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Large stiff systems solved by Chebyshev methods

Chebyshev methods (also called stabilized methods) are explicit Runge-Kutta methods with extended stability domains along the negative real axis. These methods are intended for large mildly stiff problems, originating mainly from parabolic PDEs. We present here new Chebyshev methods of second and fourth order called ROCK, which can be seen as a combination and a generalization of van der Houwen-Sommeijer-type methods and Lebedev-type methods.

1. Parabolic equations, stiff ODE's and Chebyshev methods

Let us consider the following reaction-diffusion problem which is based on a chemical reaction between two substances, called the Brusselator (Lefever and Nicolis 1971),

$$\frac{\partial u}{\partial t} = 1 + u^2 v - 4u + \alpha \frac{\partial^2 u}{\partial x^2}, \qquad \frac{\partial v}{\partial t} = 3u - u^2 v + \alpha \frac{\partial^2 v}{\partial x^2}, \tag{1}$$

with $0 \leq x \leq 1$, $0 \leq t \leq 10$, $\alpha = 1/50$, and boundary conditions

$$u(0,t) = u(1,t) = 1, \quad v(0,t) = v(1,t) = 3, \quad u(x,0) = 1 + \sin(2\pi x), \quad v(x,0) = 3.$$

The spatial derivative is discretized by finite differences on a grid of $N = 40$ points. We integrate the resulting ODE with a standard explicit method, say DOPRI5 (method of Dormand & Prince of order 5 implemented by Hairer and Wanner, see [4]) and with ROCK2 and ROCK4 (Orthogonal Runge-Kutta Chebyshev methods of order 2 and 4 respectively). The following table shows the obtained results at $t = 10$. We see that DOPRI5 uses a huge number of steps due to the lack of stability along the negative axis.

Table 1: Results for the Brusselator (dimension $2N = 80$)

codes	tol	error	# steps(rejected)	# F-evals	Max # stages
DOPRI5	$0.5 \cdot 10^{-2}$	$8.12 \cdot 10^{-4}$	406(3)	2438	-
ROCK2	$0.5 \cdot 10^{-2}$	$3.34 \cdot 10^{-3}$	39(1)	273	11
ROCK4	$0.5 \cdot 10^{-2}$	$1.46 \cdot 10^{-3}$	16(1)	283	26

Chebyshev methods differ from “standard” Runge-Kutta methods in the following way: while in the classical theory one tries to fix a stage number and construct an integration formula with an order as large as possible, here we fix the order and vary the number of stages so as to satisfy the stability condition. The good performance of such methods is due to the property that the size of the stability domain, along $\mathbb{R}^-$, increases *quadratically* with the stage number. Thus, they are applicable to ODEs with a Jacobian possessing large eigenvalues around the negative real axis. Up to now, there exist two types of second order Chebychev methods: those of van der Houwen-Sommeijer [5], which possess a three-term recurrence relation but no optimal stability, and those of Lebedev [6], which are built upon optimal stability polynomials but without recurrence relation. ROCK methods *combine* these two strategies, i.e., they possess nearly optimal stability polynomials and a three-term recurrence relation. This new strategy is generalized to fourth order.

2. Orthogonal stability polynomials and ROCK methods

Existence and uniqueness of polynomials of order p, i.e. $R_s^p(z) - e^z = \mathcal{O}(z^{p+1})$, and degree s which remain bounded as long as possible along $\mathbb{R}^-$ are known (see [8]). In the case of $p = 1$, they are shifted Chebyshev polynomials. In [1] it was shown, using order stars, that for arbitrary p and s, we have the decomposition

$$R_s^p(z) = w_p(x) P_{s-p}(x),$$

where $w_p(x)$, polynomial of degree p, has p complex zeros ($p-1$ if p is odd) and $P_{s-p}(x)$, polynomial of degree $s-p$, possesses only real zeros. Using a theorem of Bernstein (1930) we can see that for p even, the orthogonal polynomials with respect to $w_p(x)^2/\sqrt{1-x^2}$ are very close to $P_{s-p}(z)$ (see [2]). This leads to the idea to construct new stability functions in the following way: for an even order p and a given degree s, we search for a positive approximation $\widetilde{w}_p(x)$ of $w_p(x)$ and $\widetilde{P}_{s-p}(x)$ an orthogonal polynomial with respect to the weight function $\widetilde{w}_p(x)^2/(\sqrt{1-x^2})$ such that

$$\widetilde{R}_s^p(x) = \widetilde{w}_p(x)\widetilde{P}_{s-p}(x)$$

is of order p and nearly optimal. The three-term recurrence relation of the orthogonal polynomials $\widetilde{P}_{s-p}(x)$ is then used to construct new numerical methods. They are implemented in a code called ROCK2 for $p = 2$ (see [2]) and ROCK4 for $p = 4$ (see [3]). In the latter case, the construction require the Butcher group (composition methods) to realize fourth order also for nonlinear problems.

Example of a large stiff system. We take the problem (1) but now in two spatial variables. We increase the number of grid points from $N = 40$ to $N = 128$ and the coefficient α to 0.1. We obtain an ODE of dimension $2N^2 = 32768$ with a spectral radius of the Jacobian close to $\rho \simeq 13200$. The following picture is the work-precision diagram for several tolerances (starting from 10^{-2} with integer exponent tolerances represented by enlarged symbols). We made comparisons between the following codes: ROCK2 and ROCK4, RKC (second order Chebyshev code of Sommeijer, Shampine and Verwer see [9]), RADAU5 (implicit code of order 5 by Hairer and Wanner see [4]) and DUMKA4 (fourth order code of Medovikov, an extension of Lebedev's methods, see [7]). We emphasize that Chebyshev methods are as simple to use as the Euler explicit method, while implicit methods applied, say, to the 2-dimensional Brusselator, require expensive linear algebra. We see that even compared to an optimized stiff code (use of FFT methods for the linear algebra), ROCK methods show a nice behavior. Source codes for ROCK are available at http://www.unige.ch/math/folks/hairer/software.html

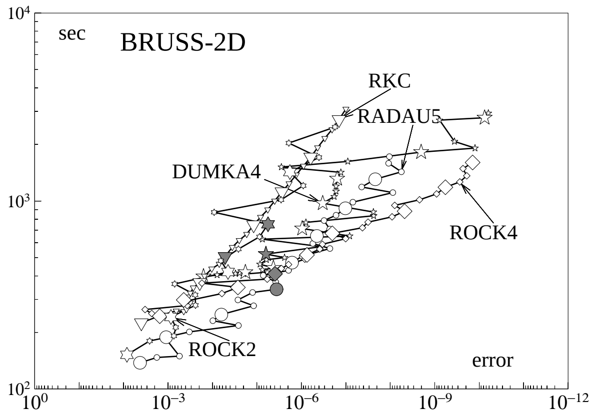

Figure 1: Work-precision diagram for the 2-dim. Brusselator problem

Acknowledgements

The author is grateful to Gerhard Wanner and Ernst Hairer for helpful discussions.

3. References

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