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A real distinct poles Exponential Time Differencing scheme for reaction–diffusion systems

E.O. Asante-Asamani [a], A.Q.M. Khaliq [b], B.A. Wade [a,*]

[a] Department of Mathematical Sciences, University of Wisconsin-Milwaukee, Milwaukee, WI 53201-0413, USA

[b] Department of Mathematical Sciences, Middle Tennessee State University, Murfreesboro, TN 37132, USA

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ABSTRACT

A second order Exponential Time Differencing (ETD) method for reaction–diffusion systems which uses a real distinct poles discretization method for the underlying matrix exponentials is developed. The method is established to be stable and second order convergent. It is demonstrated to be robust for problems involving non-smooth initial and boundary conditions and steep solution gradients. We discuss several advantages over competing second order ETD schemes.

1. Introduction

Time-dependent reaction–diffusion–advection equations are mathematical models of the form

$$u_t + \nabla \cdot (\vec{a}u) = \nabla(D\nabla u) + f(u)$$

used in many applications, *cf.* [1–3]. The advection term in this equation can be handled with our methods, according to whether the resulting abstract operator remains sectorial. Generally, these can be classified as semilinear parabolic IVP

$$u_t + Au = f(t,u) \quad \text{in } X,\ t \in (0,T),$$
$$u(0,\cdot) = u_0,$$

where $-A$ generates an analytic semigroup $E(t) = e^{-At}$ in X and f a sufficiently smooth nonlinear reaction term. We assume X is a Banach space and $A : \mathcal{D}(A) \to X$ is a sectorial operator. For details and bounds for the semigroup $E(t)$ see [4,5].

Among many time stepping methods developed to solve such parabolic PDE's are the class of Exponential Time Differencing (ETD) schemes. These schemes search for solutions to the integral formulation of the IVP, i.e.

$$u(t) = e^{-tA}u_0 + \int_0^t e^{-(t-s)A} f(s,u(s))ds \quad \forall t \in [0,T].$$

The major attraction of ETD schemes is the separate treatment of the linear part by the discretization of the exponential operator and using the advantage of the one-step variation of constants integral formula to avoid the necessity of iteration of the nonlinearity, which reduces computational time and preserves accuracy.

In 2002, Cox and Matthews [6] introduced a class of exponential time differencing schemes, ETD Runge–Kutta schemes. A major challenge in that work and for other schemes as well as more general problems has been the efficient resolution

* Corresponding author.
E-mail addresses: eoa@uwm.edu (E.O. Asante-Asamani), abdul.khaliq@mtsu.edu (A.Q.M. Khaliq), wade@uwm.edu (B.A. Wade).

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of the matrix exponentials. B. Kleefeld et al. introduced an ETD Crank–Nicolson Scheme [7] which utilizes a Padé-(1,1) rational approximation for the matrix exponential. The resulting scheme, though highly efficient, is not L-stable and hence does not damp out spurious oscillations generated by non-smooth initial and boundary conditions. A follow-up paper [8] addresses this problem by proposing the use of a Padé-(0,2) rational approximation, which is L-acceptable. However, the partial fraction decomposition of this approximation, used in deriving the scheme, has complex poles and requires complex arithmetic in all applications, which may slow the evolution process, depending on the matrices.

In this work, we propose a new Exponential Time Differencing Scheme, ETD-RDP, which utilizes a non-Padé rational approximation with real and distinct poles for approximating the matrix exponentials. The scheme is L-stable and thus damps out spurious oscillations. The added advantage of having real and distinct poles for the partial fraction decomposition is that we avoid complex arithmetic and can take advantage of parallel implementation to speed up computation.

2. ETD-schemes

Define $V = \mathcal{D}(A^\alpha) \subset X$, where $0 \leq \alpha \leq 1$ with A being a closed linear invertible operator. The linear space V is a Banach space, X_α with norm $\|v\|_V = \|A^\alpha v\|$. Our main assumption on f is the following:

Assumption 1 *([4,5])*. Let Y be an open subset of $\Re \times X_\alpha$ and $f : Y \to X$ satisfies: For every $(t, u) \in Y$ there is a neighborhood $V \subset Y$ and constants $L \leq 0$, $0 < \theta \leq 1$ such that

$$\|f(t_1, u_1) - f(t_2, u_2)\| \leq L(|t_1 - t_2|^\theta + \|u_1 - u_2\|_\alpha)$$

for all $(t_i, u_i) \in V$.

Then standard semigroup theory [4,5] yields that for every initial data $(t_0, u_0) \in Y$ the initial value problem has a unique local solution

$$u \in C([t_0, t) : X) \bigcap C^1((t_0, t_1) : X)$$

where $t_1 = t_1(t_0, u_0) > t_0$. The local, mild solution satisfies the integral formulation of our IVP, which can be reformulated into the recurrence relation

$$u(t_{n+1}) = e^{-Ak}u(t_n) + \int_{t_n}^{t_{n+1}} e^{-A(t_{n+1}-s)}f(s, u(s))ds.$$

By setting $s = t_n + \tau k$ with $t_n = nk (0 \leq k \leq k_0; 0 \leq n \leq N)$ and $\tau \in [0, 1]$ we can reduce the recurrence relation to the more useful form

$$u(t_{n+1}) = e^{-Ak}u(t_n) + k\int_0^1 e^{-Ak(1-\tau)}f(t_n + \tau k, u(t_n + \tau k))d\tau,$$

which is the basis for deriving ETD schemes.

Methods of various order and properties can be obtained by different discretizations of the integral. Here, we focus on second order ETD schemes, which employ a linear approximation of the non-linear function

$$f(t_n + s, u(t_n + s)) \approx f(t_n, u(t_n)) + s\left(\frac{f(t_{n+1}, u(t_{n+1})) - f(t_n, u(t_n))}{k}\right), \quad s = \tau k \in [0, k],$$

to obtain the semi-discrete scheme

$$u_{n+1} = e^{-Ak}u_n + A^{-1}(I - e^{-Ak})f(u_n) + \frac{A^{-2}}{k}(kA - I + e^{-Ak})[f(u_{n+1}) - f(u_n)].$$

Towards a semidiscrete scheme, a locally second order approximation of u_{n+1} will be employed:

$$u^* = e^{-Ak}u_n + A^{-1}(I - e^{-Ak})f(u_n).$$

The semi-discrete scheme then becomes

$$\begin{aligned} u_{n+1} &= e^{-Ak}u_n + A^{-1}(I - e^{-Ak})f(u_n) + \frac{A^{-2}}{k}(kA - I + e^{-Ak})[f(u^*) - f(u_n)] \\ u^* &= e^{-Ak}u_n + A^{-1}(I - e^{-Ak})f(u_n) \end{aligned} \tag{1}$$

where we assume the spatial operator A has been discretized to a matrix through any of many standard techniques such as finite differences, finite elements, spectral methods, etc.