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Special methods for the numerical integration of some ODEs systems

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Abstract

We investigate a Runge-Kutta like method of order three with two evaluations per step, for the numerical integration of separated systems of ODEs. The formula being L-stable do not require Jacobian evaluations. Some numerical examples are discussed in order to show the good performance of the new scheme when applied to stiff systems.

1 Introduction

Our aim in the present work is to describe a new L-stable method of order three, involving two function evaluations per step, for the numerical integration of separated systems of ODEs. We will consider autonomous systems given by

$$\begin{aligned}
y'_{(1)} &= f_{11}(y_{(1)}) + f_{12}(y_{(2)}) + \ldots + f_{1m}(y_{(m)}) \,, \\
y'_{(2)} &= f_{21}(y_{(1)}) + f_{22}(y_{(2)}) + \ldots + f_{2m}(y_{(m)}) \,, \\
&\vdots \\
y'_{(m)} &= f_{m1}(y_{(1)}) + f_{m2}(y_{(2)}) + \ldots + f_{mm}(y_{(m)}) \,,
\end{aligned} \tag{1}$$

that is, systems in which $f : \mathbb{R}^m \to \mathbb{R}^m$ can be put in the form $f(y) = F(y)\mathbb{1}$ with $y = (y_{(1)}, y_{(2)}, \ldots, y_{(m)})$, $\mathbb{1} = (1, 1, \ldots, 1)^T$ and where F is the matrix

$$F(y) = \begin{pmatrix} f_{11}(y_{(1)}) & f_{12}(y_{(2)}) & \cdots & f_{1m}(y_{(m)}) \\ f_{21}(y_{(1)}) & f_{22}(y_{(2)}) & \cdots & f_{2m}(y_{(m)}) \\ \vdots & \vdots & & \vdots \\ f_{m1}(y_{(1)}) & f_{m2}(y_{(2)}) & \cdots & f_{mm}(y_{(m)}) \end{pmatrix} ,$$

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with $f_{ij} : \mathbb{R} \to \mathbb{R}$. Systems of this type appear for example when solving some parabolic partial differential equations by the method of lines. We will show an example of this later, by obtaining a system of ODEs for the method of lines approach to solving the Burgers' equation.

2 Construction of the method.

In our recent paper [3], a new family of explicit and linearly implicit two-stage methods of order three for the numerical integration of scalar autonomous ODEs is proposed. These methods can be seen as a generalization of the explicit Runge-Kutta methods providing better order and stability results with the same number of stages.

The general form of a third order two-stage method of our family (see [3] for more details) is given by

$$y_{n+1} = y_n + hk_1 G(s)\,,$$

where k_1, k_2 and s are given by

$$k_1 = f(y_n)\,, \quad k_2 = f(y_n + h\,c_2 k_1)\;, \quad s = \frac{k_2 - k_1}{c_2 k_1}\,,$$

$c_2 = 2/3$ and G takes the form

$$G(s) = \frac{1 + \dfrac{1+2d_1}{2}s + \dfrac{1+3d_1+6d_2}{6}s^2 + \displaystyle\sum_{i=3}^{n^*} n_i s^i}{1 + d_1 s + d_2 s^2 + \displaystyle\sum_{i=3}^{d^*} d_i s^i}\,. \qquad (2)$$

Note at this point that the formulae do not require Jacobian evaluations. Moreover, our methods are related to Rosenbrock-type methods such as W-methods [6], MROW-methods [8] and generalized Runge-Kutta methods [7], in which the exact Jacobian is no needed. For an excellent survey of some of these methods the reader is referred to [4].

Some third order methods with special properties (such as A-stability, L-stability, order four when applied to linear problems, etc) have been developed in [2,1,3], where also some numerical experiments can be found.

From the Butcher theory we know that a Runge-Kutta method which has order q for a scalar initial value problem may have order less than q when applied to a problem involving a system of differential equations. However, when $q \leq 3$, any Runge-Kutta method has the same order applied to systems as it has when applied to the scalar autonomous problem (see [5] pp. 173–175 for more details). Unfortunately for our methods this is not true because of the nonlinearities that arise from the term s in (2) and from the function G in (2) (note that term s and function G are not defined when applied to systems). However, when considering separated systems, it is possible to implement our methods in such a way that the resulting formula works well and with the same order as in the scalar autonomous case. We will give more details later.

When extending our methods in order to apply them to separated systems of ODE's, it is desirable to consider formulas in which the denominator in (2) is given in the form $(1-as)^\alpha$ ($\alpha \in \mathbb{N}$) so that only one LU-decomposition per step is needed. Moreover, we look for a third order method being L-stable, with the previous property.

All we need for this is to take $\alpha = 3$ and let the free parameters in (2) satisfy

$$d_1 = -3a\,, \quad d_2 = 3a^2\,, \quad d_3 = -a^3\,, \tag{3}$$

where, in order to get L-stability, a is the root of the polynomial $6x^3 - 18x^2 + 9x - 1 = 0$ given by

$$a = 1 + \frac{\sqrt{6}}{2}\sin\left(\frac{1}{3}\arctan\left(\frac{\sqrt{2}}{4}\right)\right) - \frac{\sqrt{2}}{2}\cos\left(\frac{1}{3}\arctan\left(\frac{\sqrt{2}}{4}\right)\right) \tag{4}$$

$$\approx 0.435866521508459\,, \tag{5}$$

and we take $n_i = 0$ for $i \geq 3$, and $d_i = 0$ for $i \geq 4$. We obtain in this manner a method with the above properties. The associated method for problem (1) (of the same order) is given by

$$y_{n+1} = y_n + hG(S)\,k_1\,, \tag{6}$$

where

$$k_1 = f(y_n) = F(y_n)\,\mathbb{1}\,, \quad k_2 = f(y_n + hc_2k_1) = F(y_n + hc_2k_1)\,\mathbb{1}\,,$$

$c_2 = 2/3$ and S is now a matrix given by

$$\begin{pmatrix} \dfrac{f_{11}(y_{n(1)} + hc_2k_{1(1)}) - f_{11}(y_{n(1)})}{c_2\,k_{1(1)}} & \cdots & \dfrac{f_{1m}(y_{n(m)} + hc_2k_{1(m)}) - f_{1m}(y_{n(m)})}{c_2\,k_{1(m)}} \\ \vdots & & \vdots \\ \dfrac{f_{m1}(y_{n(1)} + hc_2k_{1(1)}) - f_{m1}(y_{n(1)})}{c_2\,k_{1(1)}} & \cdots & \dfrac{f_{mm}(y_{n(m)} + hc_2k_{1(m)}) - f_{mm}(y_{n(m)})}{c_2\,k_{1(m)}} \end{pmatrix}$$

where $y_n = (y_{n(1)}, y_{n(2)}, \ldots, y_{n(m)})$ and $k_1 = (k_{1(1)}, k_{1(2)}, \ldots, k_{1(m)})$.

Note that the method is linearly implicit.

It is also possible to integrate with our methods some non-autonomous scalar ODEs and separated systems. In fact, those that when rewritten in autonomous form in the usual way (that is, adding the trivial equation $x' = 1$) are given by a separated system (1). The resulting system is one dimension higher. However, noting that the last row in S has all entries equal to zero, it can be seen that our methods can be implemented without increasing this dimension.

3 Numerical experiments.

Next we will consider a numerical experiment involving the Burgers' equation

$$u_t + u\,u_x = \nu\,u_{xx} \qquad \text{or} \qquad u_t + \left(\frac{u^2}{2}\right)_x = \nu\,u_{xx}\,, \qquad \nu > 0\,, \tag{7}$$

where $u = u(x,t)$ and we take $0 \leq x \leq 1$ and $0 \leq t \leq 1$. The initial and Dirichlet boundary conditions are taken as

$$u(x,0) = (\mathrm{sen}(3\pi x))^2 \cdot (1-x)^{3/2}\,, \qquad u(0,t) = u(1,t) = 0\,. \tag{8}$$

This nonlinear parabolic problem is taken from [4] (see pp. 349 and 443) and was originally designed by Burgers (1948) as "a mathematical model illustrating the theory of turbulence". Nowadays it remains interesting as a nonlinear equation resembling the Navier-Stokes equations in fluid dynamics which possesses for ν small, shock waves and, for $\nu \to 0$ discontinuous solutions.

Now we apply the numerical method of lines to this partial differential equation as follows. We discretize along the x-axis with a uniform mesh and replace all spatial derivatives in the right equation of (7) by centered finite difference approximations. Taking

$$\Delta x = \frac{1}{N+1}\,, \qquad u_i(t) = u(i\Delta x, t) \qquad i = 0, 1, \ldots, N+1\,, \tag{9}$$

then a system of separated ODEs for the method of lines approach to solving Burgers' equation is

$$\begin{aligned} u_i' &= -\frac{u_{i+1}^2 - u_{i-1}^2}{4\Delta x} + \nu \frac{u_{i+1} - 2u_i + u_{i-1}}{(\Delta x)^2}\,, \qquad i = 1, 2, \ldots, N \\ u_i(0) &= (\mathrm{sen}(3\pi i \Delta x))^2 \cdot (1 - i\Delta x)^{3/2}\,, \qquad i = 1, 2, \ldots, N\,, \end{aligned} \tag{10}$$

where $u_i = u_i(t)$ and we have from the boundary conditions that $u_0(t) = u_{N+1}(t) = 0$. After the appropriate exclusions and substitutions we can note by inspection that the above system has a tridiagonal Jacobian matrix.

Now we will apply the method of the preceding section to this separated system of ODEs taking $N = 24$ and $\nu = 0.2$ in (10). For this values, the system becomes banded of dimension 24 and the associated Jacobian matrix is tridiagonal. It is easy to show that the problem is mildly stiff. In fact, we have that the eigenvalues of the Jacobian are all real and range between -499 and -1 (with the dominant eigenvalue being close to -498) for the integration interval considered.

First we integrate this problem with fixed stepsize $h = 0.04$. Figure 1 shows the numerical solution we obtained. With fixed step size $h = 2^{-m}$ for various $m = 2, 3, \ldots, 10$ over 2^m steps, the value of the numerical solution (for $t = 1$) was computed using our method. We also computed very carefully (taking $h = 0.0001$) the exact solution at the specified output point. The magnitude of the error E (measured in the Euclidean norm of the space $\mathbb{R}^{24}$) for the different step sizes h is shown in Figure 2 in double logarithmic scale. On the logarithmic scale used for this figure, the error is represented very closely by a straight line whose slope equals the order of the method. The figure show complete agreement with our theoretical result.

We repeat our numerical experiment taking $N = 24$ and $\nu = 0.004$ in (10). Again the system of ODEs we get for the method of lines approach to solving

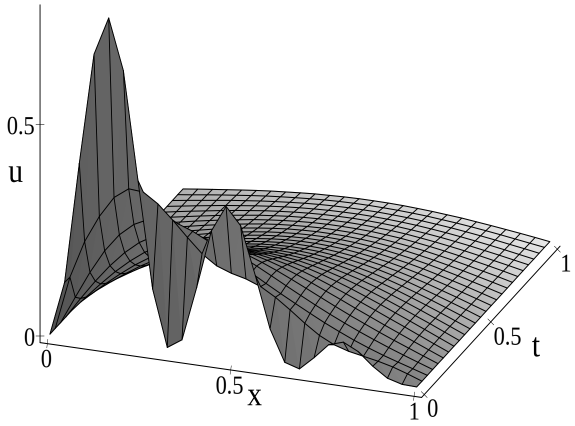

Fig. 1. Numerical solution: MOL approach to Burgers' equation taking $\nu = 0.2$, $N = 24$ and $h = 0.04$.

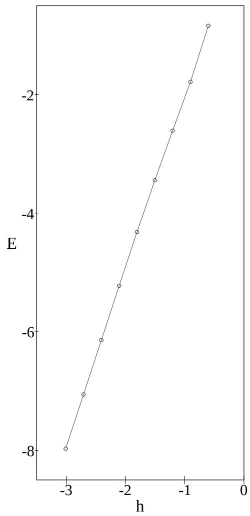

Fig. 2. Error as a function of step size (double logarithmic scale) for our method.

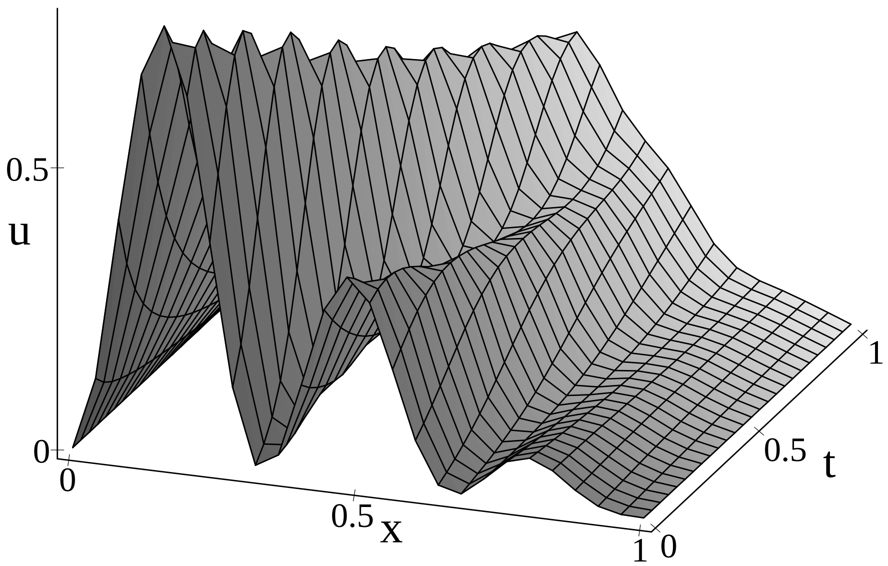

Fig. 3. Numerical solution: MOL approach to Burgers' equation taking $\nu = 0.004$, $N = 24$ and $h = 0.04$.

Burgers' equation is banded of dimension 24, but now the eigenvalues of the tridiagonal Jacobian matrix are most of them complex (with all real parts being negative and ranging between -10 and 0, and all imaginary parts ranging between -14 and 14).

Figure 3 shows the numerical solution we obtained in this way. The solution possesses shock waves that later fuse. Note at this point that Burgers' equation can be thought of as a hyperbolic problem with artificial diffusion for small ν. Note also that the imaginary parts of the eigenvalues of the Jacobian matrix introduce oscillations in the numerical solution (as can be observed in the figure).

4 Conclusions.

Our new method is primarily useful when applied to many separated stiff systems for which no accurate evaluation of a Jacobian is available or the evaluation of the Jacobian is too expensive. For some non stiff problems for which function evaluations are expensive, our explicit method might be more efficient than the usual explicit Runge-Kutta methods. This follows from the fact that for a given number of stages (or function evaluations per step), our method attain bigger order than the Runge-Kutta ones, as we have pointed out before.

Though several practical questions remain to be solved, for example, how to extend our methods in order to integrate a wider class of problems, the new method seem quite promising, for instance in the context of solving some nonlinear parabolic equations (by the method of lines).

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