Numerical Experiments for Reaction-Diffusion Equations Using Exponential Integrators

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Abstract. In this study we focus on a comparative numerical approach of two reaction-diffusion models arising in biochemistry by using exponential integrators. The goal of exponential integrators is to treat exactly the linear part of the differential model and allow the remaining part of the integration to be integrated numerically using an explicit scheme. Numerical simulations including both the global error as a function of time step and error as a function of computational time are shown.

1 Introduction

Reaction-diffusion equations are frequently encountered in mathematical biology, ecology, physics and chemistry. This type of equations leads to interesting phenomena, such as, pattern formation far from equilibrium, pulse splitting and shedding, reactions and competitions in excitable systems, nonlinear waves and spatio-temporal chaos. The efficient and accurate simulation of such systems, however, represent a difficult task. This is because they couple a stiff diffusion term with a (typically) strongly nonlinear reaction term. When discretised this leads to large systems of strongly nonlinear, stiff ODEs.

In this work we perform a comparative numerical approach of two reaction-diffusion models arising in biochemistry by using exponential integrators. The paper is organized as follows. Section 2 briefly describes the exponential integrators and their features. In Section 3 the two reaction kinetics – Gierer-Meinhardt and Thomas models, respectively – are presented on the basis of which the numerical study is carried out. Section 4 is devoted to a short description of the numerical schemes applied to the models under study, together with results of the numerical simulations. Finally, some concluding remarks are drawn in the last section.

2 Exponential Integrators

The exponential integrators represent numerical schemes specifically constructed for solving differential equations (see for details [8]), where it is possible to split the problem into a linear and a nonlinear part

$$\dot{y} = Ly + N(y,t), \qquad y(t_{n-1}) = y_{n-1}\,, \tag{1}$$

where $y \in \mathbf{C}^d$, $L \in \mathbf{C}^{d\times d}$ and $N : \mathbf{C}^d \times \mathbf{R} \to \mathbf{C}^d$. In specific applications (discretizations of PDEs) the matrix L is unbounded. Generally, solving such problems requires an implicit scheme; the goal of the exponential integrators is to treat the linear term exactly and allow the remaining part of the integration to be integrated numerically using an explicit scheme.

An exponential integrator has two main characteristics: (i) If $L = 0$, then the scheme reduces to a standard general linear scheme. This is often called the underlying general linear scheme; (ii) If $N(y,t) = 0$ for all y and t, then the scheme reproduces the exact solution of (1). To satisfy (i) the exponential function must be used within the numerical scheme. Despite the fact that L is unbounded, typically the coefficients of the scheme will be bounded.

For an s-stage exponential integrator of Runge-Kutta type, we define the internal stages and output approximation:

$$\begin{aligned} Y_i &= h\sum_{j=1}^{s} a_{ij}(hL)N(Y_j, t_{n-1} + c_j h) + u_{i1}(hL)y_{n-1}\,, \quad i = 1,\ldots,s\,,\\ y_n &= h\sum_{i=1}^{s} b_i(hL)N(Y_j, t_{n-1} + c_j h) + v_1(hL)y_{n-1}\,. \end{aligned} \tag{2}$$

The feature (i) above is satisfied if we require in (2) as $u_{i1}(0) = 1$, $a_{ij}(0) = a_{ij}$, $v_1(0) = 1$, and $b_i(0) = b_i$, where the real numbers a_{ij} and b_j represent the coefficients of the underlying Runge-Kutta scheme.

The extension to general linear schemes is carried out as follows. A step of length h in an exponential general linear scheme, requires to import r aproximations into the step, denoted as $y_i^{[n-1]}$, $i = 1,\ldots,r$. The internal stages (as in the Runge-Kutta case) are written as Y_i, $i = 1,\ldots,s$. After the step is completed, r updated approximations are computed. These are then used in the next step. Each step in an exponential general linear scheme can be written as

$$\begin{aligned} Y_i &= h\sum_{j=1}^{s} a_{ij}(hL)N(Y_j, t_{n-1} + c_j h) + \sum_{j=1}^{r} u_{ij}(hL)y_j^{[n-1]}\,, \quad i = 1,\ldots,s\,,\\ y_i^{[n]} &= h\sum_{j=1}^{s} b_{ij}(hL)N(Y_j, t_{n-1} + c_j h) + \sum_{j=1}^{r} v_{ij}(hL)y_j^{[n-1]}\,, \quad i = 1,\ldots,r. \end{aligned} \tag{3}$$

The exponential integrators of Runge-Kutta type are easily seen to be a special case when $r = 1$ with $u_{i1}(z) = a_{i0}(z)$, $v_{11}(z) = b_0(z)$ and $b_{1j}(z) = b_j(z)$.

3 Model Equations

In this section we shortly describe the models governing different reaction kinetics arising in biochemistry, which will be solved numerically in Section 4.

Gierer-Meinhardt reaction kinetics. This represents a phenomenological model suggested by Gierer and Meinhardt ([5]), whereby reaction kinetics are

chosen in such a way that one of the chemicals (termed activator) activates the production of the other chemical (the inhibitor) which, in turn, inhibits the production of the activator. The non-dimensionalised reaction-diffusion system is given by

$$\begin{aligned} \frac{\partial u}{\partial t} &= D_u \nabla^2 u + \gamma \left(a - bu + \frac{u^2}{v(1+\kappa u^2)} \right) , \\ \frac{\partial v}{\partial t} &= D_v \nabla^2 v + \gamma (u^2 - v) , \end{aligned} \tag{4}$$

where $u(x,t)$ is the concentration of the activator, $v(x,t)$ is the concentration of the inhibitor, t is time and ∇^2 is the 1-dimensional Laplacian. D_u, D_v, a, b and γ are all nondimensionalised positive parameters and k is a measure of the saturation concentration ([10]). The biological interpretation of the reaction kinetics in (4) is that u is produced at a constant rate γa and is degraded linearly at rate γb. The $\gamma \frac{u^2}{v(1+\kappa u^2)}$ term implies autocatalysis in u with saturation at high concentration values of u, and inhibition of u through the production of v. In the second equation of the system (4), v is activated (produced) by u and degraded linearly.

Thomas reaction kinetics. This model is based on a specific substrate-inhibition reaction involving the substrates oxygen $v(x,t)$, and uric acid $u(x,t)$, which react in the presence of the enzyme uricase. The reaction kinetics, derived by fitting the kinetics to experimental data ([12]), can be written in nondimensional form as

$$\begin{aligned} \frac{\partial u}{\partial t} &= D_u \nabla^2 u + \gamma \left(a - u - h(u,v) \right) , \\ \frac{\partial v}{\partial t} &= D_v \nabla^2 v + \gamma \left(\alpha b - \alpha v - h(u,v) \right) , \end{aligned} \tag{5}$$

with $h(u,v) = \frac{\rho u v}{1+u+K u^2}$. Here D_u, D_v, a, α, b, γ and ρ are positive parameters. The term $h(u,v)$ indicates the rate at which u and v are used up, in particular $h(u,v)$ exhibits what is known as substrate-inhibition, that is, for small u, $h(u,v)$ increases with u, while it decreases with large u.

4 Description of the Numerical Schemes and Computational Issues

In what follows, we briefly describe the numerical schemes defining the exponential integrators that have been used in our comparative study. All these integrators belong to the package `EXPINT` written in Matlab ([1]). In this description we will use two terms of order. The non-stiff order refers to the case when the operator L is bounded, such conditions were derived in [8]. The stiff order refers to the case when L is unbounded ([3]), for various schemes. We remark here that the stiff order convergence analysis is performed for the parabolic case only.

The first scheme that has been applied to our models is named `Lawson4`. The scheme `Lawson4` belongs to the Lawson schemes constructed by applying the Lawson transformations ([7]) to the semi-linear problem. It is based on the clasical fourth order scheme of Kutta (see [2], Eq. (235i)), and this scheme has stiff order one.

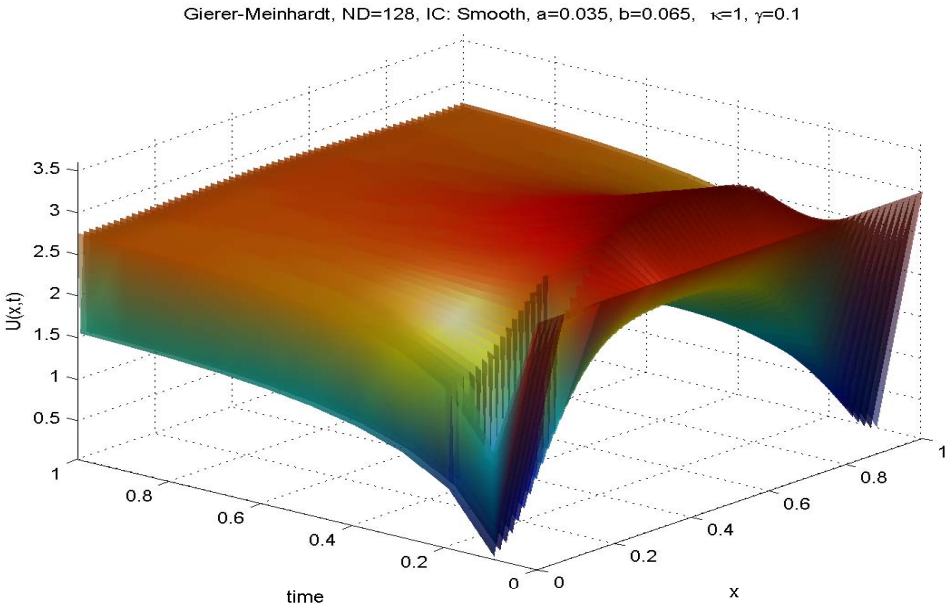

Fig. 1. The variation profile of the variable $u(x,t)$ in the model (4) representing the concentration of the activator which stimulates the production of the inhibitor denoted by $v(x,t)$ (Gierer-Meinhardt reaction kinetics).

The scheme denoted by `hochost4` was developed by Hochbruck and Ostermann. It has five-stages and is the only known exponential Runge-Kutta method with stiff order four.

Nørsett designed in [11] a class of schemes which reduced to the Adams-Bashforth methods when the linear part of the problem is zero.

`ABLawson4` has stiff order one and is based on the Adams-Bashforth scheme of order four and is represented in this way so that the incoming approximation has the form $y^{[n-1]} = [y_{n-1}, hN_{n-2}, hN_{n-3}, hN_{n-4}]^T$.

`ABNørsett4` is a stiff order four scheme of Norsett ([11]), which is implemented so that the incoming approximation has the same form as in `ABLawson4`.

`ETD` schemes are based on algebraic approximations to the nonlinear term in the variation of constants formula. `ETD` means "Exponential Time Differencing" and the name stems from [4]. The scheme `ETD4RK` due to Cox and Matthews in ([4], Eqs. (26)-(29)) started the recent focus on exponential integrators, unfortunately it has only stiff order two. `ETD5RKF` is a non-stiff fifth order scheme based on the six stage fifth order scheme of Fehlberg.

The scheme `RKMK4t` uses a convenient truncation of the $dexp^{-1}$ operator, leading to the method of Munthe-Kaas [9], which again is of stiff order two but suffers from instabilities, especially when non-periodic boundary conditions are used.

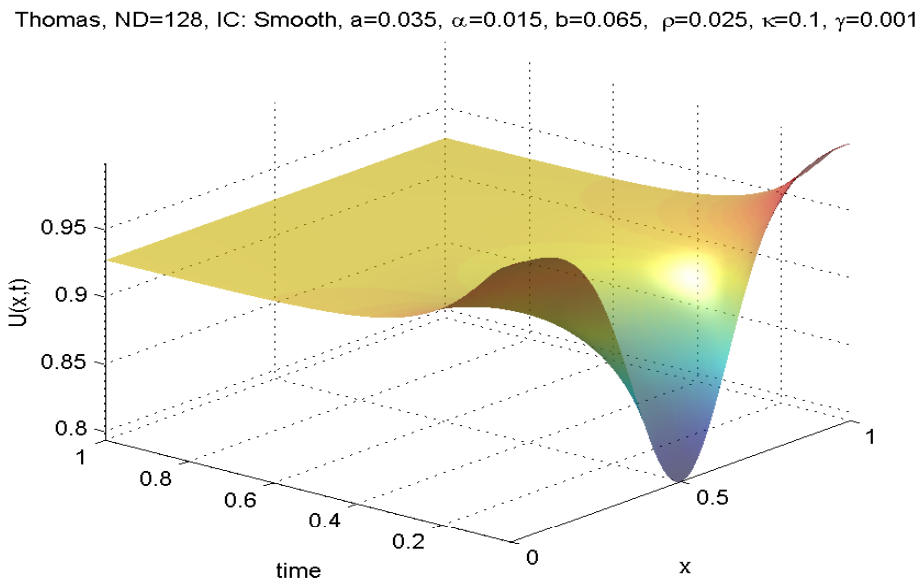

Fig. 2. The variation profile of the variable $u(x,t)$ in the model (5) representing the concentration of the uric acid in the substrate-inhibition reaction involving the substrate oxygen $v(x,t)$ (Thomas reaction kinetics).

Krogstad [6] constructed the generalized Lawson schemes as a means of overcoming some of the undesirable properties of the Lawson schemes. This class of schemes uses approximations of the nonlinear term from previous steps, resulting in an exponential general linear method. The scheme `genlawson45` included in the package mentioned above is also used for our numerical study.

Figures 1 and 2 present the variation profiles for the concentration variable of $u(x,t)$ in the two reaction kinetics, Gierer-Meinhardt and Thomas, respectively.

Figures 3 and 4 illustrate comparison results concerning the quality of the numerical schemes that have been used in this analysis. There are shown relationships between the global error and the timestep h varying from 10^{-2} to 10^{-1}. We note that for Gierer-Meinhardt model good behaviours have had the schemes `lawson4`, `hochcost4`, `etd4rk`, `ablawson4`, while the schemes `rkmk4t`, and `etd5rkf` indicated a more significant increasing rate of the global errors with respect to the computed global error (see Fig. 3). In the case of Thomas reaction kinetics, the scheme `etd5rkf` has had the best behaviour (see Fig. 4).

Figures 5 and 6 give timing results in the sense that present dependencies of the global error as a function of computational time for the two models. In this respect, good results are obtained with the schemes `lawson4`, `etd4rk` and `ablawson4` for the Gierer-Meinhardt model (see Fig. 5), and `lawson4`, `rkmk4t`, `etd5rkf` for the Thomas model (see Fig. 6).

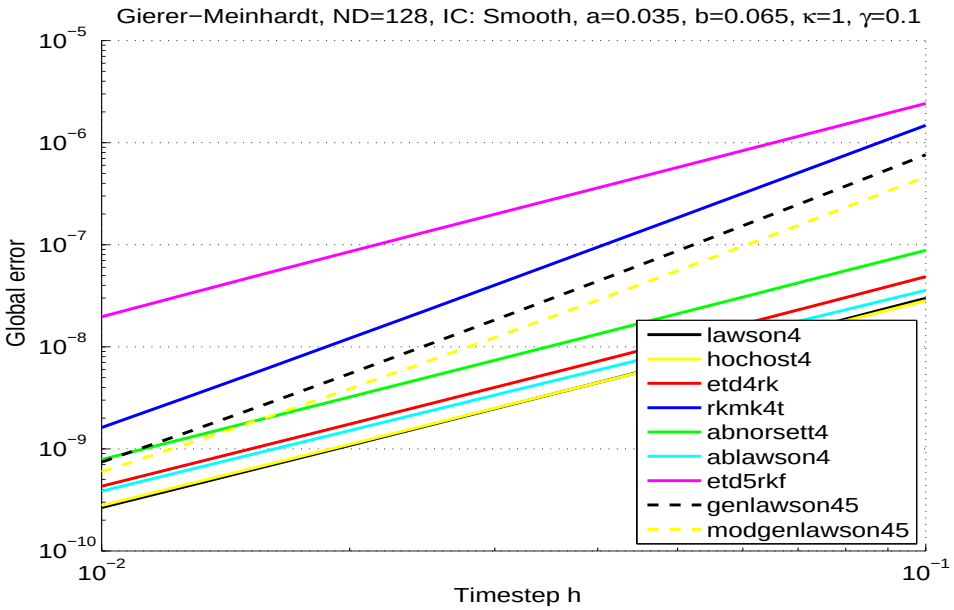

Fig. 3. Comparative results concerning the quality of the numerical schemes: the global error as a function of timestep h for the Gierer-Meinhardt reaction kinetics.

All the plots indicate in their title: "ND=128" and "IC: Smooth". This means that we have used 128 Fourier modes in the spatial direction (must be power of 2), and as initial condition for the model variables, we have chosen a set of values with a Gaussian distribution.

5 Conclusions

In this paper we focused on a comparative numerical study for two models arising in biochemsitry: Gierer-Meinhardt reaction kinetics and Thomas reaction kinetics. The numerical approach has been performed by using several exponential integrators belonging to Matlab package EXPINT ([1]). The numerical findings together with global error and timing results were presented in illustrative plots.

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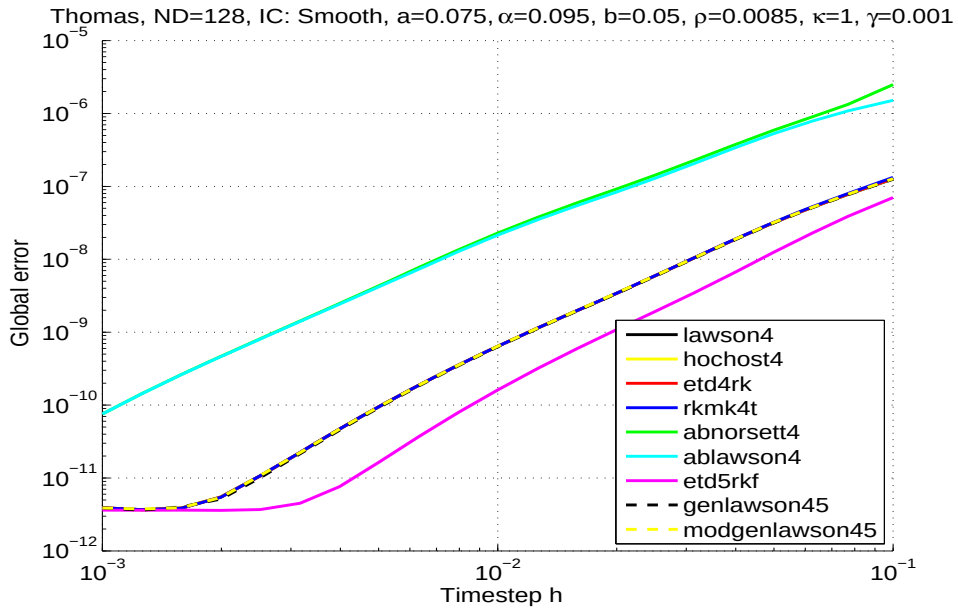

Fig. 4. Comparative results concerning the quality of the numerical schemes: the global error as a function of timestep h for the Thomas reaction kinetics.

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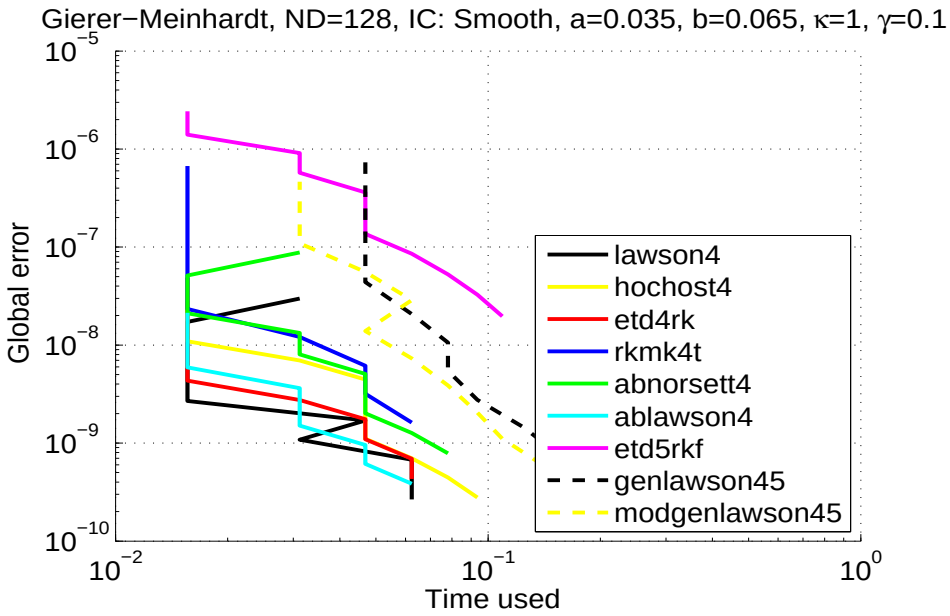

Fig. 5. Comparative results concerning the global error as a function of computational time for the Gierer-Meinhardt reaction kinetics.

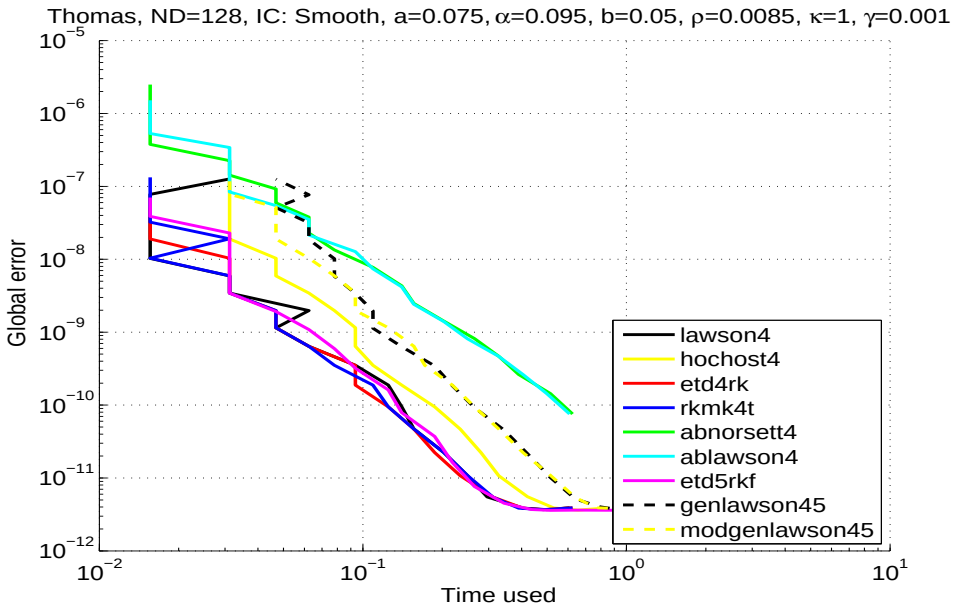

Fig. 6. Comparative results concerning the global error as a function of computational time for the Thomas reaction kinetics.