Research Journal of Applied Sciences, Engineering and Technology 4(19): 3539-3543, 2012
ISSN:2040-7467

Submitted: January 03, 2012 Accepted: February 09, 2012 Published: October 01, 2012

A Review of Time Discretization of Semi-linear Parabolic Problems

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Abstract: In this study, exponentialRunge-Kutta methods of collocation type are considered for linear and semi-linear parabolic problems. An abstract Banach space framework of sectorial operators and Lipchitz continuous nonlinearities are selected for the analysis. Exponential Runge-Kutta methods of collocation type are also employed for parabolic Cauchy problems. Moreover, numerical experiments have been presented for illustration of parabolic problems.

Keywords: Exponential integrators, exponential quadrature rules, Range-kutta methods, schrödinger equation, semi-linear parabolic problems

INTRODUCTION

In this study, the time discretization of semi-linear parabolic problems are proposed:

$$u'(t)+A\,u(t) = g(t,u) \qquad (1)$$
$$u(t_0) = u_0$$

by the exponential Runge-Kutta methods. A numerical solution of (1) based on the variation of constants formula has been presented. Besides that, the well-known construction of collocation methods for ordinary differential equations is considered. Lawson (1967) deliberated the formula of Exponential Time Differencing (ETD) schemes that are based on integrating the linear parts of the differential equations exactly and approximating the nonlinear terms by polynomials that are integrated. Lubich and Ostermann (1993, 1995) argued a stability and error analysis of linearly implicit one-step for time discretization of nonlinear parabolic equation. Cox and Matthews (2002) studied a clear derivation of the explicit Exact Linear Part (ELP) method, which they have been submitted to the methods as Exponential Time Differencing (ETD) and their implementation of the ETD methods. The exponential Runge-Kutta methods of collocation type for solving linear and semi-linear Cauchy problems on the d-dimension torus were claimed by Dujardin (2009). Hochbuck and Ostermann (2005) considered the explicit exponential Runge-Kutta methods for the time integration of semi-linear parabolic problems and a new derivation of the classical (nonstiff) order was also classified for Runge-Kutta methods. Other papers on this subject include (Hochbruck and Lubich, 1999; Berland *et al*., 2007; Boyd, 2001; Certaine, 1960; Sheen *et al*., 2000; Berland *et al*., 2007).

A numerical analysis of exponential Runge-Kutta methods of collocation type applied to the linear and semi-linear Schrödinger equation has been proposed on a d-dimension torus. Moreover, linear and semi-linear problems have been presented with two examples and numerical experiments.

METHODOLOGY

Exponential Runge-kutta methods of collocation type: The main idea behind exponential integrators of collocation type is to replace the function g in the variation of constants formula:

$$u(t_n+h) = u(t_n)e^{-hA} + \int_0^h e^{-(h-\tau)A} g\big(t_n+\tau, u(t_n+\tau)\big)d\tau \qquad (2)$$

by a collocation polynomial $\hat{g}_n$ which that yields:

$$u(t_n+h) \approx u(t_n)e^{-hA} + \int_0^h e^{-hA}\hat{g}_n(\tau)d\tau \qquad (3)$$

Choosing non-confluent collocation nodes $c_1, c_2, \ldots, c_s$ and it is assumed that approximations are given:

$$u_n \approx u(t_n)$$
$$U_{n,i} \approx u(t_n + c_i h)$$

The collocations:

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$$\hat{g}_n(c_i h) = g(t_n + c_i h, U_{n,i})G_{n,i} \tag{4}$$

is defined so that:

$$\hat{g}_n(\tau) = \sum_{j=1}^{s} L_j(\tau) G_{n,i} \tag{5}$$

where, L_i is the Lagrange interpolation polynomial:

$$L_j(\tau) \prod_{m \neq j} \frac{\tau / h - c_m}{c_j - c_m} \tag{6}$$

replacing $u(t_n)$ in (3) by the given approximation u_n, the evaluation of the integral yields an approximation to the exact solution at time t_{n+1}:

$$u_{n+1} = u_n e^{-hA} + h \sum_{i=1}^{s} b_i(-hA) G_{n,i} \tag{7}$$

where,

$$b_i(-hA) = \frac{1}{h}\int_0^h e^{-(h-\tau)A} L_i(\tau) d\tau \tag{8}$$

$U_{n,i}$ can be defined by substituting h with $c_i h$ in (3), it is obtained:

$$U_{n,i} = u_n e^{-c_i hA} + h \sum_{j=1}^{s} a_{ij}(-hA) G_{n,i} \tag{9}$$

where,

$$a_{ij}(-hA) = \frac{1}{h}\int_0^{c_i h} e^{-(c_i h-\tau)A} L_j(\tau) d\tau \tag{10}$$

Since L_j is a polynomial of degree at most $s-1$, the coefficients b_i $(-hA)$ and a_{ij} $(-hA)$ are linear combinations of the functions (Hochbruck and Ostermann, 2005; Minchev and Wright, 2005):

$$\varphi_j(-tA) = \frac{1}{t^j}\int_0^t e^{-(t-\tau)A} \frac{\tau^{j-1}}{(j-1)!} d\tau \qquad 1 \leq j \leq s \tag{11}$$

The schemes (7), (8), (9) and (10) are called exponential Runge-Kutta methods of collocation type. Moreover, it is noted that for later use:

$$\varphi_{k+1}(Z) = \frac{\varphi_k(Z) - \frac{1}{k!}}{Z}, \ \varphi_k(Z) = \frac{1}{k!} \tag{12}$$

If the limit A→ 0 is considered, this construction reduces to the construction of Runge-Kutta methods $b_i = b_i(0)$ and $a_{ij} = a_{ij}(0)$ and also the underling Runge-Kutta method has been obtained by the limiting method.

Linear problems: In this part, the error bounds for exponential Runge-Kutta discretization of linear parabolic problems (13) have been presented (Hochbruck and Ostermann, 2005; Henry, 1981; Nie *et al*., 2006):

$$u'(t)+Au(t) = f(t) \qquad u(0) = u_0, \tag{13}$$

where, A is time-invariant operator.

Note that for such problems, exponential Runge-Kutta methods reduce to exponential quadrature rules:

$$u_{n+1} = u_n e^{-hA} + h \sum_{i=1}^{s} b_i(-hA) f(t_n + c_i h) \tag{14}$$

with

$$b_i(-hA) = \frac{1}{h}\int_0^h e^{-(h-\tau)A} L_i(\tau) d\tau \tag{15}$$

The analysis of (14) is based on an abstract formulation of (13) as an evolution in a Banach space (X, $\|.\|$) .

Let $D(A)$ denotes the domain of A in X . The basic assumption on the operator A is that of (Henry, 1981; Gallopoulos and Saad, 1992).

Assumption 1: Let $A{:}D(A) \to X$ be sectorial, i.e., A is a densely defined and closed operator on X to satisfy the resolvent condition:

$$\left\| (\lambda I - A)^{-1} \right\| \leq \frac{M}{|\lambda - a|} \tag{16}$$

on the sector

{є¢: $\theta \leq |\arg(\lambda - a)| \leq \pi$, $\lambda \neq a$} for $M \geq 1$, $a \in R$ and $0 < \theta < \pi / 2$.

Note that under this assumption, the operator $-A$ is the infinitesimal generator of an analytic semigroup $\{e^{-tA}\}$. For $\omega > -a$, the fractional powers of $\tilde{A} = A + \omega I$ are well-defined.

The convergence results have been shown (Hochbruck and Ostermann, 2005).

Example 1: To demonstrate the sharpness of the bounds in theorem 3 (Hochbruck and Ostermann, 2005), the linear parabolic problem is considered:

Table 1: Numerically observed temporal orders of convergence in different norms for discretizations with N spatial degrees of freedom and h = 1/128

N	H^1	L^1	L^2	L^∞
50	2.80	3.53	3.27	3.00
100	2.76	3.50	3.26	3.01
200	2.75	3.50	3.25	3.00

Table 2: Numerically observed temporal orders of convergence in the maximum norm with 200 grid points and h = 1/32

Gauβ	Gauβ	Radau	Radau
s =1	s = 2	s = 2	s = 3
2.02	3.01	3.03	4.06

$$\frac{\partial U}{\partial t}(x,t) - \frac{\partial^2 U}{\partial x^2}(x,t) = \left(2 + x(1+x)\right)e^t \qquad (17)$$

for $x \in [0,1]$ and $t \in [0,1]$, subject to homogenous Dirichlet boundary conditions. For initial value $x(1-x)$, the exact solution is $U(x, t) = x\,(1- x)e^x$.

The problem is discretized in space by standard finite differences and in time by the exponential 2-stag Gauss method, respectively. The numerically observed temporal orders of convergence in different norms are shown in Table 1.

The attainable value of β in Theorem 3 (Hochbruck and Ostermann, 2005) relies on the characterization of the domains of fractional powers of elliptic operators. The source function in (17) is spatially smooth but does not satisfy the boundary condition. For the choice $X = L^2$, the best value is $\beta = \frac{1}{4} - \varepsilon$ (Fujiwara, 1967). This explains the observed orders in the discrete L^2-norm in Table 1. The results in other norms can be shown in a similar way (Lubich and Ostermann, 1993).

Semi-linear problems: In this part, the convergence properties of exponential Runge-Kutta methods for parabolic problems (1) have been considered. As the abstract of Banach space has been proposed, it is assumed that the linear operator A satisfies the assumption 1.

The basic assumption on g are determined. So, $V = D(\tilde{A}^{\propto})$ is defined where, is the shifted operator $\tilde{A} = A + \omega I$ and $0 \le \propto < 1$. The linear space V is a Banach space with norm $\|\upsilon\|_V = \|\tilde{A}^{\propto}\upsilon\|$.

Note that this definition does not depend on ω, since choices of ω give rise to equivalent norms.

Assumption 2: Let $g : [0, 1] \times V \to X$ be locally Lipschitez-continuous. Thus, there is a real number $L(R,T)$ such that:

$$\| g(t, \upsilon) - g(t, \omega)\| \le L\|\upsilon - \omega\|_v$$

for all $t \in [0,T]$ and Max $(\|\upsilon\|_v, \|\omega\|_v) \le R$.

Note that the convergence results have been demonstrated (Hochbruck and Ostermann, 2005).

Example 2: To demonstrate the bounds in theorem 5 (Hochbruck and Ostermann, 2005), the semi-linear parabolic problem is considered:

$$\frac{\partial U}{\partial t}(x,t) - \frac{\partial^2 U}{\partial x^2}(x,t) = \frac{1}{1+U(x,t)^2} + \varnothing(x,t) \qquad (18)$$

for $x \in [0,1]$ and $t \in [0, 1]$, subject to homogenous Dirichlet boundary conditions. The source function $\varnothing$ is chosen in such way that the exact solution is $U(x,t) = x(1-x)e^x$.

The problem is discretized in space by standard finite differences with 200 grid points and in time by the various methods with step size 1/200, respectively. The numerically observed temporal orders of convergence in the maximum norm are shown in Table 2.

Note that the temporal order of convergence can be improved further under slightly stronger assumptions on the spatial regularity (Lubich and Ostermann, 1993).

NUMERICAL EXPERIMENTS

In this section, two kinds of numerical experiments are considered. Both of them have been performed with s = 2collocation points.

- The first method is defined by $c_1 = 1/2$ and $c_2 = 1$. This method does not satisfy reaction (Dujardin, 2009).Moreover, its underlying Runge-Kuttamethod is exactly of order 2.
- The second method is defined by $c_1 = 1/3$ and $c_2 = 1$. This method satisfies reaction (Dujardin, 2009).Therefore, its underlying Runge-Kutta is exactly of order 3.

Linear problems: In order to calculate numerical solutions of the linear parabolic Cauchy problems.

$$\begin{aligned} &\partial_t u(t, x) + Au(t, x) = f(t, x) && (t, x) \in [0, T] \times T^d \\ &u(0, x) = u_0(x) && x \in T^d, \end{aligned} \qquad (19)$$

where, $T > 0$, $A = -i\Delta (i^2 = -1)$ u_0 and f are given, the numerical exponential Runge-Kutta methods of collocation type have been presented .

In the problem (19), T is one-dimensional torus $R / 2\pi Z$. For all given positive integer, T^d is the d-dimensional torus.

A linear problem (19) with dimension $d = 1$ is considered. The functions u_0 and f are selected in such a way that the exact solution of the problem is:

$$u(t,x) = e^{i\left(\frac{t}{2}\right)\sin(x)}.$$

The final time is considered $T = 2\pi$. Method 1 and 2 to this problem for different time steps $h > 0$ are utilized (T/h is an integer). Logarithmic scalesofthe L^2 -norm of the final error $e_{T/h}$ as a function of h on Fig. 1 are plotted.

Computations are implemented with Fast Fourier Transforms whit 2^8 nodes. In both cases, the error plot lies between two different straight lines with same slope. The upper line is reached when $\frac{T}{h} = \frac{2\pi}{h}$ is close to the square of an integer, that is to say when the time step is resonant (for example, when $\frac{T}{h} = \frac{2\pi}{10^{-1.2019}} \sim 100 = 10^2$).

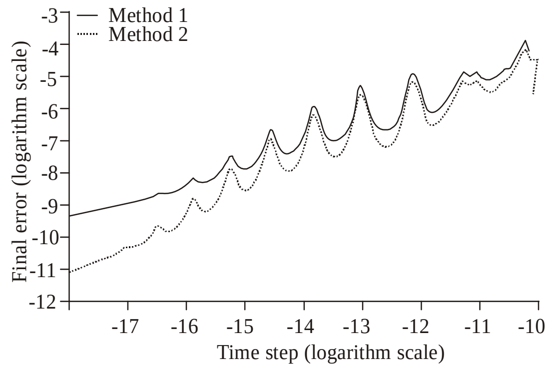

Fig. 1: Final error as a function of the time step for a linear Schrödinger problem. Method 1 (upper dotted line) and 2 (lower starred line). Logarithmic scales

Semi-linear problems: In order to compute solution of the semi-linear parabolic Cauchy problem:

$$\partial_t u(t, x) + Au(t, x) = g(t, u(t, x)) \qquad (t, x) \in [0,T] \times \mathrm{T}^d \quad (20)$$
$$u(0, x) = u_0(x) \qquad x \in \mathrm{T}^d$$

where, $T > 0$, $A = -i\Delta$ ($i^2 = -1$), $r \geq 0$, $u_0 \in H^r(\mathrm{T}^d)$ and g are given, the numerical exponential Runge-Kutta methods of collocation type have been proposed

In many applications, for all $t \in [0,1]$, $g(t)$ result from a nonlinear function from ¢ to ¢. For instance, the Cubic nonlinear Schrödinger, $g(t, u) = g(t)(u) = i|u|^2 u$.

A nonlinear problem (20) with dimension $d = 1$ is demonstrated. The nonlinearity is $g(u) = i\,|u|^2 u$ and the initial datum is:

$$u_0 = \frac{1 + e^{2ix}}{2 + \sin(x)}$$

The final time is considered $T = 2\pi$. Method 1 and 2 to this problem for different time steps $h > 0$ are applied (T/h is an integer). Logarithmic scales of the L^2-norm of the final error $e_{T/h}$ as a function of h on Fig. 2 are plotted.

Computations are implemented with Fast Fourier Transforms with 2^8 nodes. No one can see that resonance occurs for time steps between 10^{-3} and 10^{-1}, even when T / h is the square of an integer and both methods have a numerical order . The upper straight line has a numerical slope close to 2, while the lower straight line of a numerical slope is close to 3.

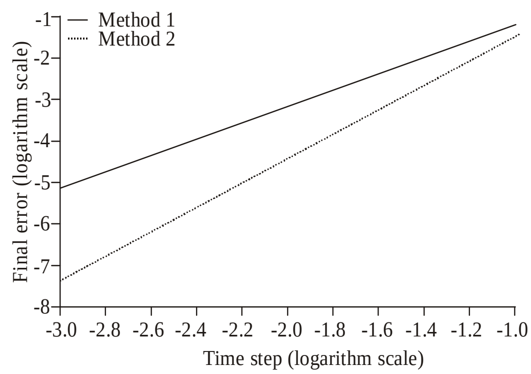

Fig. 2: Final error as a function of the time step for the cubic Schrödinger equation. Method 1 (upper dotted line, numerical slope 1.9932) and Method 2 (lower starred line, numerical slope 2.9874). Logarithmic scales

CONCLUSION

This study has discussed a numerical analysis of exponential Runge-Kutta methods of collocation type utilized to the linear and semi-linear Schrödinger equation on a d-dimension torus. These methods have been argued when used in parabolic problems.

In the Eq. (7) and (8), the numerical schemes are described implicitly in the internal stage $U_{n,\ i}$ and furthermore the evaluation of products of matrix functions with vectors has been involved. In contrast to fully implicit Runge-Kutta methods, the nonlinear Eq. (9) can be resolved by a few steps of fix-point iteration. Products of matrix functions with vectors can also be calculated by Fast Fourier transformations.

In Fig. 1 and 2, implementation of the calculations has been illustrated using the Fast Fourier Transforms (FFT) with 2^8 nodes in Matlab.

REFERENCES

Boyd, J.P., 2001. Chebyshev and Fourier Spectral Methods. 2nd Edn., Dover, New York.

Berland, H., B. Skaestad and W.M. Wright, 2007. EXPINT-A Matlab Package for Exponential Integrators. ACM Transactions on Mathematical Software, 33: Article Number 4.

Berland, H., A.L. Islas and C.M. Schober, 2007. Conservation of phase space propertiesusing exponential integrators on the cubic Schrödinger equation. J. Computat. Phys., 255(1): 284-299.

Certaine, J., 1960. The Solution of Ordinary Differential Equations with Large Time Constants. In: Ralston, A. and H.S. Wilf, (Eds.), Mathematical Methods for Digital Computers, wiley, New York, pp: 128-132.

Cox, S.M. and P.C. Matthews, 2002. Exponential time differencing for stiff systems. J. Computat. Phys., 176: 430-455.Dujardin, G., 2009. Exponential Runge-Kutta methods for the Schrödinger equation. Appl. Numer. Math., 59(8): 1839-1857.

Dujardin, G., 2009. Exponential Runge-Kutta methods for the Schrödinger equation. Appl. Numer. Math., 59(8): 1839-1857.

Fujiwara, D., 1967. Concrete characterization of the domains of fractionalpowers ofsome elliptic differential operators of the second order. Proc. Japan Acad., 43: 82-86.

Gallopoulos, E. and Y. Saad, 1992. Efficient solution of parabolic equations by Krylov approximation methods. SIAM J. Sci. Statist. Comput., 13: 1236-1264.

Hochbruck, M. and A. Ostermann, 2005. Exponential Runge-Kutta methods for parabolic problems. Appl. Numer. Math., 53(2): 323-339.

Hochbruck, M. and A. Ostermann, 2005. Explicit exponential Runge-Kutta methods for semi linear parabolic problems. SIAM J. Numer. Anal., 43(3): 1069-1090.

Hochbruck, M. and C. Lubich, 1999. A Gautschi-type method for oscillatory second order differential equations. Numer. Math., 83: 403-426.

Henry, D., 1981. Geometric Theory of Semilinear Parabolic Equations. Vol. 840 of Lecture Notes inMathematics, Springer, Berlin, Heidelberg.

Lubich, C. and A. Ostermann, 1995. Runge-Kutta approximation of quasi-linearparabolic equations. Math. Comp., 64: 603-627.

Lawson, J.D., 1967. Generalized Runge-Kutta processes for stable systems with large Lipschitz constants. SIAM J. Numer. Anal., 4: 372-380.

Lubich, C. and A. Ostermann, 1993. Runge-Kutta methods for parabolic equations and convolution quadrature. Math. Comp., 60: 105-131.

Lubich, C. and A. Ostermann, 1995. Linearly implicit time discretization of non-linear parabolic equations. IMA J. Numer. Anal., 15: 555-583.

Minchev, B.V. and W.M. Wright, 2005. A Review of Exponential Integrators forFirst Order Semi-Linear Problems. Tech. Rep, NTNU, Preprint.

Nie, Q., Y.T. Zhang and R. Zhao, 2006.Efficient semi-implicit schemes for stiff systems. J. Computat. Phys., 214: 521-537.

Sheen, D., I.H. Sloan and V. Thom´ee, 2000. A parallel method for time discretization of parabolic equationsbased on Laplace transformation and quadrature. Math. Comp., 69: 177-195.