



Centrum voor Wiskunde en Informatica

**REPORTRAPPORT**

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Modelling, Analysis and Simulation (MAS)

**MAS-R0001 January 31, 2000**

Report MAS-R0001  
ISSN 1386-3703

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SMC is sponsored by the Netherlands Organization for Scientific Research (NWO). CWI is a member of ERCIM, the European Research Consortium for Informatics and Mathematics.

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# A Numerical Study of Mixed Parabolic-Gradient Systems

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## Abstract

This paper is concerned with the numerical solution of parabolic equations coupled to gradient equations. The gradient equations are ordinary differential equations whose solutions define positions of particles in the spatial domain of the parabolic equations. The vector field of the gradient equations is determined by gradients of solutions to the parabolic equations. Such mixed parabolic-gradient systems are for example used in neurobiological studies of the formation of axonal connections in the nervous system. We discuss a numerical approach for solving parabolic-gradient systems on a grid. The basic ingredients are 4th-order spatial finite-differencing for the parabolic equations, piecewise cubic Hermite interpolation for approximating the gradient equations, and explicit time-stepping by means of a Runge-Kutta-Chebyshev method.

*1991 Mathematics Subject Classification:* Primary: 65D05, 65L05, 65M06. Secondary: 62P10.

*1991 ACM Computing Classification System:* G.1.1, G.1.7 and G.1.8.

*Keywords and Phrases:* Parabolic equations, gradient equations, computational neuroscience.

*Note:* Work carried out under subtheme MAS1.3 - Applications from the Life Sciences

## 1 Introduction

The mathematical model motivating our work emanates from a neurobiological study in Hentschel & Van Ooyen [6] on the development of neuronal connections in the nervous system, in particular outgrowth of axons from neurons in a development phase. Growth of axons to their targets is partly guided by concentration gradients of biochemical molecules in the extracellular space. These gradients arise from diffusion and chemical interactions and vary in space and time. The diffusion processes, the chemical interactions and the positions of the growth cones of axons, are modelled by systems of parabolic equations with source terms coupled with gradient equations. The gradient equations are ordinary differential equations and define positions of the axonal growth cones.

This paper deals with numerical methods. We discuss a general approach for solving parabolic-gradient systems on a grid. For spatial discretization we use 4th-order finite-differencing for the parabolic equations and piecewise cubic Hermite interpolation for approximating the gradient equations. This spatial discretization leaves us with a semi-discrete system whose time integration is the main subject of our study. Because the semi-discrete gradient equations are nonstiff, and locally defined and nonlinear, explicit integration is attractive. On the other hand, the semi-discrete parabolic problems are stiff and therefore cannot be efficiently solved with a standard explicit method.

For time integration we examine the explicit Runge-Kutta-Chebyshev (RKC) method. This method originates from [7] and has been designed for the time integration of systems of ordinary differential equations which possess a 'close-to-normal' Jacobian matrix with eigenvalues located in a long, narrow band along the negative axis in the complex plane (see also [10, 13]). Many semi-discrete parabolic partial differential equations fulfil this property. RKC is based on a family of 2nd-order consistent Runge-Kutta-Chebyshev formulas with a real stability boundary approximately

equal to  $0.65s^2$ , where  $s \geq 2$  denotes the number of stages. Hence the real stability boundary is quadratic in  $s$ . Noteworthy is that  $s$  can vary and that it can be made arbitrarily large to fulfil the stability requirement for a chosen step size. This makes it possible for RKC to select at each step the most efficient step size (maximal) defined by local error control [10], as well as the most efficient stable formula (minimal  $s$ ). This also makes it possible to use RKC for a march to steady state, provided  $s$  can be kept within reasonable bounds for efficiency. Moreover, RKC evaluates the explicit formulas in just a few vectors of storage. These characteristics of the method make it especially attractive for parabolic problems in several spatial variables. Because we wish to integrate the gradient equations explicitly, it is interesting to examine RKC for mixed parabolic-gradient systems.

The contents is as follows. In Section 2 we outline the mixed parabolic-gradient system taking the system from [6] as an example. Section 3 is devoted to the Hermite interpolation procedure. Since in this paper we restrict ourselves to numerical illustrations in two spatial dimensions, we only discuss the 2D interpolant adopting the style of [11]. Spatial discretization aspects are dealt with in Section 4. In Section 5 we derive a simple model for linear time stepping stability for which we examine power boundedness for Runge-Kutta methods. Section 6 is devoted to the RKC method. We examine its stability, briefly discuss its convergence for the approximate gradient equations, and illustrate its performance as a variable stepsize solver using the code from [10]. In the final Section 7 we mention possibilities for future research on parabolic-gradient systems.

## 2 A mixed parabolic-gradient system

The model from [6] has been designed to admit an analytical-numerical treatment. It should be considered as a first prototype for more realistic models which undoubtedly will require a full numerical approach. In this section we will briefly outline the model from [6], in particular some properties of the gradient equation. The numerical methods discussed in later sections are applicable to this special model and easily allow generalizations on the model side.

The model contains parabolic equations of the type

$$\frac{\partial \rho_m}{\partial t} = d_m \Delta \rho_m - \delta_m \rho_m + S_m, \quad t > 0, \quad \mathbf{x} \in \Omega \subset \mathbb{R}^{dim}, \quad (1)$$

where  $\rho_m(\mathbf{x}, t)$  represents the concentration of a chemical  $m$  at the spatial point  $\mathbf{x}$  and time  $t$ . The chemical  $m$  is either a chemoattractant or a chemorepellant. For further use we introduce the notations  $\rho_{m,a}$  and  $\rho_{m,r}$  for attractants and repellants, respectively. Boundary conditions play no special role so that we may assume that we have a pure initial value problem or periodic boundary conditions. For numerical convenience we impose periodicity and put  $\Omega = [0, 1]^{dim}$ . The coefficients  $d_m$  and  $\delta_m$  are positive constants and  $S_m$  is a source flux. The source flux may depend on other chemicals, released at so-called fixed target points  $\mathbf{x} \in \Omega$  or at moving points  $\mathbf{r}_n(t) \in \Omega$  representing the position of the growth cone of axon  $n$  at time  $t$ . Omitting the index  $n$  for convenience of notation,  $\mathbf{r}(t)$  is a solution of the gradient equation

$$\frac{d\mathbf{r}}{dt} = \sum_m \lambda_{m,a} \nabla \rho_{m,a}(\mathbf{r}(t), t) - \sum_m \lambda_{m,r} \nabla \rho_{m,r}(\mathbf{r}(t), t), \quad t > 0, \quad \mathbf{r}(0) = \mathbf{r}_0, \quad (2)$$

where  $\lambda_{m,a}$  and  $\lambda_{m,r}$  are positive constants. For given concentration gradients, (2) is a standard initial value problem for an autonomous system of ordinary differential equations  $\dot{\mathbf{r}} = \mathbf{f}(\mathbf{r})$ . The parabolic equations (1) and the gradient equations (2) are coupled through the sources  $S_m$ . More general parabolic or gradient equations leading to stronger coupling are conceivable. For example, the coefficients  $\lambda_{m,a}$  and  $\lambda_{m,r}$  could be made dependent on concentrations and positions.

Let us recall some properties of gradient equations. Consider, for simplicity, the equation

$$\frac{d\mathbf{r}}{dt} = \lambda \nabla \rho(\mathbf{r}(t), t), \quad t > 0, \quad \mathbf{r}(0) = \mathbf{r}_0, \quad (3)$$

based on a single concentration  $\rho$  and a constant  $\lambda$  being either positive or negative. The Jacobian matrix is the symmetric  $dim \times dim$  matrix composed of second order spatial derivatives of  $\rho$ . Hence if  $\rho$  is at least twice continuously differentiable, we have Lipschitz continuity guaranteeing existence and uniqueness of solutions. From (3) we deduce

$$\frac{d}{dt}\rho(\mathbf{r}(t), t) = \lambda \nabla \rho(\mathbf{r}(t), t) \cdot \nabla \rho(\mathbf{r}(t), t) + \frac{\partial}{\partial t}\rho(\mathbf{r}(t), t) = \lambda \|\nabla \rho(\mathbf{r}(t), t)\|^2 + \frac{\partial}{\partial t}\rho(\mathbf{r}(t), t). \quad (4)$$

Consequently, for negative (positive)  $\lambda$  the concentration will eventually decrease (increase) along a solution of the gradient equation in the approach to a stationary concentration field. Hence, for a stationary concentration field, extremal points (zero gradient vector) are limit points. Maxima are stable if  $\lambda > 0$  and unstable if  $\lambda < 0$ . At minima the situation is reversed, stability if  $\lambda < 0$  and instability if  $\lambda > 0$ . Saddle points are always unstable. In the application one assumes that solutions  $\rho$  of the parabolic equations converge to a stationary solution so that the above observations apply.

The gradient equation (2) describes the combined effect of a growth cone growing up gradients of attractants and growing down gradients of repellants. Associate to (2) the auxiliary concentration

$$\Phi = \sum_m \lambda_{m,a} \rho_{m,a} - \sum_m \lambda_{r,m} \rho_{m,r}. \quad (5)$$

Then (2) is rewritten as

$$\frac{d\mathbf{r}}{dt} = \nabla \Phi(\mathbf{r}(t), t), \quad t > 0, \quad \mathbf{r}(0) = \mathbf{r}_0. \quad (6)$$

Hence in the approach to steady state, maxima of  $\Phi$  are stable limit points of (6) and minima are always unstable. For an extensive discussion on gradient equation properties, see [12].

## 2.1 Example

The model in [6] is based on three species, a target derived attractant  $\rho_1$ , an axon derived attractant  $\rho_2$  and an axon derived repellant  $\rho_3$ . The target derived attractant is released at  $N_t$  fixed target points  $\mathbf{x}_n$ . The two axon derived species are released at  $N_a$  moving positions  $\mathbf{r}_n(t)$ . Typically, in simulations  $N_a$  and  $N_t$  range from about 10 to 50. Hence we have three coupled parabolic equations

$$\frac{\partial \rho_1}{\partial t} = d_1 \Delta \rho_1 - \delta_1 \rho_1 + S_1(\mathbf{x}, \{\mathbf{x}_n\}, \rho_1, \rho_2, \rho_3), \quad (7)$$

$$\frac{\partial \rho_2}{\partial t} = d_2 \Delta \rho_2 - \delta_2 \rho_2 + S_2(\mathbf{x}, \{\mathbf{r}_n\}, \rho_1, \rho_2, \rho_3), \quad (8)$$

$$\frac{\partial \rho_3}{\partial t} = d_3 \Delta \rho_3 - \delta_3 \rho_3 + S_3(\mathbf{x}, \{\mathbf{r}_n\}, \rho_1, \rho_2, \rho_3), \quad (9)$$

subjected to given initial functions at  $t = 0$  and coupled to the  $N_a$  initial value problems

$$\frac{d\mathbf{r}_n}{dt} = \lambda_1 \nabla \rho_1(\mathbf{r}_n(t), t) + \lambda_2 \nabla \rho_2(\mathbf{r}_n(t), t) - \lambda_3 \nabla \rho_3(\mathbf{r}_n(t), t), \quad \mathbf{r}_n(0) = \mathbf{r}_{n,0}, \quad n = 1, \dots, N_a. \quad (10)$$

For the sake of generality we here let the  $S_k$  depend on all three concentrations. The target derived attractants serve to control guidance of axons to the target points. The axon derived attractants and repellants serve to control axon bundling and debundling, respectively. In a simulation one should start from given initial concentration fields and given initial positions  $\mathbf{r}_n(0)$  appropriately chosen in  $\Omega$ , one for each axon. The simulation is then to be continued up to a time at which all growth cones have found a target point  $\mathbf{x}_n$  (for innervation) and the attractant and repellant fields have become stationary. Van Ooyen [8] estimates the maximal distance between start positions and targets in axonal growth during development to be about 1.0 *mm*. At greater distances the growth cones cannot sense gradients of target derived chemoattractants. Hence 1.0 *mm* is a reasonable unit as length scale for the spatial domain  $\Omega$ . The various diffusion constants approximately vary

between  $10^{-5}$  and  $10^{-3} \text{ mm}^2 \text{ s}^{-1}$ . The growth rates for the axons approximately lie between  $10^{-6}$  and  $10^{-4} \text{ mm s}^{-1}$ , yielding maximal periods of  $10^4$  to  $10^6$  seconds to travel a distance of  $1 \text{ mm}$ . Hence axonal growth simulation may involve very long time intervals.

We should remark that axonal growth simulation models are still in an early state of development. Biologically, the process of target derived attraction is now fairly well established. The working of axon derived attractions and repellants seems plausible, but there is less direct evidence. Hentschel and Van Ooyen [8] give a nice example of a successful simulation of axon development in the presence of all three diffusible fields (see their Figure 1). This simulation is based on a quasi-steady state approximation for the parabolic equations and on an analytical solution of the resulting elliptic equations. The quasi-steady state approximation makes sense if the axonal growth is much slower than the speed at which the concentration gradients are set up. This often seems to be true. The use of analytical solutions is of course a genuine restriction. As it is, the model seems rather sensitive for simulating bundling and debundling. The various coefficients and source terms must be chosen with real care to obtain, subsequently, bundling, debundling, target point attraction and finally complete steady state. Imposing the quasi-steady state approximation of course simplifies matters somewhat.

### 3 Hermite interpolation

Let  $\Omega_h$  denote a uniform space grid on  $\Omega$  with grid size  $h$  and knots  $(x_i, y_j)$  (assuming two space dimensions). We wish to interpolate  $\rho(\mathbf{x}, t)$ ,  $\mathbf{x} = (x, y)$ , in grid cells

$$\Omega_{ij} = \{(x, y) \mid x_{i-1} \leq x \leq x_i, y_{j-1} \leq y \leq y_j\} \quad (11)$$

by means of two-dimensional Hermite interpolation. The Hermite interpolant on  $\Omega_{ij}$  is the unique bicubic polynomial [4, 11]

$$P_{\rho, ij}(\mathbf{x}, t) = \sum_{m,n=0}^3 \gamma_{mn}(t)(x - x_{i-1})^m (y - y_{j-1})^n, \quad (12)$$

which at the four corner points fits the values of

$$\rho, \frac{\partial \rho}{\partial x}, \frac{\partial \rho}{\partial y}, \frac{\partial^2 \rho}{\partial x \partial y}. \quad (13)$$

That means that the matrix  $\gamma = (\gamma_{mn})$  is given by  $\gamma = H K H^T$ , where ([11], p. 31)

$$K = \begin{pmatrix} B_{i-1, j-1} & B_{i-1, j} \\ B_{i, j-1} & B_{i, j} \end{pmatrix}, \quad B_{l, k} = \begin{pmatrix} \rho(\mathbf{x}_{lk}, t) & \rho_y(\mathbf{x}_{lk}, t) \\ \rho_x(\mathbf{x}_{lk}, t) & \rho_{xy}(\mathbf{x}_{lk}, t) \end{pmatrix}, \quad \mathbf{x}_{lk} = (x_l, y_k),$$

and

$$H = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ -3h^{-2} & -2h^{-1} & 3h^{-2} & -h^{-1} \\ 2h^{-3} & h^{-2} & -2h^{-3} & h^{-2} \end{pmatrix}.$$

Let  $\theta = (x - x_{i-1})/h$  and  $\eta = (y - y_{j-1})/h$ . Taylor expansion at  $(x_{i-1}, y_{j-1})$  gives

$$\rho(\mathbf{x}, t) - P_{\rho, ij}(\mathbf{x}, t) = \frac{1}{24} (\theta^2(\theta - 1)^2 \rho_{xxxx} + \eta^2(\eta - 1)^2 \rho_{yyyy}) h^4 + O(h^5),$$

revealing order four if  $\rho$  is sufficiently differentiable. The leading error constant is rather small, being bounded by the cell center maximum  $(1/384)(|\rho_{xxxx}| + |\rho_{yyyy}|)$ . The error depends on the location in the grid cell, implying that upon grid refinement the order behaviour will be somewhat erratic when examining a fixed location. The Taylor expansion reveals that in the remainder term only derivatives of order five and higher are present. It also reveals that in the leading error

term the derivatives  $\rho_{xyyy}$ ,  $\rho_{xxxx}$  and  $\rho_{xyxy}$  are eliminated. A 4-th order error bound valid for nonuniform Cartesian grids can be found in [11]. In this bound the derivatives  $\rho_{xxxx}$ ,  $\rho_{yyyy}$  and  $\rho_{xyxy}$  are present.

Let  $P_\rho(\mathbf{x}, t)$  denote the piecewise bicubic polynomial on  $\Omega$  obtained by connecting all cell polynomials  $P_{\rho,ij}(\mathbf{x}, t)$ . The functions

$$P_\rho, \frac{\partial P_\rho}{\partial x}, \frac{\partial P_\rho}{\partial y}, \frac{\partial^2 P_\rho}{\partial x \partial y}$$

are continuous across grid cells, so that  $P_\rho$  is  $C^1$  on  $\Omega$ . When  $\rho$  is four times continuously differentiable in space, the interpolant  $P_\rho$  is 4th-order accurate and  $\partial P_\rho / \partial x$  and  $\partial P_\rho / \partial y$  provide 3rd-order approximations. In 3D the same procedure can be applied using a 3D Hermite interpolant. In exactly the same manner Hermite interpolation can be used on nonuniform Cartesian grids (see [11]). Hence a uniform grid  $\Omega$  is not necessary allowing the possibility of locally refined Cartesian grids.

Next consider, for simplicity, again the gradient equation (3) and write

$$\frac{d\mathbf{r}}{dt} = \lambda \nabla P_\rho(\mathbf{r}(t), t) + (\lambda \nabla \rho(\mathbf{r}(t), t) - \lambda \nabla P_\rho(\mathbf{r}(t), t)) = \lambda \nabla P_\rho(\mathbf{r}(t), t) + O(h^3). \quad (14)$$

Omitting the  $O(h^3)$ -term yields the approximate gradient equation

$$\frac{d\mathbf{r}}{dt} = \lambda \nabla P_\rho(\mathbf{r}(t), t), \quad (15)$$

using the same notation for solution  $\mathbf{r}$  for convenience. This approximate gradient equation approximates its original counterpart (3) with 3rd-order spatial accuracy. It is obvious that the more general gradient equation (2) can be approximated in the same way and that the gradient equation property (4) carries over to  $P_\rho$ . The approximate solution  $\mathbf{r}$  and its first derivative are continuous in the whole of  $\Omega$  yielding a smooth trajectory at the passing of grid cell boundaries. We note that global interpolation, e.g. cubic splines, would yield an even smoother trajectory. However, global interpolation is more expensive, and redundant, since we only need to approximate the gradient equation at a few single cells  $\Omega_{ij}$ .

## 4 Spatial discretization

Consider the parabolic problem (1) (for convenience of notation we here omit the index  $m$ ). On  $\Omega_h$  the Laplacian is approximated using the 4th-order difference stencil

$$[-1 \ 16 \ -30 \ 16 \ -1]/(12h^2). \quad (16)$$

This stencil can also be used near the boundaries due to the periodic boundary conditions. By spatial discretization we thus approximate (1) on  $\Omega_h$  by the ordinary differential equation

$$\frac{d\rho_h}{dt} = d\Delta_h \rho_h - \delta \rho_h + S_h, \quad (17)$$

where  $\rho_h$  is the approximation to  $\rho$  on  $\Omega_h$  and  $S_h$  represents the source term  $S$  on the grid. In the Hermite interpolated gradient equation (15) we have to replace, at the corner points of grid cells, the true values (13) by approximate values defined from the grid function  $\rho_h$ . This incurs a second approximation error for the gradient equation. We use the 4th-order difference stencil

$$[1 \ -8 \ 0 \ 8 \ -1]/(12h), \quad (18)$$

and denote the resulting, spatially discrete, gradient equation by

$$\frac{d\mathbf{r}_h}{dt} = \lambda \nabla P_{\rho_h}(\mathbf{r}_h(t), t). \quad (19)$$

The 3rd-order accuracy is maintained. Also the gradient equation property carries over. Because of the cross derivative, 36 grid points are involved (in 2D) in computing  $P_{\rho_h}$  for a grid cell. Convenient is that the periodic boundary conditions allow the use of stencil (18) also at cells near boundaries.

To sum up, the use of the cubic Hermite interpolation procedure and the 4th-order difference stencils (16) and (18) provides us with 3rd-order spatial accuracy for the mixed, semi-discrete system (17), (19), i.e.,

$$\rho_h(\mathbf{x}, t) - \rho(\mathbf{x}, t) = O(h^3), \quad \mathbf{r}_h(t) - \mathbf{r}(t) = O(h^3).$$

In the gradient equation we lose one order because we differentiate the interpolant. In the parabolic equation we lose one order through the  $\mathbf{r}$ -dependence of the source term. This order result extends to more general mixed parabolic-gradient systems. When assessing spatial accuracy, one should keep in mind that due to the interpolation the spatial order behaviour will normally be somewhat erratic upon grid refinement. For time integration it is important to note that only the solution  $\mathbf{r}_h$  and its first derivative are continuous across grid cells. We pay attention to this point in Section 6.4.1.

## 4.1 Numerical illustration

We will illustrate the spatial accuracy behaviour for the single-species system

$$\frac{\partial \rho}{\partial t} = 2 \cdot 10^{-4} \Delta \rho - 10^{-4} \rho + 0.2 e^{-200(x-0.5)^2 - 200(y-0.5)^2}, \quad t > 0, \quad 0 \leq x, y \leq 1, \quad (20)$$

$$\frac{d\mathbf{r}_n}{dt} = 10^{-2} \nabla \rho(\mathbf{r}_n(t), t), \quad t > 0, \quad n = 1, \dots, 10, \quad (21)$$

with zero initial function for  $\rho$  and the initial solutions for  $\mathbf{r}_n$  positioned on a circle with center point  $(\frac{1}{2}, \frac{1}{2})$  and radius 0.34,

$$\mathbf{r}_n(0) = \left( \frac{1}{2} + 0.34 \cos\left(\frac{1}{5}n\pi\right), \frac{1}{2} + 0.34 \sin\left(\frac{1}{5}n\pi\right) \right), \quad n = 1, \dots, 10.$$

The solution  $\rho(\mathbf{x}, t)$  is circle symmetric. The constant source creates a bell shaped profile with a maximum at  $(\frac{1}{2}, \frac{1}{2})$ . We consider the solution on the time interval  $[0, 100]$  during which  $\rho$  remains practically zero on the boundary. The maximum at  $(\frac{1}{2}, \frac{1}{2})$  acts as target point for all  $\mathbf{r}_n(t)$ . Due to the circle symmetry, all solutions  $\mathbf{r}_n(t)$  travel along straight lines from their initial circle position to their joint target point and hence frequently cross cell boundaries with a slope. Due to the bell shaped profile, initially they move very slowly. At time  $t = 100$  the target point has been reached. Observe that the  $r_n$  are not present in the source term. For the current illustration this means no restriction. Figure 1 shows all ten positions at times  $t = 40, 45, 100$  and the corresponding trajectories.

We have solved system (20)-(21) in high temporal accuracy for grid sizes  $h = 1/20, 1/40, 1/80$  and  $h = 1/320$ . The resulting  $\rho_h$ -fields and  $\mathbf{r}_{n,h}(t)$ -values for the coarse grids were then compared with their counterparts for the fine grid, considering these as reference solutions. Table 1 lists maximum norm spatial errors at times  $t = 40$  and  $t = 45$ . The errors for  $\rho_h$  reveal the common 4th-order convergence (the source term does not depend on the solutions of the gradient equations). Noteworthy is that the gradient equations are solved in high accuracy, in spite of the somewhat erratic convergence behaviour upon grid refinement. As mentioned in Section 3, this behaviour is inherent to interpolation. Note that at  $t = 40$  the errors in the gradient equation solutions are much smaller than at  $t = 45$ . This is due to the fact that at  $t = 40$  the positions are still close to the boundary, where  $\nabla \rho$  is much smaller than at  $t = 45$ .

## 5 Stability analysis

We are now ready to discuss the time integration and begin with some stability considerations. For that purpose we use the coupled system (7)-(10) with a few simplifying assumptions. To begin with



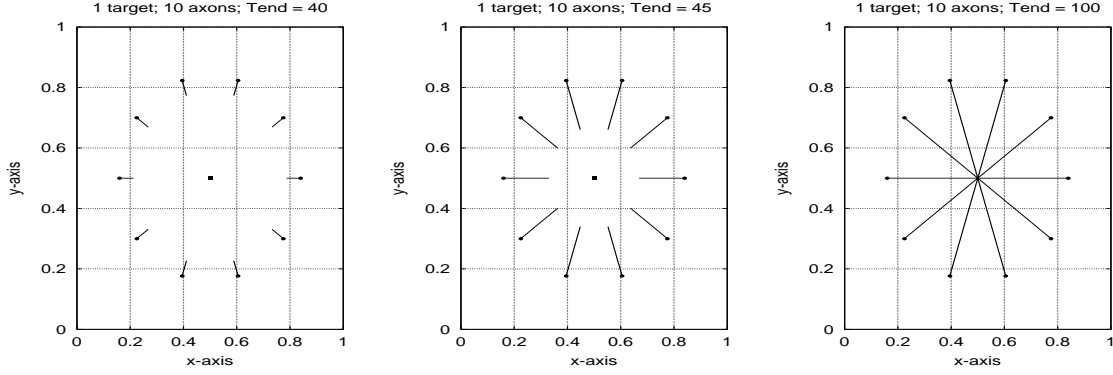


Figure 1: Gradient equation solutions for the test problem of Section 4.1.

h	$\ (\rho - \rho_h)(40)\ $	$\ (\mathbf{r}_n - \mathbf{r}_{n,h})(40)\ $	$\ (\rho - \rho_h)(45)\ $	$\ (\mathbf{r}_n - \mathbf{r}_{n,h})(45)\ $
1/20	$.274 \cdot 10^{-1}$	$.254 \cdot 10^{-2}$	$.277 \cdot 10^{-1}$	$.234 \cdot 10^{-1}$
1/40	$.192 \cdot 10^{-2}$	$.137 \cdot 10^{-3}$	$.194 \cdot 10^{-2}$	$.116 \cdot 10^{-2}$
1/80	$.126 \cdot 10^{-3}$	$.778 \cdot 10^{-6}$	$.127 \cdot 10^{-3}$	$.970 \cdot 10^{-5}$

Table 1: Maximum norm spatial errors at  $t = 40, 45$  for the test problem of Section 4.1.

we suppose zero decay terms, equal diffusion coefficients and consider one gradient equation. These restrictions are non-essential for what follows. Denote  $\vec{\rho} = (\rho_1, \dots, \rho_3)^T$  and  $\vec{S} = (S_1, \dots, S_3)^T$  and rewrite system (7)-(10) as

$$\frac{\partial \vec{\rho}}{\partial t} = d \Delta \vec{\rho} + \vec{S}(\mathbf{r}, \vec{\rho}), \quad (22)$$

$$\frac{d\mathbf{r}}{dt} = \lambda_1 \nabla \rho_1(\mathbf{r}(t), t) + \lambda_2 \nabla \rho_2(\mathbf{r}(t), t) - \lambda_3 \nabla \rho_3(\mathbf{r}(t), t), \quad (23)$$

where we have suppressed the dependence of  $\vec{S}$  on the independent variables  $t$  and  $\mathbf{x}$ . We rely on standard linear stability arguments, hence linearize along a given solution, freeze coefficients and drop constant terms. An elementary calculation yields the following constant coefficient model system for linear stability,

$$\frac{\partial \vec{\rho}}{\partial t} = d \Delta \vec{\rho} + \mathbf{G} \cdot \mathbf{r} + \mathbf{S}' \vec{\rho}, \quad (24)$$

$$\frac{d\mathbf{r}}{dt} = J \mathbf{r}, \quad (25)$$

where  $\vec{\rho}$  and  $\mathbf{r}$  now stand for perturbation solutions,  $\mathbf{G} = \nabla \vec{S}$  with respect to  $\mathbf{r}$ ,  $\mathbf{S}'$  is the Jacobian matrix of  $\vec{S}$  with respect to  $\vec{\rho}$ , and  $J$  denotes the Jacobian matrix of the right-hand side of (23). For example, in 3D we have the symmetric matrix

$$J = \begin{pmatrix} \zeta_{xx} & \zeta_{xy} & \zeta_{xz} \\ \zeta_{xy} & \zeta_{yy} & \zeta_{yz} \\ \zeta_{xz} & \zeta_{yz} & \zeta_{zz} \end{pmatrix}, \quad \zeta = \lambda_1 \rho_1 + \lambda_2 \rho_2 - \lambda_3 \rho_3.$$

Because  $J$  is composed of bounded second derivatives, it makes sense to assume that  $\tau \|J\| \leq 1$  for step sizes  $\tau$  which are realistic with respect to accuracy. Hence we can say that the gradient equation is nonstiff and can be integrated explicitly. A practical reason to always choose for explicit

integration of the semi-discrete gradient equation is the use of local piecewise interpolation. A consequence of local interpolation is that during integration we have to make updates when we pass a grid cell boundary. Updating renders no problem for an explicit method, but is not advocated within implicit integration using modified Newton iteration because the Jacobian matrix of the semi-discrete system is not continuous across grid cell boundaries.

In spite of the fact that  $\|J\|$  is of moderate size, a standard explicit integrator may eventually become inefficient in a march to steady state during which we should like to steadily increase  $\tau$ . This holds even stronger for the parabolic problem because the Laplacian gives rise to stiffness, something which manifests itself already in the transient phase. Hence the parabolic problem cannot be efficiently integrated with a standard explicit method. In the current application we may assume that both  $\|\mathbf{S}'\|$  and  $\|\mathbf{G}\|$  are of moderate size, similar as  $\|J\|$ .

Next we will impose two further simplifying assumptions on (24)-(25). First we assume that we may decouple the three parabolic equations. Specifically, the Jacobian matrix  $\mathbf{S}'$  is supposed to be similar to a real-valued diagonal matrix with a real-valued, well-conditioned eigensystem. For stability investigations we then may replace (24)-(25) by

$$\frac{\partial \rho}{\partial t} = d \Delta \rho + G \cdot \mathbf{r} + S_\rho \rho, \quad (26)$$

$$\frac{d\mathbf{r}}{dt} = J \mathbf{r}, \quad (27)$$

where  $\rho$  is a scalar,  $S_\rho$  represents an eigenvalue of  $\mathbf{S}'$  and  $G$  a transformed gradient vector, both real-valued and of moderate size. Second, we also assume that we may diagonalize  $J$  and replace (26)-(27) by the model system

$$\frac{\partial \rho}{\partial t} = d \Delta \rho + G \cdot \mathbf{s} + S_\rho \rho, \quad (28)$$

$$\frac{d\mathbf{s}}{dt} = D \mathbf{s}, \quad (29)$$

where  $D$  is the eigenvalue matrix of  $J$  and, using the same notation,  $G$  a new transformed gradient vector, still real-valued and of moderate size.

The same exercise can be carried out for the associated semi-discrete problems. Using the same notations  $G$  and  $S_\rho$ , the semi-discrete version of model (28)-(29) is written as

$$\frac{d\rho_h}{dt} = (d\Delta_h + S_\rho) \rho_h + G \cdot \mathbf{s}_h, \quad (30)$$

$$\frac{d\mathbf{s}_h}{dt} = D \mathbf{s}_h, \quad (31)$$

where the entries of  $D$  now represent derivatives of the interpolant  $P_{\rho_h}$ . Finally, we decompose  $\rho_h$  in Fourier modes,

$$\begin{pmatrix} \rho_h(\mathbf{x}, t) \\ \mathbf{s}_h(t) \end{pmatrix} = \begin{pmatrix} c(t) \\ \mathbf{u}(t) \end{pmatrix} \cos(\omega \cdot \mathbf{x}),$$

so that we end up with the following model for linear time stepping stability,

$$\frac{dc}{dt} = d_0 c + G \cdot \mathbf{u}, \quad (32)$$

$$\frac{d\mathbf{u}}{dt} = D \mathbf{u}, \quad (33)$$

where  $d_0 = d\kappa + S_\rho$ ,  $\kappa$  being an eigenvalue of the discrete Laplacian  $\Delta_h$ . Due to (16),

$$-\frac{64}{12} \frac{dim}{h^2} \leq \kappa \leq 0. \quad (34)$$

In the remainder we will denote the entries of  $D$  and  $G^T$  by  $d_k$  and  $g_k$  and hence use the notations  $D = \text{diag}(d_1, \dots, d_{dim})$  and  $G^T = [g_1, \dots, g_{dim}]$ .

Albeit simple, any method for mixed parabolic-gradient systems must pass the stability test for this model. Herein,  $c \in \mathbb{R}$  represents a concentration and  $\mathbf{u} \in \mathbb{R}^{dim}$  a position. For the sake of the stability analysis we assume that all eigenvalues  $d_k$  ( $0 \leq k \leq dim$ ) are nonpositive. Of importance is that  $d_0$  can take on very large negative values according to (34) (stiffness), while the gradient vector  $G$  and the diagonal matrix  $D$  are of moderate size. During transient phases stiffness thus only emerges from the 'parabolic' term  $d_0 c$ .

## 5.1 Power boundedness for Runge-Kutta methods

In what follows we write the real-valued, linear model system (32)-(33) as

$$\frac{dU}{dt} = AU, \quad U = \begin{pmatrix} c \\ \mathbf{u} \end{pmatrix}, \quad A = \begin{pmatrix} d_0 & G^T \\ \mathbf{0} & D \end{pmatrix}. \quad (35)$$

The Runge-Kutta-Chebyshev method discussed later on in the paper belongs to the class of explicit Runge-Kutta methods. Hence, when applied to (35), it yields a linear recurrence relation

$$U_{n+1} = R(\tau A) U_n, \quad n = 0, 1, \dots, \quad R(\tau A) = \sum_{j=0}^s c_j (\tau A)^j, \quad (36)$$

where  $U_n$  is the approximation at time  $t = t_n$ ,  $\tau$  is the step size, and  $R$  is the stability polynomial, assuming  $s$  stages. We associate stability with the concept of power boundedness. For a given step size  $\tau$ , the matrix  $R(\tau A)$  is power bounded if there exists a constant  $C$  such that

$$\|R(\tau A)^n\| \leq C \quad \text{for all } n \geq 1. \quad (37)$$

Hence  $C$  should exist independent of  $n$  and for practice  $C$  should of course be of moderate size. Trivially, power boundedness implies  $\|Y_n\| \leq C \|Y_0\|$  uniformly in  $n$  for the value of  $\tau$  under consideration (stability).

We will derive a general expression for  $R(\tau A)$ , where  $R(z)$  can be any polynomial or rational function or the exponential function. Consequently, the derived expression is also valid for stability functions generated by implicit Runge-Kutta or linearly implicit Runge-Kutta-Rosenbrock methods, as well as for the exact solution operator  $\exp(\tau A)$ . First, let  $d_0$  be distinct from all entries  $d_k$  of the diagonal matrix  $D$  and compute the eigenvector-eigenvalue decomposition  $A = X \Lambda X^{-1}$ ,

$$\Lambda = \begin{pmatrix} d_0 & \mathbf{0}^T \\ \mathbf{0} & D \end{pmatrix}, \quad X = \begin{pmatrix} 1 & G^T(D - d_0 I)^{-1} \\ \mathbf{0} & I \end{pmatrix}, \quad X^{-1} = \begin{pmatrix} 1 & -G^T(D - d_0 I)^{-1} \\ \mathbf{0} & I \end{pmatrix}. \quad (38)$$

Elaborating  $R(\tau A) = X R(\tau \Lambda) X^{-1}$  gives

$$R(\tau A) = \begin{pmatrix} R(\tau d_0) & V^T \\ \mathbf{0} & R(\tau D) \end{pmatrix}, \quad V^T = [v_1, \dots, v_{dim}], \quad (39)$$

where

$$v_k = \tau g_k (\tau d_k - \tau d_0)^{-1} (R(\tau d_k) - R(\tau d_0)). \quad (40)$$

With the mean value theorem we can write  $v_k$  also as  $v_k = \tau g_k R'(\tau \tilde{d}_k)$  where  $d_0 \leq \tilde{d}_k \leq d_k$ . Next suppose that  $d_0$  equals one or more of the entries  $d_k$  of  $D$ . The above derivation then still can be used when accompanied with a standard limit argument. Specifically, if  $d_0 = d_k$ , then

$$v_k = \tau g_k R'(\tau d_k). \quad (41)$$

The powers of  $R(\tau A)$  read

$$R(\tau A)^n = \begin{pmatrix} R(\tau d_0)^n & W^T \\ \mathbf{0} & R(\tau D)^n \end{pmatrix}, \quad W^T = [w_1, \dots, w_{dim}], \quad (42)$$

where

$$w_k = v_k \sum_{i=0}^{n-1} R(\tau d_k)^i R(\tau d_0)^{n-i-1}. \quad (43)$$

Inserting expressions (40) and (41) yields

$$w_k = \begin{cases} \tau g_k (\tau d_k - \tau d_0)^{-1} (R^n(\tau d_k) - R^n(\tau d_0)) & \text{if } d_0 \neq d_k, \\ n\tau g_k R'(\tau d_k) R^{n-1}(\tau d_k) & \text{if } d_0 = d_k, \end{cases} \quad (44)$$

or

$$w_k = \begin{cases} n\tau g_k R'(\tau \tilde{d}_k) R^{n-1}(\tau \tilde{d}_k), & d_0 \leq \tilde{d}_k \leq d_k \text{ if } d_0 \neq d_k, \\ n\tau g_k R'(\tau d_k) R^{n-1}(\tau d_k) & \text{if } d_0 = d_k. \end{cases} \quad (45)$$

These inequalities are valid for  $R(\tau A) = e^{\tau A}$  and for  $R(\tau A)$  generated by stability functions  $R(z)$ . Due to consistency,  $R(z) = e^z + O(z^2)$  for  $z \rightarrow 0$ . Hence for  $z = \tau d_k$  ( $0 \leq k \leq \dim$ ) close to zero,  $R(n\tau A)$  will be close to  $e^{n\tau A}$  in the sense that the bound  $C$  introduced in definition (37) will be close. For values not close to zero the situation is different because stability functions decay much slower than the exponential, or don't decay at all. However, for power boundedness decay is not necessary. With a minor exception it is sufficient (see Theorem 1) that all values  $\tau d_k$  ( $0 \leq k \leq \dim$ ) belong to the real stability interval  $[-\beta, 0]$ ,  $\beta = \max(z_\beta : |R(z)| \leq 1, -z_\beta \leq z \leq 0)$ , which is the common (scalar) stability requirement.

**Lemma 1** *Suppose  $R(z)$  is damped for  $\tau d_0 \leq z \leq \tau d_k$ , i.e.,  $|R(z)| \leq \eta < 1$ . Then, for all  $n \geq 1$ ,*

$$|w_k| \leq \left| \frac{\tau g_k R'(\tau \tilde{d}_k)}{e \eta \ln(\eta)} \right|, \quad d_0 \leq \tilde{d}_k \leq d_k. \quad (46)$$

**Proof** Imposing  $|R(z)| \leq \eta$  in (45) yields  $|w_k| \leq n\tau \eta^{n-1} |g_k R'(\tau \tilde{d}_k)|$ , where  $d_0 \leq \tilde{d}_k \leq d_k$ . The positive function  $f(x) = x\eta^{x-1}$ ,  $x \geq 1$ , vanishes for  $x \rightarrow \infty$  and has a maximum at  $x = -1/\ln(\eta)$ . This maximum is given by  $-1/(e \eta \ln(\eta))$ .  $\square$

**Theorem 1** *The amplification matrix  $R(\tau A)$  is power bounded if all values  $\tau d_k$  ( $0 \leq k \leq \dim$ ) belong to the real stability interval  $[-\beta, 0]$  and none of the pairs  $\tau d_0, \tau d_k$  ( $1 \leq k \leq \dim$ ) coalesce at the boundary.*

**Proof** Because  $|R(\tau d_k)| \leq 1$  ( $0 \leq k \leq \dim$ ), we have power boundedness if the entries  $w_k$  are bounded uniformly in  $n$ . First suppose  $d_0 \neq d_k$ . Boundedness of  $w_k$  then follows immediately from (44). Second, suppose  $d_0 = d_k$ . By assumption,  $z = \tau d_0$  then lies in the interior of the stability interval. Now two situations can occur, either  $|R(z)| \leq \eta < 1$  or  $|R(z)| = 1$ . If  $|R(z)| \leq \eta < 1$ , Lemma 1 applies so that  $w_k$  is bounded. If  $|R(z)| = 1$ , then  $R'(z) = 0$  because  $z$  belongs to the interior of the stability interval and  $|R(z)| = 1$  is an extremum. In this situation  $w_k = 0$ .  $\square$

**Remark** Suppose that  $\tau > 0$  and that  $d_0 = d_k = 0$ . Then  $\tau d_0, \tau d_k$  coalesce at the boundary point  $z = 0$ . Because  $R(0) = R'(0) = 1$ , we then get  $w_k = n\tau g_k$  (cf. (45)) which increases without bound with  $n$ . However, also the exact solution increases linearly with time and hence the case  $d_0 = d_k = 0$  is of no interest and should be excluded in a stability analysis. Next suppose that  $\tau d_0, \tau d_k$  coalesce at the other boundary point  $z = -\beta$  and that  $\beta$  is finite. By definition, then  $|R(-\beta)| = 1$  so that in this case  $|w_k| = n\tau |g_k R'(-\beta)|$  which is also unbounded. Hence in this special case uniform boundedness of  $R(\tau A)$  does not exist. Theorem 1 therefore excludes it. Would  $\beta$  be infinite and  $|R(-\beta)| = 1$ , the eigenvalues are allowed to coalesce because at infinity  $R'$  vanishes.  $\square$

## 6 The Runge-Kutta-Chebyshev method

We proceed with the explicit Runge-Kutta-Chebyshev (RKC) method. This method is intended for solving systems of ordinary differential equations

$$\frac{dU}{dt} = F(U), \quad t > 0, \quad U(0) = U_0, \quad (47)$$

which possesses a 'close-to-normal' Jacobian matrix  $F'(U)$  with eigenvalues located in a long, narrow band along the negative axis in the complex plane. Many semi-discrete parabolic partial differential equations fulfil this property. Because we wish to integrate the gradient equations explicitly, it is interesting to examine RKC. In this section we will discuss the integration formula, its stability properties, and we will discuss two numerical tests.

## 6.1 The integration formula

RKC is based on the  $s$ -stage formula

$$\begin{aligned} Y_0 &= U_n, \\ Y_1 &= Y_0 + \tilde{\mu}_1 \tau F_0, \\ Y_j &= (1 - \mu_j - \nu_j)Y_0 + \mu_j Y_{j-1} + \nu_j Y_{j-2} + \tilde{\mu}_j \tau F_{j-1} + \tilde{\gamma}_j \tau F_0, \quad j = 2, \dots, s, \\ U_{n+1} &= Y_s, \end{aligned} \tag{48}$$

where  $F_j = F(Y_j)$ . All the coefficients are available in analytical form for arbitrary  $s \geq 2$ . They are defined as follows. Let  $T_j$  be the Chebyshev polynomial of the first kind of degree  $j$  satisfying the three-term recursion  $T_0(x) = 1, T_1(x) = x, T_k(x) = 2xT_{k-1}(x) - T_{k-2}(x), 2 \leq k \leq j$ . Defining

$$\epsilon = 2/13, \quad w_0 = 1 + \epsilon/s^2, \quad w_1 = \frac{T'_s(w_0)}{T'_s(w_0)}, \quad b_j = \frac{T''_j(w_0)}{(T'_j(w_0))^2} \quad (2 \leq j \leq s), \quad b_0 = b_2, \quad b_1 = b_2,$$

the coefficients are given by

$$\tilde{\mu}_1 = b_1 w_1, \quad \mu_j = \frac{2b_j w_0}{b_{j-1}}, \quad \nu_j = \frac{-b_j}{b_{j-2}}, \quad \tilde{\mu}_j = \frac{2b_j w_1}{b_{j-1}}, \quad \tilde{\gamma}_j = -(1 - b_{j-1} T_{j-1}(w_0)) \tilde{\mu}_j \quad (2 \leq j \leq s).$$

The stage formula computing  $Y_j$  is reminiscent of the three-term Chebyshev recursion [7]. All approximations  $Y_j$  ( $2 \leq j \leq s$ ) are second order consistent [13] and the real stability boundary  $\beta$  is very close to  $0.65s^2$ . Hence  $\beta$  is quadratic in  $s$ . Noteworthy is that  $s$  can vary and that  $s$  can be made arbitrarily large so as to fulfil the linear stability requirement for a chosen step size  $\tau$ . This makes it possible for RKC to select at each step the most efficient step size (maximal  $\tau$ ) defined by local error control [10], as well as the most efficient stable formula (minimal  $s$ ). This also makes it attractive to use RKC for a march to steady state, provided  $s$  can be kept within reasonable bounds for efficiency. Moreover, RKC evaluates the explicit formulas in just a few vectors of storage, which can be of interest for parabolic problems in several spatial variables. For more details we refer to the original paper [7], the survey paper [13], and the software paper [10] where a FORTRAN code is discussed. We will illustrate this code in Section 6.4.2.

## 6.2 The stability polynomial

The stability polynomial of the  $s$ -stage RKC method is the Bakker-Chebyshev polynomial  $R(z) = 1 - b_s T_s(w_0) + b_s T_s(w_0 + w_1 z)$  [13] for which

$$\beta = \frac{(w_0 + 1)T''_s(w_0)}{T'_s(w_0)} \approx \frac{2}{3}(s^2 - 1)\left(1 - \frac{2}{15}\epsilon\right). \tag{49}$$

The parameter  $\epsilon$  has been introduced to obtain damping. Would we choose  $\epsilon = 0$ , then  $R(z)$  alternates between  $\approx 1/3$  and 1 as long as  $z$  lies in the stability interval  $[-\beta, 0]$ . That means that at isolated points  $z$  we have  $R(z) = 1$ . For  $0 < \epsilon \ll 1$ , the RKC polynomial is damped, i.e.,  $|R(z)| \leq \eta < 1$  on a subinterval  $[-\beta_l, -\beta_r] \subset [-\beta, 0]$  such that  $\beta_l \approx \beta$  and  $\beta_r \approx 0$ . The value  $\epsilon = 2/13$  gives approximately 5% damping (see Section 6.3), letting  $R(z)$  alternate between  $\approx 1/3$  and  $\eta = 0.95$  for  $z \in [-\beta_l, -\beta_r]$ . For this value of  $\epsilon$ , the boundary  $\beta \approx 0.65s^2$ . Fig. 2 illustrates this damped case for  $s = 10$ . Note that  $\beta_l$  and  $\beta_r$  are the values of  $z$  where  $R(z)$  intersects the upper dashed line.

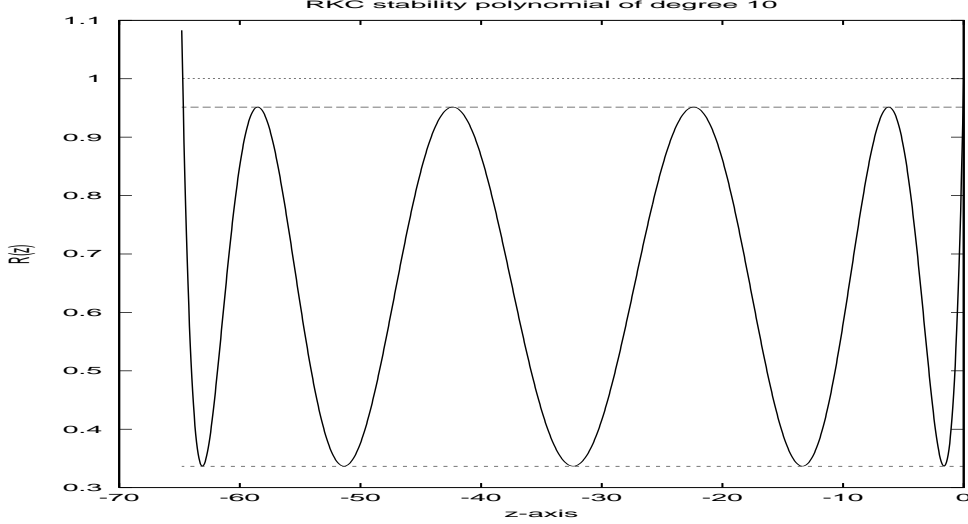


Figure 2: The stability polynomial  $R(z)$  of degree 10 along the stability interval  $-65 \leq z \leq 0$ .

### 6.3 Power boundedness

According to Theorem 1, RKC will be power bounded as long as  $z = \tau d_k$  ( $0 \leq k \leq \dim$ ) belongs to the stability interval  $[-\beta_l, 0]$ , which is only slightly smaller than  $[-\beta, 0]$  (see e.g. Figure 2). To be more specific about RKC, we now wish to apply Lemma 1 and are therefore going to specify the exact amount of damping over  $[-\beta_l, 0] = [-\beta_l, -\beta_r] \cup [-\beta_r, 0]$ .

By construction, the point  $\beta_r$  is determined by the condition  $R(-\beta_r) = \eta$  at the right end point of the Chebyshev interval  $[-1, 1]$ . Hence,

$$\beta_r = \frac{w_0 - 1}{w_1} = \frac{\epsilon T_s''(w_0)}{s^2 T_s'(w_0)}.$$

Inserting  $T_s'(1) = s^2$ ,  $T_s''(1) = \frac{1}{3}s^2(s^2 - 1)$ ,  $T_s'''(1) = \frac{1}{15}s^2(s^2 - 1)(s^2 - 4)$  and expanding in  $\epsilon$  yields

$$\beta_r = \frac{1}{3} \frac{s^2 - 1}{s^2} \epsilon \left[ 1 - \epsilon \frac{2s^2 + 7}{15s^2} + O(\epsilon^2) \right] \approx \frac{1}{3} \epsilon.$$

Let  $\eta = 1 - \mu$ . By construction,  $a_s + b_s = 1 - \mu$ . Hence

$$\mu = \frac{T_s''(w_0)}{(T_s'(w_0))^2} (T_s(w_0) - 1).$$

Expanding in  $\epsilon$ , similar as for  $\beta_r$ , yields

$$\mu = \frac{1}{3} \frac{s^2 - 1}{s^2} \epsilon \left[ 1 - \epsilon \frac{3s^2 + 3}{10s^2} + O(\epsilon^2) \right] \approx \frac{1}{3} \epsilon.$$

We see that for  $s \geq 2$  and  $\epsilon$  sufficiently small,  $\mu/\beta_r < 1$  (this holds for  $\epsilon = 2/13$ ). Specifically,

$$\frac{\mu}{\beta_r} = 1 - \frac{1}{6} \epsilon \frac{s^2 - 1}{s^2} + O(\epsilon^2).$$

Because  $R'(0) = 1$  and  $R(z)$  is convex for  $z \in [-\beta_r, 0]$ , on this interval we can bound  $R(z)$  by the straight line  $1 + (\mu/\beta_r)z$ . On the whole of the stability interval  $[-\beta_l, 0]$  this results in

$$|R(z)| \leq \eta = \begin{cases} \approx 1 - \epsilon/3 \approx 0.95 & \text{for } -\beta_l \leq z \leq -\beta_r, \\ 1 + (\mu/\beta_r)z \approx 1 + z & \text{for } -\beta_r \leq z \leq 0. \end{cases} \quad (50)$$

This result enables us to specify bounds for the entries  $w_k$  occurring in  $R(\tau A)^n$ . First, suppose  $\tau d_0$  and  $\tau d_k$  both belong to the interval  $[-\beta_l, -\beta_r]$ . We then can apply Lemma 1 with  $\eta \approx 1 - \epsilon/3 \approx 0.95$ . By also taking into account  $|R'(z)| \leq 1$  for  $z$  in the stability interval, we obtain

$$|w_k| \leq \left| \frac{\tau g_k R'(\tau \tilde{d}_k)}{e \eta \ln \eta} \right| \leq \left| \frac{\tau g_k}{e \eta \ln \eta} \right| \approx 7.6 \tau |g_k|. \quad (51)$$

Of interest is that this bound applies for the greater part of the stability interval, since  $\beta_r \approx \epsilon/3 \approx 0.05$  is very close to the origin.

Obviously, on the remaining small interval  $[-\beta_r, 0]$ , all consistent Runge-Kutta methods have a bound for  $R(\tau A)^n$  very close to that of the true solution operator  $e^{n\tau A}$ . Suppose  $z = \tau d_0$  or  $z = \tau d_k$  belongs to this small interval and that they do not coalesce at  $z = 0$ . Let  $z = \tau d_k$  be the value closest to the origin. We then can apply Lemma 1 with  $\eta = 1 + (\mu/\beta_r)z$ . This yields

$$|w_k| \leq \left| \frac{\tau g_k R'(\tau \tilde{d}_k)}{e \eta \ln \eta} \right| \leq \left| \frac{\tau g_k}{e \eta \ln \eta} \right| \approx \left| \frac{g_k}{e d_k} \right|. \quad (52)$$

This bound gets larger as  $d_k$  is closer to the origin. The bound is strict if  $d_0 = d_k$ , reflecting the lack of boundedness if the eigenvalues coalesce at the origin.

### 6.3.1 Example

On fine space grids the largest eigenvalue is  $d_0$ . According to (34),  $d_0 \approx -\frac{64}{12} \frac{d \dim}{h^2}$ , so that for (32)-(33) we have power boundedness if

$$\tau \leq \frac{0.65 s^2}{|d_0|} \approx \frac{7.8 h^2 s^2}{64 d \dim}. \quad (53)$$

The test problem from Section 4.1 has  $d = 2.0 \cdot 10^{-4}$  and  $\dim = 2$ . Hence when using the  $80 \times 80$  space grid, we have to satisfy the inequality  $\tau \leq s^2/21.005$ . The  $320 \times 320$  grid yields the inequality  $\tau \leq s^2/336.08$ . A very valuable property of RKC is that it can be applied with any value of  $s$ . For actual computation we may therefore suppose that  $\tau$  is determined by accuracy considerations based on local error control [10] and that  $s$  is adjusted for stability. For the two mentioned grids this means  $s \approx \sqrt{21.005\tau}$  and  $s \approx \sqrt{336.08\tau}$ . These numbers of derivative evaluations give an indication for the amount of work that RKC will need per time step in axonal growth calculations.

## 6.4 Numerical illustrations

### 6.4.1 Convergence for the gradient equations

The ODE system  $\dot{U} = F(U)$  to which RKC is applied contains all semi-discrete parabolic and gradient equations present in the model. The gradient equation components of  $F(U)$  are defined by the piecewise Hermite interpolation procedure discussed in Sections 3 and 4. Let equation (19) be such a component. By construction, its solution  $\mathbf{r}_h$  and the first derivative  $\dot{\mathbf{r}}_h$  exist and are continuous in  $t$ . Also the second derivative  $\ddot{\mathbf{r}}_h$  exists, but this second derivative is discontinuous at the crossing of a grid cell. When this happens, the 2nd-order consistency of RKC reduces to one, causing some loss of accuracy. Because on a given grid the number of grid cell crossings is finite, the effect of the order reduction will diminish when the number of time steps increases. Specifically, for  $\tau \rightarrow 0$  the method is still 2nd-order convergent, because only a finite number of local errors of  $O(\tau^2)$  exist. When the spatial grid size is reduced, the number of grid cell crossings will increase, resulting in a larger order reduction.

We illustrate the temporal convergence behaviour of RKC for the test problem of Section 4.1. To emphasize the (minor) order reduction phenomenon, the very fine  $320 \times 320$  grid has been used. Table 2 shows temporal errors for a number of fixed step sizes and associated convergence orders. We have also listed  $s$ , the number of stages, which can be computed from (53). It can be

concluded that RKC converges as expected. Because the source term of the parabolic equation does not depend on the gradient equation solutions, the convergence behaviour for  $\rho_h$  is standard. For the gradient equations the order is only slightly smaller than two and the minor reduction diminishes when the number of time steps increases.

# steps	$s$	$\ (\rho - \rho_h)(45)\ $	order	$\ (\mathbf{r}_n - \mathbf{r}_{n,h})(45)\ $	order
50	18	.463 $10^{-4}$		.622 $10^{-2}$	
100	13	.116 $10^{-4}$	1.99	.197 $10^{-2}$	1.66
200	9	.295 $10^{-5}$	1.98	.567 $10^{-3}$	1.80
400	7	.762 $10^{-6}$	1.95	.155 $10^{-3}$	1.87

Table 2: Maximum norm errors for RKC for the test problem of Section 4.1,  $t = 45$ ,  $h = 1/320$ .

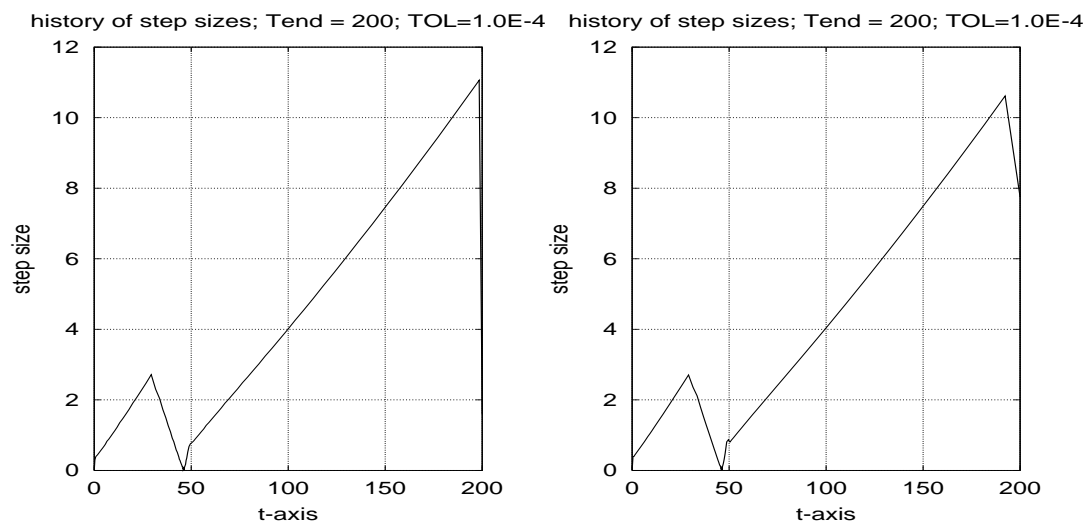


Figure 3: Step size plots for the experiment of Section 6.4.2; at the left for the  $80 \times 80$  grid, at the right for the  $320 \times 320$  grid. Close to  $t = 200$  the step size  $\tau$  has been automatically reduced to hit this end point exactly.

### 6.4.2 The FORTRAN code RKC illustrated

RKC has been coded in a FORTRAN program, also named RKC [10]. This code works as a variable step size ODE solver using local error control. In addition, to minimize work, at each step it selects the minimal number of stages  $s$  for stability. In the actual application  $s$  may increase to very large values. Algorithmically,  $s$  is only constrained by internal growth of round-off proportional to  $s^2$ . For a very large number of stages, RKC can of course no longer be considered efficient. A great advantage is that it is explicit. Hence programming is easy and adding or deleting equations in a model is straightforward for implementations.

Focusing again on target attraction, we have applied the code to the test problem of Section 4.1, except that now the source is switched off when the target has nearly been reached. Our purpose is to illustrate the code's ability to approach a complete steady state with larger and larger step sizes. For switching off the source, we have used the condition

$$\sum_{n=1}^{10} \text{dist}(\mathbf{r}_{n,h}(t) - (\frac{1}{2}, \frac{1}{2})) < 0.1,$$



which is satisfied at  $t \approx 46$ . The integration is continued up to  $t = 200$  which is sufficiently far. The effect of switching off the source is that the bell shaped solution for  $\rho$  slowly smooths out.

To illustrate the reliability of RKC's variable  $(\tau, s)$ -strategy, we have used two space grids,  $80 \times 80$  and  $320 \times 320$ . Figure 3 shows for both grids the step size history for a tolerance value  $TOL = 10^{-4}$ . Hardly any difference exists, indicating that the  $(\tau, s)$ -strategy works fine. This is further exemplified by Table 3 which contains maximum norm temporal errors <sup>1</sup> at  $t = 45$  for different values of  $TOL$ . The table also contains standard integration statistics. One can see that there is hardly any difference in temporal accuracy and number of time steps for the coarse and the fine grid. On the fine grid the number of function evaluations is about four times larger, completely in accordance with (53). On the fine grid the average number of (explicit derivative) evaluations per time step is, for example, equal to 14 for  $TOL = 10^{-5}$ . In view of the fact that we are solving a parabolic equation and gradient equations, this work load is still moderate. Of further interest is that the step size and local error control can be seen to obey the theory given in Shampine [9], p. 339. This theory says that upon reducing  $TOL$  by 10, the global error will asymptotically decrease by  $10^{p/(p+1)}$ . For  $p = 2$ , the order of consistency of RKC, this gives a factor of about 5, which we can trace in Table 3.

Maximum norm errors and integration statistics on $80 \times 80$ grid								
$t_{end}$	$TOL$	$\ \rho - \rho_h\ $	$\ \mathbf{r}_n - \mathbf{r}_{n,h}\ $	# Steps	# Acc.	# Rej.	# F-evals	$s_{max}$
45	$10^{-2}$	$.386 10^{-2}$	$.482 10^{-1}$	13	11	2	128	16
	$10^{-3}$	$.835 10^{-3}$	$.204 10^{-1}$	23	22	1	159	12
	$10^{-4}$	$.172 10^{-3}$	$.550 10^{-2}$	48	47	1	237	8
	$10^{-5}$	$.385 10^{-4}$	$.138 10^{-2}$	103	103	0	365	6
200	$10^{-2}$			34	31	3	354	29
	$10^{-3}$			64	58	6	468	21
	$10^{-4}$			126	118	8	684	16
	$10^{-5}$			261	250	11	1052	11
Maximum norm errors and integration statistics on $320 \times 320$ grid								
45	$10^{-2}$	$.376 10^{-2}$	$.473 10^{-1}$	13	11	2	490	65
	$10^{-3}$	$.800 10^{-3}$	$.188 10^{-1}$	23	22	1	591	49
	$10^{-4}$	$.161 10^{-3}$	$.499 10^{-2}$	47	46	1	833	32
	$10^{-5}$	$.341 10^{-4}$	$.118 10^{-2}$	97	97	0	1187	21
200	$10^{-2}$			34	30	4	1373	106
	$10^{-3}$			64	56	8	1746	86
	$10^{-4}$			115	111	4	2388	60
	$10^{-5}$			251	238	13	3496	43

Table 3: Integration results for the experiment of Section 6.4.2. At time  $t = 200$  the solution is very close to steady state so that the temporal errors are extremely small at this point of time. Therefore we only give the temporal errors for  $t = 45$ .

## 7 Possible future research

This paper deals with migration in gradient fields described by a model from neuroscience. In this model the gradient fields are solutions of parabolic equations with source terms representing

<sup>1</sup>The code described in [10] uses the weighted Euclidean norm for the local error estimation. For the current test we have adapted the code to use the maximum norm to impose a more stringent test for the gradient equations. Observe that the factor  $1/15$  in the formula for  $Est_{n+1}$  in [10] must be replaced by  $1/27$  to have  $Est_{n+1} = Le(t_{n+1}) + O(\tau^4)$ . This correction is not essential for the application of the code. Our tests have been carried out with the factor  $1/15$ .

concentrations of biochemicals. Conceivable is that similar migration problems occur in other biological applications. The numerical solution we have discussed rests on a combination of efficient existing techniques, piecewise cubic Hermite interpolation, 4th-order finite differencing, and 2nd-order time integration by an explicit Runge-Kutta-Chebyshev method especially designed for parabolic problems. We have shown that this combination works well and that it can be used for solving a wide range of mixed parabolic-gradient systems.

This paper is the first in a co-operation with the Netherlands Institute for Brain Research in the field of computational neuroscience. The long term goal is further model and algorithm development focusing on axonal growth. What comes to mind for further numerical research includes (1) treatment of highly localized source terms on grids, (2) biquadratic or even quintic piecewise Hermite interpolation or global spectral or spline collocation methods [3, 5] for obtaining smoother gradient equation solutions, (3) higher order time stepping methods to exploit this, e.g. special purpose implicit-explicit methods [1, 2] or Rosenbrock methods using approximate or factorized Jacobian matrices [14], (4) adaptivity and local refinement in the vicinity of steep gradients and near the trajectories, and (5) the efficient treatment of systems assuming a quasi-steady state for the parabolic equations.

**Acknowledgement** We thank Arjen van Ooyen and Jaap van Pelt from the Netherlands Institute for Brain Research for helpful discussions on the kind of models used in studying axonal growth.

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