(\rho_j - \delta_{kj}/A_j)A_j$ of the new state, and that of the old state $f_k(\rho_k)A_k + f_j(\rho_j)A_j$ (neglecting the gradient term): temporary opportunities are averaged out. At each time step, the elements tends to reorder themselves in a configuration which coincides with a maximum of the total attractiveness $-V(\rho)$.

With respect to the HW model two questions arise: is it possible to allow for averaging out individual, with respect to the model random,

behavior and at the same time restricting to single transitions? Secondly, when applying the model to empirical data, can the time scale of the model in anyway be compatible with the time scale of data acquisition? Both questions can be answered by no. The averaging out process presumes not only a grain spatial structure but also a time scale on which individual behavior can be neglected which means at the least a time scale on which not only single transitions occur. The continuous time formulation is a shorthand for a discrete time notation (Haken, 1978). Moreover, the time scale of data measurement is in most cases rather long. Note that the single transition aspect of the H-W model has disappeared from the final equations: $f_j(\bar{n}_j)$ instead of $f_j(\bar{n}_j + 1)$.

The most probable configurations of the AD system are given by the minima of the 'free energy' (= maxima of the total attractiveness). The concept of the AD model is, of course, strongly related to entropy-maximizing models. In that case the most probable spatial configuration possesses the greatest number of states associated with it; it is the situation in which an element of the system can be everywhere with equal probability. The uncertainty with respect to the position is maximal (Wilson, 1970; Nijkamp and Paelinck, 1974). We recall that minimization of the free energy is maximization of the entropy for isolated systems (chapter I) and also that in open systems, the minimum of the free energy is not necessarily given by the disordered state.

Based on the assumption that the attractiveness of a domain is a function of the population number or density only, the mezoscopic migration dynamics are directly linked with the macroscopic pattern in both system descriptions. The essential difference is given by the time scales used, on which the mezoscopic modeling is based. As a consequence the relation between attractiveness and probability to migrate is defined differently. We think that the AD approach is consistent with the basic assumption of a mezoscopic description that all elements of a cell (domain) behave identically.

X.3.1 Model specification and parameter estimation

The model formulation (X.7a) with equation (X.8) was based on the general form derived in chapter IV, section 5. In this case the specification of the transition δ_{kj} allows for the identification of the terms in the summation of equation (X.7a) with the net migration flows between the different domains; denoting the net mass flow between subdomain j and k in the direction of k by M_{kj}, one gets

$$M_{kj} = -M \cdot \Psi(k,j)\left\{\frac{1}{A_k}\cdot\frac{\delta V}{\delta \rho_k} - \frac{1}{A_j}\cdot\frac{\delta V}{\delta \rho_j}\right\} \qquad (X.9a)$$

Define NB(k) as consisting of those indices j such that domain j has a common boundary with domain k; let D(j,k) be the distance between the centers of domain k and domain j and let furthermore the length of the common boundary between domain j, $j \in NB(k)$, and domain k be given as $\Gamma(j,k)$, then the flux term in equation (X.8) is approximated as follows:

$$\frac{1}{A_k}\int_{\Gamma}\frac{\partial}{\partial \nu}\rho_k d\Gamma = \frac{1}{A_k}\sum_{j\in NB(k)}\left[\Gamma(j,k)(\rho_j - \rho_k)/D(j,k)\right] \qquad (X.9b)$$

The right hand side of (X.9b) shall be denoted as flux(k).
No-flux boundary conditions are tacitly assumed since only fluxes between neighboring domains contribute to the summation; the model describes only redistribution of the population.
The weighting factor Ψ is identified as a discount based on the distance D(j,k). The attractiveness differences motivating a migration are discounted for spatial distance modeling cost effects. In the so called Gravity Models, the migration flow between two locations j and k is proportional to the product of number of people at location j and the number of people at location k, and inversely proportional to the distance between these locations raised to the s-the power, see Zipf (1946). An exponential form is chosen as in the gravity migration models (see also entropy maximization models, for example, Nijkamp and Paelinck (1974)):

$$\Psi(j,k) = \exp[\delta D(j,k)], \quad j,k = 1,..,L \qquad (X.9c)$$

where δ is parameter measuring the cost effect. The expected sign of δ

will be negative.
Finally the (homogeneous) attractiveness function $-f(\rho)$ is specified as before in polynomial form:

$$f(\rho) = \tfrac{1}{2}\beta_1\rho^2 + \tfrac{1}{3}\beta_2\rho^3 + \tfrac{1}{4}\beta_3\rho^4 \qquad (X.9d)$$

hence $\phi(\rho)$ in (X.8) is

$$\phi(\rho) = \beta_1\rho + \beta_2\rho^2 + \beta_3\rho^3 \qquad (X.9e)$$

Since all terms in (X.9a) are differences, any homogeneous distribution is a solution and the model can be written in the deviation u of the mean value of ρ, defined as:

$$u_1(t) = (\rho_1(t) - \bar{\rho}(t))/400 \qquad (X.10a)$$

where

$$\bar{\rho}(t) = \left(\sum (A_1\rho_1(t)\right)/\sum A_1 \qquad (X.10b)$$

with summations over all $1 = 1,..,L$; $\bar{\rho}(t)$ is the mean value of all $\rho_1(t)$ (over the chosen period). (This mean value is approximately 400.)
In that case, neglecting the cohesion term (X.9b), the dynamics will give a clustering process if β_1 is negative (see chapter II and III). The quadratic term stands for the cooperative factors: the possibility of encounters is proportional to ρ^2 and the outcome will depend on economic factors as income, rent, skilled labor force, transport facilities, etc. The trend parameter β_1 takes account of these factors. Assuming limited carrying capacity, the growth of a region is bounded; there are bounds on the growth if β_3 is positive. Saturation effects will inhibit further growth, hence we expect that β_3 will be positive if β_1 is negative.
The flux term (X.9b) has a smoothing effect. The model assumes a constant population density in a specific domain and this term adjust the data at the boundary of a domain. Since the fourth order term sets the bounds on the carrying capacity of a domain and the gradient term will smooth the data, it is to be expected that these terms play complementary roles if the bounds are active (negative β_1).

Including the positive constants τ and M in the linear parameters β, γ the net migration flows are modeled as follows

$$M_{lj} = -\Psi(l,j)\Big[\beta_1(u_l - u_j) + \beta_2(u_l^2 - u_j^2) + \beta_3(u_l^3 - u_j^3) + -\gamma(\text{flux}(l) - \text{flux}(j))\Big] \quad 1 \le l < j \le L \qquad (X.11)$$

with $\text{flux}(l) = \frac{1}{A_l} \sum_{k \in NB(l)} \Big[\Gamma(l,k)(u_k - u_l)/D(l,k)\Big]$,

and $\Psi(j,l) = \exp[\delta\, D(j,l)]$ and $\Gamma(j,k)$ the length of common boundary between area j and k. $NB(l) = \{k \in (1,..,L) \mid \Gamma(l,k) \neq 0 \;\&\; l \neq k\}$.

The basic model equations were obtained as the most probable path equations of a stochastic process (see chapter IV). The population change in an area l was based on the net migration flows between all other areas j, $j \neq l$. In accordance with this specification, deviations from the deterministic path were considered by adding a stochastic term to each of the migration flows (see equation IV.30d in chapter IV.) Since $M_{lj} = -M_{jl}$, this stochastic term was given as S_{lj} with $S_{lj} = -S_{jl}$ and $S_{lj} = R_n$ with $n = j-l + (l-1)\cdot L$ for $1 \le l < j$, $l = 1,2,..,L-1$ and R is a $0.5(L^2 - L)$ dimensional vector of random variables with

$$\langle R(t) \rangle = 0 \qquad (X.12a)$$

$$\langle R_n(t) R_m(t^1) \rangle = Q(n,m)\cdot\delta(t - t^1) \qquad (X.12b)$$

As in chapter IV, paragraph 8, Q is taken diagonal, especially $Q = \sigma^2 \cdot I$. Furthermore it assumed that the stochastic process is Gaussian.

In the following estimation procedure, an error term is assumed of the form (X.12) with Q diagonal and the addition that σ is time dependent. In the formulation of equation (IV.30d), chapter IV, the deterministic part has constant, time independent coefficients. Here, the parameters β, γ and δ are assumed to be time dependent reflecting changes in the economical environment between the periods.

Define for $n = j - l + (l-1)\cdot L$, $1 \le l < j \le L$, $n = 1,..,N$,

$M(n) = M_{lj}$: net migration flow,

and the explanatory variables

$\Psi(n;\delta) = \Psi(l,j)$: distance discount factor,

$R(n,1) = u_l - u_j$: difference of deviations from density mean-value,

$R(n,2) = u_l^2 - u_j^2$

$R(n,3) = u_l^3 - u_j^3,$

$div(n) = flux(l) - flux(j)$: difference of fluxes through boundary,

$D(n) = D(l,j)$: distance,

$\Gamma(n) = \Gamma(l,j)$: length of common boundary between area l and j,

and the error structure:

$E(\cdot) = N(0,\sigma^2 I)$: Gaussian error term.

and

$N = 0.5L(L-1)$: Number of observations where L is given by the number of areas.

With the above defined variables the model, for each n, is written as

$$M(n) = -\Psi(n;\delta)\Big[\sum_{k=1}^{3}\beta_k R(n,k) - \gamma\, div(n) + E(n)\Big] \qquad (X.13)$$

The model parameters are β_1, β_2, β_3, γ, δ and σ.

The data are net (= inflow-outflow) internal migration flows between the eleven Dutch provinces. The recently formed province "Flevoland" is excluded. Hence for each year, there are 55 independent net migration flows (N = 55). The measurement period is one year. The data were collected for the years 1970-1985 (source C.B.S.). The same source has supplied the population densities ρ_l and the area A_l of the provinces. For the distance variable D(l,j) is taken the distance by railway between central places of the provinces. The variable $\Gamma(l,j)$ which is the length of the common boundary between two provinces j and l has to be constructed. Of course, $\Gamma(j,l)$ is zero if the provinces are not neighbors. In other cases $\Gamma(j,l)$ is approximated by the sum over the distance between places lying on the vertices of the common boundary. The variables D(j,l) and $\Gamma(j,l)$ are taken constant over time and scaled down to units of 100 km.

Since the model is written in u, the deviation from the mean density $\bar{\rho}$, parameter β_1 determines whether the state with $\rho_l = \bar{\rho}$, $l = 1,..,L$, is stable or not. Neglecting γ, the uniform state $u = 0$ is stable if β_1 is

positive, otherwise this state is unstable. The former case means that the migration flows are from high density areas to low density ones; the migration process tends to smooth out density differences. If β_1 is negative, the density differences are retained and may be enhanced. So a change in the sign of β_1 indicates a structural change in the migration process and will be viewed as a phase transition.

In table X.1 the total net migration is given for some years. The first column gives the provinces code names, the second one the mean population density over the estimation period. In the following columns a negative value means a decrease, a positive value an increase in population by migration.

Area	mean ρ	total net migration 1974	1976	1978	1980	1982	1984	1985
DR	155.38	4376	1637	1012	849	-37	736	770
FR	171.38	2978	2399	2555	1367	46	-1730	-2077
ZE	190.43	2022	1828	2712	1309	-6	-1039	-1037
GR	234.96	400	1901	1559	232	284	-1271	-2173
OV	263.80	861	498	538	1	-174	-1411	-2337
GE	333.33	7229	3594	2273	1838	1027	2389	3682
NB	407.80	11942	8686	4141	2137	-1381	-321	2
LI	489.05	-1171	-1152	131	-844	-915	-1617	-1330
UT	667.75	1644	402	1301	3422	2708	2538	2765
NH	863.84	-10852	-5795	-6942	-4943	-707	2905	3769
ZH	1065.63	-19321	-13998	-9280	-5377	-923	-1179	-2052

Table X.1: Total net migration. The second column ρ gives population density of provinces (column Area).

The data in table X.1 indicate a direction reversal of the migration flow in the period 1974-1985. Typical low density areas (except area DR) have a negative migration surplus in the second part of the period; the two highest density areas, taken together, have a positive surplus in the same period. This could give a sign reversal of the coefficient β_1.

Given the Gaussian error structure of E, the values of the parameters δ, β_i, $i = 1,2,3$, γ and σ can be estimated by means of maximum likelihood.

Let $\theta = (\delta,\beta_1,\beta_2,\beta_3,\gamma,\sigma)$ then the likelihood function $L(\theta)$ of (X.13) is given by

$$L(\theta) = L(\delta,\beta_1,\beta_2,\beta_3,\gamma,\sigma) = (2\pi)^{-N/2}\sigma^{-N}\cdot\prod_{n=1}^{N}\Psi^{-1}(n;\delta)\cdot\exp\left[-\frac{1}{2}\sigma^{-2}\cdot URSS\right]$$

with

$$URSS = \sum_{n=1}^{N}\left\{M(n)\Psi^{-1}(n;\delta) + \sum_{k=1}^{3}\beta_k R(n,k) - \gamma div(n)\right\}^2 \qquad (X.14)$$

and maximum likelihood (ML) estimates of θ are those values which maximize $L(\theta)$] (see for example Maddala (1977)). The ML-estimates will be denoted by $\hat{\theta}$, and the estimated migration flows calculated on the base of the estimators will be denoted by $\hat{M}$.

Instead of maximizing the likelihood function $L(\theta)$ it is convenient to maximize the log of the likelihood function, $\log[L(\theta)]$,

$$\text{Log}[L(\theta)] = -\frac{N}{2}\log(2\pi) - \frac{N}{2}\log(\sigma^2) - \sum_{n=1}^{N}\log(\Psi(n;\delta)) - \frac{1}{2}\sigma^{-2}URSS \qquad (X.15a)$$

with URSS defined in (X.14).

The estimators of θ are denoted by $\hat{\theta}$; $\hat{\sigma}$ can be solved directly from (X.15) by the condition $\frac{\partial}{\partial\sigma}\log[L(\theta)] = 0$ in the optimum, hence

$$\hat{\sigma}^2 = \frac{1}{N}URSS \qquad (X.15b)$$

which is called the maximum-likelihood estimate of σ^2 if URSS is evaluated at $\theta = \hat{\theta}$. Inserting (X.15b) in (X.15a), suppressing the constant, one has to maximize $ML(\theta|\sigma)$:

$$ML(\theta|\sigma = \hat{\sigma}) = -\frac{N}{2}\log(URSS) - \sum_{n=1}^{N}\log(\Psi(n;\delta)) \qquad (X.16)$$

Since the estimation procedure involves only one non-linear parameter (δ), a golden section search method (GS) on the parameter δ combined with ordinary least-squares estimates of $(\beta_1,\beta_2,\beta_3,\gamma)$ given δ, is applied. The stop criterion of this GS-method is formulated in terms of the length of final search interval for parameter δ. As a second method a Quasi-Newton (Variable Metric) procedure based on the algorithm of Davidon-Fletcher-Powell (DFP) was used. In this case the stop criterion was formulated in terms of the norm of the gradient of $ML(\theta|\sigma)$

(Luenberger, 1973; Minoux, 1986). Implementations of the methods can be found in Press et al. (1986). The GS-method is very practical in searching over large intervals and supplies reasonable starting values for the variable metric method. The results from both methods are checked with respect to each other.

The information matrix $I(\hat{\theta})$ is defined by the expected value of minus the Hessian of $\log[L(\theta)]$ in $\theta = \hat{\theta}$. The ML-estimators $\hat{\theta}$ are asymptotically normally distributed with variance $[I(\hat{\theta})]^{-1}$. Approximations of the bounds of confidence intervals of the estimators are obtained by approximating $I(\hat{\theta})$ by $-\frac{\partial^2}{\partial\theta^2}\log[L(\theta)]\Big|_{\theta=\hat{\theta}}$ (Maddala, 1977).

Finally, to test whether a variable contributes significantly to the value of $\log[L(\theta)]$ or not, the generalized likelihood ratio test can applied:

Let S be the parameter index set. To test a hypothesis

$$\mathcal{H}_0\colon\ \theta_k = 0,\ \theta_l \neq 0 \text{ for all } k \in S_k \text{ and } l \in S_l \text{ with } S_k \oplus S_l = S \tag{X.17a}$$

against the alternative hypothesis

$$\mathcal{H}_1\colon\ \theta_k \neq 0 \quad \text{for all } k \in S, \tag{X.17b}$$

define

$$\lambda = L(\hat{\theta}|\mathcal{H}_0)/L(\hat{\theta}|\mathcal{H}_1) \tag{X.18}$$

where $L(\hat{\theta}|\mathcal{H}_0)$ is the value of $L(\theta)$ in the optimum if $\mathcal{H}_0$ is true. Then $-2\log(\lambda)$ is (asymptotically) chi-square distributed with $\#(S_k)$ degrees of freedom (≡ number of restrictions) (Mood et al., 1974; Maddala, 1977). Let $\chi^2_{1-\alpha}(r)$ denote the $(1-\alpha)$-th quantile of the chi-square distribution with r degrees of freedom, then

$$\text{reject } \mathcal{H}_0 \text{ if and only if } -2\log(\lambda) > \chi^2_{1-\alpha}(r).$$

In the tables below, the column denoted by -2LR will give the value of $-2\log(\lambda)$ with respect to the tested $\mathcal{H}_0$ hypothesis.

Any decision with respect to inclusion or exclusion of variables must be taken considering the theoretical background of the model. For instance, the variable $R(\cdot,1)$ is not to be excluded since it determines

essentially the qualitative properties of the model; and if β_1 is negative, boundedness of solution needs the inclusion of the third order term R(·,3) (with positive coefficient).

With respect to the explanatory variables, table X.2 gives the correlation coefficients between the linear variables R(·,k), k = 1,2,3 and the div(·) variable as calculated for the year 1977. (Similar results for all other years.) A strong correlation will result in rather large changes in the estimated parameter values after exclusion, c.q. inclusion of one of those linear variables.

variables	R(·,1)	R(·,2)	R(·,3)	div(·)
R(·,1)	1.000	0.8190	0.8663	0.6792
R(·,2)		1.0000	0.9703	0.8203
R(·,3)			1.0000	0.8864

Table X.2: correlation between linear explanatory variables.

Table X.3 gives the results of the estimation procedure with no restriction on any of the parameters.

The column -2LR in table X.3 gives the value of $-2\log[L(\hat{\theta}|\mathcal{H}_0)/L(\hat{\theta}|\mathcal{H}_1)]$ with $\theta = (\delta,\beta_1,\beta_2,\beta_3,\gamma,\sigma)$; the null hypothesis $\mathcal{H}_0$ is $\beta_1 = \beta_2 = \beta_3 = \gamma = 0$, all other parameters free, the alternative hypothesis $\mathcal{H}_1$ is that all parameters are free.

The 95-the quantile of the chi-square distribution with 4 degrees of freedom, $\chi_{95}(4)$, is 9.48773 (Pearson et al., 1970). Hence, at a significance level of 0.05 in all years except 1982, the hypothesis $\mathcal{H}_0$ is rejected; recall that this hypothesis says that the migration flow data are just realizations of a stochastic process with zero mean-value and covariance $\sigma^2\cdot\Psi(n)\Psi(m)\cdot\delta(n-m)$, n,m = 1,..,N. Since $\chi_{99}(4) = 13.2767$ the null hypothesis is not rejected in 1981 and 1982.

The column denoted by r^2 gives the square of the correlation coefficient between M(·) and $\hat{M}(\cdot)$, the estimated value of M. Again, in 1982 the estimated values are not correlated in any way with the observed data.

year	parameters					σ^2	-2LR $\beta=0,\gamma=0$	r^2
	δ	β_1	β_2	β_3	γ			
1970	-0.28 (0.03)	1.51 (0.72)	4.69 (1.50)	-2.95 (1.20)	1.43 (0.63)	5.53	44.68	0.69
1971	-0.27 (0.03)	2.30 (0.83)	3.45 (1.41)	-2.04 (1.18)	1.19 (0.61)	6.82	56.90	0.53
1972	-0.27 (0.03)	1.24 (0.74)	2.42 (1.33)	0.03 (1.17)	0.47 (0.56)	7.86	75.52	0.59
1973	-0.23 (0.02)	1.63 (0.77)	3.64 (1.40)	-0.52 (1.21)	-0.10 (0.61)	9.51	73.08	0.57
1974	-0.17 (0.02)	1.33 (0.46)	2.00 (0.81)	-0.58 (0.69)	0.22 (0.35)	4.13	74.36	0.62
1975	-0.25 (0.03)	1.82 (0.50)	2.11 (0.81)	-0.98 (0.69)	0.66 (0.36)	4.96	84.72	0.63
1976	-0.18 (0.03)	0.77 (0.31)	0.59 (0.53)	0.11 (0.50)	0.00 (0.24)	3.31	67.38	0.55
1977	-0.19 (0.02)	1.07 (0.28)	0.69 (0.47)	0.12 (0.42)	-0.00 (0.21)	1.85	97.82	0.68
1978	-0.23 (0.02)	1.23 (0.35)	1.08 (0.56)	-0.17 (0.50)	-0.01 (0.26)	1.53	81.84	0.70
1979	-0.20 (0.03)	0.67 (0.28)	0.68 (0.44)	-0.51 (0.39)	0.54 (0.23)	0.87	49.90	0.63
1980	-0.23 (0.03)	0.54 (0.35)	0.26 (0.62)	0.03 (0.55)	0.27 (0.29)	1.59	35.76	0.43
1981	-0.20 (0.03)	-0.06 (0.26)	-0.43 (0.49)	0.23 (0.40)	0.29 (0.23)	0.88	10.35	0.14
1982	-0.17 (0.03)	-0.17 (0.18)	-0.39 (0.35)	0.27 (0.28)	0.13 (0.16)	0.43	8.28	0.04
1983	-0.18 (0.03)	-0.38 (0.17)	-0.42 (0.31)	0.28 (0.26)	0.28 (0.15)	0.37	17.92	0.25
1984	-0.16 (0.03)	-0.68 (0.23)	-0.47 (0.35)	0.37 (0.29)	0.30 (0.19)	0.45	26.26	0.33
1985	-0.16 (0.03)	-0.85 (0.28)	-0.23 (0.40)	0.21 (0.34)	0.46 (0.22)	0.72	28.24	0.38

Table X.3: estimated values of parameters; standard errors between brackets; column -2LR gives $-2\log(\lambda)$ (X.18) with respect to the hypothesis: $\beta_i = 0, i = 1,2,3$ and $\gamma = 0$; r^2 is square of correlation coefficient between M and $\hat{M}$.

year	parameters δ	β_1	β_2	β_3	σ^2	-2LR $\gamma=0$	r^2
1970	-0.28 (0.03)	0.73 (0.64)	3.27 (1.30)	-1.02 (0.85)	5.75	6.56	0.68
1971	-0.27 (0.03)	1.68 (0.75)	2.38 (1.35)	-0.42 (0.96)	7.64	4.01	0.52
1972	-0.28 (0.03)	1.00 (0.68)	2.01 (1.25)	0.67 (0.93)	8.17	0.66	0.59
1973	-0.23 (0.02)	1.68 (0.72)	3.72 (1.33)	-0.66 (0.89)	9.52	0.02	0.57
1974	-0.18 (0.02)	1.23 (0.43)	1.82 (0.77)	-0.28 (0.54)	4.28	0.42	0.62
1975	-0.25 (0.03)	1.49 (0.46)	1.55 (0.77)	-0.12 (0.55)	5.29	3.54	0.63
1976	-0.18 (0.03)	0.77 (0.30)	0.58 (0.50)	0.12 (0.37)	3.31	0.00	0.55
1977	-0.19 (0.02)	1.07 (0.27)	0.69 (0.44)	0.12 (0.32)	1.85	0.00	0.68
1978	-0.23 (0.02)	1.24 (0.34)	1.09 (0.54)	-0.20 (0.37)	1.53	0.00	0.70
1979	-0.19 (0.03)	0.39 (0.24)	0.26 (0.41)	0.15 (0.31)	0.91	6.98	0.62
1980	-0.24 (0.03)	0.42 (0.33)	0.06 (0.60)	0.36 (0.45)	1.64	0.86	0.43
1981	-0.20 (0.03)	-0.19 (0.24)	-0.61 (0.48)	0.55 (0.34)	0.88	1.78	0.11
1982	-0.17 (0.03)	-0.22 (0.17)	-0.47 (0.33)	0.40 (0.24)	0.43	0.66	0.04
1983	-0.17 (0.03)	-0.47 (0.18)	-0.57 (0.31)	0.56 (0.23)	0.36	3.60	0.17
1984	-0.15 (0.03)	-0.78 (0.25)	-0.65 (0.35)	0.69 (0.27)	0.46	3.35	0.26
1985	-0.16 (0.03)	-1.01 (0.30)	-0.53 (0.40)	0.70 (0.29)	0.76	5.42	0.27

Table X.4: estimated parameter values (γ = 0). Standard errors between brackets. Column -2LR gives $-2\log(\lambda)$ with respect to the hypothesis: γ = 0. r^2 is square of correlation coefficient M and $\hat{M}$.

The main question is the stability of the null solution u = 0. If $\gamma = 0$ then the stability depends only on the sign of β_1. Estimating under the condition $\gamma = 0$ will give evidence about the stability of the null solution. The column in table X.4 denoted by -2LR gives the values of $-2\log[L(\hat{\theta}|\mathcal{H}_0)/L(\hat{\theta}|\mathcal{H}_1)]$ with $\mathcal{H}_0$: $\gamma = 0$, all other parameters free and $\mathcal{H}_1$: all parameters free.

Since $\chi_{95}(1)$ is 3.84146 (Pearson et al., 1970), the hypothesis is rejected in four years (1970, 1971, 1979 and 1985); in these years γ is "significant" , see also table X.3.

The time path of the estimated parameter values of β_1 indicates a change in the migration process at the end of the period. Estimating subject the condition that $\beta_1 = 0$ implies that the hypothesis $\mathcal{H}_0$: $\beta_1 = 0$ versus the alternative $\mathcal{H}_1$: all parameters free, is rejected at a significance level of 0.05 in all years except 1981. With a significance level of 0.01 the $\mathcal{H}_0$ hypothesis is rejected in all years but 1972, 1973, 1981 and 1982. Only in 1981 we have found a sign reversal of β_1.

The generalized likelihood ratio test can be applied to test homogeneity hypotheses on the parameters of the model. By pooling together data of two or more years t_1, $t_2,..,t_T$ with model parameters θ^1, $\theta^2,..,\theta^T$ where the super indices denote different years, the null hypothesis is formulated as:

$$\mathcal{H}_0(\theta): \delta^j = \delta^1 \;\&\; \beta_i^j = \beta_i^1,\ i = 1,..3 \;\&\; \gamma^j = \gamma^1 \text{ for } j = 2,3,..,T$$

whereas the alternative hypothesis $\mathcal{H}_1$ is that all parameters θ^j are free. (The variance parameters $(\sigma^j)^2$ are unrestricted under the null hypothesis). $-2\log[L(\hat{\theta}|\mathcal{H}_0)/L(\hat{\theta}|\mathcal{H}_1)]$ is asymptotically chi-square distributed with 5(T -1) degrees of freedom.

Comparing these values with $\chi^2_{95}(5(T - 1))$, results in not rejecting the null hypothesis for the combination 1979 and 1980. For the model with $\gamma = 0$ the homogeneity hypothesis is again not rejected for the years 1979 and 1980. In table X.5 we give the results of parameter estimation for three group of years: 1985-1981, 1980-1979 and 1978-1975.

years	parameters δ	β_1	β_2	β_3	γ	σ^2	-2LR	r^2
1975 .. 1978	-0.21 (0.01)	1.11 (0.17)	0.91 (0.28)	-0.01 (0.21)	0	3.97	31.81	0.15
1979 .. 1980	-0.22 (0.02)	0.42 (0.20)	0.18 (0.36)	0.24 (0.27)	0	1.28	9.08	0.41
1981 .. 1985	-0.17 (0.01)	-0.51 (0.10)	-0.57 (0.17)	0.57 (0.13)	0	1.08	44.37	0.10
1975 .. 1978	-0.21 (0.01)	1.15 (0.18)	1.00 (0.30)	-0.14 (0.26)	0.10 (0.13)	3.88	34.78	0.16
1979 .. 1980	-0.22 (0.02)	0.64 (0.22)	0.54 (0.38)	-0.32 (0.33)	0.46 (0.18)	1.17	10.12	0.42
1981 .. 1985	-0.17 (0.01)	-0.41 (0.10)	-0.39 (0.17)	0.27 (0.15)	0.29 (0.10)	1.07	47.50	0.10

Table X.5: parameter estimation for (1975-1978), (1979-1980) and (1981-1985). Column -2LR gives $-2\log(\lambda)$ (X.18) with respect to the hypothesis: equal parameters for the period in column one (years). $\chi_{95}(4)=9.49$; $\chi_{95}(5)=11.07$.

Is it possible to conclude something from these estimations? We first note that if β_1 is negative then β_3 is positive. In this case, the upper- and lower bounds of stationary solutions can be calculated (see chapter III). For all years 1981-1985 the scaled population density values u, defined in (X.10a, X.10b) lie between these bounds except for one province, Zuid-Holland (ZH) which has the highest population density. This means that the density values u lie in the domain of bounded solutions and the estimated parameter values seem to be feasible. In the case β_1 is positive, the state u = 0 is a minimum of the functional V. In the years 1976, 1977, 1979 and 1980 this is also the only extremum. In all other years except 1972, $f(\rho)$, as defined in (X.9d), has one minimum at u = 0 and two maxima. In this case all the u-values lie inside the u = 0 attraction basin. The estimated parameters for 1972 give a maximum of $f(\rho)$ at u = -0.63 (and a second minimum at u = -2.37); only one u-value is smaller than -0.63.
So in the years 1976, 1977, 1979 and 1980 the state u = 0 is the only

stable state whereas from 1981 till 1985 this state is unstable and there exists a nonconstant bounded stable population distribution.
The rejection of equal model parameters combined with the significant negativity of the parameter β_1 in 1983 and the significant positivity of β_1 in 1978, with $\gamma = 0$ (table X.4), this allows of expressing the conjecture that in that period, especially between 1978 and 1983, the migration process has undergone a phase transition in the way explained above.
Moreover, the deterministic part of the model is insignificant in 1981 and 1982: in the vicinity of a bifurcation point the fluctuations in the system are enhanced ("there exists no dominant time evolution direction") (Nicolis and Prigogine, 1977; Nicolis, 1981). Initially the model was applied only to the data of 1982 with very bad results. Finally it became clear that the almost total lack of sensitivity with respect to the parameters of the model should be seen as a 'positive' result in connection with a sign reversal of the β_1 parameter, i.e. the presence of a qualitative change in behavior (phase transition).

If this conjecture is true, then since 1980 the migration process tends to enhance, or at the least to sustain, the higher density areas (provinces) whereas in foregoing years the tendency was to spread out. This observation is in accordance with the observation that Dutch governmental policies are not fervently supporting anymore the diffusion of governmental, or semi-governmental, organizations outside the Randstad which globally includes the provinces Zuid-Holland (ZH) and (part of) Noord-Holland (NH). Those two provinces have the highest population densities. As an example can be taken the very slow and now only partial transition of the Dutch Post, Telegraph and Telephone institute from The Hague (Zuid-Holland (ZH)) to Groningen (GR).
Another example of not succeeding in transferring activities outside the Randstad, is the famous Eems-Dollard project at the boundary of the province Groningen (GR) and Germany. The failure of this project, with the pressure of under-employment, which is one of the constituents of (negative) attractiveness of a region, will enhance the need for seeking opportunities elsewhere. And this need will be much stronger with low employment rates. In the Netherlands, the data show a slow

increase of unemployment since 1972; however since 1977 and especially since 1981, the unemployment rates are increasing fast and dramatically (source: CBS).

The model formulation is rather crude: all motivation factors are represented by the polynomial form in the density ρ. However, the model allows for an exact definition of a structural change in the form of a sign change of parameter β_1 and even with the coarse spatial structure given by the provinces, the model seems to be capable to detect such a singularity in the migration process.

Appendix A

In the first paragraph we present the procedure to find approximations of stationary solutions bifurcating from the trivial null solution at a simple eigenvalue for a general one dimensional evolution system. In the same context, exchange of stability at the bifurcation point is treated in section two.
In the last two sections, these notions are applied to the anti-diffusion and migration equation derived in chapter IV.

A.1 Bifurcation equations by Poincaré-Lindstedt series

Let the system be given as:

$$\frac{\partial u}{\partial t} = G(u;\gamma) \tag{A.1a}$$

with appropriate boundary conditions; $u \in M$, M is a Hilbert space and $\gamma \in I \subset \mathbb{R}$ and

$$G(u;\gamma) = Bu - \gamma Au + N(u;\gamma) \tag{A.1b}$$

where B, A are linear operators on M. $N(0;\gamma) = 0$ and $d_u N(0;\gamma) = 0$ for all $\gamma \in I$, (d_u is Fréchet derivative in u (see appendix E.) then $u = 0$ will be a stationary solution of (A.1) for all γ. Suppose G is m-times Fréchet differentiable in u and γ ($m \geq 2$), thus $G \in C^m(I \times M, Z)$ with M and Z real Hilbert spaces.
In this section the innerproduct in M will be denoted by $\langle \cdot, \cdot \rangle$.
The stability of $u = 0$ is given by the spectral problem:

$$\omega(\gamma)v(\gamma) = d_u G(0;\gamma)v(\gamma), \quad v(\gamma) \in M \tag{A.2}$$

with eigenvalues $\omega(\gamma)$, eigenvectors $v(\gamma)$ and $d_u G(0;\gamma)$ is the Fréchet derivative in u at $(0,\gamma)$.
Suppose for $\gamma = \gamma_c$ an isolated, simple, real eigenvalue $\omega_c(\gamma)$ crosses strictly the imaginary axis (see appendix E). The strict crossing or

transversality condition reads:

$$\frac{d\omega_c}{d\gamma}(\gamma_c) \neq 0 \tag{A.3}$$

In the following the (Fréchet) derivatives in $(0,\gamma_c)$ shall be denoted by $G_u := d_u G(0;\gamma_c)$, $G_\gamma := d_\gamma G(0;\gamma_c)$ and so on.
Since $u = 0$ is a solution for all γ, $d_\gamma N(0;\gamma) = 0$ and $d_{\gamma\gamma} N(0;\gamma) = 0$.
Using (A.1b) gives

$$(B - \gamma_c A) = G_u \tag{A.4a}$$

and

$$-Au = G_\gamma \tag{A.4b}$$

The adjoint operator of G_u is denoted by G_u^*; the eigenvector of G_u with eigenvalue $\omega_c = 0$ is u_c; the adjoint eigenvector is given as u_c^*, thus

$$G_u u_c = 0 \text{ and } G_u^* u_c^* = 0 \tag{A.4c}$$

By theorem 5.1 of Chow e.a. (1982) there exists a bifurcating stationary solution branch (u,γ) in a small neighborhood of $(0,\gamma_c)$ given by:

$$\gamma(\varepsilon) = \gamma_c + O(|\varepsilon|) \tag{A.5a}$$

$$u(\varepsilon) = \varepsilon u_c + O(\varepsilon^2) \tag{A.5b}$$

(see also theorem A.1 formulated below).
The equations (A.5a-5b) are given by the Poincaré-Lindstedt series which are expansions of the solution (u,γ) in powers of a small parameter ε:

$$u(\varepsilon) = 0 + \varepsilon u_1 + \varepsilon^2 u_2 + \ldots\ldots\ldots \tag{A.6a}$$

$$\gamma(\varepsilon) = \gamma_c + \varepsilon\gamma_1 + \varepsilon^2\gamma_2 + \ldots\ldots\ldots \tag{A.6b}$$

where $u_i \in M$ and $\gamma_i \in \mathbb{R}$, $i = 1,2,3,\ldots\ldots$
The stability of the bifurcating branch $(u(\varepsilon),\gamma(\varepsilon))$ is determined by the eigenvalue problem:

$$\omega(\varepsilon)v(\varepsilon) = d_u G(u(\varepsilon),\gamma(\varepsilon))v(\varepsilon) \tag{A.7}$$

where

$$v(\varepsilon) = v_c + \varepsilon v_1 + \varepsilon^2 v_2 + \ldots\ldots\ldots \tag{A.6c}$$

$$\omega(\varepsilon) = \omega_c + \varepsilon\omega_1 + \varepsilon^2\omega_2 + \ldots\ldots\ldots \tag{A.6d}$$

The convergence of the series (A.6a) and (A.6b) is given by the following theorem found in Sattinger (1973):

Theorem A.1:

Under the assumption of satisfying the transversality condition (A.3), the equation $G(u;\gamma) = 0$ with G defined in (A.1b) has a nontrivial solution (u,γ) which may be expressed parametrically in the form $u = u(\varepsilon)$, $\gamma = \gamma(\varepsilon)$, where $u(0) = 0$ and $\gamma(0) = \gamma_c$. The functions u and γ are power series in ε (A.6a and A.6b), convergent for sufficiently small $|\varepsilon|$ with $\varepsilon = \langle u, u_c^* \rangle$ and $u_1 \in [u_c]$ where $[u_c]$ is the null space of G_u.

Proof: see Sattinger (1973), page 85.

The proof of the convergence of the series (A.6c) and (A.6d) can be found also in Sattinger (1973), page 99.

Now we will describe the construction procedure for the bifurcating solution (Sattinger (1973); Iooss et al. (1980)). In the course of the description, some additional assumptions will be made which are valid for the anti-diffusion system.

Insert (A5a-5b) in $G(u;\gamma) = 0$ and collect the terms with the same order in ε to find:

to the zeroth order in ε ($O(1)$):

$$G(0;\gamma_c) = 0 \tag{A.8a}$$

to the first order ($O(\varepsilon)$):

$$G_u \cdot u_1 = 0 \tag{A.8b}$$

to the second order ($O(\varepsilon^2)$):

$$G_u \cdot u_2 + \gamma_1 G_{u\gamma} \cdot u_1 + \frac{1}{2} G_{uu} \cdot u_1 \cdot u_1 = 0 \tag{A.8c}$$

to the third order ($O(\varepsilon^3)$):

$$G_u \cdot u_3 + \gamma_1 G_{u\gamma} u_2 + \gamma_2 G_{u\gamma} \cdot u_1 + \frac{1}{2}\gamma_1^2 G_{u\gamma\gamma} \cdot u_1 +$$
$$+ G_{uu} \cdot u_1 \cdot u_2 + \frac{1}{6} G_{uuu} \cdot u_1 \cdot u_1 \cdot u_1 + \frac{1}{2}\gamma_1 G_{uu\gamma} \cdot u_1 \cdot u_1 = 0 \tag{A.8d}$$

etc.

Equation (A.8a) is just the equation for the reference state u = 0;
From (A.8b) it is obvious that u_1 must belong to the null space $[u_c]$ of G_u. Thus

$$u_1 = A_1 u_c. \tag{A.9}$$

with the amplitude $A_1 \in \mathbb{R}$.
Next $\gamma_1, ..$ and $u_2, ..$ are calculated. The condition under which equations as (A.8c) and (A.8d) are solvable if G_u is singular are given by the so-called Fredholm alternative: the equation $(\lambda - A)x = y$ has a solution if y is perpendicular to the null space of the adjoint operator $(\lambda - A)^*$. In appendix E the conditions of the Fredholm alternative are given. In this section it is assumed that G_u satisfies these conditions. The Fredholm alternative gives the necessary and sufficient condition for the solvability of

$$G_u . u_k = (B - \gamma A) \cdot u_k = z, \text{ with } u_k \in M \tag{A.10a}$$

as

$$\langle z, v^* \rangle = 0 \tag{A.10b}$$

for all v^* such that $G_u^* \cdot v^* = 0$ where G_u^* is the adjoint operator of G_u. If $\langle v, v^* \rangle = 1$ then the solution u_k can be taken orthogonal to v^* since $w_k = u_k - \langle u_k, v^* \rangle v$ is also a solution and $\langle w_k, v^* \rangle = 0$. We assume that the normalization $\langle v, v^* \rangle = 1$ is possible. (In the case of the anti-diffusion model G_u is self-adjoint.)
Using (A.9) and writing $v_{11} = G_{uu} \cdot u_c \cdot u_c$ to find:

$$G_u \cdot u_2 = -\gamma_1 A_1 . G_{u\gamma} \cdot u_c - \frac{1}{2} A_1^2 v_{11} \tag{A.11}$$

The Fredholm condition for a solution u_2 of (A.11) is

$$-\gamma_1 A_1 P_1 + A_1^2 P_2 = 0 \tag{A.12a}$$

where

$$P_1 = \langle G_{u\gamma} \cdot u_c, u_c^* \rangle \tag{A.12b}$$

$$P_2 = -\frac{1}{2} \langle v_{11}, u_c^* \rangle \tag{A.12c}$$

with $[u_c^*]$ is null space of G_u^*. (The case of a simple eigenvalue.)
Using the general spectral formulation (A.2) and some normalization $\langle u_c, u_c^* \rangle = 1$, to find that

$$P_1 = \frac{d\omega_c}{d\gamma}(\gamma_c) \neq 0 \tag{A.12d}$$

where the inequality value follows from the transversality or strict crossing assumption.

Assumption A.2: $P_2 = 0.$ (A.12e)

(This assumption is satisfied by the systems considered below.)
Then

$$\gamma_1 = 0 \tag{A.12f}$$

and the vector v_{11} belongs to the range of G_u. Let G_u^{-1} be the inverse operator of G_u restricted to the range of G_u. Then u_2 can be solved as

$$u_2 = -\frac{1}{2} A_1^2 G_u^{-1} v_{11} \tag{A.12g}$$

and the procedure is continued with equation (A.8d).

$$G_u \cdot u_3 = -\gamma_2 A_1 G_{u\gamma} \cdot u_c - A_1^3 v_{111} \tag{A.13a}$$

where

$$v_{111} = -\frac{1}{2} G_{uu} \cdot u_c \cdot (G_u^{-1} v_{11}) + \frac{1}{6} G_{uuu} \cdot u_c \cdot u_c \cdot u_c \tag{A.13b}$$

The solvability condition becomes:

$$-\gamma_2 A_1 P_1 + A_1^3 P_3 = 0 \tag{A.13c}$$

where

$$P_3 = -\langle v_{111}, u_c^* \rangle \tag{A.13d}$$

Now the following assumption is made:

Assumption A.3.: $P_3 \neq 0$ (A.13e)

In phase transition terminology, the assumptions A.2 and A.3 define a second order (continuous) transition, see equation (A.13g) below.
Subject to this assumption, γ_2 is equal to

$$\gamma_2 = A_1^2 (P_3/P_1) \tag{A.13f}$$

Since

$$\gamma = \gamma_c + \varepsilon^2 \gamma_2 + O(\varepsilon^3) \tag{A.13g}$$

an approximate solution is

$$u(x) = \pm \beta u_c + O(\varepsilon^2) \tag{A.14a}$$

with

$$\beta^2 = P_1 (\gamma - \gamma_c)/P_3 \tag{A.14b}$$

Given the sign of P_1 the branching direction is given by the sign of P_3 and in this way subcritical- c.q. supercritical branching can be distinguished.

A.2 Exchange of stability at a simple eigenvalue

By using the expansion equation for the eigenvector $v(\varepsilon)$ of the spectral problem (A.7), the stability qualities of the branching solution can be established (Iooss et al., 1980).
Inserting of (A.6c-6d) in (A.7), using the same notations as above, yields to the zeroth order in ε:

$$G_u \cdot v_c = \omega_c v_c \tag{A.15}$$

which is nothing else than the spectral problem for the reference state $u = 0$;
to the first order in ε:

$$G_u \cdot v_1 + G_{uu} \cdot u_1 \cdot v_c + \gamma_1 G_{u\gamma} \cdot v_c = \omega_1 v_c \tag{A.16}$$

We are looking at the critical eigenvalue $\omega(\varepsilon)$ with $\omega(0) = \omega_c$ where $\omega_c = \omega(\gamma_c)$ is the eigenvalue which causes the loss of stability, hence $\omega_c = 0$ and by equation (A.15), $v_c = a_1 u_c$.
Given the assumptions (A.1) and (A.2), we have found that $\gamma_1 = 0$ and $u_1 = A_1 u_c$ (see (A.9) and (A.12f). Then again by assumption (A.2)the Fredholm alternative for (A.16a) gives:

$$\omega_1 = 0 \tag{A.17a}$$

and

$$G_u v_1 = -a_1 A_1 G_{uu} \cdot u_c \cdot u_c \tag{A.17b}$$

(Compare (A.16) with (A.11)). Note that we can find v_1 such that $\langle v_1, u_c^* \rangle = 0$.

Let $d_u^* G(u(\varepsilon), \gamma(\varepsilon))$ be the adjoint operator of $d_u G(u(\varepsilon), \gamma(\varepsilon))$; denote the eigenvector of $d_u^* G(u(\varepsilon), \gamma(\varepsilon))$ by $v^*(\varepsilon)$, the adjoint eigenvalue problem of (A.7) is

$$\bar{\omega}(\varepsilon) v^*(\varepsilon) = d_u^* G(u(\varepsilon), \gamma(\varepsilon)) \cdot v^*(\varepsilon) \tag{A.18}$$

Since $\omega_c(\gamma_c)$ is a simple eigenvalue, the eigenvalue $\omega(\varepsilon)$ in (A.5d) must be real for small ε otherwise there would exist a pair of complex conjugate eigenvalues becoming zero at $\gamma = \gamma_c$. So $\bar{\omega}(\varepsilon) = \omega(\varepsilon)$ for small ε.

The equation for the non trivial solution $u(\varepsilon)$ (A.5a) can be written as:

$$u(\varepsilon) = \varepsilon A_1 u_c + \varepsilon^2 W_u \quad \text{with } \langle W_u, u_c^* \rangle = 0 \tag{A.19}$$

and similar the equation of the eigenvector $v(\varepsilon)$ (A.5c):

$$v(\varepsilon) = a_1 u_c + \varepsilon^2 W_v \quad \text{with } \langle W_v, u_c^* \rangle = 0 \tag{A.20}$$

Similar $v^*(\varepsilon)$ can be decomposed:

$$v^*(\varepsilon) = a_1^* u_c^* + \varepsilon^2 W_v^* \quad \text{with } \langle W_v^*, u_c \rangle = 0 \tag{A.21}$$

Since $(u(\varepsilon), \gamma(\varepsilon))$ satisfies $G(u;\gamma) = 0$, the derivative in ε of $G(u(\varepsilon);\gamma(\varepsilon))$ equals to

$$d_u G(u(\varepsilon);\gamma(\varepsilon)) \cdot u_\varepsilon + \gamma_\varepsilon . d_\gamma G(u(\varepsilon);\gamma(\varepsilon)) = 0 \tag{A.22}$$

Then

$$\langle d_u G(u(\varepsilon);\gamma(\varepsilon)) u_\varepsilon, v^*(\varepsilon) \rangle = -\gamma_\varepsilon \langle d_\gamma G(u(\varepsilon);\gamma(\varepsilon)), v^*(\varepsilon) \rangle \tag{A.23}$$

where the subindex ε denotes derivatives in ε.

For small ε, with real $\omega(\varepsilon)$, equation (A.23) becomes:

$$\omega(\varepsilon) \langle u_\varepsilon, v^*(\varepsilon) \rangle = -\gamma_\varepsilon \langle d_\gamma G(u(\varepsilon);\gamma(\varepsilon)), v^*(\varepsilon) \rangle \tag{A.24}$$

Note that

$$u_\varepsilon = A_1 u_c + \varepsilon W \quad \text{with } \langle W, u_c^* \rangle = 0 \tag{A.25a}$$

and

$$\gamma_\varepsilon = 2\varepsilon\gamma_2 + O(\varepsilon^2) \tag{A.25b}$$

with $\gamma_2 = A_1^2 (P_3/P_1)$ (see (A.13f)) and P_1 is given by transversality condition (A.3).

Inserting (A.21) and (A.25a) in (A.24) and expanding $d_\gamma G$ around $(u,\gamma) = (0,\gamma_c)$ we find:

$$\omega(\varepsilon) \langle A_1 u_c + \varepsilon W, a_1^* u_c^* + \varepsilon^2 W_v^* \rangle = -\gamma_\varepsilon \langle F(u;\gamma), a_1^* u_c^* + \varepsilon^2 W_v^* \rangle$$

where

$$F(u;\gamma) = G_{u\gamma}(\varepsilon A_1 u_c + \varepsilon^2 W_u) + G_{\gamma\gamma}(\varepsilon^2 \gamma_2 + O(\varepsilon^3)) + C(u^2(\varepsilon), \gamma^2(\varepsilon)) \tag{A.26}$$

where the notations are as defined before: all the derivatives in (A.26) are evaluated at $(u,\gamma) = (0,\gamma_c)$.
Now using orthogonality and normalization one obtains to the smallest order in ε:

$$\omega(\varepsilon)A_1 a_1^* = -\gamma_\varepsilon \varepsilon A_1 a_1^* \langle G_{u\gamma}\cdot u_c, u_c^*\rangle \qquad (A.27a)$$

Noting that $\langle G_{u\gamma}\cdot u_c, u_c^*\rangle = \frac{d\omega_c}{d\gamma}(\gamma_c) = P_1$ ((A.3), (A.12d)) and $\gamma_\varepsilon = 2\varepsilon\gamma_2 + O(\varepsilon^2)$, equation can be written as:

$$\omega(\varepsilon)A_1 a_1^* = -2\varepsilon^2 A_1 a_1^* P_1 \gamma_2 + O(\varepsilon^2) \qquad (A.27b)$$

which ties the sign of the eigenvalue $\omega(\varepsilon)$ to that of γ_2, given the sign of P_1.
So, if $P_1 < 0$ and $\gamma_2 < 0$ the bifurcating branch is stable if the reference state was stable for $\gamma > \gamma_c$ since (for small ε) all eigenvalues will have a negative real part (**supercritical bifurcation**). In general this type of bifurcation means that the bifurcating branch has one "unstable" eigenvector (eigenmode) less than the number of unstable eigenvectors of the reference state. For $P_1 < 0$ and $\gamma_2 > 0$ the bifurcating branch is unstable (**subcritical branching**).

A.3 Bifurcation of the one-dimensional anti-diffusion system

The one-dimensional anti-diffusion system defined on $x \in \Omega$, $\Omega = [0,L] \subset \mathbb{R}$ is

$$\frac{\partial u}{\partial t} = G(u;\gamma) \qquad (A.28a)$$

with

$$G(u;\gamma) = \frac{\partial^2}{\partial x^2}\phi(u) - \gamma\frac{\partial^4 u}{\partial x^4}, \quad \gamma > 0 \qquad (A.28b)$$

and no-flux boundary conditions:

$$\frac{\partial u}{\partial x} = \frac{\partial^3 u}{\partial x^3} = 0 \text{ at } x = 0 \text{ and } x = L \qquad (A.28c)$$

where

$$\phi(u) = -u + r_1 u^2 + r_2 u^3, \quad r_2 > 0 \qquad (A.28d)$$

The initial condition is given by some u_o with $\int u_o(x)dx = 0$.

So we can write (A.28b) as

$$G(u;\gamma) = Bu - \gamma Au + N(u)$$

with $N(u) = r_1\frac{\partial^2}{\partial x^2}u^2 + r_2\frac{\partial^2}{\partial x^2}u^3$ and

$$Bu = -\frac{\partial^2 u}{\partial x^2}, \qquad Au = \frac{\partial^4 u}{\partial x^4} \tag{A.28e}$$

As noted in chapter III, stationary solutions of (A.28) must satisfy

$$\phi(u) - \gamma\frac{\partial^2 u}{\partial x^2} - \beta = 0 \tag{A.29a}$$

with

$$\beta = \frac{1}{L}\int\phi(u)dx \text{ and } \int u(x)dx = 0 \tag{A.29b}$$

Now $u = 0$ is a solution of (A.28) with $\beta = 0$. Let $v(x)$ be a small disturbance of $u = 0$ then the first order approximation is:

$$\frac{\partial v}{\partial t} = -\frac{\partial^2}{\partial x^2}v - \gamma\frac{\partial^4 v}{\partial x^4} = (B - \gamma A)u \tag{A.30}$$

Let

$$d_u G(0;\gamma)\cdot v = \frac{\partial^2}{\partial x^2}\left[-1 - \gamma\frac{\partial^2}{\partial x^2}\right]v \tag{A.31}$$

then

$\langle d_u G(0;\gamma)\cdot v, w\rangle_0$ is well defined for all $v,w \in H^2_*$ with

$$H^2_* = \left\{ u \in H^2 \mid \langle u, 1\rangle_2 = 0 \right\} \tag{A.32}$$

where the symbol 1 denotes a constant function equal to 1 for all x. (See for the definition of the function space H^2 appendix E.) So as solution space is chosen H^2_*. The operator $d_u G(0;\gamma_c)$ is symmetric.

The eigenvectors of $\frac{\partial^2}{\partial x^2}$ are orthogonal and form a complete set in $L^2(\Omega)$; the eigenvalues are real and simple (Coddington e.a., 1955).

Given the boundary conditions these eigenvectors are

$$u_k(x) = \cos(k\pi x/L) \quad , \; k = 0,1,2,.... \tag{A.33}$$

which are also the eigenvectors of $d_u G(0;\gamma)$ as defined in (A.31) except that $k \neq 0$ since the solution space is restricted by the condition $\int u(x)dx = 0$. The corresponding eigenvalues are:

$$\omega_k = p_k^2(1 - \gamma p_k^2), \; p_k^2 = \left(\frac{\pi k}{L}\right)^2 \quad k = 1,2,3,... \tag{A.34}$$

An eigenvalue ω_k becomes zero if $\gamma = 1/p_k^2$ and such a value γ is a simple eigenvalue of the pair (B,A) defined in (A.28e) since we can write $(B - \gamma A) = \gamma(-A + (1/\gamma)B) = -\gamma B(B - (1/\gamma)I)$ for $\gamma \neq 0$ and $(1/\gamma)$ is a simple eigenvalue of (B,I)(see appendix E).
The stability of the null solution follows from the spectral form (A.2) in the weak sense:

$$\langle \omega(\gamma)v(\gamma), w\rangle_o = \langle d_u G(0;\gamma)v(\gamma), w\rangle_o \text{ all } w \in H_*^2 \tag{A.35}$$

In the following γ is taken such that one of the eigenvalues ω_k is zero; to get in line with the notations used in section A.1 and A.2, this eigenvalue and the eigenvector will be denoted by ω_c and u_c respectively. Hence:

$$\gamma_c = 1/p_k^2 \tag{A.36a}$$

$$u_c = \cos(k\pi x/L) \tag{A.36b}$$

$$\omega_c(\gamma) = p_k^2(1 - \gamma p_k^2) \tag{A.36c}$$

$$G_u = d_u G(0;\gamma_c) = \frac{\partial^2}{\partial x^2}\left[-1 - \gamma_c \frac{\partial^2}{\partial x^2}\right] \tag{A.36d}$$

$$G_{uu} = d_{uu} G(0;\gamma_c) = 2r_1 \frac{\partial^2}{\partial x^2} \tag{A.36e}$$

$$G_{u\gamma} = d_{u\gamma} G(0;\gamma_c) = -\frac{\partial^4}{\partial x^4} \tag{A.36f}$$

The eigenvector u_c^* of the adjoint operator G_u^* of G_u is given by

$$u_c^* = \cos(k\pi x/L)/N_k \tag{A.37}$$

with N_k a normalization factor such that $\langle u_c, u_c^*\rangle_2 = 1$, hence $N_k = \frac{1}{2}L(1 + p_k^2 + p_k^4)$. $(G_u^* = G_u.)$

Let ε be a small parameter; the expansions of u and γ are

$$u(\varepsilon) = 0 + \varepsilon u_1 + \varepsilon^2 u_2 + \ldots\ldots \tag{A.38a}$$

$$\gamma(\varepsilon) = \gamma_c + \varepsilon\gamma_1 + \varepsilon^2\gamma_2 + \ldots\ldots \tag{A.38b}$$

where $u_i \in H_*^2$ and $\gamma_i \in \mathbb{R}$, $i = 1,2,3,\ldots\ldots$
It is clear that the transversality condition holds since

$$\frac{d\omega_c}{d\gamma}(\gamma_c) = -(p_k^2)^2 < 0 \quad (k>0) \tag{A.39}$$

To apply the above exposed construction procedure one needs a similar solvability condition as in (A.10b) with respect to (A.10a). Since G_u is unbounded G_u satisfies not the condition of the Fredholm alternative since this is only valid for compact operators (see appendix E). But at the same place is shown that the solvability condition is similar to the Fredholm alternative (see appendix E: self-adjoint operators with compact resolvent).

The main object is to find the values of the constants P_1, P_2 and P_3 as defined in (A.12b), (A.12c) and (A.13d).

P_1 is given by equation (A12b); using (A.36f) with (A.37) one finds:

$$P_1 = -(p_k^2)^2 \tag{A.40}$$

which is equal to the transversality condition (A.39).

Then (A.9) with the definition of u_c gives:

$$u_1 = A_1 \cos(k\pi x/L) \tag{A.41}$$

Write again $v_{11} = G_{uu} \cdot u_c \cdot u_c$ then one finds that

$$v_{11} = 2r_1 \frac{\partial^2}{\partial x^2}(\cos(k\pi x/L))^2 = -4r_1 p_k^2 \cos(2k\pi x/L) \tag{A.42a}$$

and thus

$$P_2 = -\frac{1}{2}\langle v_{11}, u_c^* \rangle_2 = 0 \tag{A.42b}$$

Hence the first conclusion is

$$\gamma_1 = 0. \tag{A.43}$$

Using the completeness of the set of eigenvectors (A.33) (see appendix E, theorem E.12) to set

$$u_2 = \sum_{\substack{m=1 \\ m \neq k}}^{\infty} \mathcal{A}_m \cos(m\pi x/L) \tag{A.44}$$

where the term belonging to the null space of G_u is omitted. The equation (A.11) with $\gamma_1 = 0$ can be solved

$$G_u \cdot u_2 = -\frac{1}{2} A_1^2 v_{11} \tag{A.45a}$$

using the orthogonality of the eigenvectors (A.33):

$$\mathcal{A}_j = 0 \text{ for all } j \neq 2k \tag{A.45b}$$

and

$$\mathcal{A}_{2k}(4 - 16\gamma_c p_k^2) = 2r_1 A_1^2 \tag{A.45c}$$

In the following $\mathcal{A}_{2k}$ is denoted by A_2.

Using (A.36a) one gets:

$$A_2 = -r_1 A_1^2/6 \tag{A.46a}$$

and

$$u_2 = (-r_1 A_1^2/6)\cos(2k\pi x/L) \text{ (modulo } [u_c]) \tag{A.46b}$$

The solvability condition (A.13c) gives

$$-\gamma_2 A_1 P_1 + A_1^3 P_3 = 0 \tag{A.47a}$$

where

$$P_3 = -\langle v_{111}, u_c^* \rangle_2 \tag{A.47b}$$

with

$$v_{111} = \left\{-2r_1 \frac{\partial^2}{\partial x^2}(u_1 u_2) + r_2 \frac{\partial^2}{\partial x^2} u_1^3\right\}/A_1^3 \tag{A.47c}$$

Use u_2 as given by (A.46b) to find that

$$P_3 = \frac{1}{6}(r_1^2 - \frac{9}{2}r_2)p_k^2 \tag{A.48a}$$

$$\gamma_2 P_1 = A_1^2 P_3 \tag{A.48b}$$

Since $P_1 < 0$ the bifurcation direction depends only on the sign of $r_1^2 - \frac{9}{2}r_2$ (assuming this term is not zero). So if

$$r_1^2 - \frac{9}{2}r_2 < 0 \text{ then the bifurcation is supercritical} \tag{A.49a}$$

and if

$$r_1^2 - \frac{9}{2}r_2 > 0 \text{ then the bifurcation is subcritical} \tag{A.49b}$$

Setting β as in (A.14b)

$$\beta^2 = P_1(\gamma - \gamma_c)/P_3 \tag{A.50a}$$

to find an approximate solution

$$u(x) = \pm\beta\cos(k\pi x/L) - \frac{r_1}{6}\beta^2\cos(2k\pi x/L) + O(\beta^3) \tag{A.50b}$$

Suppose the reference state $u = 0$ is stable for $\gamma > \gamma_c$ and loses its stability at $\gamma = \gamma_c$, then $\gamma_c = L^2/\pi^2$; according to (A.27b) the bifurcating solution will be

stable if $r_1^2 - \frac{9}{2}r_2 < 0$ (A.51a)

and

unstable if $r_1^2 - \frac{9}{2}r_2 > 0$. (A.51b)

For $r_2 < 0$ the bifurcation is always subcritical and the bifurcating branch is unstable.

The case that $r_1^2 - \frac{9}{2}r_2 = 0$ is not followed further since the principal construction procedure is not changed, except when all higher order terms are zero.

A.4 Stability of the null solution of the general migration system

The system equation can be written as (see chapter IV, section 7)

$$\tau\frac{\partial u}{\partial t} = -M\int_0^L K(x,y)\left(\phi(u(y)) - \gamma\frac{\partial^2}{\partial y^2}u(y)\right)dy \qquad (A.52)$$

where $K(x,y) = \delta(x,y) - \Psi(x,y)$, with δ the Dirac delta function; the operator Ψ defined by $(\Psi u)(x) = \int_0^L \Psi(x,y)u(y)dy$ is symmetric with eigenvalues less or equal to 1. The boundary conditions are of no-flux type. (M and τ are positive constants.)

With ϕ as in (A.28d), $u = 0$ is a solution of (A.52). Let $v(x)$ be a disturbance satisfying (A.52) then the first order approximation is:

$$\tau\frac{\partial v}{\partial t} = -M\int K(x,y)\left(-v - \gamma\frac{\partial^2 v}{\partial y^2}\right)dy \qquad (A.53)$$

Using again completeness and orthogonality of the eigenvectors of the Laplace operator by writing

$$v(x,t) = \sum_{k=1}^{\infty} a_k(t)\cos(k\pi x/L) \qquad (A.54a)$$

to find

$$\tau\dot{a}_l(t) = M\left[\frac{2}{L}\sum_{k=1}^{\infty}\omega_k a_k(t)\left\{\iint\cos(l\pi x/L)K(x,y)\cos(k\pi y/L)dydx\right\}\right] \qquad (A.54b)$$

where

$$\omega_k = (1 - \gamma p_k^2) \text{ for } k = 1,2,\ldots \qquad (A.54c)$$

Substituting $\delta(x,y) - \Psi(x,y)$ for $K(x,y)$ in (A.54b), to find that the right hand side of (A.54b) is equal to

$$M\omega_1 a_1(t) - M\left[\frac{2}{L}\sum_{k=1}^{\infty}\omega_k a_k(t)\left\{\iint\cos(l\pi x/L)\Psi(x,y)\cos(k\pi y/L)dydx\right\}\right] \tag{A.54d}$$

If $\Psi(x,y) = 1/L$ then (A.54d) becomes equal to $M\omega_1 a_1(t)$, hence the stability properties are the same as for the anti-diffusion system. However, in this case, the fastest growing mode (= mode corresponding with the largest eigenvalue) is given always for $k = 1$, the monotone mode. This is not necessarily true for the anti-diffusion system where the eigenvalues are given by (A.34): $\omega_k = p_k^2(1 - \gamma p_k^2)$. For γ small the fastest growing mode is not the monotone mode. The initial evolution of a small perturbation will be different in the migration system and the anti-diffusion system if the null solution is unstable in more than one mode.

Appendix B

In this appendix some properties of the two wave amplitude system given in chapter VI, will be deduced. The system is given by the following equations:

$$\dot{a}_1 = \left\{a_1 - \gamma_o a_1 - a_1 a_2 r_1 - r_2\left[\tfrac{3}{4}a_1^3 + \tfrac{3}{2}a_1 a_2^2\right]\right\}p_k^2 \qquad \text{(B.1a)}$$

$$\dot{a}_2 = \left\{a_2 - 4\gamma_o a_2 - \tfrac{1}{2}a_1^2 r_1 - r_2\left[\tfrac{3}{2}a_1^2 a_2 + \tfrac{3}{4}a_2^3\right]\right\}4p_k^2 \qquad \text{(B.1b)}$$

where $p_k^2 = \left(\frac{k\pi}{L}\right)^2$, for some integer $k > 0$. Define $V(a_1, a_2)$ as follows:

$$V(a_1, a_2) = -\tfrac{1}{2}\left[(1 - \gamma_o)a_1^2 + (1 - 4\gamma_o)a_2^2\right] + \tfrac{1}{2}r_1 a_1^2 a_2 +$$
$$+ \tfrac{3}{16}r_2\left[a_1^4 + a_2^4 + 4a_1^2 a_2^2\right] \qquad \text{(B.2)}$$

The system equations can be written as:

$$\dot{a}_k = -V_k(a_1, a_2)k^2 p_k^2, \qquad k = 1,2 \qquad \text{(B.3)}$$

where V_k denotes the partial derivative with respect to a_k.
Stationary solutions for $r_2 \neq 0$ are given by the following sets:

$$S1 = \left\{(a_1, a_2)\,\middle|\,(a_1, a_2) = (0,0)\right\} \qquad \text{(B.4a)}$$

$$S2 = \left\{(a_1, a_2)\,\middle|\,(a_1, a_2^2) = (0, \tfrac{4}{3r_2}(1-4\gamma_o))\right\} \qquad \text{(B.4b)}$$

$$S3 = \left\{(a_1, a_2)\,\middle|\,a_1^2 = \tfrac{4}{3r_2}\left(1 - \gamma_o - a_2 r_1 - \tfrac{3}{2}a_2^2 r_2\right)\ \&\right.$$
$$\left. 9r_2 a_2^3 + 12r_1 a_2^2 + \left(-4 - 8\gamma_o + \frac{8r_1^2}{3r_2}\right) - \frac{8r_1}{3r_2}(1 - \gamma_o) = 0\right\} \qquad \text{(B.4c)}$$

In the first paragraph the first terms of the Poincaré-Lindstedt expansions are calculated and used to determine the type of branching at $\gamma_o = 1$. The result is an exact replica of the statements with respect to branching from the null solution for the complete

(anti-diffusion) system.
Paragraph two is restricted to the case $r_2 < 0$, especially $r_2 = -1$. It is shown that all non-trivial solutions $(a_1, a_2) \neq (0,0)$ are unstable.
In the last paragraph, the case of positive r_2 with subcritical branching is examined. It will be shown that the subcritical branch has a turning point at which stability is changed.

B.1 Poincaré-Lindstedt approximations

The solution $(a_1, a_2) = (0,0)$ loses its stability at $\gamma_{oc} = 1$. The expansions of (a_1, a_2, γ_o) at $(0,0,\gamma_{oc})$ in a small parameter ε are:

$$a_1 = \varepsilon a_{11} + \varepsilon^2 a_{12} + \varepsilon^3 a_{13} + \ldots\ldots \tag{B.5a}$$
$$a_2 = \varepsilon a_{21} + \varepsilon^2 a_{22} + \varepsilon^3 a_{23} + \ldots\ldots \tag{B.5b}$$
$$\gamma_o = \gamma_{oc} + \varepsilon\gamma_{o1} + \varepsilon^2\gamma_{o2} + \varepsilon^3\gamma_{o3} + \ldots\ldots \tag{B.5c}$$

Inserting (B.5) in (B.1) and collecting the terms with the same ε order yields:
to $O(\varepsilon)$:
$$\dot{a}_{11} = p_k^2(1 - \gamma_{oc})a_{11} \tag{B.6a}$$
$$\dot{a}_{21} = 4p_k^2(1 - 4\gamma_{oc})a_{21} \tag{B.6b}$$

to $O(\varepsilon^2)$:
$$\dot{a}_{12} = p_k^2\left\{(1 - \gamma_{oc})a_{12} - \gamma_{o1}a_{11} - r_1 a_{11}a_{21}\right\} \tag{B.6c}$$
$$\dot{a}_{22} = 4p_k^2\left\{(1 - 4\gamma_{oc})a_{22} - \gamma_{o1}a_{21} - \tfrac{1}{2}r_1 a_{11}\right\} \tag{B.6d}$$

to $O(\varepsilon^3)$:
$$\dot{a}_{13} = p_k^2\left\{(1 - \gamma_{oc})a_{13} - \gamma_{o2}a_{11} - r_1\left[a_{11}a_{22} + a_{12}a_{21}\right] + -\tfrac{3}{4}r_2\left[a_{11}^3 + 2a_{11}a_{21}^2\right]\right\} \tag{B.6e}$$
$$\dot{a}_{23} = 4p_k^2\left\{(1 - 4\gamma_{oc})a_{23} - \gamma_{o2}a_{21} - \tfrac{1}{2}r_1 a_{11}a_{22} - \tfrac{3}{4}r_2\left[a_{21}^3 + 2a_{11}^2 a_{21}\right]\right\} \tag{B.6f}$$

For stationary solutions the left hand side of the equations must be

zero. Equations (B.6a) and (B.6b) defines nothing else than the eigenvector corresponding with the zero eigenvalue at $\gamma_{oc} = 1$ of the linearized system: $a_{11} = 1$ and $a_{21} = 0$.
Equation (B.6c) gives now : $\gamma_{o1} = 0$ and subsequently equation (B.6d) gives: $a_{22} = -r_1/6$.
Equation (B.6e) is now reduced to:

$$\gamma_{o2} = -r_1 a_{11} a_{22} - \frac{3}{4} r_2 a_{11}^3 = (r_1^2 - \frac{9}{2} r_2)/6 \qquad (B.7)$$

Inserting (B.7) in (B.5c) gives:

$$\gamma_o = \gamma_{oc} + \varepsilon^2 (r_1^2 - \frac{9}{2} r_2)/6 + O(\varepsilon^3) \ldots\ldots \qquad (B.8)$$

And thus analogously to the original complete system, the following theorem can be formulated:

Theorem B.1

For the system (B.1) the branching solutions at $(\gamma_o, a_1, a_2) = (1,0,0)$ exist for
$\gamma_o > \gamma_{oc}$ if $r_1^2 > \frac{9}{2} r_2$ (subcritical (unstable) branching) and for
$\gamma_o < \gamma_{oc}$ if $r_1^2 < \frac{9}{2} r_2$ (supercritical (stable) branching).

Note that the conclusions for the bifurcations are only valid for $\gamma_o = 1$. The same conclusions were obtained for all branching solutions from the null solution for the complete anti-diffusion system (of course apart from the stability aspects) (see the conclusions in Appendix A: (A.49a-b)). For this two wave system the branching at $\gamma_o = \frac{1}{4}$ is rather straightforward and depends only on the sign of r_2.

B.2 Instability of the non-trivial solutions for $r_2 < 0$

In this paragraph it will be shown that all non-trivial solutions of the system (B.1) with $r_2 < 0$ are unstable.

The stability of a solution (a_1, a_2) is given by the eigenvalues of the Jacobian matrix J. Using (B.3) one finds that J is given by

$$J = \begin{bmatrix} -V_{11} & -V_{12} \\ -4V_{21} & -4V_{22} \end{bmatrix} \tag{B.9}$$

where $V_{ij} = \dfrac{\partial^2}{\partial a_i \partial a_j} V(a_1, a_2)$.

Just as for a pure gradient system where J is the Hessian of the function V in (a_1, a_2), the eigenvalues of J are real.

In the following r_2 will be negative and without reducing the generality, is taken to be -1. Then

$$-V_{11} = 1 - \gamma_o - r_1 a_2 + \tfrac{9}{4} a_1^2 + \tfrac{3}{2} a_2^2 \tag{B.10a}$$

$$-V_{12} = -V_{21} = -r_1 a_1 + 3 a_1 a_2 \tag{B.10b}$$

$$-V_{22} = 1 - 4\gamma_o + \tfrac{9}{4} a_2^2 + \tfrac{3}{2} a_1^2 \tag{B.10c}$$

Now it is clear that all solutions belonging to solution set S2 (B.4b) are unstable, since $V_{12} = 0$ and $-V_{22} = -2(1 - 4\gamma_o) > 0$ for $\gamma_o > \frac{1}{4}$.

Solutions belonging to the third solution set S3 (B.4c) must satisfy the following equations:

$$1 - \gamma_o = r_1 a_2 - \left\{ \tfrac{3}{4} a_1^2 + \tfrac{3}{2} a_2^2 \right\} \tag{B.11a}$$

$$(1 - 4\gamma_o) a_2 = \tfrac{1}{2} r_1 a_1^2 - a_2 \left\{ \tfrac{3}{2} a_1^2 + \tfrac{3}{4} a_2^2 \right\} \tag{B.11b}$$

If $a_2 = 0$ then the non-trivial solution exists only for $\gamma_o > 1$ with $a_1^2 = -\frac{4}{3}(1 - \gamma_o)$. Inserting this solution in the matrix J (B.9) gives: $V_{11} = 2(1 - \gamma_o)$, $V_{22} = 1 + 2\gamma_o$ and $V_{12}^2 = -\frac{4}{3}(1 - \gamma_o) r_1^2$ so the determinant of the matrix J becomes equal to:

$$\det(J) = 8(1 - \gamma_o)(1 + 2\gamma_o) + \tfrac{16}{3}(1 - \gamma_o) r_1^2$$

and $\det(J) < 0$ if $\gamma_o > 1$. Hence the product of the eigenvalues is negative. So J must have at least one positive eigenvalue, and the solutions are unstable.

If $a_2 \neq 0$ then $(1 - 4\gamma_o)$ can be solved from equation (B.11b). Inserting (B.11a) in V_{11} and (B.11b), after dividing by a_2, in V_{22} yields:

$$-V_{11} = \frac{3}{2}a_1^2$$

$$-V_{22} = \frac{1}{2}r_1 a_2 \frac{a_1^2}{a_2^2} + \frac{3}{2}a_2^2$$

If $r_1 a_2 \geq 0$ then the trace of J is positive; hence the sum of the eigenvalues is positive and J must have at least one positive eigenvalue. The solution is unstable.

If $r_1 a_2 < 0$ then the determinant of J is equal to:

$$6a_1^2\left\{\frac{1}{2}r_1 a_2 \frac{a_1^2}{a_2^2} + \frac{3}{2}a_2^2\right\} - 4a_1^2\left\{r_1 - 3a_2\right\}^2 = r_1 a_2\left\{3\frac{a_1^2}{a_2^2} + 24a_1^2\right\} - 4a_1^2 r_1^2 - 27a_1^2 a_2^2$$

which is clearly negative for $r_1 a_2 < 0$; so J must have at least one positive eigenvalue, hence the solution is unstable.

The only remaining solutions are the trivial ones; so each non-trivial solution is unstable if $r_2 < 0$.

B.3 The subcritical solutions for $r_2 > 0$ with $r_1^2 \geq \frac{9}{2}r_2$

For $r_2 > 0$ and $r_1^2 \geq \frac{9}{2}r_2$ the bifurcating branch at $\gamma_o = 1$, $(a_1, a_2) = (0,0)$ is subcritical. The following theorem will be proved:

Theorem B.2:

For $r_2 > 0$ and $r_1^2 \geq \frac{9}{2}$ the subcritical solution branch bifurcating at $(\gamma_o, a_1, a_2) = (1,0,0)$ has a turning point.

Proof:

Let $r_2 = 1$. Define $f(a_2)$ as follows:

$$f(a_2) = a_2^3 + \frac{4}{3}r_1 a_2^2 + a_2\left\{\frac{4-8\gamma_o}{9} + \frac{8r_1^2}{27}\right\} - \frac{8r_1(1-\gamma_o)}{27} \qquad (B.12)$$

Then the solutions S3 (B.4c) are equivalent with

$$f(a_2) = 0 \;\&\; -\frac{3}{2}a_1^2 = \frac{3}{2}a_2^2 + r_1 a_2 - (1 - \gamma_o) \leq 0 \qquad (B.13)$$

Assume $r_1 > 0$.

Define $a_L(\gamma_o) = \dfrac{-r_1 - \sqrt{r_1^2 + 6(1-\gamma_o)}}{3}$ (B.14a)

and $a_R(\gamma_o) = \dfrac{-r_1 + \sqrt{r_1^2 + 6(1-\gamma_o)}}{3}$ (B.14b)

then the inequality constraint in (B.13) is equivalent with:

$$a_L(\gamma_o) \leq a_2 \leq a_R(\gamma_o) \tag{B.15}$$

Each non-zero a_2 -solution generates a pair $(\pm a_1, a_2)$ -solutions of (B.1). To proof that each of these solutions is connected with solutions branching at $\gamma_o = 1$, or that the solutions (B.13) have a turning point, means to proof that for some $\gamma_o > 1$, there exists an a_2 which satisfies the condition (B.13) with $f'(a_2) = 0$. The last conditions are equivalent with demanding that $f(a_2) = 0$ has two coinciding roots which satisfy (B.15). The proof is based on the following observations:

i) $f(0) = -\dfrac{8r_1}{27} + \dfrac{8r_1\gamma_o}{27}$

$$f(-\tfrac{2}{3}r_1) = \tfrac{8}{81}r_1^3 - \tfrac{16}{27}r_1 + \tfrac{24}{27}r_1\gamma_o$$

So at both ends of the interval $[a_L(1), a_R(1)]$ the function values are linear monotone increasing in γ_o.

ii) The zero's of $f(a_2)$ depend continuously on γ_o and for sufficiently high γ_o, there exist only one real zero. See e.g. the explicit formulas for the solutions of the roots of a polynomial equation of degree 3 (v/d Waerden, page 193 (1964)).

iii) If $\gamma_o = 1$, then (B.13) has exactly two solutions if $r_1^2 \geq \frac{9}{2}$; one solution is $a_2 = 0$ representing the branch bifurcating from the null solution at $\gamma_o = 1$; for r_1 with $r_1^2 \geq \frac{9}{2}$, the derivative of f in $a_2 = 0$ is always positive. (Note that $r_1^2 \geq \frac{9}{2}$ is just the condition for subcritical branching in the complete system, see Appendix A: (A.49a-b)). So for $\gamma_o = 1$ the function $f(a_2)$ has two zeros lying in the interval $[-\frac{2}{3}r_1, 0] = [a_L(1), a_R(1)]$.

By ii) there exists γ_o ($\gamma_o > 1$) such that $f(a_2)$ has exactly two roots

and by observation iii) the double root must lie in the interval $[-\frac{2}{3}r_1, 0] = [a_L(1), a_R(1)]$.

Suppose this double root does not satisfy the constraint (B.15). But then, there must exist $\gamma_o > 1$ such that a root of $f(a_2) = 0$ satisfies exactly the constraint (B.13):

$$-\frac{3}{2}a_1^2 = \frac{3}{2}a_2^2 + r_1 a_2 - (1 - \gamma_o) = 0$$

hence $a_1 = 0$ and $a_2 \neq 0$ because $\gamma_o \neq 1$. It follows from (B.1b) that a stationary solution of (B.1a-b) with $a_1 = 0$ and $a_2 \neq 0$, must satisfy

$$\frac{3}{4}a_2^2 = 1 - 4\gamma_o \text{ which is impossible for } \gamma_o > 1.$$

Hence the double root will satisfy the constraint (B.15) which completes the proof of the existence of a turning point on the subcritical branch.

The stability exchange is checked by calculating that the non-zero solution branch at $\gamma_o = 1$ is stable. Since the branch bifurcating from the null solution at $\gamma_o = 1$ is unstable, we must have an exchange of stability at the turning point.

The proof for $r_1 \leq 0$ is similar.

Appendix C

C.1 Most probable path equations

The method of finding the most probable path equation from the master equation

$$\tau\frac{\partial P}{\partial t} = -\sum_{\delta} W\{\rho \to \rho + \delta\}P(\rho,t) + \sum_{\delta} W\{\rho - \delta \to \rho\}P(\rho - \delta, t) \qquad (C.1)$$

can be found in Metiu et al. (1979); in this appendix the same procedure is applied apart from the handling of the constrained case.
Let $\delta = (\delta_1,\ldots,\delta_N) \in \mathbb{R}^N$ be the array of changes; let $\rho = (\rho_1,\ldots,\rho_N) \in \mathbb{R}^N$ be the density array.
The followings notations are introduced: $\alpha = (\alpha_1,\ldots,\alpha_N)$ is a multi-index if all α_n are nonnegative integers. Denote $|\alpha| = \sum_{n=1}^{N} \alpha_N$ and $\alpha! = \prod_{n=1}^{N} \alpha_n!$. The differential operator D^α is defined as

$$D^\alpha \equiv (\partial^{\alpha_1}/\partial\rho_1^{\alpha_1})\ldots(\partial^{\alpha_N}/\partial\rho_N^{\alpha_N}) \qquad (C.2a)$$

and in consequence we use the notation

$$\rho^\beta D^\alpha f(\rho) \equiv \rho_1^{\beta_1}\ldots\rho_1^{\beta_1}(\partial^{\alpha_1}/\partial\rho_1^{\alpha_1})\ldots(\partial^{\alpha_N}/\partial\rho_N^{\alpha_N})f(\rho_1,..\rho_N) \qquad (C.2b)$$

With respect to $W\{\rho \to \rho + \delta\}$ and $P(\rho,t)$ the assumptions are made that both are infinitely differentiable functions satisfying the condition $\sup|\rho^\beta D^\alpha f(\rho)| < \infty$ with the supremum being over all $\rho \in \mathbb{R}^N$ and all possible multi-indices α and β to secure that all manipulations on Fourier transforms are correct (Kawata, 1972).
The master equation (C.1) can be written as

$$\tau\frac{\partial P}{\partial t} = H(D,\rho)P(\rho,t) \qquad (C.3a)$$

with

$$H(D,\rho)P(\rho,t) = \sum_{\delta}\sum_{\alpha} \frac{(-1)^{|\alpha|}}{\alpha!}\delta^{\alpha}D^{\alpha}W\{\rho \to \rho + \delta\}P(\rho,t) \qquad (C.3b)$$

where D acts on the product WP. The summing is over all possible δ and all possible α. A path integral formula is derived by taking a short time (Δt) solution of (C.3):

$$P(\rho,t^0 + \Delta t) = P(\rho,t^0) + \frac{\Delta t}{\tau} H(D,\rho)P(\rho,t^0) \qquad (C.4)$$

The Fourier transform $\mathcal{F}(P)(k,t^0 + \Delta t)$ is defined by

$$P(\rho,t^0 + \Delta t) = (2\pi)^{-N/2}\int \exp(-i\langle k,\rho\rangle)\mathcal{F}(P)(k,t^0 + \Delta t)dk \qquad (C.5)$$

with $dk \equiv dk_1 \ldots dk_N$ and $\langle k,\rho\rangle \equiv \sum_{n=1}^{N} k_n \rho_n$, the innerproduct in $\mathbb{R}^N$ which notations shall be used throughout this appendix. Using (C.4) one gets:

$$\mathcal{F}(P)(k,t^0 + \Delta t) =$$
$$= (2\pi)^{-N/2}\int \left[\exp(i\langle k,\rho^0\rangle)\left\{1 + \frac{\Delta t}{\tau}H(D,\rho^0)\right\}P(\rho^0,t^0)\right]d\rho^0 \qquad (C.6)$$

where $\rho^0 = (\rho_1^0,\ldots,\rho_N^0)$ is ρ at time t^0.
Applying Fourier transform properties for derivatives (Kawata, 1972) and using (C.6), one finds:

$$\mathcal{F}(P)(k,t^0 + \Delta t) =$$
$$= \mathcal{F}(P)(k,t^0) + \frac{\Delta t}{\tau}\sum_{\alpha}\sum_{\delta}\left\{\frac{(-1)^{|\alpha|}}{\alpha!}\delta^{\alpha}k^{\alpha}(-i)^{|\alpha|}\mathcal{F}(WP)(k,\rho)\right\} \qquad (C.7)$$

where $WP = W\{\rho \to \rho + \delta\}P(\rho,t)$. Use (C.5) to see that (C.7) can be written as

$$\mathcal{F}(P)(k,t^0 + \Delta t) =$$
$$= (2\pi)^{-N/2}\int \left[\exp(i\langle k,\rho^0\rangle)\left\{1 + \frac{\Delta t}{\tau}H(-ik,\rho^0)\right\}P(\rho^0,t^0)\right]d\rho^0 \qquad (C.8)$$

where $H(-ik,\rho^0)$ is obtained from (C.3b).
For small $\frac{\Delta t}{\tau}$ the term between curly brackets in (C.8) may be approximated by an exponential; introducing (C.8) in (C.5) to find

$$P(\rho,t^0 + \Delta t) =$$
$$= (2\pi)^{-N/2}\int_{\rho}\int_{k} \exp\left[-\frac{\Delta t}{\tau}\left\{\langle ik,\frac{\tau(\rho - \rho^0)}{\Delta t}\rangle - H(-ik,\rho^0)\right\}\right]P(\rho^0,t^0)dkd\rho^0 \qquad (C.9)$$

Define the conditional probability $G(\rho,t|\rho^0,t^0)$ by

$$P(\rho,t) = \int G(\rho,t|\rho^0,t^0)P(\rho^0,t^0)d\rho^0 \qquad (C.10)$$

then by successive use of (C.9) for small time stapes Δt the conditional probability G can be written as a path integral:

$$G(\rho,t|\rho^0,t^0) =$$
$$= \int_\rho \int_k \exp\left[-\int_0^t \left\{ <ik(t'),\tau\dot{\rho}(t')> - H(-ik(t'),\rho(t')) \right\}\right] \mathcal{D}(k)\mathcal{D}(\rho) \qquad (C.11a)$$

where the notation of (C.11a) means the limit of the multiple integrals:

$$\int_\rho \ldots \int_\rho \int_k \ldots \int_k (2\pi)^{-NL/2} \times$$
$$\times \exp\left[-\Delta t \sum_{l=0}^{L-1} \left\{ <ik^l, \tau\frac{(\rho^{l+1} - \rho^l)}{\Delta t}> - H(-ik^l,\rho^l) \right\}\right] dk^0 \ldots dk^{L-1} d\rho^0 \ldots d\rho^{L-1} \qquad (C.11b)$$

where $L \equiv \frac{t - t^0}{\Delta t} \to \infty$ if $\Delta t \to 0$.

The most probable path is the path for which $G(\rho,t|\rho^0,t^0)$ is maximal. Compute $H(-ik,\rho)$ from (C.3b) for general δ to get

$$H(-ik,\rho) = i\int <k,\delta> W\{\rho \to \rho + \delta\}d\delta - \frac{1}{2}\int <k,\delta>^2 W\{\rho \to \rho + \delta\}d\delta + \ldots \qquad (C.12)$$

where the first term is obtained for $|\alpha| = 1$ and the second term for $|\alpha| = 2$. The first term gives the 'expectation' $E(<k,\delta>)$ of $<k,\delta>$ which is equal to $<k,E(\delta)>$. Denoting the 'covariance matrix' of δ by Q_δ then gives the second term $<k,Q_\delta k>$. The matrix Q_δ is symmetric and strictly positive. So we will $H(-ik,\rho)$ approximate by:

$$H(-ik,\rho) = i<k,E(\delta)> - \frac{1}{2}<k,Q_\delta k> \qquad (C.13)$$

Inserting (C.13) in (C.11b) integration over k can be performed: since Q_δ is symmetric and strictly positive, the positive square root A of Q_δ exists. A new variable η of integration (in the notation of (C.11a) is given by

$$k = iQ_\delta^{-1}(\tau\dot{\rho}(t')-E(\delta)) + A^{-1}\eta \qquad (C.14)$$

where Q_δ^{-1} denotes the inverse of Q_δ and A^{-1} the inverse of A. Using

$$\int \exp(-<\eta,\eta>d\eta = \left(\int_{-\infty}^{\infty} \exp(-s^2)ds\right)^N = \pi^{-N/2},$$

one finds (in the notation of (C.11a)):

$$G(\rho,t|\rho^0,t^0) = \int_{\rho} \exp\left[-\frac{3}{2}\int_0^t \left\{<\tau\dot{\rho}(t') - E(\delta), Q_\delta^{-1}(\tau\dot{\rho}(t') - E(\delta))>\right\}\right] \mathcal{D}'(\rho) \qquad (C.15)$$

with $\mathcal{D}'(\rho)$ is $\mathcal{D}(\rho)$ scaled by some constants.

The path integral is now over ρ only and the most probable path from ρ^0 to ρ is defined by the minimum of the integrand over t'. As Q_δ is strictly positive, this minimum is obtained if

$$\tau\dot{\rho}_n = E(\delta)_n, \qquad n = 1,\ldots,N \qquad (C.16)$$

In chapter IV (equation IV.2) the transition probability W is given as:

$$W\{\rho \to \rho + \varepsilon\} = \alpha \exp(-\frac{<\varepsilon,\varepsilon>}{\Delta})\cdot\exp\left[-\frac{\beta}{2}\left\{V(\rho+\varepsilon) - V(\rho)\right\}\right] \qquad (C.17)$$

where $\varepsilon \in \mathbb{R}^N$ (ε is unrestricted) and α, β, Δ are positive constants.

For Δ is small only small ε values contribute significantly. Therefore it is reasonable to expand V in a power series of ε and retain only the first order approximation:

$$V(\rho+\varepsilon) - V(\rho) = <\frac{\delta V}{\delta\rho}, \varepsilon> \qquad (C.18)$$

where $\frac{\delta V}{\delta\rho}$ is the gradient of V and $W\{\rho \to \rho + \varepsilon\}$ is approximated by

$$W\{\rho \to \rho + \varepsilon\} = \alpha \exp(-\left\{<\varepsilon + \frac{\beta}{2}\sqrt{\Delta}\,\frac{\delta V}{\delta\rho}, \varepsilon + \frac{\beta}{2}\sqrt{\Delta}\,\frac{\delta V}{\delta\rho}>/\Delta\right\} \qquad (C.19)$$

For ε unrestricted, the 'expected' value $E(\varepsilon) = \int \varepsilon W\{\rho \to \rho + \varepsilon\}d\varepsilon$ is given by

$$E(\varepsilon) = -M\frac{\delta V}{\delta\rho} \qquad (C.20)$$

where $M = \frac{1}{2}\alpha\beta(2\pi\Delta)^{N/2}\Delta$.

For restricted δ defined as $\delta = K\varepsilon$ the 'expected' value $E(\delta) = K\cdot E(\varepsilon)$. Hence the most probable path is given as:

$$\tau\dot{\rho}_n = -M\left(K\frac{\delta V}{\delta\rho}\right)_n, \qquad n = 1,..N \qquad (C.21)$$

with K is a symmetric positive matrix and τ and M are positive constants. Note that $\dot{\rho}_n$ must be conceived as a short notation of $\left(\frac{\rho^{l+1} - \rho^l}{\Delta t}\right)_n$ where the super index l denotes successive time steps Δt. The continuous time notation is an 'approximation' of the discrete time notation; the same holds for the spatial coordinates.

Appendix D

This appendix deals with the discrete version of the one dimensional anti-diffusion system and migration system as used in chapter VIII.

D.1 Bifurcation in the discrete anti-diffusion system

The discrete anti-diffusion system is

$$u_n^{j+1} = u_n^j + r\,\delta_x^2\left[\phi(u_n^j) - (\gamma/\Delta x^2)\delta_x^2 u_n^j\right] \tag{D.1}$$

where $r = \Delta t/\Delta x^2$, and $n = 1,..,N$ (spatial indices), $j = 1,...$ (time indices) with no-flux boundary conditions. We recall from chapter VIII that

$$\delta_x^2 u_n = u_{n+1} - 2u_n + u_{n-1} \tag{D.2a}$$

and that the no-flux boundary conditions are approximated by introducing artificial grid points u_o, u_{-1}, u_{N+1} and u_{N+2} with for all time steps j

$$u_o^j = u_1^j,\ u_{-1}^j = u_2^j,\ u_{N+1}^j = u_N^j \text{ and } u_{N+2}^j = u_{N-1}^j \tag{D.2b}$$

The function ϕ is

$$\phi(u) = -u + r_1 u^2 + r_2 u^3 \tag{D.3}$$

Let $G(u;\gamma)_n$, $n = 1,..,N$ be defined by

$$G(u;\gamma)_n = \delta_x^2\left[\phi(u_n) - (\gamma/\Delta x^2)\delta_x^2 u_n\right] \tag{D.4}$$

then stationary solutions of (D.1) must satisfy $G(u;\gamma)_n = 0$ all n. By the no-flux boundary conditions (D.2b), such a stationary solution satisfies

$$\phi(u_n) - (\gamma/\Delta x^2)\delta_x^2 u_n = \beta \text{ for } n = 1,..,N \tag{D.5a}$$

with

$$\beta = \frac{1}{N} \sum_{n=1}^{N} \phi(u_n) \tag{D.5b}$$

The eigenvectors of the operator δ_x^2, subject to the no-flux boundary conditions, are

$$u_k(n) = a_k \cos(k\pi(n - \tfrac{1}{2})/N), \quad k = 0,..N-1 \tag{D.6}$$

Using

$$\delta_x^2 \cos(k\pi(n - \tfrac{1}{2})/N) = -4\sin^2(k\pi/2N) \cdot \cos(k\pi(n - \tfrac{1}{2})/N) \tag{D.7}$$

we find that the eigenvalues ω_k of $-\delta_x^2 - (\gamma/\Delta x^2)\delta_x^4$ are

$$\omega_k = 4\sin^2(\tfrac{1}{2}p_k)\left(1 - (\gamma/\Delta x^2)4\sin^2(\tfrac{1}{2}p_k)\right) \tag{D.8}$$

with $k = 1,..,N-1$ and $p_k = k\pi/N$ ($k = 0$ is excluded by the mass-conservation property of (D.1)).

The eigenvalues of the right hand side of (D.1) linearized at the null solution are $1 + r\omega_k$. In chapter VIII an upperbound r_b of r is found such that for bounded stationary solutions of (D.1), the eigenvalues of the system linearized at such a solution are always greater than -1 if $r < r_b$ (see section VIII.1.1). Hence for $0 < r < r_b$, the stability properties of bounded solutions depend only on the sign of the eigenvalues (D.8). In the following we assume that $0 < r < r_b$ holds.

Let $\gamma = \gamma_c$ be such that for some k, an eigenvalue (D.8) becomes zero; this eigenvalue is simple hence $\gamma = \gamma_c$ is a bifurcation point. Thus

$$1 - (\gamma_c/\Delta x^2)4\sin^2(\tfrac{1}{2}p_k) = 0 \text{ for some } k, \quad k = 1,..N-1 \tag{D.9}$$

Now we apply the same procedures as in appendix A to find the Poincaré-Lindstedt series of the bifurcation parameter γ and the bifurcating branches. Let the expansions of the bifurcating stationary solution be written as

$$u_n = \varepsilon u_{1n} + \varepsilon^2 u_{2n} + O(\varepsilon^3) \tag{D.10a}$$

and

$$\gamma = \gamma_c + \varepsilon\gamma_1 + \varepsilon^2\gamma_2 + O(\varepsilon^3) \tag{D.10b}$$

Define $G(u;\gamma)_n$ as

$$G(u;\gamma)_n = \left[-\delta_x^2 - (\gamma_c/\Delta x^2)\delta_x^4\right]u_n - ((\gamma - \gamma_c)/\Delta x^2)\delta_x^4 u_n + \\ + r_1\delta_x^2 u_n^2 + r_2\delta_x^2 u_n^3 \qquad (D.11)$$

then by identifying the terms with the same order in ε one obtains to the first order ($O(\varepsilon)$):

$$\left[-\delta_x^2 - (\gamma_c/\Delta x^2)\delta_x^4\right]u_{1n} = 0 \qquad (D.12a)$$

to the second order ($O(\varepsilon^2)$):

$$\left[-\delta_x^2 - (\gamma_c/\Delta x^2)\delta_x^4\right]u_{2n} - (\gamma_1/\Delta x^2)\delta_x^4 u_{1n} + r_1\delta_x^2 u_{1n}^2 = 0 \qquad (D.12b)$$

to the third order ($O(\varepsilon^3)$):

$$\left[-\delta_x^2 - (\gamma_c/\Delta x^2)\delta_x^4\right]u_{3n} - (\gamma_1/\Delta x^2)\delta_x^4 u_{2n} - (\gamma_2/\Delta x^2)\delta_x^4 u_{1n} + \\ + 2r_1\delta_x^2 u_{1n}u_{2n} + r_2\delta_x^2 u_{1n}^3 = 0 \qquad (D.12c)$$

From (D.12a) it follows that

$$u_{1n} = A_1\cos(p_k(n - \tfrac{1}{2})), \quad n = 1,2,\ldots,N \qquad (D.13a)$$

and the Fredholm alternative for the existence of a solution u_{2n} of (D.12b) (see appendix E) gives that

$$\sum_{n=1}^{N}\left[(\gamma_1/\Delta x^2)\delta_x^4 u_{1n} - r_1\delta_x^2 u_{1n}^2\right]u_{1n} = 0 \qquad (D.13b)$$

Using (D.7) one finds that

$$\gamma_1 = 0 \qquad (D.13c)$$

By writing u_{2n} as series in the eigenvectors (D.6)

$$u_{2n} = \sum_{\substack{m=1\\ m\neq k}}^{N} \mathcal{A}_m\cos(m\pi(n - \tfrac{1}{2})/N) \qquad (D.14a)$$

and inserting (D.14a) in (D.12b) one finds that

$$\mathcal{A}_m = 0 \text{ all } m \neq 2k \text{ and } \mathcal{A}_{2k} = -A_1^2 r_1/(2 + 4\cos(p_k)) \qquad (D.14b)$$

Applying again the Fredholm alternative for the existence of a solution u_{3n} of (D.12c), one gets:

$$\gamma_2 = A_1^2\left\{\frac{r_1^2}{2(1+2\cos(p_k))} - \frac{3}{4}r_2\right\}\frac{\Delta x^2}{(2-2\cos(p_k))} \qquad (D.15)$$

Since the bifurcation direction depends on the sign of γ_2, the bifurcation is

supercritical for $\frac{r_1^2}{(1+2\cos(p_k))} - \frac{3}{2}r_2 < 0$; (D.16a)

subcritical for $\frac{r_1^2}{(1+2\cos(p_k))} - \frac{3}{2}r_2 > 0$. (D.16b)

In the first case, the bifurcating branch is stable if the reference branch (the null solution) was stable for $\gamma > \gamma_c$ (see appendix A, section 2)).

For $(1 + 2\cos(p_k))$ is positive, the conclusions (D.16a-b) are similar to those obtained for the continuous model (see appendix A). If $(1 + 2\cos(p_k))$ is negative, supercritical branching is possible even if $r_2 < 0$ which has no equivalent in the continuous case. But for some k_o with $(1 + 2\cos(p_{k_o}))$ negative and supercritical branching, the branching solution is unstable since all modes with $k < k_o$ are also unstable including modes with subcritical branching. This means this type of supercritical branching for $r_2 < 0$ will never be observed in numerical simulations.

Note that for $N \to \infty$, $4\sin^2(\frac{1}{2}p_k)/\Delta x^2 \to (k\pi/L)^2$ with $L = (N-1)\Delta x$ and also $p_k \to 0$. Hence the conditions (D.16a-b) for super- or subcritical branching become equal to those for the continuous model, see appendix A, conditions (A.49a-b). The same holds for the parameter values γ_1 and γ_2 (compare (D.15) with (A.48a-b)).

The eigenvalues ω_k, $k = 1,..N-1$, change sign at $\gamma = \gamma_k$ with $\gamma_k = \Delta x^2/(4\sin^2(\frac{1}{2}p_k))$, $p_k = k\pi/N$, see (D.8). The null solution becomes unstable at $\gamma = \gamma_1$. At points γ with $\gamma < \gamma_2$ at least two modes are unstable. In such case the evolution of a perturbation of the null solution will be initially dominated by the fastest growing mode(s), i.e. mode(s) k with eigenvalue ω_k maximal. And the fastest growing mode

is (approximately) given for k with

$$1 - 2(\gamma/\Delta x^2)4\sin^2(\tfrac{1}{2}p_k) = 0 \qquad (D.17)$$

Hence for small γ, the fastest growing mode is not identical with the mode k = 1, the monotone one.

D.2 The discrete migration system

The system equations are:

$$u_n^{j+1} = u_n^j + r\left[-\phi(u_n^j) + (\gamma/\Delta x^2)\delta_x^2 u_n^j - \frac{1}{N}\sum_{n=1}^{N} -\phi(u_n^j)\right] \qquad (D.18)$$

Using (D.6) the above results apply also for the discrete migration model (D.11). Define $G(u;\gamma)_n$ as

$$G(u;\gamma)_n = -\phi(u_n) + (\gamma/\Delta x^2)\delta_x^2 u_n - \frac{1}{N}\sum_{n=1}^{N} -\phi(u_n) \qquad (D.19)$$

Assume that r satisfies the upperbound r_b defined in chapter VIII, section VIII.3, equation (VIII.44c) then there is no difference between system (D.1) and (D.18) with respect neither to stability properties of a stationary solution (see also chapter V) nor to the Poincaré-Lindstedt series since the constant β involved in (D.5a) is just $\frac{1}{N}\sum_{n=1}^{N}\phi(u_n)$. However the eigenvalues ω_k of $G(u;\gamma)_n$ (D.19) linearized in the null solution are not given by (D.8) but by

$$\omega_k = 1 - (\gamma/\Delta x^2)4\sin^2(\tfrac{1}{2}p_k) \quad k = 1,..N-1 \qquad (D.20)$$

As a consequence, in contrast to the anti-diffusion system (see (D.17)) the fastest growing mode is always the mode with the longest wavelength (k = 1). This result is identical with that of the continuous case (see Appendix A, section A.4).

Appendix E

Definitions and Theorems

This appendix contains some definitions and basic theorems from the functional analysis. The object is to give conditions under which properties of the finite dimensional case are transferable to the infinite dimensional one. The information is not ordered alphabetically but packed in coherent groups. The first part deals with vector spaces and gives the justification for writing a disturbance v(x) as a series in the eigenvectors of the Laplace operator (see appendix A); here one also finds that the solvability condition for the equation $A(I - \gamma A)x = y$ with A the Laplace operator, is given by the Fredholm alternative: y must be perpendicular to the null space of $\left(A(I - \gamma A)\right)^T$. The second part gives the definition of convergence, continuity and derivatives of operators.
The main references for the first part are Kato (1966), Gohberg and Goldberg (1981), Taylor and Lay (1980) and Zaanen (1964). Most of the second part can be found in Kato (1966), Coolen (1978), Groesen (1978) and Lang (1969).

E.1 Operators on Linear vector spaces

Normed vector space

The vector space X is called a normed space if there exists a non-negative function $\|x\|$ on X such that for x and $y \in X$ hold:

i) $\|\alpha x\| = |\alpha| \cdot \|x\|$, α real (complex).

ii) $\|x + y\| \leq \|x\| + \|y\|$.

iii) $\|x\| > 0$ for $x \neq 0$.

From i) and iii) follows $\|x\| = 0 \Leftrightarrow x = 0$.

Completeness, Complete vector space, Completion

Suppose X is normed vector space. The vector space X is called complete if for any sequence $\{x_n\} \subset X$ satisfying the condition $\lim \|x_m - x_n\| = 0$ as $m,n \to \infty$, there exists an element $x \in X$ such that $\lim \|x - x_n\| = 0$ as $n \to \infty$. The sequence $\{x_n\}$ with $\lim \|x_m - x_n\| = 0$ as $m,n \to \infty$, is called a Cauchy sequence.

Completeness is comparable with extension from rational numbers to real numbers. Its means that every Cauchy sequence is convergent in X.

Every finite-dimensional normed linear space is complete.

An incomplete normed linear space X may be enlarged to form a complete space $\hat{X}$ in which X is dense. This completion is essentially unique.

Banach space

A Banach space is a complete normed vector space, i.e. every Cauchy sequence has a limit.

If the scalar field is $\mathbb{R}$ then X is called a real Banach space.

Banach space examples

1) $\mathbb{R}^N$ is real Banach space if supplied with the norm $\|x\| = \left(\sum_{n=1}^{N} |x_n|^2 \right)^{1/2}$.

2) Let $[0,1] \subset \mathbb{R}$ and let $C^o([0,1])$ be the class of continuous functions on $[0,1]$ with values in $\mathbb{R}$. $C^o([0,1])$ is a vector space over $\mathbb{R}$. Define as norm on B: $\|f\| = \sup_{x \in [0,1]} |f(x)|$, for all $f \in C^o([0,1])$, then $C^o([0,1])$ is complete, i.e., $C^o([0,1])$ is a real Banach space.

3) Let $C^p([0,1])$ be the class of functions having p continuous derivatives. Define the norm on C^p as $|f|_p = \sup_{|k| \le p} |D^k f|$, then $C^p([0,1])$ is complete.

4) Let $C_o^\infty(\Omega)$ be the class of functions with compact support in $\Omega \subset \mathbb{R}^N$ which are infinitely times differentiable.

Define as norm for $f \in C_o^\infty(\Omega)$

$$\|f\|_0 = \left\{ \int_\Omega f^2(x)dx \right\}^{1/2},$$

where elements are identified which differ only on a set of measure zero. $C_o^\infty(\Omega)$ is not complete under this norm (see Sobolev spaces,

discussed below).

Define as norm, with the same identification procedure,

$$\|f\|_p = \left\{ \sum_{k=0}^{p} \|D^k f\|^2 \right\}^{1/2},$$

where $D^k f$ is k-the derivative of f, then C_0^∞ is not complete.

Hilbert space

Suppose X is vector space over the real (complex) numbers. Suppose that with every pair $x, y \in X$ corresponds a real (complex) number (x,y), called the inner product of x and y, with the properties

i) $\langle \alpha x, y \rangle = \alpha \langle x, y \rangle$, α real (complex).

ii) $\langle x + y, z \rangle = \langle x, z \rangle + \langle y, z \rangle$.

iii) $\langle x, y \rangle = \overline{\langle y, x \rangle}$, where $\overline{\langle y, x \rangle}$ is the complex conjugate of $\langle x, y \rangle$.

iv) $\langle x, x \rangle > 0$ for $x \neq 0$.

The non-negative number $\langle x, x \rangle^{1/2}$ is called the norm of x. If with this norm X is complete then X is called a Hilbert space.

If the scalar field is $\mathbb{R}$ then X is called a real Hilbert space.

Hilbert space examples

1) The n-dimensional real vector space $\mathbb{R}^N$ supplied with the Euclidean inner product.

2) Let $[0,1] \subset \mathbb{R}$. Consider the class of square integrable real valued functions on the interval $[0,1]$, $L^2([0,1])$. Functions only differing in value on a set of measure zero are identified. Define the inner product $\langle f, g \rangle_0$ as

$$\langle f, g \rangle_0 = \int_0^1 f(x)g(x)dx$$

with the corresponding norm

$$\|f\|_0 = \left\{ \int_0^1 |f(x)|^2 dx \right\}^{1/2}$$

then $L^2([0,1])$ is a Hilbert space.

Linear mapping (linear operator, linear functional)

Suppose X and Y are vector spaces over the same scalar field ϕ. A mapping $T: X \to Y$ is called linear if

$$T(\alpha x + \beta y) = \alpha T(x) + \beta T(y).$$

Often Tx is written in stead of T(x).

If T: $X \to \phi$ and T is linear then T is called a linear functional.
The set of all linear functionals on X will be denoted as X^f.

Continuous mapping

Suppose X and Y are normed vector spaces. An operator F: $X \to Y$ is called continuous at a point $x \in X$ if for any sequence $\{x_n\}$ in X converging to x the sequence $\{F(x_n)\}$ converges to F(x).
F is called continuous on a open set $A \subset X$, if it is continuous at each point of A.

Bounded

Suppose X and Y are normed vector spaces. An operator F: $X \to Y$ is called bounded if it maps bounded sets in X into bounded sets of Y.
The set of bounded linear operators which map X into Y is denoted by $L(X,Y)$. If X = Y, we write $L(X)$ instead of $L(X,X)$.

Bounded linear functional
Dual (adjoint) space

The normed vector space $L(X,\mathbb{R})$ or $L(X,\mathbb{C})$ of all bounded linear functionals on the normed vector space X is called the dual (adjoint) space of X and denoted as X^*. Elements of X^* will be written as x^*; the value of x^* at $x \in X$, $x^*(x)$, is written as (x,x^*), the symmetric notation.
In the finite dimensional case X^f, the space of all linear functionals, is equal to X^*, the space of all bounded linear functionals.

Bounded linear operator

(Theorem) A linear operator T of a normed vector space X into a normed vector space Y is continuous if and only if it is bounded.

Riesz representation theorem:

Let x^* be a bounded linear functional on a Hilbert space H. Then there exists a unique $y \in H$, such that

$$x^*(x) = \langle x,y \rangle$$

for all $x \in H$. Moreover, $\|x^*\| = \|y\|$. The mapping defined by $x^* \to y$ is called the duality map.

(*Finite dimensional*: Consider a n-dimensional linear space $\mathbb{R}^N$, let $(e_1,\ldots,e_N)$ form a basis for $\mathbb{R}^N$, then $x = \sum_{n=1}^{N} x_n e_n$ for some $x_1,..,x_N$. Let f be a linear functional on $\mathbb{R}^N$ then

$$f(x) = f\left(\sum_{n=1}^{N} x_n e_n\right) = \sum_{n=1}^{N} x_n f(e_n) = \sum_{n=1}^{N} x_n f_n.$$

Conversely, an expression of the form

$$f(x) = \sum_{n=1}^{N} x_n f_n,$$

is a linear functional on $\mathbb{R}^N$. ($f_n \in \mathbb{R}$).
Now, consider $\mathbb{R}^N$ as the Hilbert space with the Euclidean inner product, then a linear functional f can be represented by $\langle x,f\rangle$, where $f \in \mathbb{R}^N$ is uniquely determined by $f(e_n) = f_n$.)

Compact operator

Suppose X and Y are normed linear spaces. Let T be a linear operator with domain $D(T)$ is X and range in Y. The operator T is called compact if for each bounded sequence $\{x_n\}$ in X, the sequence $\{Tx_n\}$ contains a subsequence converging to some limit in Y.
The set of all compact linear operators will be denoted as $C(X,Y)$.
The set $C(X,Y)$ is a subspace of $L(X,Y)$, the set of all bounded linear operators.

Let X, Y, Z be normed linear spaces and suppose $T \in L(X,Y)$, $S \in L(Y,Z)$ then ST is compact whenever S or T is compact.

If T is a compact operator whose domain X is infinite dimensional then T cannot have a bounded (continuous) inverse. (The identity operator I is not compact if X is infinite dimensional.)

Closed operator

Let T be an operator from X to Y. T is said to be closed if for any sequence $\{x_n\} \in D(T)$ such that $x_n \to x$ and $Tx_n \to y$, x belongs to $D(T)$ and $Tx = y$.

Adjoint operator

Suppose X is a Hilbert space. If T is bounded linear mapping on X into X there exists a unique bounded linear mapping T^* such that

$\langle Tx, y\rangle = \langle x, T^* y\rangle$ for all $x, y \in X$. Furthermore, T^* satisfies $\|T^*\| = \|T\|$. The mapping T^* is called the adjoint mapping of T.

Symmetric operator

A linear operator T with domain $D(T)$ and range $R(T)$ in the inner product space X is said to be symmetric if the closure of $D(T)$ is X and $T^* \supset T$. Thus $T^* x = Tx$ for all $x \in D(T)$

Selfadjoint operator

A symmetric operator is selfadjoint if $T^* = T$.

A linear bounded operator T on X into X with X is a Hilbert space with $\langle Tx, y\rangle = \langle x, Ty\rangle$ is selfadjoint.

Clearly a selfadjoint operator is symmetric, but the reverse need not be true. *For finite dimensional spaces symmetric and self adjoint are always identical.*

Annihilator

Let S be a subset of a linear space X. The annihilator of S in X^*, is the set $S^{\perp}$ of all $x^* \in X^*$ such that $(x, x^*) = 0$ if $x \in S$.

It is possible to define the annihilator for X^f in stead of X^* on the same way. This set will be denoted as $S_f^{\perp}$. *For finite dimensional spaces the two definitions are identical.*

Transposed operator

Let X and Y linear spaces and let A be a linear operator on X into Y. For each $y^f \in Y^f$ corresponds an element $x^f \in X^f$, defined by

$(x, x^f) = (Ax, y^f)$; denote the function so defined by A^T; thus: $A^T y^f = x^f$. The operator A^T is called the transpose of A.

Solvability of Ax = y (*finite dimensional*).

(Theorem (Taylor and Lay, 1980)): Let A a linear operator on X into Y, where X and Y are linear spaces with the same scalar field. Then the range $R(A)$ is characterized as follows:

i) $\{R(A)\}_f^{\perp} = N(A^T)$

ii) $R(A) = \{N(A^T)\}_f^{\perp}$

iii) $R(A) = Y$ if and only if $(A^T)^{-1}$ exists.

Solvability of Ax = y for finite dimensional spaces is now given by ii) since $X^f = X^*$ *and* $S_f^\perp = S^\perp$. *The space* X^f *is again finite dimensional and* A^T *is represented by the transposed matrix.*

For infinite spaces the conditions above are not very useful: the space of all linear functionals is not an amenable space to study. Furthermore the representation is only for bounded functionals.

Spectrum, Resolvent

Let T be an operator from X into X. The identity operator is denoted by I. For each scalar λ the operator $\lambda I - T$ shall be denoted as T_λ.

The resolvent set of T is the set $\rho(T)$ of all λ such that the range of $\lambda I - T$ is dense in X and $\lambda I - T$ has a continuous (bounded) inverse. For $\lambda \in \rho(T)$, the operator $(\lambda I - T)^{-1}$ is called the *resolvent operator* and is denoted as R_λ.

The spectrum of T is the set $\sigma(T)$ of all scalar values not in $\rho(T)$.

The spectrum is divided into three mutually exclusive parts:

$C\sigma(T)$ = the continuous spectrum

$R\sigma(T)$ = the residual spectrum

$P\sigma(T)$ = the point spectrum = eigenvalues.

If X is finite dimensional and domain D(T) of T is X, then the spectrum of T is all λ *which are roots of the equation del*$(\lambda I - T) = 0$. *Each* $\lambda \in \sigma(T)$ *is an eigenvalue of T. Thus* $\sigma(T) = P\sigma(T)$ $(C\sigma(T) = R\sigma(T) = \varnothing)$.

Codimension

Let M be a subspace of X which is complemented by a finite dimensional subspace N. The dimension of N is called the *codimension* of M and is written codim M.

Eigenvalues

Let A be an operator from X into Y and B be an operator from Y into X, and let D and K be invertible operators acting on the spaces X and Y, respectively. Then

$$\begin{bmatrix} D-BK^{-1}A & -BK^{-1} \\ K^{-1}A & K^{-1} \end{bmatrix}^{-1} = \begin{bmatrix} D^{-1} & D^{-1}B \\ -AD^{-1} & K-AD^{-1}B \end{bmatrix} \tag{E.1}$$

Theorem E.2: The eigenvalues of AB and BA are the same except eventually zero eigenvalues; if A and B are acting on the same finite dimensional spaces then all eigenvalues of AB and BA are the same. (E.2)

Theorem (E.2) can be proved by using the following theorem:
Theorem (theorem 1.1 in Bart et al. (1984): Assume T is an operator from X_1 into Z_1 and S is an operator from Z_2 into X_2 such that

$$\begin{bmatrix} T & A_{12} \\ A_{21} & A_{22} \end{bmatrix}^{-1} = \begin{bmatrix} B_{11} & B_{12} \\ B_{21} & S \end{bmatrix}.$$

Then

$$\begin{bmatrix} T & 0 \\ 0 & I_{X_2} \end{bmatrix} = E \begin{bmatrix} S & 0 \\ 0 & I_{Z_1} \end{bmatrix} F,$$

where E and F are invertible 2×2 operator matrices

$$E = \begin{bmatrix} -A_{12} & TB_{11} \\ I_{X_2} & B_{21} \end{bmatrix}, \quad F = \begin{bmatrix} A_{21} & A_{22} \\ T & A_{12} \end{bmatrix}$$

with inverses

$$E^{-1} = \begin{bmatrix} -B_{21} & SA_{22} \\ I_{Z_1} & A_{12} \end{bmatrix}, \quad F^{-1} = \begin{bmatrix} B_{12} & B_{11} \\ S & B_{21} \end{bmatrix}.$$

Proof of (E.2):

Let $D = I_X$, $K = \lambda I_Y$ with $\lambda \neq 0$; let $T = D - BK^{-1}A$ and $S = K - AD^{-1}B$ then use (E.1) to see that T and S satisfy the condition of the above theorem. Since $\lambda \neq 0$ we find:

$$\frac{1}{\lambda} \begin{bmatrix} \lambda I_X - BA & 0 \\ 0 & \lambda I_X \end{bmatrix} = E \begin{bmatrix} \lambda I_Y - AB & 0 \\ 0 & I_Y \end{bmatrix} F,$$

The operators E and F are invertible. Hence, if $\lambda \neq 0$ is an eigenvalue of BA then λ is an eigenvalue of BA, and vice versa which proves the first part of (E.2).

Suppose A and B are acting on finite dimensional spaces $\mathbb{R}^N$ and we now only have to prove that AB has a zero eigenvalue if and only if BA has a zero eigenvalue. If the eigenvalues of AB are not zero then A and B have right inverses which on finite dimensional spaces are equal to the left inverses; hence BA is invertible and BA does not have a zero eigenvalue.

Suppose AB has a zero eigenvalue with eigenvector $w \in \mathbb{R}^N$ then at least either A or B must have a zero eigenvalue. If both A and B have a zero eigenvalue then also has BA. If A has a zero eigenvalue then also has BA. If A does not have a zero eigenvalue then A is invertible and $Bw = 0$. Hence there exists $v \in \mathbb{R}^N$ such that $Av = w$ and $BAv = Bw = 0$.

Eigenvalues of (B,A)

Suppose $B, A: X \to Z$ are bounded linear operators.

The resolvent set $\rho(B,A)$ of the pair (B,A) is the set of $\lambda \in \mathbb{C}$ such that $B - \lambda A$ has a bounded inverse (Chow and Hale, 1982).

The spectrum $\sigma(B,A)$ of the pair (B,A) is the set of all scalar values not in $\rho(B,A)$.

A point $\lambda \in \sigma(B,A)$ is an *eigenvalue of (B,A)* if zero is an eigenvalue of $B - \lambda A$.

If $A = I$ then λ is a *I-simple* eigenvalue of (B,I) if and only if zero is a simple eigenvalue of $B - \lambda I$; that is

$$\dim N(B - \lambda I) = 1 = \operatorname{codim} R(B - \lambda I)$$

$$[IN(B - \lambda I)] \oplus R(B - \lambda I) = Z.$$

The point λ is called an *A-simple* eigenvalue of (B,A) if

$$\dim N(B - \lambda A) = 1 = \operatorname{codim} R(B - \lambda A)$$

$$[AN(B - \lambda A)] \oplus R(B - \lambda A) = Z.$$

Solvability of $(\lambda I - T)x = y$.

Separation of the spectrum

Isolated eigenvalues

The next theorem (theorem 6.17 in Kato) gives a decomposition of the spectrum which generalizes the decomposition of the spectrum for finite dimensional spaces.

Let T be a closed operator. Suppose the spectrum $\sigma(T)$ contains a bounded part $\sigma^1(T)$ separated from the rest $\sigma^2(T)$ in such a way that a rectifiable, simple closed curve Γ can be drawn as to enclose an open set containing $\sigma^1(T)$ in its interior and $\sigma^2(T)$ in its exterior. Now the decomposition theorem is formulated:

Theorem E.3: Let $\sigma(T)$ be separated into $\sigma^1(T)$ and $\sigma^2(T)$ as described above. Then there exists a decomposition of T given by a decomposition $X = M^1 \oplus M^2$ of the space in such a way that the spectra of the parts T_{M1}, T_{M2} coincide with $\sigma^1(T)$, $\sigma^2(T)$ respectively and $T_{M1} \in L(M^1)$. (T_M: the restriction of T to M, $T_M x = Tx$ for all $x \in M$.)

(E.3)

Suppose λ is an isolated point in the spectrum $\sigma(T)$. Then according to the theorem (E.3) there exists a decomposition and an operator T_{M1} whose spectrum consists of the single point λ. Suppose now that M^1 is finite dimensional then λ is an eigenvalue of T_{M1} and thus of T. In this case $\dim(M^1)$ is called the algebraic multiplicity of the eigenvalue λ.

An isolated eigenvalue λ of T with finite multiplicity m has properties quite similar to an eigenvalue of a finite dimensional operator. Thus e.g. $\bar{\lambda}$ is an eigenvalue of T^* with algebraic multiplicity m. Moreover,

$(T - \lambda I)x = y$ is solvable if and only if $y \perp N(T^* - \bar{\lambda} I^*)$

and

$(T^* - \bar{\lambda} I^*)g = f$ is solvable if and only if $f \perp N(T - \lambda I)$.

The similarity follows from the fact that the problem is reduced to the finite-dimensional problem for the parts T_{M1} and $T^*_{M1^*}$. (see Kato page 184.).

Spectrum of a bounded operator

The spectrum $\sigma(T)$ of a bounded linear operator is closed and bounded and hence compact.

Spectrum of a compact operator

The null spaces $N(T_\lambda^n)$, n = 1,2,.. with $T_\lambda^n = (\lambda I - T)^n$, are finite dimensional. (Theorem 7.6, page 299, in Taylor and Lay) (E.4a)

The spectrum of a compact operator in $L(X)$ contains at most a countable set of points and these have no accumulation point except possible the $\lambda = 0$. Each nonzero point of the spectrum $\sigma(T)$ is an eigenvalue. (Theorem 6.26 in Kato) (E.4b)

Hence the point $\lambda = 0$ can belong to $P\sigma(T)$, $C\sigma(T)$ or $R\sigma(T)$ but not to $\rho(T)$, the resolvent set of T, if X is infinite dimensional.

If λ and μ are distinct eigenvalues of the compact linear operator T, then the corresponding eigenvectors are linearly independent.

Solvability condition of $(\lambda I - T)x = y$ if T is compact

The solvability condition is given by the following characterization of the range of T_λ (see also the decomposition at isolated eigenvalues (E.3)):

$$R(T_\lambda) = N(T_\lambda^*)^\perp \qquad (E.5)$$

Fredholm alternative for compact operators

Let X be a normed linear space, let T be a compact linear operator on X into X, and consider the equations

$$(\lambda I - T)x = y \qquad (1)$$

in X and

$$(\lambda I^* - T^*)x^* = y^* \qquad (2)$$

in X^*.

Then one of the following two statements is true.

i) There exists a uniquely determined solution of (1) for each $y \in X$ and of (2) for each $y^* \in X^*$.

ii) The homogeneous equations

$$(\lambda I - T)x = 0 \qquad (3)$$

and

$$(\lambda I^* - T^*)x^* = 0 \qquad (4)$$

have a finite and equal number, say m, of linearly independent solutions. In this case equation (1) has a solution (not uniquely determined) if and only if $y \in N(\lambda I^* - T^*)^\perp$, and (2) has a solution if and only if $y^* \in N(\lambda I - T)^\perp$.

Orthogonal, orthonormal

A set of vectors in a inner product space is called an orthogonal set if $\langle x,y\rangle = 0$ for every $x, y \in S$, $x \neq y$. If, in addition, $\|x\| = 1$ for every $x \in S$, the set is called an orthonormal set.

Complete set

An orthonormal set S in the inner product space X is said to be complete if there exists no orthonormal set of which S is a proper subset; thus S is complete if it is maximal.

E.2 Spectral properties

Spectral properties of a symmetric operator

Let A be a linear operator with domain and range in the inner product space X. Let A be symmetric and define

$$m(A) = \inf_{\|x\|=1} \langle Ax,x\rangle \quad M(A) = \sup_{\|x\|=1} \langle Ax,x\rangle,$$

with the possibility that $m(A) = -\infty$, $M(A) = +\infty$.

The next theorems can be found in Taylor and Lay pages 345-346.

(Theorem E.6) If A is symmetric and λ is an eigenvalue of A then λ is real and $m(A) \leq \lambda \leq M(A)$. Eigenvectors corresponding to distinct eigenvalues are orthogonal. (E.6)

(Theorem E.7) Suppose that A is symmetric and $D(A)$ is dense in X. Suppose $y \in D(A)$, $\|y\| = 1$ and $\langle Ay,y\rangle = \lambda$ where λ is either m(A) or M(A). Then $Ay = \lambda y$ so that λ is an eigenvalue of A. (E.7)

(Theorem E.8) If A is symmetric with $D(A) = X$ then A is continuous if and only if m(A) and M(A) are both finite and in that case

$$\|A\| = \sup_{\|x\|=1} |\langle Ax,x\rangle| = \max\{|m(A)|, |M(A)|\}. \quad (E.8)$$

Spectral properties of symmetric compact operators

From (E.4) and (E.5) it is seen that compact operators have properties which are comparable with properties of linear operators in finite dimensional spaces. This statement was formulated as the Fredholm alternative.

The combination of symmetric and compact gives the following important theorems. The structure of the operator can be completely analyzed in terms of the eigenspaces corresponding to the eigenvalues. The result (see (E.10)) is a generalization of the finite dimensional case where if A is symmetric, a basis consisting of eigenvectors can be chosen in such a way that the matrix representing A is a diagonal matrix with each diagonal element an eigenvalue.

Next theorems can be found in Taylor and Lay, pages 354-357.

The space X is an inner product space not necessarily complete.

(Theorem E.9) Suppose A is compact, symmetric and $A \neq 0$. Then either $\|A\|$ or $-\|A\|$ is an eigenvalue of A, and there is a corresponding eigenvector x such that $\|x\| = 1$ and $|\langle Ax, x\rangle| = \|A\|$. (E.9)

(Theorem E.10) Suppose A is compact, symmetric and $A \neq 0$. There exists a possible terminating sequence of nonzero eigenvalues $\lambda_1, \lambda_2, \ldots$ and a corresponding orthonormal set of eigenvectors $x_1, x_2, \ldots$. If the sequence do not terminate then $|\lambda_n| \to 0$.

The expansion

$$Ax = \sum \langle Ax, x_k\rangle x_k = \sum \lambda_k \langle x, x_k\rangle x_k$$

is valid for each $x \in X$, the summation being extended over the entire sequence whether finite or infinite. Each nonzero eigenvalue of A occurs in the sequence $\{\lambda_n\}$. The eigenmanifold corresponding to a particular λ_i is finite dimensional and its dimension is exactly the number of times this particular eigenvalue is repeated in the sequence $\{\lambda_n\}$. (E.10)

(Theorem E.11) (a) Let A, $\{\lambda_n\}$ and $\{x_n\}$ be as in theorem (E.10), and let M be the closed linear manifold generated by the eigenvectors $x_1, x_2, \ldots$. Then $M^{\perp} = N(A)$. Hence the orthonormal set $\{x_n\}$ is complete if and only if 0 is not an eigenvalue of A.

(b) When X is complete then $X = M \oplus N(A)$. Also the range of A is composed of those elements y in M which are such that the series $\sum \frac{\langle y, x_k \rangle}{\lambda_k} x_k$ is convergent. (E.11)

(Theorem E.12) (Gohberg and Goldberg, 1981) Suppose $\{x_k\}$ is an orthonormal system in X and $\{\lambda_k\}$ is a sequence of real numbers which is either a finite sequence or converges to zero . The linear operator A defined on X by $Ax = \sum_k \lambda_k \langle x, x_k \rangle x_k$ is compact and self-adjoint. (E.12)

So if the Laplace operator were a compact, symmetric operator, the decomposition of a disturbance v in the eigenvectors of the Laplace operator would be allowed. Furthermore the solvability condition would be given by the Fredholm alternative. The Laplace operator is certainly symmetric with the no-flux boundary conditions (see Kato page 274) however it is not compact, not even bounded, since $\frac{d^2}{dx^2} cos(k\pi x/L) = -\left(\frac{k\pi}{L}\right)^2 cos(k\pi x/L)$.
Fortunately the Laplace operator belongs to the class of (unbounded) symmetric operators with compact resolvent, a notion discussed below.

Spectral properties of symmetric operators with compact resolvent

Theorem 6.29 in Kato gives the spectral properties:

(Theorem E.13) Let T be a closed operator in X such that the resolvent R_λ exists and is compact for some λ. Then the spectrum of T consists entirely of isolated eigenvalues with finite multiplicities and R_λ is compact for every $\lambda \in \rho(T)$, the resolvent set. (E.13)

Such an operator is called an **operator with compact resolvent.**

The solvability condition of $(T - \lambda I)x = y$ follows directly from the remarks after (E.3) on isolated eigenvalues.

If an operator in X with compact resolvent is bounded, X must be finite dimensional.

The Laplace operator $\frac{d^2}{dx^2}$ *is an operator with compact resolvent, see example 6.31 in Kato. The argument is that this operator has a inverse (resolvent) which is an integral operator with continuous*

kernel. See also Coolen (1978).

The kernel is $G(x,y)$, *determined by* $-\frac{d^2}{dx^2} G(x,y) = \delta(x - y)$. *So the problem*

$$\frac{d^2}{dx^2}\left[1 - \gamma\frac{d^2}{dx^2}\right]u(x) = v(x) \qquad \text{(E.14)}$$

can be written as

$$\left[1 - \gamma\frac{d^2}{dx^2}\right]u(x) = -\int G(x,y)v(y)dy.$$

Set $\lambda = 1/\gamma$ $(\gamma \neq 0)$. *Suppose* λ *is eigenvalue of* $\frac{d^2}{dx^2}$, *with eigenvector* $\cos(k\pi x/L)$, *(with no-flux boundary conditions). Since*

$$\int \cos(k\pi x/L)G(x,y)dx = \left(\frac{L}{k\pi}\right)^2 \cos(k\pi y/L)$$

problem (E.14) has still as solvability condition that v *must be perpendicular to the null space of* $\left[1 - \gamma\frac{d^2}{dx^2}\right]$.

The next theorem (Taylor and Lay, page 361) gives the spectral representation:

Let X be an inner product space, not necessarily complete.

(Theorem E.15) Suppose that T is a symmetric linear operator with domain and range in X and suppose that T^{-1} exists, belongs to $L(X)$ and is compact. Let $\{\lambda_n\}$, $\{x_n\}$ be the sequence of eigenvalues and eigenvectors associated with $A = T^{-1}$ as explained in connection with theorem (E.8) and let $\mu_n = 1/\lambda_n$. The sequence $\{\mu_n\}$ is infinite, and $|\mu_n| \to \infty$. The orthonormal set $\{x_n\}$ is complete, and $x = \sum_{k=1}^{\infty} \langle x, x_k\rangle x_k$ for each $x \in D(T)$.

A point μ is in $\sigma(T)$ if and only if it is one of the μ_k's. Thus $Tx_n = \mu_n x_n$. If μ is not in $\sigma(T)$, $(\mu - T)^{-1}y = \sum_{k=1}^{\infty} \frac{\langle y, x_k\rangle}{\mu - \mu_k} x_k$ for each $y \in X$. The inverse operator is compact. (E.15)

E.3 Generalized derivative, Sobolev-spaces

Let $\Omega \subset \mathbb{R}^N$ be open, let f be a square integrable function on Ω, $f \in L^2(\Omega)$; the function f is said to have a generalized (distributional) first order partial derivative with respect to x_i, if there exists a function $f^{(i)} \in L^2(\Omega)$ such that

$$\int_\Omega f(x)\frac{\partial \phi}{\partial x_i}\,dx = -\int_\Omega f^{(i)}(x)\phi(x)dx, \qquad \text{for every } \phi \in C_o^\infty(\Omega).$$

Then $f^{(i)}$ is denoted as $\frac{\partial f}{\partial x_i}$.

Sobolev spaces

Let $\Omega \subset \mathbb{R}^N$ be open; for $1 \le p < \infty$, $H^{m,p}(\Omega)$ be the space of functions f in the open domain , all of whose generalized derivatives up to order m are functions in $L^p(\Omega)$. Under the norm

$$\|f\|_{m,p} = \left\{ \sum_{|k|\le m} \int_\Omega |D^k f(x)|^p dx \right\}^{1/p} \tag{E.16}$$

$H^{m,p}$ is a Banach space. $H^{m,2}(\Omega)$ is a Hilbert space with the inner product denoted as $(.,.)_m$. If $p = \infty$, $H^{m,\infty}(\Omega)$ is the space of continuously differentiable functions f up to the order m, such that the following norm is finite:

$$\|f\|_{m,\infty} = \sup_{\substack{x\in\Omega \\ |k|\le m}} |D^k f(x)|. \tag{E.17}$$

$H^{m,p}$ is called a Sobolev space. For $p = \infty$ we write $H^{m,\infty}(\Omega) = C^m(\Omega)$, and it can be defined if Ω is not open too. If $p = 2$ one often writes $H^m(\Omega)$ with norm $\|\cdot\|_m$, and so shall we do.

Theorem E.18 (Wloka, 1969): $C^\infty(\bar{\Omega}) \cap H^{m,p}(\Omega)$ is dense in $H^{m,p}(\Omega)$, $1 \le p \le \infty$. (E.18)

Corollary E.19 (Wloka, 1969): $C^m(\bar{\Omega}) \cap H^{m,p}(\Omega)$ is dense in $H^{m,p}(\Omega)$, $1 \le p \le \infty$. (E.19)

Theorem (E.18) means that the set of functions which satisfy the definition conditions of $H^{m,p}(\Omega)$ with standard continuous derivatives, are dense in $H^{m,p}(\Omega)$.

Theorem E.19 (Wloka, 1969): Let $\Omega \subset \mathbb{R}^N$ be convex (or bounded with a C^∞-boundary. Then the following identity mappings are continuous:

I: $H^{m,1}(\Omega) \to C^r(\bar{\Omega})$, for $m \geq r + N$,

I: $H^{m,p}(\Omega) \to C^{r+\alpha}(\bar{\Omega})$ for $1 < p < \infty$, $m - r - N/p \geq \alpha > 0$ and $\alpha < 1$.

The function space $C^{r+\alpha}(\bar{\Omega})$ is the space of all continuous differentiable functions f in Ω up to order r such that the derivatives of order r are Hölder continuous in Ω with exponent α and such that the following norm is finite:

$$|f|_{r+\alpha} = \sup_{\substack{x\in\Omega \\ |k|\leq r}} |D^k f(x)| + \sup_{\substack{x,\,y\in\Omega \\ |k|=r}} |D^k f(x)-D^k f(y)|/|x-y|^\alpha$$

The continuity means that there are constants C depending on N, m, r, p and Ω such that for $f \in H^{m,p}(\Omega)$: $|f|_r \leq C\|f\|_{m,p}$.

E.4 Convergence, continuity, differentiability

Let X, Y be Banach spaces. Let $T, T_n \in L(X,Y)$, $n = 1,2,\ldots$

Uniform convergence, Convergence in norm

The convergence of $\{T_n\}$ to T in the sense of $\|T_n - T\| \to 0$ is called uniform convergence or convergence in norm.

Strong convergence

$\{T_n\}$ is said to converge strongly to T if $T_n u \to Tu$ for each $u \in X$. $\{T_n\}$ converges in norm if an only if $\{Tu_n\}$ converges uniformly for $\|u\| \leq 1$.

Weak convergence

$\{T_n\}$ is said to converge weakly if $\{T_n u\}$ converges weakly for each $u \in X$, that is, if $(T_n u, g)$ converges for each $u \in X$ and $g \in Y^*$.

$\{T_n\}$ converges in norm if and only if $(T_n u, g)$ converges uniformly for $\|u\| \leq 1$ and $\|g\| \leq 1$.

Continuity:

Let T(t) be an operator valued function $t \to T(t) \in L(X,Y)$.

Continuity in norm

T(t) is continuous in norm if $\|T(t + h) - T(t)\| \to 0$ for $h \to 0$.

Strong continuity

T(t) is strongly continuous if T(t)u is strongly continuous for each $u \in X$.

Weak continuity

T(t) is weakly continuous if T(t)u is weakly continuous for each $u \in X$, that is if $(T(t)u, g)$ is continuous for each $u \in X$ and $g \in Y^*$.

Gateaux differentiable

Suppose X and Y are real Banach spaces. An operator $F: A \subset X \to Y$ is called (linearly) Gateaux differentiable at a point $a \in A$ if there exists a linear bounded operator $T(a): X \to Y$ such that

$$\lim_{t \to 0} \frac{F(a+th) - F(a)}{t} = T(a)h$$

for every $h \in X$, where the limit is taken for real t and convergence in the norm is meant.

The operator T(a) is called the Gateaux derivative of F at the point $a \in A$ and will be denoted as DF(a).

The image of $h \in X$ under DF(a), $DF(a)h \in Y$, is called the **Gateaux** differential of F at the point a in the direction of h. F is Gateaux differentiable on a subset $A \subset X$ if F is Gateaux differentiable at each point of A. In this case, the mapping $a \mapsto DF(a)$ is called the Gateaux derivative of F on A and is denoted as DF. In some literature the Gateaux derivative in a is denoted as $\frac{\partial F}{\partial x}(a)$.

Fréchet differentiable (1)

Suppose X and Y are real Banach spaces. An operator F: $A \subset X \to Y$ is called Fréchet differentiable at a point $a \in A$ if there exists a linear bounded operator T(a): $X \to Y$ such that

$$F(a + h) - F(a) = T(a)h + w(a;h)$$

for every $h \in X$ where the remainder $w(a;\cdot)$: $X \to Y$ satisfies

$$\lim_{\|h\|_X \to 0} \frac{\|w(a;h)\|_Y}{\|h\|_X} = 0$$

The operator T(a) is called the Fréchet derivative of F at the point $a \in A$ and will be denoted by dF(a). F is Fréchet differentiable on a subset $A \subset X$ if F is Fréchet differentiable at each point of A. In this case, the mapping $a \mapsto dF(a)$ is called the Fréchet derivative of F on A and is denoted as dF.

In some literature the Fréchet derivative in a is denoted as $\frac{\delta F}{\delta x}(a)$. See variational derivative.

Fréchet differentiable (2)

If F is Fréchet differentiable at $a \in A$, then F is continuous at $a \in A$.

If F is Fréchet differentiable at $a \in A$, then F is Gateaux differentiable at $a \in A$, and DF(a) = dF(a).

If the Gateaux derivative DF exists in some neighborhood U(a) of $a \in A$, and is continuous at a, then the Fréchet derivative dF(a) exists and dF(a) = DF(a). Thus: A continuous Gateaux derivative is a Fréchet derivative.

Gradient

Suppose X is real Banach space and f: $X \to \mathbb{R}$ is functional on X. If f is Fréchet (Gateaux) differentiable on $A \subset X$ then the derivative of f at a point $a \in A$, df(a) (Df(a)), is bounded and linear functional and hence a element of the dual space X^*. The derivative of f on A is thus a mapping from A into X^*: df (Df): $A \to X^*$.
Now using the symmetric notation (see dual space), the effect of H under df (Df), df(a)h (Df(a)h), can be written as

$$df(a)h = (h, \text{grad } f(a))$$

$$Df(a)h = (h, \text{Grad } f(a))$$

respectively.

Grad f(a) is called the gradient of f at the point a.

Note that the representation of df (Df) by the gradient depends on the inner product defined on X.

If f is Gateaux differentiable at $x_o \in X$, then x_o is called a stationary point , or critical point of f if Grad $f(x_o) = 0$.

We will apply these notions to the following problem: suppose the functional V: $H^1(0,L) \to \mathbb{R}$ is given by

$$V(u) = \int_0^L f(u) + \frac{1}{2}\gamma(u_x)^2 dx, \quad \gamma > 0 \tag{E.20}$$

where $u_x = \frac{du}{dx}$ and $f(u) = \int_0^u \phi(s)ds$ with

$$\phi(u) = -u + r_1 u^2 + r_2 u^3,$$

Then

$$\lim_{t\to 0} \frac{V(u + th) - V(u)}{t} =$$

$$= \lim_{t\to 0} t^{-1}\left\{\int_0^L \left(t\phi(u)h + \frac{1}{2}t^2\phi'(u) + t\gamma u_x h_x + \frac{1}{2}t^2\gamma(h_x)^2 + \ldots\right)dx\right\}$$

$$= \int_0^L \left(\phi(u)h + \gamma u_x h_x\right)dx \tag{E.21}$$

Using Hölders's inequality, one finds:

$$\int u_x h_x dx \le \|u_x\|_0 \|h_x\|_0 \le \|u\|_1 \|h\|_1$$

and

$$\int \phi(u)h dx \le C_o L^2 \|h\|_0 \le C_o L^2 \|h\|_1$$

with $C_o = \sup_{0\le x\le L} |\phi(u(x))|$. Hence (E.21) is bounded. Thus the Gateaux derivative DV(u) of V at a point u is given by

$DV(u)h = \int_0^L \left(\phi(u)h + \gamma u_x h_x\right)dx$ and critical points of V must satisfy

$$\int_0^L \left(\phi(u)h + \gamma u_x h_x\right)dx = 0 \text{ for all } h \in H^1.$$

A classical calculus of variations problem may be written as:

$$\min_{(u(x))} V = \int_0^L I(u(x), u_x(x), x)dx \qquad \text{(E.22)}$$

$$\text{subject } u(0) = u_o,\ u(L) = u_1$$

$(u_x(x) = du(x)/dx)$.

For example, the Brachistochrone problem is to find a curve such that a particle sliding frictionless along the curve under influence of gravity moves from a given upper point to a given lower point in minimum time. A necessary condition for an extremum of V at u is that the Gateaux derivative, in this case also called the *first variation*, vanishes at u: DV(u)h = 0 for all h with h(0) = h(L) = 0.

$$DV(u)h =$$

$$= \lim_{t\to 0} t^{-1}\left\{\int_0^L \left(I(u(x)+th(x), u_x(x)+th_x(x), x) - I(u(x), u_x(x), x)\right)dx\right.$$

$$= \int_0^L \left(\frac{\partial I}{\partial u}(u(x), u_x(x), x))h(x) + \frac{\partial I}{\partial u_x}(u(x), u_x(x), x))h_x(x)\right)dx = 0$$

By partial integration one gets:

$$\int_0^L \left(\frac{\partial I}{\partial u}(u(x), u_x(x), x))h(x) - \frac{d}{dx}\left[\frac{\partial I}{\partial u_x}(u(x), u_x(x), x))\right]h(x)\right)dx +$$

$$+ \left|\frac{\partial I}{\partial u_x}(u(x), u_x(x), x))h(x)\right|_0^L = 0 \qquad \text{(E.23)}$$

Using the boundary conditions h(0) = h(L) = 0, the last term is zero. And the integral (E.23) is zero if

$$\frac{\partial I}{\partial u}(u(x), u_x(x), x)) - \frac{d}{dx}\left[\frac{\partial I}{\partial u_x}(u(x), u_x(x), x))\right] = 0 \qquad \text{(E.24)}$$

The equation (E.24) is called the Euler equation; the left hand side is also called the *variational derivative* and denoted by $\frac{\delta I}{\delta u}$.
Comparing (E.23) with (E.21) one sees that both forms are identical (given the same boundary conditions) by setting

$$I(u, u_x, x) = f(u) + \frac{1}{2}\gamma(u_x)^2$$

Then by (E.24) the variational derivative $\frac{\delta I}{\delta u}$ becomes equal to

$$\phi(u) - \gamma u_{xx}$$

with $u_{xx} = \frac{d^2u}{dx^2}$. Note that no-flux boundary conditions $u_x(0) = u_x(L) = 0$ yields the same result.

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