The energy estimate above was derived under the assumption that Dirichlet boundary conditions are given for the *transformed* variables. In fact, the boundary conditions are posed in terms of the *physical* variables $\mathbf{u} = (F, p, h)^T$. Dirichlet boundary conditions for $\mathbf{u}$ lead to a coupling of the boundary conditions for $\mathbf{v}$. Does this have any influence on the stability properties? It can be shown that the linearized system is stable if the Reynolds number is not too large. It is not known if this restriction is really necessary or not for the system considered.

Having in mind that the system is a part of a larger network it is appropriate to discretize it by the method of lines (MOL). This discretization is done in the *physical* variables. By transforming it to the canonical ones the latter become coupled. For a toy problem, by using a simple upwind discretization the following can be shown:

If the step size is restricted by $\Delta x < Cu$, then

- the numerical scheme becomes weakly unstable;
- the resulting differential-algebraic equation has the tractability index 1.

Thus, for sufficiently small step sizes, the properties of the continuous system are resembled.

References

[1] M. Hanke, K.H.A. Olsson, Magnus Strïgren: *Stability analysis of a degenerate hyperbolic system modeling a heat exchanger.* Submitted 2005

[2] M. Hanke, M. Strïgren: *MOL discretization of a degenerate hyperbolic PDAE system.* Manuscript 2006

[3] P.G. Mehta, B. Eisenhower, J. Oppelstrup: *Bifurcation analysis of the CO_2 steady state model.* Internal Report, United Technologies Research Center, Hartford, CT, 2002

[4] W. S. Martinsson, P. I. Barton: Index and characteristic analysis of linear PDE systems. *SIAM J. Sci. Comput.,* 24(3):905-923, 2002

Exponential integrators of Rosenbrock-type

Marlis Hochbruck and Alexander Ostermann

(joint work with Julia Schweitzer)

1. Introduction

We consider a system of ordinary differential equations in autonomous form

$$y'(t) = f(y), \qquad y(t_0) = y_0, \tag{1}$$

assuming that the linearisation $J = Df(y)$ is uniformly sectorial in a neighbourhood of the exact solution. Consequently, there exist constants C and ω (both independent of y) such that

$$\left\| \mathrm{e}^{tJ} \right\| \le C\, \mathrm{e}^{\omega t}, \qquad t \ge 0. \tag{2}$$

Typical examples are abstract nonlinear parabolic equations, see [4], and their spatial discretisations.

Recently, we studied a class of explicit exponential Runge–Kutta methods for similar problems, see [2]. Due to the involved structure of the order conditions, however, it seems to be difficult to construct reliable and efficient error estimates for these methods. Moreover, in contrast to classical time integrators, exponential Runge–Kutta methods are *not invariant* under linearisation. This results in an error behaviour similar to classical W-methods, see [1]. Therefore, one has to expect large errors whenever the linear part is not well chosen.

2. Method class

Motivated by the observations just mentioned, we propose to linearise the right-hand side of (1) in each step, as it is done in classical Rosenbrock methods. Thus we write

$$y' = J_n y + g_n(y), \qquad J_n = Df(y_n), \quad g_n(y) = f(y) - J_n y. \tag{3}$$

Here, y_n is the numerical approximation to $y(t_n)$.

Applying then an exponential Runge–Kutta method to (3) gives the following s-stage exponential Rosenbrock-type scheme

$$Y_{ni} = \mathrm{e}^{c_i h J_n} y_n + h \sum_{j=1}^{i-1} a_{ij}(hJ_n)\, g_n(Y_{nj}), \tag{4a}$$

$$y_{n+1} = \mathrm{e}^{h J_n} y_n + h \sum_{i=1}^{s} b_i(hJ_n)\, g_n(Y_{ni}). \tag{4b}$$

For a variable step size implementation of (4), we base the step size selection on a local error control. For that purpose, we consider the embedded error estimator

$$\widehat{y}_{n+1} = \mathrm{e}^{h J_n} y_n + h \sum_{i=1}^{s} \widehat{b}_i(hJ_n)\, g_n(Y_{ni}) \tag{5}$$

and take the difference $\|y_{n+1} - \widehat{y}_{n+1}\|$ as error estimate.

3. Stiff order conditions

As usual in exponential integrators, the functions

$$\varphi_k(hJ) = h^{-k} \int_0^h \mathrm{e}^{(h-\tau)J} \frac{\tau^{k-1}}{(k-1)!}\, \mathrm{d}\tau, \qquad k \geq 1$$

play an important role. For sectorial operators J, the bound (2) shows that these functions are well defined and bounded on compact time intervals.

It is shown in [3] that the stiff order conditions for an exponential Rosenbrock-type method are given as:

No.	Order	Order Condition
1	1	$\sum_{i=1}^{s} b_i(hJ) = \varphi_1(hJ)$
2	2	$\sum_{j=1}^{i-1} a_{ij}(hJ) = c_i\varphi_1(c_i hJ), \quad 2 \le i \le s$
3	3	$\sum_{i=2}^{s} b_i(hJ)c_i^2 = 2\varphi_3(hJ)$
4	4	$\sum_{i=2}^{s} b_i(hJ)c_i^3 = 6\varphi_4(hJ)$

The first, third, and fourth order condition are just the (exponential) quadrature conditions, the second one is the well-known $C(1)$ condition, generalised to the operator case.

It is worth noting that the exponential Euler method applied to (3) is second-order accurate. It has one stage ($s = 1$) with weight $b_1(hJ) = \varphi_1(hJ)$ and consequently satisfies the first two order conditions.

4. Examples

From the above order conditions, it is straightforward to construct pairs of embedded methods up to order 4. We consider two examples. The method `exprb32` is a third-order method with a second-order error estimator (the exponential Euler method). Its coefficients are

$$\begin{array}{c|cc} c_1 & & \\ c_2 & a_{21} & \\ \hline & b_1 & b_2 \\ & \widehat{b}_1 & \end{array} \quad = \quad \begin{array}{c|cc} 0 & & \\ 1 & \varphi_1 & \\ \hline & \varphi_1 - 2\varphi_3 & 2\varphi_3 \\ & \varphi_1 & \end{array}$$

The method `exprb43` is a fourth-order method with a third-order error estimator. Its coefficients are

$$\begin{array}{c|ccc} c_1 & & & \\ c_2 & a_{21} & & \\ c_3 & a_{31} & a_{32} & \\ \hline & b_1 & b_2 & b_3 \\ & \widehat{b}_1 & \widehat{b}_2 & \widehat{b}_3 \end{array} \quad = \quad \begin{array}{c|ccc} 0 & & & \\ \frac{1}{2} & \frac{1}{2}\varphi_1\left(\frac{1}{2}\cdot\right) & & \\ 1 & 0 & \varphi_1 & \\ \hline & \varphi_1 - 14\varphi_3 + 36\varphi_4 & 16\varphi_3 - 48\varphi_4 & -2\varphi_3 + 12\varphi_4 \\ & \varphi_1 - 14\varphi_3 & 16\varphi_3 & -2\varphi_3 \end{array}$$

5. Stability and Convergence

For proving convergence estimates, the temporal smoothness of the *exact solution* is one of our basic ingredients. Using this property, we establish by Taylor series expansion a recursion for the global errors $E_n = y_n - y(t_n)$ in terms of the defects

$$E_{n+1} = \mathrm{e}^{h_n J_n} E_n + h_n \Delta_n.$$

Here Δ_n depends on the defects and on E_n itself. The stability of this recursion is all-important. It is verified in [3] that there exist constants C and Ω such that

$$\left\| \mathrm{e}^{h_n J_n} \cdots \mathrm{e}^{h_0 J_0} \right\| \;\leq\; C\, \mathrm{e}^{\Omega(h_0+\ldots+h_n)},$$

whenever the involved step sizes are sufficiently small. We emphasise that our proof of this result does *not* require the unrealistic condition $\left\| \mathrm{e}^{h_m J_m} \right\| \leq 1$.

A method is said to have *order* p, if it fulfils the stiff order conditions up to order p. For such methods, we have the following convergence result, see [3].

Theorem (Convergence). *Under the above assumptions, for $H > 0$ sufficiently small and $T \geq t_0$, there exists a constant C such that the global error satisfies*

$$\left\| y_n - y(t_0 + nh) \right\| \;\leq\; C\, h^p,$$

uniformly for all $0 < h \leq H$ and all $n \geq 0$ with $nh \leq T - t_0$. The constant C is independent of n and h.

Methods up to order 4 can be constructed easily, see the previous section. For numerical comparisons, we refer to [3].

References

[1] E. Hairer and G. Wanner, *Solving Ordinary Differential Equations II. Stiff and Differential-Algebraic Problems*. 2nd rev. ed., Springer, Berlin, 1996.

[2] M. Hochbruck and A. Ostermann, *Explicit exponential Runge-Kutta methods for semilinear parabolic problems*. SIAM J. Numer. Anal. **43** (2005), 1069–1090.

[3] M. Hochbruck, A. Ostermann, and J. Schweitzer, *Exponential Rosenbrock-type methods*. In preparation.

[4] A. Lunardi, *Analytic Semigroups and Optimal Regularity in Parabolic Problems*. Birkhäuser, Basel, 1995.

Optimization of DAEs with applications in Optimal Control

Shivakumar Kameswaran

(joint work with Lorenz T. Biegler)

Dynamic optimization aims at optimizing systems that are governed by differential equations. From a mathematical viewpoint, a dynamic optimization problem is an optimal control problem, which formally refers to the minimization of a cost (objective) function subject to constraints that represent the dynamics of the system. The last decade has witnessed a tremendous amount of effort going into optimization of DAEs. The focus was on developing numerical algorithms and optimization platforms, and solving interesting applications.

In order to cater to the scale and the complexity of present-day applications, the following directions must be explored: design of powerful numerical methods, optimization of systems governed by PDEs, ability to handle discrete decisions, identification of problem classes that can be solved by various dynamic optimization methodologies, reliability of NLP methodologies for dynamic optimization,