Centrum voor Wiskunde en Informatica
REPORT*RAPPORT*

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NM-R9516 1995

Report NM-R9516
ISSN 0169-0388

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Abstract

We investigate the use of splitting methods for the numerical integration of three-dimensional transport-chemistry models. In particular, we investigate various possibilities for the time discretization that can take advantage of the parallelization and vectorization facilities offered by multi-processor vector computers. To suppress wiggles in the numerical solution, we use third-order, upwind-biased discretization of the advection terms, resulting in a five-point coupling in each direction. As an alternative to the usual splitting functions, such as co-ordinate splitting or operator splitting, we consider a splitting function that is based on a three-coloured hopscotch-type splitting in the horizontal direction, whereas full coupling is retained in the vertical direction. Advantages of this splitting function are the easy application of domain decomposition techniques and unconditional stability in the vertical, which is an important property for transport in shallow water. The splitting method is obtained by combining the hopscotch-type splitting function with various second-order splitting formulae from the literature. Although some of the resulting methods are highly accurate, their stability behaviour (due to horizontal advection) is quite poor. Therefore we also discuss several new splitting formulae with the aim to improve the stability characteristics. It turns out that this is possible indeed, but the price to pay is a reduction of the accuracy. Therefore, such methods are to be preferred if accuracy is less crucial than stability; such a situation is frequently encountered in solving transport problems. As part of the project TRUST (Transport and Reactions Unified by Splitting Techniques), preliminary versions of the schemes are implemented on the Cray C98/4256 computer and are available for benchmarking.

AMS Subject Classification (1991): 65M06, 65M12, 65M20
CR Subject Classification (1991): G.1.7, G.1.8
Keywords and Phrases: Transports models, shallow water, 3D, splitting methods, stability, HPCN.
Note: The investigations reported in this paper were supported by the NCF (National Computing Facility Foundation) who provided the authors with a grant (CRG 95-08) from the Cray Research University Grants Program.

1. Introduction

The mathematical model describing transport processes of salinity, pollutants, etc., combined with their chemical or bio-chemical interactions, is defined by an initial-boundary value problem for the system of 3D advection-diffusion-reaction equations

$$\text{(1.1a)} \qquad \frac{\partial c_i}{\partial t} = L(u,v,w)c_i + g_i(t,x,y,z,c_1,...,c_m), \quad i = 1, \ldots, m,$$

$$\text{(1.1b)} \qquad L(u,v,w)c_i := -\frac{\partial}{\partial x}(uc_i) - \frac{\partial}{\partial y}(vc_i) - \frac{\partial}{\partial z}(wc_i) + \frac{\partial}{\partial x}\left(\varepsilon_x \frac{\partial c_i}{\partial x}\right) + \frac{\partial}{\partial y}\left(\varepsilon_y \frac{\partial c_i}{\partial y}\right) + \frac{\partial}{\partial z}\left(\varepsilon_z \frac{\partial c_i}{\partial z}\right).$$

Here, the various quantities are defined as follows:

c_i	concentrations of the contaminants,
u, v, w	local fluid velocities in x, y, z directions (assumed to be divergence free),
$\varepsilon_x, \varepsilon_y, \varepsilon_z$	diffusion coefficients in x, y, z directions,
g_i	reaction terms (e.g. chemical interactions) and emissions from sources.

The velocities u, v, w, and the diffusion coefficients ε_x, ε_y, ε_z are assumed to be known in advance. The terms g_i describe chemical reactions, emissions from sources, etc., and therefore depend on the concentrations. The mutual coupling of the equations in the system (1.1) is due to the functions g_i.
Along the lines described in [8], we replace the physical domain by a set of N Cartesian grid points and we approximate (1.1) and its boundary conditions by the semi-discrete, mN-dimensional initial value problem (IVP)

$$(1.2) \qquad \frac{d\mathbf{C}(t)}{dt} = \mathbf{F}(t,\mathbf{C}(t)) := \mathbf{H}(t,\mathbf{C}(t)) + \mathbf{G}(t,\mathbf{C}(t)), \quad \mathbf{C}(t_0) = \mathbf{C}_0.$$

Here, $\mathbf{C}$ contains the m concentrations c_i at all N grid points, $\mathbf{C}_0$ defines the initial values, $\mathbf{H}(t,\mathbf{C}(t))$ represents the advection-diffusion terms, and $\mathbf{G}(t,\mathbf{C}(t))$ contains the reaction terms and emissions from sources. $\mathbf{H}(t,\mathbf{C})$ is linear in $\mathbf{C}$ with a matrix of coefficients which is an m-by-m block-diagonal matrix with the same N-by-N diagonal blocks. In general, $\mathbf{G}(t,\mathbf{C})$ is nonlinear in $\mathbf{C}$, but at each grid point, it only depends on the m concentrations c_i at that particular grid point.
Since the right-hand side function in (1.2) contains terms of quite a different nature (advection-diffusion terms and reaction-source terms), it is a natural approach to integrate the system by splitting methods which are tuned to the individual right-hand side terms. Such splitting methods consists of a splitting *function* and a splitting *formula*. The splitting function is determined by a partitioning of the spatial grid points. Given the splitting function, many splitting formulae are possible. These formulae take the particular properties of the right-hand side into account and determine the temporal accuracy and stability of the splitting method.
In [8, 9, 12], the numerical treatment of (1.1) has been investigated for the case of a single transport equation, i.e. m = 1. The semi-discretization was obtained by symmetric, second-order spatial finite difference discretizations and the splitting method used was the so-called Odd-Even Line Hopscotch (OELH) method. It belongs to a family of splitting methods in which the splitting function is based on grid points which are divided into two different groups arranged according to the so-called 'odd-even line hopscotch' ordering (see also Gourlay [3]). The splitting formula uses a second-order, one-step time discretization consisting of two (fractional) stages of trapezoidal rule type. It is designed such that the implicit relations to be solved in each time step are only (tridiagonally) implicit in the vertical direction. In [10] this OELH method was successfully applied to a five-species model, i.e. m = 5. The accuracy of the results is dictated by the grid sizes in space and time and not by the stability condition; in vector mode on the Cray C98/4256 computer, the speed-up is about a factor 12 with respect to the scalar mode.
A possible drawback of this OELH method is its symmetric spatial discretization that may cause unwanted wiggles in the numerical solution. This disadvantage can be suppressed by changing to an upwind-biased discretization for the advection terms. In this paper, we use a third order upwind scheme, resulting - in general - in a 5-point discretization (the so-called $\kappa = 1/3$ discretization [6]). As a consequence of this extended stencil, we can no longer apply the odd-even line hopscotch ordering. Therefore, in this paper, we introduce three groups of grid points (red, black and white points), that

are arranged according to the 'red-black-white line hopscotch' ordering. Given the associated splitting function, the time integration requires a splitting formula which allows for multi-term splitting (in our case, a four-term splitting).

We distinguish between splitting formulae based on *consistent* stages and on *fractional* stages. Unlike fractional stages, consistent stages provide approximations to the exact solution at some point on the t-axis. It turns out that formulae with only consistent stages generate more accurate methods than formulae with one or more fractional stages. Both types of multi-term splitting formulae are available in the literature. We consider the *stabilizing corrections* formula of Douglas [1], based on only consistent stages, the fractional-stage formula of *approximation corrections* suggested by Yanenko [13], and the *parallel* fractional-stage splitting formula of Lu et al. [7]. These formulae have been selected because they are all second-order accurate. Furthermore, we present two new fractional-stage splitting formulae; one is a formula based on a combination of *Forward* and *Backward Euler* stages suggested by Hundsdorfer [5]; the second one is a formula with *Trapezoidal rule* type stages (like the OELH method in [9]). All these splitting formulae will be combined with the hopscotch type splitting function and the resulting methods will be called Red-Black-White Line Hopscotch (RBWLH) methods. The verification of the time-discretization-order of these methods becomes quite difficult. To overcome this difficulty, we will formulate the (one-step) RBWLH methods as Runge-Kutta methods with fractional stages, to be referred to as Runge-Kutta Splitting (RKS) methods. For RKS methods, the order conditions up to order 3 are easily derived [4]. In this way, we can verify the order of any (one-step) splitting method, whatever complicated the method is.

As a result of our analysis of RBWLH methods, it turns out that two methods are particularly promising: the five-stage Douglas type method, showing a highly accurate behaviour, and the seven-stage trapezoidal rule type method, possessing improved stability properties. Since in shallow flow problems, stability is usually of more importance than accuracy, the trapezoidal rule type method is recommended. In this scheme, the implicit part of each of the seven stages is associated with either the red, or black, or white grid points, or with the reaction term **G**. A preliminary version of this method is implemented on the Cray C98/4256 computer and is available for benchmarking as the code TRUST (Transport and Reactions Unified by Splitting Techniques). The main properties are summarized below:

- ♦ fractional-stage method with seven stages
- ♦ third-order in space (upwind-biased $\kappa = 1/3$ discretization)
- ♦ second-order in time (Strang-type symmetry)
- ♦ linear stability condition $\Delta t\,(|u|/\Delta x + |v|/\Delta y) \leq 2.7$ (independent of the vertical mesh size)
- ♦ storage economic
- ♦ bio-chemical stage (**G**-stage) solved by functional iteration
- ♦ red, black and white stages five-diagonally, linearly implicit in vertical direction
- ♦ highly vectorizable implementation of the linear systems solver
- ♦ easy domain decomposition owing to the horizontal explicitness.

The remainder of the paper is organized as follows. The next section briefly discusses RKS methods and provides us with criteria to verify the order of accuracy in time and to reduce the number of arrays needed for storage. In Section 3, the upwind-biased $\kappa = 1/3$ discretization is described. Section 4 presents a brief survey of time discretization options and their main characteristics. Finally, in Section 5, we discuss numerical experiments and make a comparison of the various methods with respect to stability and accuracy.

2. Runge-Kutta splitting methods

For simplicity, we shall ignore the t-argument in the right-hand side function $\mathbf{F}(t,\mathbf{C}(t))$ of (1.2). In Section 4, where the actual RKS methods will be specified, we return to the nonautonomous notation.

Suppose that the right-hand side $\mathbf{F}$ is split according to the splitting function

$$\mathbf{F}(\mathbf{C}) = \sum_{k=1}^{\sigma} \mathbf{f}_k(\mathbf{C}). \tag{2.1}$$

Then the RKS formula is defined by

$$\begin{aligned} \mathbf{Y} &= (\mathbf{e} \otimes I)\, \mathbf{C}_n + \Delta t \sum_{k=1}^{\sigma} (A^{(k)} \otimes I)\, \mathbf{F}_k(\mathbf{Y}), \\ \mathbf{C}_{n+1} &= (\mathbf{e}_s^T \otimes I)\, \mathbf{Y}, \end{aligned} \tag{2.2}$$

where Δt is the integration step, $\mathbf{C}_n$ and $\mathbf{C}_{n+1}$ represent approximations to the exact solution vector $\mathbf{C}(t)$ at $t = t_n$ and $t = t_{n+1}$, $\otimes$ denotes the Kronecker product, the s-dimensional vectors $\mathbf{e}$ and $\mathbf{e}_i$ respectively are the vector with unit entries and the ith unit vector, I is the identity matrix whose dimension should be deduced from the context in which it appears (here, it equals the dimension of the IVP (1.2)). The s components $\mathbf{Y}_i$ of $\mathbf{Y}$ represent intermediate approximations to the exact solution values, $\mathbf{F}_k(\mathbf{Y})$ contains the derivative values $\left(\mathbf{f}_k(\mathbf{Y}_i)\right)$, and the s-by-s parameter arrays $A^{(k)}$ are to be determined by order and stability conditions. In the following, $A^{(k)}$ will be assumed lower triangular.

If $\sigma = 1$, then (2.2) reduces to a conventional diagonally implicit RK method (DIRK method). The method {(2.1),(2.2)} will be called a *σ-terms RKS method with s fractional stages*. RKS methods are completely defined by the splitting function (2.1) and the arrays $A^{(k)}$ defining the splitting formula.

In our case, where we want to solve transport problems, it is more convenient to present the RKS formula in an alternative form, that allows us to choose the arrays $A^{(k)}$ such that we obtain a storage economic scheme. Let T be an s-by-s nonsingular transformation matrix. Then, by premultiplication of (2.2) by the matrix $T \otimes I$, we obtain

$$\mathbf{Y} = \big((I - T) \otimes I\big)\mathbf{Y} + \big(T\mathbf{e} \otimes I\big)\, \mathbf{C}_n + \Delta t \sum_{k=1}^{\sigma} \big(\tilde{A}^{(k)} \otimes I\big)\, \mathbf{F}_k(\mathbf{Y}),\ \ \tilde{A}^{(k)} := TA^{(k)},$$

(2.3)

$$\mathbf{C}_{n+1} = \big(\mathbf{e}_s^T \otimes I\big)\, \mathbf{Y}.$$

For example, if T is defined by

(2.4)
$$T := \begin{pmatrix} 1 & 0 & 0 & \dots & 0 & 0 \\ -1 & 1 & 0 & \dots & 0 & 0 \\ . & . & . & . & . & . \\ 0 & 0 & 0 & \dots & -1 & 1 \end{pmatrix}, \quad T^{-1} := \begin{pmatrix} 1 & 0 & 0 & 0 & \dots \\ 1 & 1 & 0 & 0 & \dots \\ 1 & 1 & 1 & 0 & \dots \\ 1 & 1 & 1 & 1 & \dots \\ . & . & . & . & . \end{pmatrix},$$

then the stage values $\mathbf{Y}_i$, $i \geq 2$ are defined by the preceding stage value $\mathbf{Y}_{i-1}$ plus a linear combination of derivative values.

In [4, Table 2.1], the order conditions up to order p = 3 have been derived. Since a second-order time integration is usually sufficiently accurate in the numerical modelling of transport problems, we restrict our considerations to orders p =1 and p = 2. Using the compact notation in terms of the matrices $A^{(k)}$, we have for first-order accuracy the σ conditions

(2.5a)
$$\mathbf{e}_s^T A^{(j)} \mathbf{e} = 1, \quad j = 1, \dots, \sigma,$$

and for second-order accuracy, in addition, the σ^2 conditions

(2.5b)
$$\mathbf{e}_s^T A^{(j)} A^{(k)} \mathbf{e} = \frac{1}{2}, \qquad j, k = 1, \dots, \sigma.$$

The conditions (2.5) can be used for checking the order of accuracy of a given RKS formula (we remark that when using the representation (2.3), we should replace $A^{(k)}$ by $T^{-1}\tilde{A}^{(k)}$ in (2.5)).

The linear stability of RKS methods can be analysed by means of the linear test equation

(2.6)
$$\frac{d\mathbf{C}(t)}{dt} = \sum_{k=1}^{\sigma} J_k \mathbf{C}(t),$$

where J_k denotes the Jacobian matrix $\partial \mathbf{f}_k(\mathbf{y}_n) / \partial \mathbf{y}$, which is assumed to be constant and to have its eigenvalues in the left halfplane. From (2.2), we deduce

$$\mathbf{Y} = \mathbf{e} \otimes \mathbf{C}_n + \Delta t \sum_{k=1}^{\sigma} \big(A^{(k)} \otimes J_k\big)\, \mathbf{Y} = \big(I - \Delta t S\big)^{-1} \big(\mathbf{e} \otimes \mathbf{C}_n\big),\ \ S := \sum_{k=1}^{\sigma} \big(A^{(k)} \otimes J_k\big).$$

Hence,

$$\mathbf{C}_{n+1} = \big(\mathbf{e}_s^T \otimes I\big)\mathbf{Y} = \big(\mathbf{e}_s^T \otimes I\big)\big(I - \Delta t S\big)^{-1}\big(\mathbf{e} \otimes I\big)\mathbf{C}_n.$$

Thus, the *stability matrix* is given by

$$R = (\mathbf{e}_s^T \otimes I)\left(I - \Delta t \sum_{k=1}^{\sigma} (A^{(k)} \otimes J_k)\right)^{-1} (\mathbf{e} \otimes I). \tag{2.7}$$

Of special interest are the RKS formulae with factorizable stability functions. Let us consider the special RKS formula which has (when represented in the form (2.3)) lower bidiagonal matrices $\tilde{A}^{(k)} = \left(\tilde{a}_{ij}^{(k)}\right)$. If T is chosen according to (2.4), we have

$$\begin{aligned} \mathbf{Y}_1 &= \mathbf{C}_n + \Delta t \sum_{k=1}^{\sigma} \tilde{a}_{11}^{(k)} J_k \mathbf{Y}_1, \\ \mathbf{Y}_i &= \mathbf{Y}_{i-1} + \Delta t \sum_{k=1}^{\sigma} [\tilde{a}_{i,i-1}^{(k)} J_k \mathbf{Y}_{i-1} + \tilde{a}_{ii}^{(k)} J_k \mathbf{Y}_i], \quad i = 2, \ldots, s, \\ \mathbf{C}_{n+1} &= \mathbf{Y}_s. \end{aligned} \tag{2.8}$$

Hence, the stability matrix takes the factorized form

$$R = \prod_{i=s}^{1} (I - \Delta t \tilde{S}_{ii})^{-1} (I + \Delta t \tilde{S}_{i,i-1}), \quad \tilde{S}_{10} = O, \quad \tilde{S}_{ij} := \sum_{k=1}^{\sigma} \tilde{a}_{ij}^{(k)} J_k, \ j > 0. \tag{2.7'}$$

3. Spatial discretization

The spatial discretization of the diffusion terms in (1.1) can be approximated by symmetric differences, but the advection terms will be discretized by upwind difference formulae in order to suppress unwanted wiggles in the numerical solution. Writing

$$\frac{\partial}{\partial x}\left(\varepsilon_x \frac{\partial c_i}{\partial x}\right) = \frac{\partial \varepsilon_x}{\partial x}\frac{\partial c_i}{\partial x} + \varepsilon_x \frac{\partial^2 c_i}{\partial x^2}, \quad \frac{\partial u c_i}{\partial x} = u \frac{\partial c_i}{\partial x} + c_i \frac{\partial u}{\partial x}, \tag{3.1}$$

(and similar expressions for the derivatives with respect to y and z), we are led to use the symmetric, second-order difference stencils

$$\frac{\partial}{\partial x} \approx \frac{1}{2\Delta x}[-1 \ \ 0 \ \ 1], \quad \frac{\partial^2}{\partial x^2} \approx \frac{1}{(\Delta x)^2}[1 \ \ -2 \ \ 1] \tag{3.2}$$

for the differential operators occurring in the diffusion terms. Furthermore, assuming that the velocity field is divergence free, we may use the third-order upwind-biased discretization (so-called $\kappa = 1/3$ discretization [6])

$$\begin{aligned} u\frac{\partial}{\partial x} &\approx \frac{u}{6\Delta x}[1 \ \ -6 \ \ 3 \ \ 2 \ \ 0] \qquad \text{if } u \geq 0 \\ u\frac{\partial}{\partial x} &\approx \frac{u}{6\Delta x}[0 \ \ -2 \ \ -3 \ \ 6 \ \ -1] \qquad \text{if } u < 0 \end{aligned} \tag{3.3}$$

for the advection terms. Inserting the above approximations into (1.1), we arrive at the semi-discrete transport model (1.2).

4. Time discretization

In this section, we apply RKS methods to the transport model (1.2). In particular, we shall apply the RKS formula in the form (2.3) with lower triangular matrices $\tilde{A}^{(k)}$. On substitution of (2.4) and taking into account the triangular structure of the RKS matrices, we obtain the representation

$$\begin{aligned} \mathbf{Y}_1 &= \mathbf{C}_n + \Delta t \sum_{k=1}^{\sigma} \tilde{a}_{11}^{(k)} \mathbf{f}_k(\mathbf{Y}_1), \\ \mathbf{Y}_i &= \mathbf{Y}_{i-1} + \Delta t \sum_{k=1}^{\sigma} \sum_{j=1}^{i} \tilde{a}_{ij}^{(k)} \mathbf{f}_k(\mathbf{Y}_j), \quad i = 2, \ldots, s, \\ \mathbf{C}_{n+1} &= \mathbf{Y}_s. \end{aligned} \tag{4.1}$$

To restrict the amount of implicitness to a manageable level, we assume that for a given i at most one of the parameters $\tilde{a}_{ii}^{(k)}$ does not vanish.

Let us first consider the advection and diffusion terms. From the preceding section it follows that the semi-discretization is such that we only have coupling along the co-ordinate directions (no cross-coupling) and that in each direction we have at most a five-point coupling.

```
o  *  +  o  *  +  o  *
+  o  *  +  o  *  +  o
*  +  o  *  +  o  *  +
o  *  +  o  *  +  o  *
```

Figure 4.1. Three categories of grid points.

Let the grid points in each *horizontal* plane be grouped into three categories, red, black and white points, as indicated in Figure 4.1, such that each vertical grid line contains either red, or black, or white points. Furthermore, let

$$\mathbf{H} = \mathbf{H}(t,\mathbf{C}) = \mathbf{H}^* + \mathbf{H}^+ + \mathbf{H}^o, \tag{4.2a}$$

where $\mathbf{H}^*$, $\mathbf{H}^+$ and $\mathbf{H}^o$ have only nonzero values at the grid points $*$, + and o, respectively. Then, we may define the Red-Black-White Line Hopscotch (RBWLH) splitting by

$$\mathbf{f}_1 := \mathbf{H}^*, \quad \mathbf{f}_2 := \mathbf{H}^+, \quad \mathbf{f}_3 := \mathbf{H}^o. \tag{4.2b}$$

Owing to this splitting and to our assumption on the parameters $\tilde{a}_{ii}^{(k)}$, the implicit stages in (4.1) involving $\mathbf{f}_1$, $\mathbf{f}_2$ or $\mathbf{f}_3$ only possess implicitness in the *vertical direction*.

The reaction and source terms represented by $\mathbf{G}(t,\mathbf{C}(t))$ can be handled simply by setting

$$\mathbf{f}_4 := \mathbf{G}. \tag{4.2c}$$

Since **G** has N component vectors, each of dimension m and mutually independent, the implicitness associated with the fractional function $\mathbf{f}_4 = \mathbf{G}$ consists of N implicit systems of dimension m. In shallow water applications, this function is nonstiff, so that it is feasible to solve these systems by functional iteration.

In the following subsections, we survey a few potential RBWLH methods of the form {(4.1),(4.2)}, written in nonautonomous form, and we discuss their suitability for integrating transport problems. In Section 5, the behaviour of these RBWLH methods will be illustrated by means of a numerical example.

4.1. RBWLH method of Douglas type

Examples of RKS formulae with an arbitrary number of fractional right-hand side functions (splitting terms) are given in [4]. A well-known example is the *stabilizing corrections formula* of Douglas [1]. In the case of the splitting function (4.2), we obtain the *RBWLH method of Douglas type* defined by

$$
\begin{aligned}
&\mathbf{Y}_1 = \mathbf{C}_n,\\
&\mathbf{Y}_2 = \mathbf{Y}_1 + \Delta t\,[\mathbf{H}^*(t_n,\mathbf{Y}_1) + \mathbf{H}^+(t_n,\mathbf{Y}_1) + \mathbf{H}^o(t_n,\mathbf{Y}_1) + \mathbf{G}(t_n,\mathbf{Y}_1)],\\
&\mathbf{Y}_3 = \mathbf{Y}_2 + \tfrac{1}{2}\Delta t\,[\mathbf{H}^*(t_n+\Delta t,\mathbf{Y}_3) - \mathbf{H}^*(t_n,\mathbf{Y}_1)],\\
&\mathbf{Y}_4 = \mathbf{Y}_3 + \tfrac{1}{2}\Delta t\,[\mathbf{H}^+(t_n+\Delta t,\mathbf{Y}_4) - \mathbf{H}^+(t_n,\mathbf{Y}_1)],\\
&\mathbf{Y}_5 = \mathbf{Y}_4 + \tfrac{1}{2}\Delta t\,[\mathbf{H}^o(t_n+\Delta t,\mathbf{Y}_5) - \mathbf{H}^o(t_n,\mathbf{Y}_1)],\\
&\mathbf{Y}_6 = \mathbf{Y}_5 + \tfrac{1}{2}\Delta t\,[\mathbf{G}(t_n+\Delta t,\mathbf{Y}_6) - \mathbf{G}(t_n,\mathbf{Y}_1)],\\
&\mathbf{C}_{n+1} = \mathbf{Y}_6.
\end{aligned}
\qquad (4.3)
$$

Note that the five stages of this method are all consistent stages. This is clear for the first stage which is in fact an explicit Euler step. The second stage can be rewritten as

$$\mathbf{Y}_3 = \tfrac{1}{2}[\mathbf{Y}_1 + \mathbf{Y}_2] + \tfrac{1}{2}\Delta t\,[\mathbf{H}^*(t_n+\Delta t,\mathbf{Y}_3) + \mathbf{H}^+(t_n,\mathbf{Y}_1) + \mathbf{H}^o(t_n,\mathbf{Y}_1) + \mathbf{G}(t_n,\mathbf{Y}_1)],$$

showing that $\mathbf{Y}_3$ is a first-order approximation at $t_n + \Delta t$ (and similarly for the remaining stages). The last four stages serve to raise the first-order accuracy of the first stage to second-order accuracy (by writing (4.3) in the RKS form (2.2), the order conditions (2.5) can be verified to hold). Evidently, due to the terms $\mathbf{H}^*$, $\mathbf{H}^+$ and $\mathbf{H}^o$, the first stage is highly unstable. Hence, the next stages also serve to stabilize the method. This can be made more precise by considering the stability matrix associated with (4.3):

$$R(Z^*,Z^+,Z^o,Z^\#) = I + \left(I - \tfrac{1}{2}Z^\#\right)^{-1}\left(I - \tfrac{1}{2}Z^o\right)^{-1}\left(I - \tfrac{1}{2}Z^+\right)^{-1}\left(I - \tfrac{1}{2}Z^*\right)^{-1}Z.$$

Here, $Z = Z^* + Z^+ + Z^o + Z^\#$ with $Z^* = \Delta t J^*$, $Z^+ = \Delta t J^+$, $Z^o = \Delta t J^o$ and $Z^\# = \Delta t J^\#$, and where the Jacobians J^*, J^+, J^o and $J^\#$ correspond to $\mathbf{H}^*$, $\mathbf{H}^+$, $\mathbf{H}^o$ and **G**, respectively. In order to get some indication of the damping effect of the stability matrix, we ignore the (nonstiff) **G**-stage and we assume that Z^*, Z^+ and Z^o share the same eigensystem with eigenvalues z^*, z^+ and z^o. Then, the eigenvalues of the stability matrix are given by $R(z^*,z^+,z^o)$. In particular, we are interested in the

magnitude of $R(z^*,z^+,z^o)$ for advection dominated problems, that is, z^*, z^+ and z^o have an imaginary part that is relatively large compared to their real part. Unfortunately, it turns out that for such eigenvalues $R(z^*,z^+,z^o)$ easily assumes values outside the unit circle. Hence, even this idealized scalar case indicates a poor stability behaviour and therefore it is to be expected that the total (non-scalar) RBWLH method of Douglas type is not sufficiently stable for integrating transport problems over long time intervals. This expectation is confirmed in Section 5, where we describe numerical tests.

4.2. RBWLH method of Yanenko type

A second well-known example of a splitting formula allowing an arbitrary number of splitting terms is presented by the *approximating corrections formula* of Yanenko [13]. In the case (4.2), we obtain the *Yanenko type RBWLH method*

$$
\begin{aligned}
&\mathbf{Y}_1 = \mathbf{C}_n + \tfrac{1}{2}\Delta t\, \mathbf{H}^*(t_n+\tfrac{1}{2}\Delta t,\mathbf{Y}_1),\\
&\mathbf{Y}_2 = \mathbf{Y}_1 + \tfrac{1}{2}\Delta t\, \mathbf{H}^+(t_n+\tfrac{1}{2}\Delta t,\mathbf{Y}_2),\\
&\mathbf{Y}_3 = \mathbf{Y}_2 + \tfrac{1}{2}\Delta t\, \mathbf{H}^o(t_n+\tfrac{1}{2}\Delta t,\mathbf{Y}_3),\\
&\mathbf{Y}_4 = \mathbf{Y}_3 + \tfrac{1}{2}\Delta t\, \mathbf{G}(t_n+\tfrac{1}{2}\Delta t,\mathbf{Y}_4),\\
&\mathbf{C}_{n+1} = \mathbf{C}_n + \Delta t\,[\mathbf{H}^*(t_n+\tfrac{1}{2}\Delta t,\mathbf{Y}_4) + \mathbf{H}^+(t_n+\tfrac{1}{2}\Delta t,\mathbf{Y}_4) + \mathbf{H}^o(t_n+\tfrac{1}{2}\Delta t,\mathbf{Y}_4) + \mathbf{G}(t_n+\tfrac{1}{2}\Delta t,\mathbf{Y}_4)].
\end{aligned}
\tag{4.4}
$$

Here, the first four fractional stages are highly stable, but the last stage, which serves to obtain second-order accuracy, is a highly unstable explicit Euler step. This situation is comparable with that of the Douglas type RBWLH method. In fact, the stability matrix is given by

$$R(Z^*,Z^+,Z^o,Z^\#) = I + Z(I-\tfrac{1}{2}Z^\#)^{-1}(I-\tfrac{1}{2}Z^o)^{-1}(I-\tfrac{1}{2}Z^+)^{-1}(I-\tfrac{1}{2}Z^*)^{-1},$$

which is quite similar to the stability matrix of the RBWLH method of Douglas type. As we will see in Section 5, the stability behaviour of this scheme closely resembles that of the Douglas type scheme.

4.3. The Lu-Neittaanmäki-Tai type RBWLH method

Recently, Lu, Neittaanmäki and Tai [7] proposed a multi-term splitting formula that can take advantage of parallel computer systems. The RBWLH version takes the form

$$
\begin{aligned}
&\mathbf{Y}_1 = \mathbf{C}_n + 2\Delta t\, \mathbf{H}^*(t_n+\tfrac{1}{2}\Delta t,\mathbf{Y}_1),\\
&\mathbf{Y}_2 = \mathbf{C}_n + 2\Delta t\, \mathbf{H}^+(t_n+\tfrac{1}{2}\Delta t,\mathbf{Y}_2),\\
&\mathbf{Y}_3 = \mathbf{C}_n + 2\Delta t\, \mathbf{H}^o(t_n+\tfrac{1}{2}\Delta t,\mathbf{Y}_3),\\
&\mathbf{Y}_4 = \mathbf{C}_n + 2\Delta t\, \mathbf{G}(t_n+\tfrac{1}{2}\Delta t,\mathbf{Y}_4),\\
&\mathbf{Y}_5 = \tfrac{1}{4}\,[\mathbf{Y}_1 + \mathbf{Y}_2 + \mathbf{Y}_3 + \mathbf{Y}_4],\\
&\mathbf{C}_{n+1} = \mathbf{C}_n + \Delta t\,[\mathbf{H}^*(t_n+\tfrac{1}{2}\Delta t,\mathbf{Y}_5) + \mathbf{H}^+(t_n+\tfrac{1}{2}\Delta t,\mathbf{Y}_5) + \mathbf{H}^o(t_n+\tfrac{1}{2}\Delta t,\mathbf{Y}_5) + \mathbf{G}(t_n+\tfrac{1}{2}\Delta t,\mathbf{Y}_5)].
\end{aligned}
\tag{4.5}
$$

Evidently, the first four fractional stages can be done in parallel. By means of (2.5), the method can be verified to be second-order accurate. With respect to stability, we observe that the structure is again similar to that of the Yanenko type method, that is, a number of highly stable stages followed by a highly unstable, explicit Euler step.

4.4. RBWLH method of Forward/Backward Euler type

Hundsdorfer [5] suggested a splitting formula of a nice conceptual simplicity. It combines Forward and Backward Euler stages in a *symmetrical* way (Strang-type schemes [11]), yielding second order accuracy. In case of the splitting function (4.2), the Hundsdorfer formula has eight fractional stages and reads

$$
\begin{aligned}
&\mathbf{Y}_1 = \mathbf{C}_n + \tfrac{1}{2}\Delta t\, \mathbf{H}^*(t_n + \tfrac{1}{2}\Delta t, \mathbf{Y}_1),\\
&\mathbf{Y}_2 = \mathbf{Y}_1 + \tfrac{1}{2}\Delta t\, \mathbf{H}^+(t_n + \tfrac{1}{2}\Delta t, \mathbf{Y}_2),\\
&\mathbf{Y}_3 = \mathbf{Y}_2 + \tfrac{1}{2}\Delta t\, \mathbf{H}^o(t_n + \tfrac{1}{2}\Delta t, \mathbf{Y}_3),\\
&\mathbf{Y}_4 = \mathbf{Y}_3 + \tfrac{1}{2}\Delta t\, \mathbf{G}(t_n + \tfrac{1}{2}\Delta t, \mathbf{Y}_4),\\
&\mathbf{Y}_5 = \mathbf{Y}_4 + \tfrac{1}{2}\Delta t\, \mathbf{G}(t_n + \tfrac{1}{2}\Delta t, \mathbf{Y}_4),\\
&\mathbf{Y}_6 = \mathbf{Y}_5 + \tfrac{1}{2}\Delta t\, \mathbf{H}^o(t_n + \tfrac{1}{2}\Delta t, \mathbf{Y}_5),\\
&\mathbf{Y}_7 = \mathbf{Y}_6 + \tfrac{1}{2}\Delta t\, \mathbf{H}^+(t_n + \tfrac{1}{2}\Delta t, \mathbf{Y}_6),\\
&\mathbf{Y}_8 = \mathbf{Y}_7 + \tfrac{1}{2}\Delta t\, \mathbf{H}^*(t_n + \tfrac{1}{2}\Delta t, \mathbf{Y}_7),\\
&\mathbf{C}_{n+1} = \mathbf{Y}_8.
\end{aligned}
\tag{4.6}
$$

The stability matrix associated with this method is readily seen to be of the form

$$
\begin{aligned}
&R(Z^*, Z^+, Z^o, Z^\#) = R_F(Z^*)\, R_F(Z^+)\, R_F(Z^o)\, R_F(Z^\#)\, R_B(Z^\#)\, R_B(Z^o)\, R_B(Z^+)\, R_B(Z^*),\\
&R_F(X) := I + \tfrac{1}{2}X, \quad R_B(X) := (I - \tfrac{1}{2}X)^{-1}.
\end{aligned}
$$

Again, the fact that this method has a number of highly unstable stages makes it unlikely that the overall stability will be satisfactory.

4.5. RBWLH method of Trapezoidal type

All preceding methods have in common that their splitting formulae consists of highly stable and highly unstable stages. Alternative and more stable methods can be constructed by choosing the splitting formula such that each individual stage is (marginally) stable. Moreover, we shall design the formula such that it contains fractional right-hand side functions of just one type, so that the stability matrix is factorizable. Similar to the previous scheme, we shall arrange the stages such that the fractional right-hand side functions appear symmetrically within each step. In this way, we are led to the second-order splitting formula

$$
\begin{aligned}
&\mathbf{Y}_1 = \mathbf{C}_n,\\
&\mathbf{Y}_2 = \mathbf{Y}_1 + \tfrac{1}{4}\Delta t\,[\mathbf{H}^*(t_n,\mathbf{Y}_1) + \mathbf{H}^*(t_n + \tfrac{1}{2}\Delta t,\mathbf{Y}_2)],\\
&\mathbf{Y}_3 = \mathbf{Y}_2 + \tfrac{1}{4}\Delta t\,[\mathbf{H}^+(t_n + \tfrac{1}{2}\Delta t,\mathbf{Y}_2) + \mathbf{H}^+(t_n + \tfrac{1}{2}\Delta t,\mathbf{Y}_3)],\\
&\mathbf{Y}_4 = \mathbf{Y}_3 + \tfrac{1}{4}\Delta t\,[\mathbf{H}^o(t_n + \tfrac{1}{2}\Delta t,\mathbf{Y}_3) + \mathbf{H}^o(t_n + \tfrac{1}{2}\Delta t,\mathbf{Y}_4)],\\
(4.7)\qquad &\mathbf{Y}_5 = \mathbf{Y}_4 + \tfrac{1}{2}\Delta t\,[\mathbf{G}(t_n + \tfrac{1}{2}\Delta t,\mathbf{Y}_4) + \mathbf{G}(t_n + \tfrac{1}{2}\Delta t,\mathbf{Y}_5)],\\
&\mathbf{Y}_6 = \mathbf{Y}_5 + \tfrac{1}{4}\Delta t\,[\mathbf{H}^o(t_n + \tfrac{1}{2}\Delta t,\mathbf{Y}_5) + \mathbf{H}^o(t_n + \tfrac{1}{2}\Delta t,\mathbf{Y}_6)],\\
&\mathbf{Y}_7 = \mathbf{Y}_6 + \tfrac{1}{4}\Delta t\,[\mathbf{H}^+(t_n + \tfrac{1}{2}\Delta t,\mathbf{Y}_6) + \mathbf{H}^+(t_n + \tfrac{1}{2}\Delta t,\mathbf{Y}_7)],\\
&\mathbf{Y}_8 = \mathbf{Y}_7 + \tfrac{1}{4}\Delta t\,[\mathbf{H}^*(t_n + \tfrac{1}{2}\Delta t,\mathbf{Y}_7) + \mathbf{H}^*(t_n + \Delta t,\mathbf{Y}_8)],\\
&\mathbf{C}_{n+1} = \mathbf{Y}_8.
\end{aligned}
$$

By means of (2.5) it can be verified that this formula does have second-order accuracy. Since all stages of (4.7) are of trapezoidal type, we shall call it an *RBWLH method of Trapezoidal type*. The stability matrix associated with (4.7) is given by

$$
\begin{aligned}
&R(Z^*,Z^+,Z^o,Z^\#) = \; Q(\tfrac{1}{4}Z^*)\,Q(\tfrac{1}{4}Z^+)\,Q(\tfrac{1}{4}Z^o)\,Q(\tfrac{1}{2}Z^\#)\,Q(\tfrac{1}{4}Z^o)\,Q(\tfrac{1}{4}Z^+)\,Q(\tfrac{1}{4}Z^*),\\
&Q(X) := (I - X)^{-1}(I + X).
\end{aligned}
$$

Since Q(X) has its eigenvalues on the unit disk for any matrix X with eigenvalues in the left halfplane and recalling that J^*, J^+, J^o and $J^\#$ are assumed to have their eigenvalues in the left halfplane, we conclude that each stage of (4.7) is unconditionally stable, which is a much better starting point than we have seen for the preceding methods. Of course, this 'stage-stability' does not imply that the combination of all the Q-matrices results in overall stability, since the matrices Z^*, Z^+, Z^o and $Z^\#$ do not share the same eigensystem for our RBWLH splitting. Therefore, a more sophisticated stability analysis is needed. This can be done along the lines of the analysis given in [12] for the OELH method and will be subject of future research.

Finally, we observe that in practice, it may be attractive to implement a modification of (4.7) that is less costly in actual computation. This modification is given by

$$
\begin{aligned}
&\mathbf{Y}_1 = \mathbf{C}_n,\\
&\mathbf{Y}_2 = \mathbf{Y}_1 + \tfrac{1}{4}\Delta t\,[\mathbf{H}^o(t_n,\mathbf{Y}_1) + \mathbf{H}^*(t_n + \tfrac{1}{2}\Delta t,\mathbf{Y}_2)],\\
&\mathbf{Y}_3 = \mathbf{Y}_2 + \tfrac{1}{4}\Delta t\,[\mathbf{H}^*(t_n + \tfrac{1}{2}\Delta t,\mathbf{Y}_2) + \mathbf{H}^+(t_n + \tfrac{1}{2}\Delta t,\mathbf{Y}_3)],\\
&\mathbf{Y}_4 = \mathbf{Y}_3 + \tfrac{1}{4}\Delta t\,[\mathbf{H}^+(t_n + \tfrac{1}{2}\Delta t,\mathbf{Y}_3) + \mathbf{H}^o(t_n + \tfrac{1}{2}\Delta t,\mathbf{Y}_4)],\\
(4.8)\qquad &\mathbf{Y}_5 = \mathbf{Y}_4 + \tfrac{1}{2}\Delta t\,[\mathbf{G}(t_n + \tfrac{1}{2}\Delta t,\mathbf{Y}_4) + \mathbf{G}(t_n + \tfrac{1}{2}\Delta t,\mathbf{Y}_5)],\\
&\mathbf{Y}_6 = \mathbf{Y}_5 + \tfrac{1}{4}\Delta t\,[\mathbf{H}^o(t_n + \tfrac{1}{2}\Delta t,\mathbf{Y}_5) + \mathbf{H}^+(t_n + \tfrac{1}{2}\Delta t,\mathbf{Y}_6)],\\
&\mathbf{Y}_7 = \mathbf{Y}_6 + \tfrac{1}{4}\Delta t\,[\mathbf{H}^+(t_n + \tfrac{1}{2}\Delta t,\mathbf{Y}_6) + \mathbf{H}^*(t_n + \tfrac{1}{2}\Delta t,\mathbf{Y}_7)],\\
&\mathbf{Y}_8 = \mathbf{Y}_7 + \tfrac{1}{4}\Delta t\,[\mathbf{H}^*(t_n + \tfrac{1}{2}\Delta t,\mathbf{Y}_7) + \mathbf{H}^o(t_n + \Delta t,\mathbf{Y}_8)],\\
&\mathbf{C}_{n+1} = \mathbf{Y}_8.
\end{aligned}
$$

It can be verified that this scheme again has second-order accuracy. It is less costly than (4.7) because the various stages have a number of terms in common (so-called *fast form*), but its stability matrix is not factorizable anymore.

5. Numerical experiments

The RBWLH methods described in the preceding subsections will be applied to the test problem

$$\text{(5.1a)} \qquad \begin{aligned} \frac{\partial c_1}{\partial t} + \mathbf{U}\cdot\nabla c_1 &= \varepsilon \Delta c_1 + g_1(t,x,y,z) - k_1 c_1 c_2, \\ \frac{\partial c_2}{\partial t} + \mathbf{U}\cdot\nabla c_2 &= \varepsilon \Delta c_2 + g_2(t,x,y,z) - k_1 c_1 + k_2(1 - c_2), \end{aligned}$$

defined on the region $0 \le x, y \le L_h$, $-L_v \le z \le 0$ and for $0 \le t \le T$. Here, $\mathbf{U} = (u, v, w)$ denotes the divergence free velocity field, given in analytical form (see [2])

$$\text{(5.1b)} \qquad \begin{aligned} u(t,x,y,z) &= \{ \ \tilde{y} + 3(\tilde{z} + 1/2)[(\tilde{x} - 1/2)^2 + (\tilde{y} - 1/2)^2 - r^2] \} \, d(t), \\ v(t,x,y,z) &= \{ -\tilde{x} + 3(\tilde{z} + 1/2)[(\tilde{x} - 1/2)^2 + (\tilde{y} - 1/2)^2 - r^2] \} \, d(t), \\ w(t,x,y,z) &= -3 L_v \tilde{z}(\tilde{z} + 1)\{(\tilde{x} - 1/2)/L_h + (\tilde{y} - 1/2)/L_h\} \, d(t), \end{aligned}$$

where we used the scaled co-ordinates $\tilde{x} := x/L_h$, $\tilde{y} := y/L_h$, $\tilde{z} := z/L_v$, and $r = 1/3$ and $d(t) = \cos(2\pi t/T_p)$. The Neumann boundary conditions, the initial condition and the functions g_1 and g_2 are chosen in accordance with the prescribed analytical solution, which is of the form

$$\text{(5.1c)} \qquad c_i(t,x,y,z) = \exp\{ \tilde{z}/i - f_i(t) - \gamma_i [(\tilde{x} - r(t))^2 + (\tilde{y} - s(t))^2]\}, \quad i = 1, 2,$$

with $f_2(t) = t/(T_b + t)$, $f_1(t) = 4 f_2(t)$, $r(t) = [2 + \cos(2\pi t/T_p)]/4$, and $s(t) = [2 + \sin(2\pi t/T_p)]/4$.
In our experiments, we take the following values for the parameters: $L_h = 20\,000$, $L_v = 100$, $\varepsilon = 0.5$, $\gamma_1 = 80$, $\gamma_2 = 20$, $T_b = 32400$, and $T_p = 43200$. The length of the integration interval $T = 36000$. Realistic values for the reaction rate constants are: $k_1 = k_2 = 10^{-4}$.
The accuracy is measured by

$$cd_i := \text{minimum over all grid points } (-^{10}\log |\text{absolute error for } c_i|), \quad i = 1, 2.$$

In the experiments, we use a grid with 81 points in each horizontal direction and 11 points in the vertical. The stage involving the (bio-chemical) **G**-function has been solved by functional iteration; it turns out that 2 iterations suffices to reduce the maximum norm of the residual below 10^{-5}.
For various values of Δt, the cd-values are given in Table 5.1. Furthermore, for each method we list the experimentally determined CFL number; these numbers have been included to give an indication of the stability behaviour of the various schemes when applied to advection dominated problems (to that end we set $\varepsilon = k_1 = k_2 = 0$ in (5.1a) and use constant u, v and w). Especially for the methods (4.3), (4.4), and (4.5), we do not claim that these numbers are very precise, since for these methods the instability is of a rather mild nature if the CFL condition is not obeyed. Even for experiments using a large number of steps it is difficult to classify a result as stable or unstable. A Fourier analysis along the lines as described in [12] should be performed to obtain the exact CFL numbers. For (4.6)

and the trapezoidal type methods however, we observe a sharp distinction between various time steps; violating the CFL condition results in severe instabilities. A common characteristic of all methods is that the stability behaviour is independent of Δz, which is a nice property in the current application of transport in *shallow* seas. Moreover, all methods behave unconditionally stable for diffusion dominated versions of the model (i.e., $k_1 = k_2 = 0$, $\varepsilon >> \|\mathbf{U}\|$). As a consequence, the time step is only restricted by the horizontal advection, and anticipating a similar stability condition as theoretically obtained for the OELH method [12], the stability condition of the RBWLH methods is conjectured to be of the form

$$\Delta t \left(\frac{|u|}{\Delta x} + \frac{|v|}{\Delta y} \right) \leq \text{CFL number.}$$

The number of stages is not the same for all schemes, resulting in different CPU times per step. Taking the computational effort of method (4.8) as unity, the corresponding factors for the other methods are listed in Table 5.1 (here, the parallel features of (4.5) have not been taken into account). These factors should be taken into consideration in selecting a method. For example, if the spatial grid is chosen as coarse as possible to achieve a certain requested accuracy, then the time integration error should not reduce the accuracy, and the Douglas type scheme (4.3) seems to be the most efficient choice. However, if the spatial grid is dictated by 'geometrical' reasons and full precision on this grid is not necessary, then also the time step can be enlarged; in this situation, the scheme (4.8) is the most efficient one, since it has the largest CFL number. Finally, we remark that the temporal error can always be reduced by applying Richardson extrapolation. Since Richardson extrapolation can be done in parallel, the accuracy of the Trapezoidal type method can be improved without increasing the effective computational costs.

Table 5.1. cd_1/cd_2-values for problem (5.1) at T=36000. For this problem, the cd_1/cd_2-values corresponding to $\Delta t \to 0$ (i.e., the spatial accuracy) are given by 3.4/3.5

Scheme	Δt=T/70	Δt=T/140	Δt=T/280	Δt=T/560	CFL	costs/step
Douglas (4.3)	*	3.1/3.1	3.4/3.5	3.4/3.5	0.6	0.8
Yanenko (4.4)	*	2.9/2.3	3.2/2.9	3.4/3.3	0.6	0.8
Lu-Neittaanmäki-Tai (4.5)	*	*	*	3.0/3.0	0.2	0.8
Hundsdorfer (4.6)	*	2.1/1.2	2.6/1.8	3.1/2.4	1.8	0.8
Trapezoidal (4.7)	*	1.9/1.5	2.5/2.1	2.9/2.7	2.2	1.6
Trapezoidal, fast form (4.8)	1.6/0.9	2.2/1.8	2.7/2.4	3.1/2.9	2.7	1.0

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