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Letter to the Editor

Note on the time integration of 3D advection–reaction equations ☆

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Abstract

We consider triangularly implicit methods for integrating advection–reaction equations in which the reaction part is highly stiff. Stability boundaries are derived if the implicit relations are solved by approximately factorized Newton.

Keywords: Time integration; Advection–reaction equations; Newton

1. Introduction

If the method of lines is applied to an initial-boundary value problem for advection–reaction equations, then we obtain an initial-value problem (IVP) for a large system of first-order ordinary differential equations (method of lines):

$$\frac{dy}{dt} = f(t,y), \quad y(t_0) = y_0. \tag{1.1}$$

We shall assume that the initial-boundary value problem is defined in three spatial dimensions. Then the right-hand side function can be split according to

$$f(t,y) := f_1(t,y) + f_2(t,y) + f_3(t,y), \tag{1.2}$$

where f_1 and f_2 contain the spatial derivative terms with respect to the horizontal directions x_1 and x_2 and where f_3 represents both the spatial derivative terms with respect to the vertical direction x_3 and the reaction and emission terms. In this paper, we consider the case where the reaction terms are highly stiff, so that f_3 is also highly stiff. The functions f_1 and f_2 are considerably less stiff.

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2. Time integration

In order to cope with the stiffness of the IVP (1.1), we shall use an *implicit* time integration formula which is at least A-stable and preferably L-stable.

Our approach is based on the iterative solution of the implicit relations by the approximately factorized Newton Method (AFN method). This method was used in [1] for solving the implicit relations obtained in the implicit time integration of shallow water transport problems. The AFN method applies to a large class of implicit integration methods. In this paper, we shall consider methods that can be written in the form

$$\boldsymbol{M}_n(\Delta t, \boldsymbol{Y}_{n+1}) = \boldsymbol{0}, \tag{2.1}$$

where $\boldsymbol{M}_n$ is a function depending on Δt and $\boldsymbol{Y}_{n+1}$ such that the Jacobian of $\boldsymbol{M}_n$ with respect to $\boldsymbol{Y}_{n+1}$ satisfies the relation

$$\frac{\partial \boldsymbol{M}_n}{\partial \boldsymbol{Y}_{n+1}} = I - \Delta t \left(T \otimes \frac{\partial \boldsymbol{f}(t_n, \boldsymbol{y}_n)}{\partial \boldsymbol{y}_n} \right) + \mathrm{O}((\Delta t)^2). \tag{2.2}$$

Here, Δt denotes the timestep $t_{n+1} - t_n$ and $\boldsymbol{Y}_{n+1} = (\boldsymbol{y}_{n+1,1}^{\mathrm{T}}, \ldots, \boldsymbol{y}_{n+1,r}^{\mathrm{T}})^{\mathrm{T}}$ is the so-called stage vector with r components $\boldsymbol{y}_{n+1,i}$ representing approximations to the solution $\boldsymbol{y}(t)$ of (1.1) at the points $t_n + c_i \Delta t$, where the c_i, $i = 1, \ldots, r$, are given positive numbers with $c_r = 1$. Furthermore, $\otimes$ denotes the Kronecker product (direct matrix product), T is an arbitrary diagonal or *lower triangular* $r \times r$ matrix with nonnegative diagonal entries, and I is the $rN \times rN$ identity matrix (in the sequel, identity matrices of arbitrary order will be denoted by I, but its order will always be clear from the context). The class of methods {(2.1), (2.2)} contains all linear multistep, all diagonally implicit Runge–Kutta methods, and many other useful integration methods.

Our starting point for solving (2.1) is the modified Newton process:

$$N(\boldsymbol{Y}^j - \boldsymbol{Y}^{j-1}) = -\boldsymbol{M}_n(\Delta t, \boldsymbol{Y}^{j-1}), \quad N := I - \Delta t T \otimes \boldsymbol{J}, \quad \boldsymbol{J} := \frac{\partial \boldsymbol{f}(t_n, \boldsymbol{y}_n)}{\partial \boldsymbol{y}_n}, \quad j \geqslant 1, \tag{2.3}$$

where $\boldsymbol{Y}^0$ is an initial approximation to be provided by some predictor formula. The solution of the linear Newton systems in (2.3) is extremely costly. Therefore, following [1], we replace (2.3) by

$$\begin{aligned} &\Pi(\boldsymbol{Y}^j - \boldsymbol{Y}^{j-1}) = -\boldsymbol{M}_n(\Delta t, \boldsymbol{Y}^{j-1}), \quad j \geqslant 1, \\ &\Pi := (I - \Delta t D \otimes J_1)(I - \Delta t D \otimes J_2)(I - \Delta t D \otimes J_3), \quad D = \mathrm{diag}(T), \quad \boldsymbol{J}_k \approx \frac{\partial \boldsymbol{f}_k(t_n, \boldsymbol{y}_n)}{\partial \boldsymbol{y}_n}. \end{aligned} \tag{2.4}$$

The matrix Π is an approximate factorization of the matrix $I - \Delta t T \otimes \partial \boldsymbol{f}(t_n, \boldsymbol{y}_n)/\partial \boldsymbol{y}_n$, explaining our terminology 'approximately factorized Newton iteration' or AFN iteration. Although AFN iteration requires the solution of three linear systems instead of the one linear Newton system in (2.3), the block structure of the system matrices $\boldsymbol{I} - \Delta t D \otimes \boldsymbol{J}_k$, $k = 1, 2, 3$, is such that solving these linear systems is not costly. For a discussion of computational costs we refer to [4].

3. Convergence of AFN iteration

We shall discuss the convergence of the AFN process (2.4) for the model problem

$$\frac{\mathrm{d}\boldsymbol{y}}{\mathrm{d}t} = \boldsymbol{J}\boldsymbol{y} = (\boldsymbol{J}_1 + \boldsymbol{J}_2 + \boldsymbol{J}_3)\boldsymbol{y}, \tag{3.1}$$

where the matrices J_k are the Jacobians of the function f_k which are assumed to be commuting (normal mode analysis).

For this model problem, the error recursion associated with (2.4) becomes

$$Y^j - Y_{n+1} = Z(Y^{j-1} - Y_{n+1}), \quad Z := I - \Pi^{-1}N, \quad j \geqslant 1. \tag{3.2}$$

Recalling that T is lower triangular, it follows from (2.3) and (2.4) that the eigenvalues of Z are

$$\lambda(Z) = 1 - \frac{1 - \Delta t\lambda(T)\lambda(J)}{(1 - \Delta t\lambda(T)\lambda(J_1))(1 - \Delta t\lambda(T)\lambda(J_2))(1 - \Delta t\lambda(T)\lambda(J_3))}. \tag{3.3}$$

In the following, we split f_3 into a reaction part $f_3^{(r)}$ and an advection part $f_3^{(a)}$, so that $J_3 = J_3^{(r)} + J_3^{(a)}$. Furthermore, we assume that the eigenvalues $\lambda(J_1), \lambda(J_2)$ and $\lambda(J_3^{(a)})$ of J_1, J_2 and $J_3^{(a)}$ are purely imaginary and that $\lambda(J_3^{(r)}) < 0$. Let us write

$$\Delta t\lambda(T)\lambda(J_k) = \mathrm{i}\eta_k, \quad k = 1,2, \qquad \Delta t\lambda(T)\lambda(J_3^{(a)}) = \mathrm{i}\eta_3, \qquad \Delta t\lambda(T)\lambda(J_3^{(r)}) = -\xi_3, \tag{3.4}$$

where the η_k are real and $\xi_3 > 0$. Then, it follows from (3.3) that

$$\lambda(Z) = 1 - \frac{1 + \xi_3 - \mathrm{i}(\eta_1 + \eta_2 + \eta_3)}{(1 - \mathrm{i}\eta_1)(1 - \mathrm{i}\eta_2)(1 + \xi_3 - \mathrm{i}\eta_3)}. \tag{3.3'}$$

We shall call the values $\alpha(\eta_1, \eta_2, \eta_3, \xi_3) := |\lambda(Z)|$ the amplification factors of the iterated AFN method. Evidently, the convergence region is defined by the points $(\eta_1, \eta_2, \eta_3, \xi_3)$ where these amplification factors are less than 1. Let us consider convergence regions of the type

$$\mathbb{C}(\xi_3) := \{(\eta_1, \eta_2, \eta_3, \xi_3) \colon |\eta_k| < \gamma(\xi_3),\ k = 1,2,3\}, \tag{3.5}$$

where the function γ is to be determined.

Since ξ_3 assumes extremely large negative values, we are particularly interested in the minimal value of $\gamma(\xi_3)$ on the interval $0 < \xi_3 \leqslant \infty$. Using Maple [3], we found that for given (ξ_3, η_3) the function $\alpha(\eta_1, \eta_2, \eta_3, \xi_3)$ increases most rapidly along the line $\eta_1 = \eta_2$. Hence, for given (ξ_3, η_3) the real solution of smallest magnitude of the equation $\alpha(\eta, \eta, \eta_3, \xi_3) = 1$ determines the square in the (η_1, η_2)-plane where we have convergence. Furthermore, it turned out that for given ξ_3, this solution is positive and decreases monotonically with η_3. Therefore, we may draw the conclusion that the function $\gamma(\xi_3)$ in (3.5) is determined by the solution of $\alpha(\eta, \eta, \eta, \xi_3) = 1$. This leads to:

Theorem 3.1. *AFN iteration converges in the region* (3.5) *for*

$$\gamma(x) = \tfrac{1}{6}(9 + 12x - 6x^2 + 3(33 + 72x + 28x^2 - 16x^3 + 4x^4)^{1/2})^{1/2}.$$

In Fig. 1, the function $\gamma(x)$ is plotted. At $x = 0$ it starts with the value $(1/6)\sqrt{9 + 3\sqrt{33}} \approx 0.85$, increases to $(1/2)\sqrt{6} \approx 1.22$ at $x = 2$, and then decreases to $(1/2)\sqrt{2} \approx 0.70$ at infinity. Thus, we have convergence for all $\xi_3 > 0$ if $|\eta_k| < (1/2)\sqrt{2}$, $k = 1,2,3$. From (3.4) we derive the condition

$$\Delta t < \frac{\sqrt{2}}{2\rho(D)\max\{\rho(J_1), \rho(J_2), \rho(J_3^{(a)})\}}. \tag{3.6}$$

If the underlying integration method {(2.1),(2.2)} is A-stable, then this condition is also sufficient for stability of the AFN iterated method. Hence $\beta := \frac{1}{2}\sqrt{2}\rho^{-1}(T)$ may be interpreted as a stability

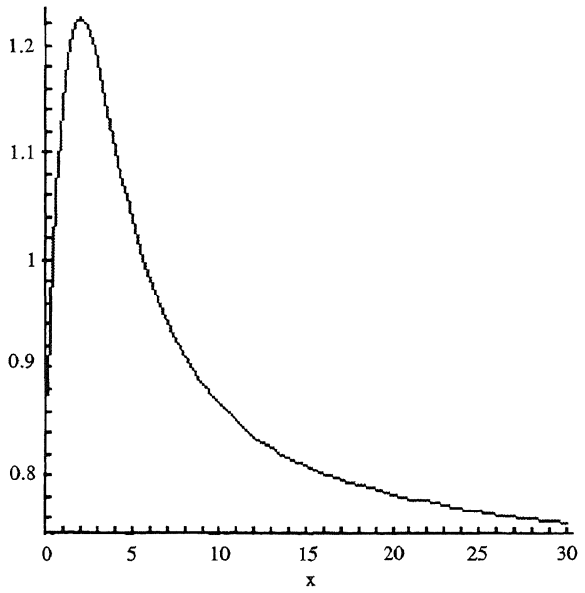

Fig. 1. The function $\gamma(x)$ in (3.5).

boundary. For example, the second-order, L-stable backward differentiation formula with $\rho(T) = \frac{2}{3}$ yields $\beta \approx 1.06$. Two other methods from the literature, whose factorized versions are popular in air pollution modeling, are the second-order Rosenbrock methods ROS2 [5] with two implicit stages and the third-order RODAS3 with four implicit stages (see [6, p. 13]). They are both L-stable. The stability boundary of ROS2 (with $\rho(T) = 1 - \frac{1}{2}\sqrt{2}$) and RODAS3 (with $\rho(T) = \frac{1}{2}$) are respectively given by $\beta \approx 2.41$ and $\beta \approx 1.41$. Finally, we mention two L-stable, diagonally implicit Runge–Kutta methods which were constructed such that $\rho(T)$ is minimal (see [2]). The first is second-order accurate with four implicit stages and $\rho(T) \approx 0.13$, i.e. $\beta \approx 5.44$, the second one is third-order accurate with four implicit stages and $\rho(T) \approx 0.33$, i.e. $\beta \approx 2.19$.

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