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Explicit Stabilized Integration of Stiff Determinisitic or Stochastic Problems

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Abstract. Explicit stabilized methods for stiff ordinary differential equations have a long history. Proposed in the early 1960s and developed during 40 years for the integration of stiff ordinary differential equations, these methods have recently been extended to implicit-explicit or partitioned type methods for advection-diffusion-reaction problems, and to efficient explicit solvers for stiff mean-square stable stochastic problems. After a short review on the basic stabilized methods we discuss some recent developments.

Keywords: stiff differential equation, advection-diffusion-reaction, stochastic problem, mean-square stability, explicit orthogonal Runge-Kutta Chebyshev method, ROCK
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EARLY DEVELOPMENT

The basic idea for constructing explicit stabilized methods goes back to the 1960s (Saul'ev, Yuan Chzao Din, Franklin, Guillou and Lago, Gentsch and Schlüter, see [8, IV.2]) and consists in considering a composition of s explicit Euler steps with step sizes h_i (the internal stages of the method) and requiring stability after each "super step size" of length $\Delta t = h_1 + \ldots + h_s$. For a given s the optimal step sizes are given by $h_i = -\Delta t/p_i,\ i = 1,\ldots,s$, where p_i are the zeros of $R_s(p) = T_s(1 + p/s^2)$ and $T_s(\cdot)$ is the Chebyshev polynomial of degree s that can be defined recursively as $T_0(p) = 1,\ T_1(p) = z,\ T_j(p) = 2pT_{j-1}(p) - T_{j-2}(p),\ j \geq 2$.

It has quickly been realized that the ordering of the Euler internal steps is crucial to also guarantee the stability *within* a "super step size" (internal stability). Indeed, unlike traditional Runge-Kutta (RK) methods, Chebyshev methods can have a large number of internal stages (e.g., 100, 200). An efficient implementation of such methods (that controls also internal stability) for the ordinary differential equations $\frac{dX}{dt} = F(X),\ X(0) = X_0,\ F : \mathbb{R}^d \to \mathbb{R}^d$ (an autonomous form is considered here for simplicity), first given in [9], reads

$$X_1 = K_s, \quad K_j = 2\Delta t \frac{T_{j-1}(\omega_0)}{T_j(\omega_0)} F(K_{j-1}) + 2\omega_0 \frac{T_{j-1}(\omega_0)}{T_j(\omega_0)} K_{j-1} - \frac{T_{j-2}(\omega_0)}{T_j(\omega_0)} K_{j-2}, \quad j = 2,\ldots,s, \tag{1}$$

where $K_0 = X_0,\ K_1 = X_0 + h\frac{\omega_1}{\omega_0} F(K_0),\ \omega_0 = 1 + \frac{\eta}{s^2},\ \omega_1 = \frac{T_s(\omega_0)}{T_s'(\omega_0)}$. The integer s is the stage number of the RK method. Applied to the standard test problem to analyze linear stability of a RK methods, namely $dX/dt = \lambda X$, on obtains after one step $X_1 = \frac{T_s(\omega_0 + \omega_1 p)}{T_s(\omega_0)} X_0 = Q_{s,\eta}(p) X_0$, where $p = \lambda \Delta t$. The property $Q_{s,\eta}(p) = 1 + p + \mathcal{O}(p^2)$ ensures that the methods (1) are first order accurate (for linear and nonlinear problems). One ensures $|X_1| \leq |X_0|$, i.e., stability for the test problem, whenever p belongs to the stability domain $S_{s,\eta} = \{p \in \mathbb{C}; |Q_{s,\eta}(p)| \leq 1\}$. One can show that the Chebyshev method (for a given s) is stable in the real negative interval $[-c(\eta) \cdot s^2, 0]$, $(c(\eta) \leq 2)$. Thus, for stiff dissipative problems (when the Jacobian of the right-hand side of the ODE has large real negative eigenvalues) the stability/work ratio of Chebyshev methods behaves like $c(\eta) \cdot s$, while for the explicit Euler method this ratio is equal to 2. This represents a tremendous computational improvement for stiff problems compared to standard explicit methods. The parameter η plays a crucial role. For $\eta = 0$ we have $Q_{s,0}(p) = T_s(1 + p/s^2)$ and $c(0) = 2$. However, at the s extrema of a Chebyshev polynomial along the negative real axis, the corresponding stability domain has no extension in the imaginary direction and there is no damping of higher frequencies. Introducing a damping for the methods (1) forces the local extrema to be strictly less that one and keeps the stability domains at a safe distance of the negative real axis.

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HIGHER ORDER METHODS, PARTITIONED AND IMEX METHODS

Explicit stability functions with rth order accuracy, i.e, $1+p+\ldots+p^r/r!+\mathcal{O}(p^{r+1})$ bounded in a strip as long as possible around the negative real axis are not available in an explicit analytical form for $r>1$ (existence and uniqueness of such functions are however established in [12]). Various strategies have been proposed to approximate such polynomials. We mention DUMKA methods of order two [11] and the Runge-Kutta-Chebyshev methods [9] based on a linear combination of Chebyshev polynomials. The stability domains of the DUMKA methods include the optimal interval ($\simeq [-0,82\cdot s^2,0]$) along the negative real axis, while the stability domains of RKC methods cover only 80% of these interval. However, the RKC methods are more convenient to implement thanks to the three-term recurrence relation of the Chebyshev polynomials. The third strategy leading to the orthogonal Runge-Kutta Chebyshev methods (ROCK) [1, 2] combines the optimality of DUMKA stability functions and the three-term recurrence relation of the RKC stability functions. The stability functions of ROCK methods (given here for order $r=2$) are based on the approximation of the optimal stability polynomials by functions of the form

$$R_s(p)=w_2(p)P_{s-2}(p), \tag{2}$$

where $P_{s-2}(p)$ (a polynomial of degree $s-2$) is a member of the family of polynomials $\{P_j(p)\}_{j\geq 0}$ (of degree j normalized such that $P_j(0)=1$) orthogonal with respect to the weight function $w_2(p)^2/\sqrt{1-p^2}$. The polynomials $w_2(p)$ with complex zeros (that depend on s) are adjusted so that $R_s(p)=1+p+\frac{p^2}{2}+\mathcal{O}(p^3)$ and to ensure at the same time a large stability interval along the negative real axis. The recurrence relation of the orthogonal polynomials $\{P_j(p)\}_{j\geq 0}$ (that gives the parameters μ_j,ν_j,κ_j below), yields a family of methods based on recurrence formula [2]

$$\begin{aligned} K_j &= \alpha\mu_j hF(K_{j-1})-\nu_j K_{j-1}-\kappa_j K_{j-2}, \quad j=2,\cdots,s-2,\\ K_{s-1} &= K_{s-2}+\sigma_\alpha hF(K_{s-2}),\\ X_1 &= K_{s-2}+\Delta t(2\sigma_\alpha-\frac{\tau_\alpha}{\sigma_\alpha})F(K_{s-2})+\Delta t\frac{\tau_\alpha}{\sigma_\alpha}F(K_{s-1}), \end{aligned} \tag{3}$$

where $K_0=X_0,\ K_1=K_0+\alpha\mu_1 hF(K_0)$. The original ROCK2 methods are based on (3) with $\alpha=1$ and the $R_s(p)$ polynomial oscillates around the negative real axis with absolute value of the local extrema fixed to $\simeq 0.95$ (see Figure 1, left picture). The parameter α introduced in [5] allows to adjust the damping of the method and the value of σ_α and τ_α can be adjusted to obtain second order accuracy. Although a simple idea, this new way of introducing variable damping in the ROCK2 methods allows for interesting extension to stochastic problems and advection diffusion reaction problems.

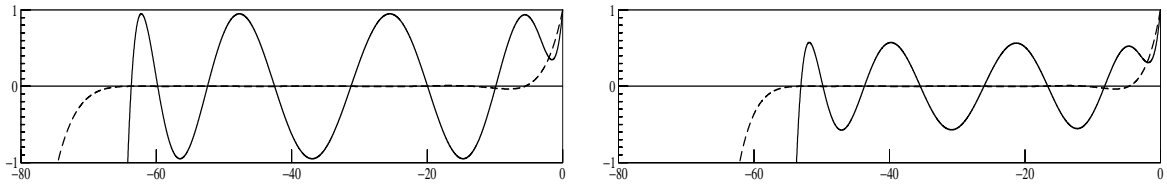

FIGURE 1. Solid line: ROCK2 stability functions $\alpha=1$ (left Fig.), $\alpha=1.2$ (right Fig). Dashed line: polynomial $P_{s-2}(\alpha p)$.

Chebyshev methods have also been recently used for designing partitioned Runge-Kutta methods for ODEs of the form

$$\frac{dX}{dt}=F_D(X)+F_G(X), \quad X(0)=X_0, \tag{4}$$

where $F_D(X)$ corresponds to a diffusion term and $F_G(X)$ to an advection or reaction term. In [15], the RKC methods have been combined with an explicit starting and finishing procedure that integrates the F_G term. The resulting methods are explicit partitioned Runge-Kutta methods of second order (that needs only four evaluations of the F_G function) suitable for problems where F_G is non-stiff but potentially expensive to evaluate. These methods have also a better stability along the imaginary axis than the original RKC method. Another extension of the RKC methods is the implicit-explicit (IMEX) methods proposed in [14]. There, the idea is to treat implicitly (via the implicit Euler method) the F_G part within each RKC internal stage in order to treat problems that are very stiff in the F_G term. The

gain compared to standard implicit method arises in the situation when the F_G term alone is much cheaper to treat implicitly. Solving implicitly for F_G amounts to solve a large number (e.g., proportional to the degrees of freedom of the partial differential equation) of small decoupled implicit systems. Notice that in the IMEX RKC methods, these implicit systems have to be solved in each internal stage.

STABILIZING EXPLICIT STOCHASTIC INTEGRATORS

We briefly explain the extension of Chebyshev methods for stochastic problems. Consider the Itô stochastic system of differential equations

$$dX(t) = F(X(t))dt + \sum_{r=1}^{m} g^r(X(t))dW_r(t), \quad X(0) = X_0, \tag{5}$$

where $X(t)$ is a random variable with values in $\mathbb{R}^d$, $F : \mathbb{R}^d \to \mathbb{R}^d$ is the drift term, $g^r : \mathbb{R}^d \to \mathbb{R}^d,\ r = 1,\ldots,m$ are the diffusion terms, and $W_r(t),\ r = 1,\ldots,m$ are independent one-dimensional Wiener processes. The simplest method to approximate solutions to (5) is the so-called Euler-Maruyama method $X_{n+1} = X_0 + hF(X_n) + \sum_{r=1}^{m} g^r(X_n)\Delta W_{n,r}$, where $\Delta W_{n,r} \sim \mathcal{N}(0,h),\ r = 1,\ldots m$ are independent Wiener increments. This method has strong order $1/2$ and weak order 1 for general systems of Itô SDEs. In practice besides the order of convergence optimizing stability properties of a numerical method is also an important issue. We focus here on mean-square stability. To gain insight on the stability behavior of a numerical method, a widely used problem is the linear scalar test problems ($d = m = 1$) [13] $dX = \lambda X dt + \mu X dW(t)$, $X(0) = 1$, with fixed complex scalar parameters λ, μ. The exact solution of the test problen, given by $X(t) = \exp((\lambda + \frac{1}{2}\mu^2)t + \mu W(t))$, is mean-square stable if and only if

$$\lim_{t\to\infty} \mathbb{E}\big(|X(t)|^2\big) = 0 \iff (\lambda,\mu) \in \mathcal{S}^{MS}_{\mathrm{SDE}} := \left\{ (\lambda,\mu) \in \mathbb{C}^2 \ ;\ \Re(\lambda) + \frac{1}{2}|\mu|^2 < 0 \right\}. \tag{6}$$

A stochastic integrator applied to the test problem gives the one step difference equation $X_{n+1} = R(p,q,\xi_n)X_n$, where $p = \lambda h, q = \mu\sqrt{h}$, and ξ_n is a random variable. The numerical method is said to be mean-square stability if

$$\lim_{t\to\infty} \mathbb{E}(|X_n|^2) = 0 \iff \mathcal{S}^{MS}_{num} := \left\{ (p,q) \in \mathbb{C}^2 \ ; \mathbb{E}|R(p,q,\xi)|^2 < 1 \right\}. \tag{7}$$

For the Euler-Maruyama method, we have $R(p,q,\xi_n) = 1 + p + q\xi$ and the corresponding stability domain (restricting to real p,q) is a disc of radius 1 centered in -1, which covers only a small region of the stability domain of the exact solution. To explain the concept of explicit stabilization, we introduce (again for p,q real) the "portion of the true mean-square stability region" $\mathcal{S}^{MS}_{num,a} = \{(p,q) \in [-a,0) \times \mathbb{R} \ ;\ p + \frac{1}{2}|q|^2 < 0\}$, and define for a given method $\ell = \sup\{a > 0 \ ;\ \mathcal{S}_{SDE,a} \subset \mathcal{S}^{MS}_{num}\}$. The goal is now to derive a method with ℓ as large as possible. The idea for stabilizing the Euler-Maruyama method is now simply to damp its stability function $R(p,q,\xi) = 1 + p + q\xi$ with the stability functions of 1st order Chebyshev methods $Q_{s,\eta}(p)$ with a value of the damping parameter η optimized for each stage number s, see [3, 4]. The corresponding Runge-Kutta type methods read [4]

$$X_1 = K_s + \sum_{r=1}^{m} g^r(K_s)\Delta W_r, \tag{8}$$

where K_s is given by (1). Applied to the linear test problem it yields $R(p,q,\xi_n) = Q_{s,\eta}(p)(1 + q\xi)$, hence the Euler-Maruyama method is stabilized by the polynomial with appropriate "damping" $Q_{s,\eta}(p)$. The method (8), denoted by S-ROCK(1/2,1) has strong order 1/2 (for general non-commutative problems) and weak order 1. Another family of methods of strong order 1 and weak order 1 has been considered in [4] written here in a derivative free form as

$$X_1 = K_s + \sum_{r=1}^{m} g^r(K_s)\Delta W_r + \frac{1}{2}\sum_{r=1}^{m}\left(g^r\Big(K_s + \sum_{q=1}^{m} g^q(K_s)I_{q,r}\Big) - g^r\Big(X_0 - \sum_{q=1}^{m} g^q(K_s)I_{q,r}\Big)\right), \tag{9}$$

where $I_{q,r} = \int_{t_0}^{t_1}\int_{t_0}^{t} dW_q(s)dW_r(t)$ are multiple stochastic integrals. It turns out that S-ROCK(1/2,1) and S-ROCK(1,1) include a portion of the true mean-square stability domain that scale like $\ell_{\mathrm{S-ROCK(1/2,1)}} = 0.33 \cdot s^2$ and $\ell_{\mathrm{S-ROCK(1,1)}} = 0.19 \cdot s^2$, respectively.

Using the ROCK methods (3), appropriate damping and considering further two additional orthogonal polynomials $P_{s-1}(p), P_s(p)$ (to enhance the damping of the noise terms) weak second order methods (S-ROCK2) have been constructed in [5]. They can be seen as a stabilized version of the derivative free Talay-Milstein method. The cost per time step of the methods is $s+2$ evaluations of the drift function F, 6 (independent of m) evaluations of the diffusion functions g^r and $2m$ simulations of independent discrete random variables. The portion of the true mean-square stability domain included in the stability domain of the S-ROCK2 methods scales as $\ell_{\mathrm{S-ROCK(1,1)}} = 0.42 \cdot (s+2)^2$. These methods are shown to be more efficient than the weak second order stochastic extension of the ROCK2 methods proposed in [10]. It is also more efficient (except for the small noise regime) than the diagonally drift-implicit weak second order method proposed in [7].

TOWARDS SWISS KNIFE INTEGRATORS

Combining the ROCK2 methods with damping (3) and the idea of damping enhancement through additional orthogonal polynomials $P_{s-1}(p), P_s(p)$, partitioned implicit-explicit methods (PI-ROCK) are constructed in [6] for the problem

$$\frac{dX}{dt} = F_D(t,X) + F_A(t,X) + F_R(t,X), \quad X(0) = X_0, \tag{10}$$

where $F_D(t,X)$ represents diffusion terms with eigenvalues close to the negative real axis, $F_A(t,X)$ corresponds to advection terms with eigenvalues close to the imaginary axis, and $F_R(t,X)$ represents stiff reaction terms. For $F_A = F_R = 0$, the method is identical to the ROCK2 method. PI-ROCK methods are more efficient than RKC IMEX methods for problem with stiff reaction as they require only 2 resolution of a nonlinear system (independently of the stage number s), whereas s nonlinear systems are solved in the RKC IMEX methods. It is more efficient than the PRKC methods as PI-ROCK methods include larger stability domains in the imaginary direction an can handle problems with dominated advection efficiently (similarly as for the PRKC methods, stiff costly reaction term are evaluated only a few time per time step). PI-ROCK methods are implemented with variable step size and with the flexibility of turning on and off the various terms in (10). Finally, these methods can also handle problems (10) with noise, e.g.,

$$dX = (F_D(t,X) + F_A(t,X) + F_R(t,X))dt + \sum_{r=1}^{m} g^r(X(t))dW_r(t), \; X(0) = X_0. \tag{11}$$

For such problems, the PI-ROCK methods become a family of weak first order integrators including even even larger portions of the true mean-square stability regions than the S-ROCK(1/2,1) or the S-ROCK(1,1) methods.

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