Second Order Numerical Operator Splitting for 3D Advection–Diffusion-Reaction Models

Riccardo Fazio and Alessandra Jannelli

Abstract In this paper, we present a numerical operator splitting for time integration of 3D advection-diffusion-reaction problems. In this approach, three distinct methods of second order accuracy are proposed for solving, separately, each term involved in the model. Numerical results, obtained for advection – reported in [Fazio and Jannelli, IAENG Int. J. Appl. Math., **39**, 25–35, 2009] –, diffusion, and reaction terms, show the efficiency of proposed schemes.

1 Introduction

This paper concerns numerical methods for three dimensional advection–diffusion-reaction (ADR) models governed by the following system of equations

$$\frac{\partial \mathbf{c}}{\partial t} + \nabla \cdot (\mathbf{vc}) - \nabla \cdot (\mathrm{D}\nabla \mathbf{c}) = \mathbf{R}(\mathbf{c}) \,, \tag{1}$$

where $\mathbf{c} = \mathbf{c}(\mathbf{x}, t) \in \mathbb{R}^m$, $\mathbf{x} \in \Omega \subset \mathbb{R}^3$ are the space variables and t denotes the time. The diffusion coefficient matrix $\mathrm{D} = diag[d_{11}, d_{22}, \ldots, d_{mm}]$ and the velocity field $\mathbf{v}(\mathbf{x}) \in \mathbb{R}^3$ are, usually, supposed to be given. Several phenomena of relevant interest can be described by model (1). Among others, we can quote the applications to a chemotaxis model [8], the pollutant transport in atmosphere [11], mucilage dynamics [4], ash-fall from volcano [5], and groundwater and surface water [9]. The governing system takes into account physical and biological processes modelled by three distinct terms: transport of each component due to the velocity field $\mathbf{v}$, described by the advection terms; random motion of each component due to the turbulent nature of the flow field, modelled by the (turbulent) diffusion terms; interaction of the involved species described by reaction terms (e.g., chemical reactions,

AQ1 R. Fazio (✉) and A. Jannelli
Department of Mathematics, University of Messina, Salita Sperone 31, 98166 Messina, Italy
e-mail: rfazio@dipmat.unime.it, jannelli@dipmat.unime.it

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growth of species, consumption of nutrients, etc.). From the numerical view-point, for the time integration of different terms of the model (1), we propose a fractional step approach. This method consists in separating in the discretized equations the part that accounts for hydrodynamics, described by advection term, usually linear, and the diffusion term on the left hand side, from the part accounting for biology, described by nonlinear reaction term on the right hand side. This splitting is reasonable when a loose coupling exists between the different phenomena and when they evolve with different characteristic times. The coupling between the components in each grid point, and not over the grid points, appears only in the solution of the reaction equations. In this contest such assumptions holds and the use of a fractional step seems promising.

2 The Operator Splitting Approach

In this section, we describe an efficient algorithm for solving ADR models (1) written in the following form

$$\frac{\partial \mathbf{c}}{\partial t} = A(\mathbf{c}) + D(\mathbf{c}) + R(\mathbf{c}). \tag{2}$$

We propose the use the Strang splitting [7] approach: if $\mathbf{c}^n$ is the approximate solution at time t^n, we obtain the solution $\mathbf{c}^{n+1}$ at next time $t^{n+1} = t^n + \Delta t$ by the following sequence of five steps:

$$\mathbf{c}^{n+1} = \mathscr{A}(\Delta t/2)\mathscr{D}(\Delta t/2)\mathscr{R}(\Delta t)\mathscr{D}(\Delta t/2)\mathscr{A}(\Delta t/2)\,\mathbf{c}^n,$$

where $\mathscr{A}(\cdot)$, $\mathscr{D}(\cdot)$ and $\mathscr{R}(\cdot)$ represent the discretized advection, diffusion and reaction operators, respectively. The advantage of the fractional step method is that, for each term, a different time integration method can be chosen. For the time integration of the advection part, explicit methods are usually more efficient than the implicit ones. On the other hand, the reaction part is sometimes very stiff and this requires the use of implicit methods, used also for the diffusion term. As far as accuracy is concerned, by using this splitting technique we get second order accuracy provided that each subproblem is solved by a second order accurate method.

2.1 Advection Solver

In this section, we consider the homogeneous hyperbolic equations

$$\frac{\partial \mathbf{c}}{\partial t} + \nabla \cdot (\mathbf{v}\mathbf{c}) = 0, \tag{3}$$

with given initial condition and appropriate boundary conditions (for instance: Dirichlet conditions at the inflow and no conditions at the outflow boundaries, or periodic boundary conditions, etc.). We set an uniform Cartesian grid $\Omega_J \in \mathbf{R}^3$. Let $\mathbf{c}^n_{ijk}$ be the average value of $\mathbf{c}$ over cell (x_i, y_j, z_k) at current time t^n, and $\mathbf{c}^{n+1}_{ijk}$ the average value of $\mathbf{c}$ at time $t^n + \Delta t$. For time integration, we use a high-resolution finite volume method written in the conservative form

$$\mathbf{c}^{n+1}_{ijk} = \mathbf{c}^n_{ijk} + \\ -\frac{\Delta t}{\Delta x}\left[\mathbf{F}^n_{i+\frac{1}{2}jk} - \mathbf{F}^n_{i-\frac{1}{2}jk}\right] - \frac{\Delta t}{\Delta y}\left[\mathbf{G}^n_{ij+\frac{1}{2}k} - \mathbf{G}^n_{ij-\frac{1}{2}k}\right] - \frac{\Delta t}{\Delta z}\left[\mathbf{H}^n_{ijk+\frac{1}{2}} - \mathbf{H}^n_{ijk-\frac{1}{2}}\right]$$

where $\mathbf{F}$, $\mathbf{G}$ and $\mathbf{H}$ are intercell numerical fluxes. A recent study on first and second order positive numerical methods for the advection equation is developed in [1] where several test problems are solved.

2.2 Diffusion Solver

The diffusion term is discretized implicitly to avoid using small time steps when are not dictated by accuracy reasons in detecting the correct dynamics of the concentration. We use the Crank–Nicolson scheme because it is second order accurate in space and time,

$$\mathbf{c}^{n+1}_{i,j,k} - \frac{\Delta t}{2\Delta x \Delta y \Delta z}\mathbf{w}^{n+1}_{i,j,k} = \mathbf{c}^n_{i,j,k} + \frac{\Delta t}{2\Delta x \Delta y \Delta z}\mathbf{w}^n_{i,j,k} \tag{4}$$

where

$$\mathbf{w}^n_{i,j,k} = -\Big\{\Delta y \Delta z\left(\widehat{\mathbf{F}}^n_{i+\frac{1}{2},j,k} - \widehat{\mathbf{F}}^n_{i-\frac{1}{2},j,k}\right) \\ + \Delta x \Delta z\left(\widehat{\mathbf{G}}^n_{i,j+\frac{1}{2},k} - \widehat{\mathbf{G}}^n_{i,j-\frac{1}{2},k}\right) + \Delta x \Delta y\left(\widehat{\mathbf{H}}^n_{i,j,k+\frac{1}{2}} - \widehat{\mathbf{H}}^n_{i,j,k-\frac{1}{2}}\right)\Big\} \tag{5}$$

with

$$\widehat{\mathbf{F}}_{i+\frac{1}{2},j,k} = -d_{i+\frac{1}{2},j,k}\frac{\mathbf{c}_{i+1,j,k} - \mathbf{c}_{i,j,k}}{\Delta x}, \\ \widehat{\mathbf{G}}_{i,j+\frac{1}{2},k} = -d_{i,j+\frac{1}{2},k}\frac{\mathbf{c}_{i,j+1,k} - \mathbf{c}_{i,j,k}}{\Delta y}, \\ \widehat{\mathbf{H}}_{i,j,k+\frac{1}{2}} = -d_{i,j,k+\frac{1}{2}}\frac{\mathbf{c}_{i,j,k+1} - \mathbf{c}_{i,j,k}}{\Delta z}. \tag{6}$$

As far as stability is concerned, the Crank–Nicolson scheme is an unconditionally stable one. We have no restriction on the time step but the extra labour involved is

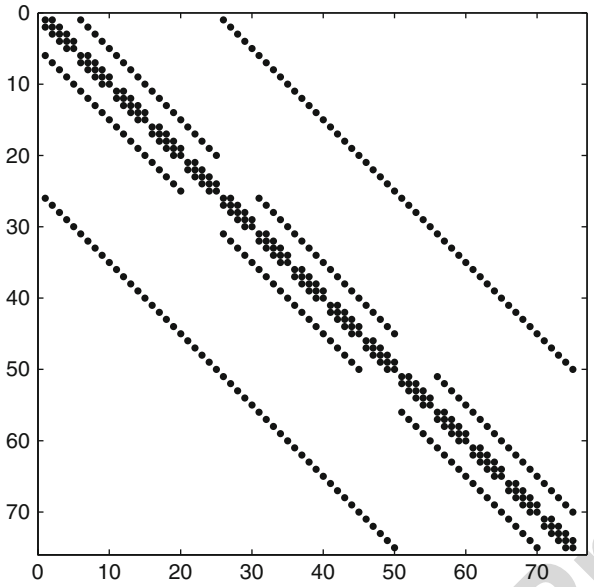

Fig. 1 Example of matrix of coefficients for the Crank–Nicolson method

very considerable. We have to solve a system of linear equations. These equations have a regular structure, each involving at most seven unknowns. The matrix of the system consists of zeroes, but it has not tridiagonal form. The linear system obtained is solved by the bi-conjugate gradient method of Van der Vorst [10] (for a simple description of the method see [2, pp. 362–379]). Figure 1 shows the matrix of coefficients on a sample domain of $5 \times 5 \times 3$ mesh-points. Note that there could be some instability in coupling with the reaction term. The presence of diffusion term in the system may cause some instabilities. When we individually test each step in the Strang splitting procedure, they are stable for reasonable time step intervals. When we test the coupled diffusion and reaction steps they could be unstable. When the full model is solved numerically, the time step interval necessary to prevent instability is very small when the diffusion term is discretized with Crank–Nicolson. A much longer time step is possible when diffusion step is discretized with the TR-BDF2, as Tyson et al. have done in [8], here TR stands for Trapezoidal Rule and BDF2 for the second order Backward Difference Formula.

2.2.1 Test Problem: Heat Equation

As an example, we consider the heat equation

$$\frac{\partial c}{\partial t} = \frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial y^2} \tag{7}$$

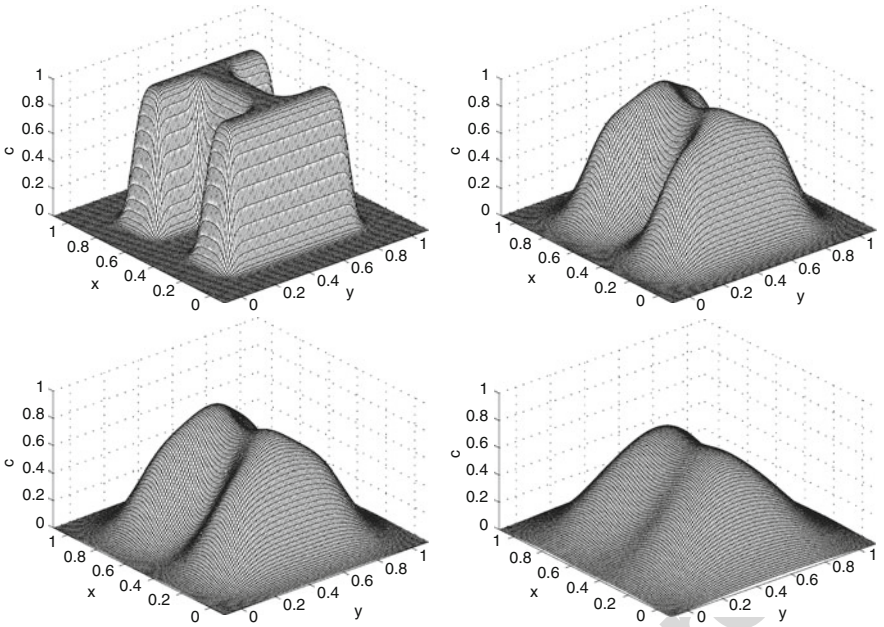

Fig. 2 The numerical solution and at time $t = 0.001$, $t = 0.003$, $t = 0.005$, and final time $t = 0.01$

on the unit square $0 < x < 1$, $0 < y < 1$, with homogeneous Dirichlet boundary conditions $c = 0$ on the boundary of the unit square. The initial condition is $c(x, y, 0) = f(x, y)$ with $f(x, y) = 1$ within the region shaped like the letter H, and $f(x, y) = 0$ in the rest of the square. In a narrow band surrounding the H, the function increases from 0 to 1, so that $f(x, y)$ is continuous; its derivatives are not continuous, being zero everywhere outside the narrow band and being greater than zero inside the band. The results of the implicit method are shown in Fig. 2. It shows the way in which the initial function diffuses throughout the square. This numerical results are obtained using $\Delta x = \Delta y = 0.01$ and $\Delta t = 0.001$ with $t_{max} = 0.01$.

2.3 Reaction Solver

The reaction step consists of solving a coupled system of ordinary differential equations in each grid cell. There are no spatial derivatives and hence no spatial coupling of different cells in this step. Moreover, the reaction equations are sometimes very stiff, requiring the use of implicit methods for stability reasons. In this contest, we propose the use of an adaptive procedure implemented with stiff solvers at low accuracy and complexity. In particular, we use the Milne device for the estimation of the local error, that is the error incurred in the integration from t^n to t^{n+1} under the

assumption that the approximate solution at time t^n is exact. In order to implement the Milne device, we use two different convergent multistep methods of same order of accuracy p in order to decide whether the numerical value is an acceptable approximation to exact solution evaluated at time t^{n+1}. Let us denote by $\mathbf{c}^{n+1}$ and $\tilde{\mathbf{c}}^{\,n+1}$ the two computed numerical approximations, and with C and $\widetilde{C}$ the corresponding local error constants. A naive approach is to require that the local error LE satisfies

$$\mathrm{LE} = \left| \frac{C}{\widetilde{C} - C} \right| ||\mathbf{c}^{n+1} - \tilde{\mathbf{c}}^{\,n+1}|| \leq tol, \tag{8}$$

with $||\cdot||$ a suitable norm.

2.3.1 Numerical Results: Robertson Problem

As sample numerical test, we consider the problem given by a stiff system of three non-linear differential equations with suitable initial conditions

$$\begin{cases} c_1' = -P_1 c_1 + P_3 c_2 c_3 \\ c_2' = P_1 c_1 - P_3 c_2 c_3 - P_2 c_2^2 \\ c_3' = P_2 c_2^2 \\ c_1(0) = 1, c_2(0) = 0, c_3(0) = 0, \end{cases} \tag{9}$$

where $P_1 = 0.04$, $P_2 = 3 \cdot 10^7$ and $P_3 = 10^4$. The model describes the kinetics of an auto-catalytic reaction described by Robertson [6]. The structure of reaction is reported in (10), where A, B and C represent the chemical species involved

$$\begin{aligned} A &\xrightarrow{P_1} B, \\ B + B &\xrightarrow{P_2} C + B, \\ B + C &\xrightarrow{P_3} A + C. \end{aligned} \tag{10}$$

This problem is sometimes used as a test problem for stiff solvers. The large difference among the reaction rate constants P_i, with $i = 1, 2, 3$, is the reason for the stiffness. As usual in problems arising in chemical kinetics, this system has a small very quick initial transient. This phase is following by a very smooth variation of the components where a large step-size would be appropriate for a numerical method. The problem (9) is integrated within the range $t \in [0, 10^6]$. Figure 3 shows the numerical solution of the species involved.

The numerical results are obtained in 267 steps (with 3 rejected steps) by Milne device implemented with the TR with $\widetilde{C} = -1/12$, and BDF2 with variable time steps, see [3], with

$$C = -\frac{(k^n + 1)^2}{6k^n(2k^n + 1)},$$

where $k^n = \Delta t^n / \Delta t^{n-1}$. Figure 4 shows the adaptive numerical results. In the top frame, we show the step-size selection Δt^n, in the bottom one the local error LE.

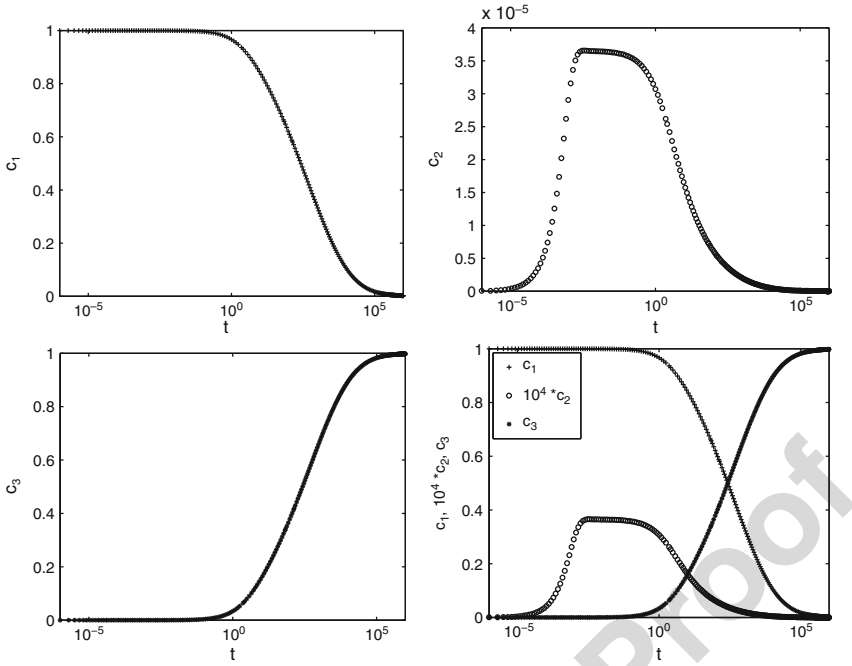

Fig. 3 Semi-log scale plot of numerical solution for the Robertson problem

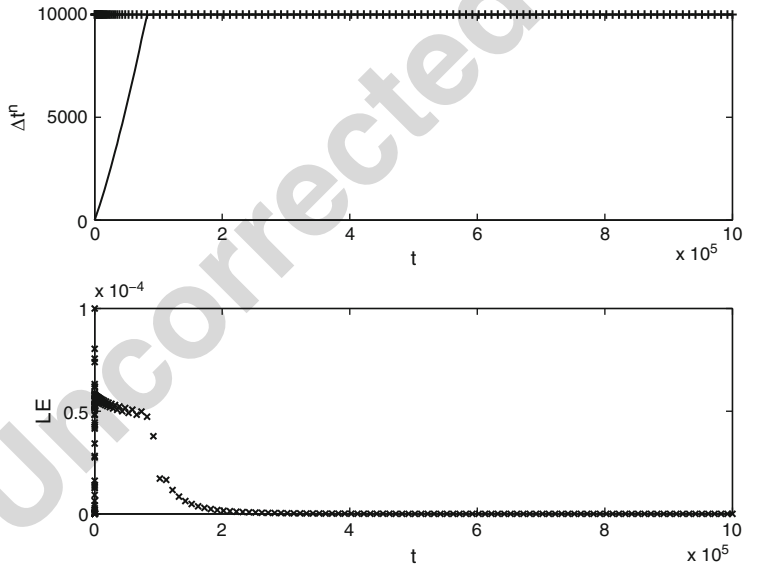

Fig. 4 Adaptive numerical results for the Robertson problem

It is easy to note, how, the adaptive procedure modifies the time step in relation to the value of the the local error for the solution second component. Initially, at the beginning of the process, the adaptive procedure sets a small Δt^n corresponding to fast transitory of the second component. Then, when this component becomes smooth, the procedure amplifies the step-size. A maximum value for step-size is set and this represents its upper bound.

For the adaptive procedure, we set: $\Delta t_{\min} \leq \Delta t^n \leq \Delta t_{\max}$ with $\Delta t_{\min} = 10^{-6}$ and $\Delta t_{\max} = 10^4$, $LE_{\min} \leq LE \leq LE_{\max}$ with $LE_{\min} = 10^{-5}$ and $LE_{\max} = 10\ LE_{\min}$. The time-step Δt^n is modified in the following cases: if $LE_{min} \leq LE \leq LE_{max}$, then $\Delta t^{n+1} = 0.9\ \Delta t^n\ (tol/LE)^{1/(p+1)}$, $p = 2$ in our case; if $LE < LE_{\min}$ then $\Delta t^{n+1} = 1.2\ \Delta t^n$; if $LE > LE_{\max}$ then the step is repeated with $\Delta t^n = 0.5\ \Delta t^n$.

References

1. R. Fazio, A. Jannelli: Second order positive schemes by means of flux limiters for the advection equation. IAENG Int. J. Appl. Math., **39**, 25–35, 2009
2. G. H. Golub, C. F. van Loan: *Matrix computations*, 2nd ed. Hopkins University Press, London, 1989
3. A. Jannelli, R. Fazio: Adaptive stiff solvers at low accuracy and complexity. J. Comp. Appl. Math., **191**, 246–258, 2006
4. A. Jannelli, R. Fazio, D. Ambrosi: A 3D mathematical model for the prediction of mucilage dynamics. Comput. Fluids, **32**, 47–57, 2003
5. R. McKibbin, L. L. Lim, T. A. Smith, W. L. Sweatman: A model for dispersal of eruption ejecta. In *Proceedings World Geothermal Congress*. 24–29 April 2005, Antalya, Turkey
6. H. H. Robertson: *The solution of a set of reaction rate equations*. Academic Press, London, 178–182, 1966
7. G. Strang: On the construction and comparison of difference schemes. SIAM J. Num. Anal., **5**, 506–517, 1968
8. R. Tyson, L. G. Stern, R. J. LeVeque: Fractional step methods applied to a chemotaxis model. J. Math. Biol., **41**, 455–475, 2000
9. M. Toro, L. C. van Rijn, K. Meijer: Three-dimensional modelling of sand and mud transport in currents and waves. Technical Report No. H461/Q407/Q791, Delft Hydraulics, Delft, The Netherlands, 1989
10. H. A. Van der Vorst: Bi-CGSTAB: A fast and smootly converging variant of Bi-CG for the solution of nonsymmetric linear systems. SIAM J. Sci. Stat. Comput., **13**, 631–644, 1992
11. J. G. Verwer, W. H. Hundsdorfer, J. G. Blom: Numerical time integration for air pollution models. Sur. Math. Ind., **2**, 107–174, 2002

AUTHOR QUERY

AQ1. First author has been identified as corresponding author. Please check.