EFFICIENT SEMI-IMPLICIT SCHEMES FOR STIFF SYSTEMS VIA NEWTON'S FORM

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In stiff reaction–diffusion equations, whiles explicit time discretization schemes are utilized, the stability constraint on the time step depends on two terms: the diffusion and the reaction terms. If the linear diffusion has been treated exactly by applying the integration factor (IF) or exponential time differencing (ETD) methods, then the part of the stability constraint due to diffusion can be completely eliminated. For systems with strictly stiff reactions, these methods are not efficient as the reaction term in IF or ETD is still estimated with explicit schemes. In this work, a new class of semi-implicit schemes are established, which treats the linear diffusions exactly and explicitly, and the nonlinear reactions implicitly. The stability region for this class of methods is much larger than the existing methods using an explicit treatment of reaction terms. Especially, the one with second order accuracy is completely linearly stable with respect to both diffusion and reaction.

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1. Introduction

The following equation is considered for many physical and biological applications,

$$\frac{\partial u}{\partial t} = D\Delta u + F(u)\,, \tag{1}$$

where $u \in R^m$ represents a group of physical or biological species, $D \in R^{m\times m}$ is diffusion constraint matrix, Δu is the Laplacian which is associated with the diffusion of species u, and $F(u)$ illustrates chemical or biological reactions. If the method of lines is utilized for solving the equation numerically, reaction-diffusion (1) can be reduced to a system of ODEs:

$$u_t = Lu + G(u), \tag{2}$$

where Lu is a finite difference approximation of $D\Delta u$. Let N shows the number of spatial grid points (independent of number of spatial dimensions) for the approximation of Laplacian Δu.Thus $u(t) \in R^{N\times m}$ and L is a $(N.m) \times (N.m)$ matrix representing a spatial discretization of the diffusion. The size of the time-step for a time integrator for solving (2), is constrained by the inverse of the eigenvalues of the diffusion matrix D as well as the stiffness of the nonlinear reaction term $G(u)$. As N increases, the diffusion constants in the system (1) become large or the

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spatial resolution is better, the stability restriction becomes very rigorous because of diffusion [1-3].

Moreover, the part of the linear diffusion has been reduced to the evaluation of an exponential function of the matrix L, after that an approximation of an integral relating the nonlinear term $G(u)$. Different approximations of the integral involving nonlinear term $G(u)$ give rise to either the integration factor (IF) method or the exponential time differencing (ETD) method. For ETD methods, special treatments for a variety of operations on L (e.g., its inverse) are needed in order to maintain a consistent order of accuracy [4-6]. Leo *et al.* [7] studied the fixed points for the original systems which are not precisely conserved in the numerical scheme, and as a result, further terms have to be included in the standard IF methods in order to preserve such conservation. Cox and Matthew [8] discussed one way of improving the stability region for a stiff reaction is to take in a Runge–Kutta type estimate for the term involving $G(u)$ in the ETD scheme.

In general, the exponential time differencing Runge–Kutta method (ETDRK) has a larger stability region than the standard ETD while the multi-stage nature of Runge–Kutta methods need more function evaluations [3]. On the other hand, it is still not efficient enough for systems with highly stiff reactions, since often is the case for several biological applications, such as the morphogen gradient scheme in which the reaction rate constants in $F(u)$ can be different by four to five order of magnitude [11-14]. Aziz *et al.* [18] studied a new review of exponential integrator, which is related to the numerical methods for solving stiff problems.

In this study, we obtain the implicit integrating factor method (IIF). For this purpose, a numerical solution is acquired by approximating the function $g(\tau)$ with the Newton's form of the interpolating polynomial $P(\tau)$. Moreover, we present a stability analysis of this implicit integrating factor (IIF), where the Matlab codes are applied to this stability region.

2. Implicit integrating factor methods

Let us consider the derivation of the new temporal schemes for the scalar case of the semi-discrete system (2) of the form

$$\frac{du}{dt} = cu + f(u) \ , \qquad t > 0 \ , \qquad u(0) = u_o \ , \tag{3}$$

where c is a constant representing the diffusion, and f is a nonlinear function representing the reaction. Multiplying (3) by the integrating factor e^{-ct}

$$\frac{du}{dt}\, e^{-ct} = cu\, e^{-ct} + e^{-ct} f(u), \text{ or}$$
$$\frac{d}{dt}(u(t)\, e^{-ct}) = e^{-ct} f(u) .$$

To integrate the equation over one time step from t_n and $t_{n+1} = t_n + \Delta t$, we have

$$\int_{t_n}^{t_{n+1}} \frac{d}{d\tau}(u(\tau)e^{-c\tau})d\tau = \int_{t_n}^{t_{n+1}} e^{-c\tau} f(u(\tau))d\tau, \text{ or}$$
$$u(t_{n+1})e^{-ct_{n+1}} - u(t_n)e^{-ct_n} = \int_{t_n}^{t_{n+1}} e^{-c\tau} f(u(\tau)d\tau \text{ , or}$$
$$u(t_{n+1}) = u(t_n)e^{-c(t_n - t_{n+1})} + e^{ct_{n+1}} \int_{t_n}^{t_{n+1}} e^{-c\tau} f(u(\tau))d\tau \text{ , or}$$
$$u(t_{n+1}) = u(t_n)e^{c\Delta t} + e^{ct_{n+1}} \int_{t_n}^{t_{n+1}} e^{-c\tau} f(u(\tau))d\tau,$$

and substituting $\tau = t_n + \Delta t$ into the integral, we have

$$u(t_{n+1}) = u(t_n)e^{c\Delta t} + e^{c\Delta t} \int_0^{\Delta t} e^{-c\tau} f(u(t_n + \tau))d\tau \ , \tag{4}$$

where u_n is considered as a numerical solution for $u(t_n)$ and $g(\tau)$ is proposed to be

$$g(\tau) = e^{-c\tau} f(u(t_n + \tau)). \tag{5}$$

In order to construct a scheme of *r*-th order truncation, we approximate $g(\tau)$ with the Newton's form of the interpolating polynomial,$P(\tau)$, with interpolation points $t_{n+1}, t_n, \dots, t_{n+2-r}$, i.e.

$$P(\tau) = \sum_{i=-1}^{r-2} e^{ic\Delta t} f(u_{n-i})\left[\varphi(\varepsilon_{-1}) + \sum_{j=0}^{r-2} \varphi[\varepsilon_{-1}, \varepsilon_0, \dots, \varepsilon_j] \prod_{k=-1}^{j-1}(\tau - \varepsilon_k)\right]$$
$$0 \le \tau \le \Delta t \ . \tag{6}$$

In the above equation, we identify

$$\varepsilon_j = j\Delta t \ , \qquad -1 \le j \le r-2 \tag{7}$$
$$\varphi[\varepsilon_j, \varepsilon_{j+1}, \dots, \varepsilon_k] = \frac{\varphi[\varepsilon_{j+1}, \varepsilon_{j+2}, \dots, \varepsilon_k] - \varphi[\varepsilon_j, \varepsilon_{j+1}, \dots, \varepsilon_{k-1}]}{\varepsilon_k - \varepsilon_j}$$

with this approximation to $g(\tau)$, and (4) can be discretized as

$$u_{n+1} = e^{c\Delta t} u_n + e^{c\Delta t} \int_0^{\Delta t} P(\tau) d\tau \ . \tag{8}$$

As a result, a direct evaluation of the integral in (8) leads to the new *r*-th order implicit scheme, i.e.

$$u_{n+1} = e^{c\Delta t} u_n + \Delta t(\alpha_{n+1} f(u_{n+1}) + \sum_{i=0}^{r-2} \alpha_{n-i} f(u_{n-i})) \ , \tag{9}$$

with $\alpha_{n+1}, \alpha_n, \alpha_{n-i}, \dots, \alpha_{n-r+2}$ defined as

$$\alpha_{n-i} = \frac{e^{(i+1)c\Delta t}}{\Delta t} \int_0^{\Delta t} \left[\varphi(\varepsilon_{-1}) + \sum_{j=0}^{r-2} \varphi[\varepsilon_{-1}, \varepsilon_0, \dots, \varepsilon_j] \prod_{k=-1}^{j-1}(\tau - \varepsilon_k)\right] d\tau \ , -1 \le i \le r-2. \tag{10}$$

To obtain the order of $r = 2$, we must take the following forms of α in Table 1.

Table 1: Coefficients α for implicit IF schemes with localized nonlinear systems.

order	α_{n+1}	α_n	α_{n-1}	α_{n-2}
1	0	0	0	0
2	$-\frac{1}{2}$	$-\frac{1}{2}e^{c\Delta t}$	0	0

Thus the second order scheme (IIF2) is derived in the following form

$$u_{n+1} = e^{c\Delta t}\left(u_n - \tfrac{\Delta t}{2} f(u_n)\right) - \tfrac{\Delta t}{2} f(u_{n+1}) \ . \tag{11}$$

To obtain the order of $r = 3$, we must take the following forms of α in Table 2.

Table 2: Coefficients α for implicit IF schemes with localized nonlinear systems.

order	α_{n+1}	α_n	α_{n-1}	α_{n-2}
3	$-\frac{1}{2}$	$-\frac{1}{2}e^{c\Delta t}$	$-\frac{1}{2}e^{2c\Delta t}$	0

Thus the third- order scheme (IIF3) is obtained in the following form

$$u_{n+1} = e^{c\Delta t} u_n + \Delta t(-\tfrac{1}{2} f(u_{n+1}) - \tfrac{1}{2} e^{c\Delta t} f(u_n) - \tfrac{1}{2} e^{2c\Delta t} f(u_{n-1})) \ .$$

Then the second, third, fourth order approximations to $g(\tau)$ are of the following forms:

1. Given $g(0) = f(u_n)$,$g(\Delta t) = e^{-c\Delta t} f(u_{n+1})$, the second order approximation to $g(\tau)$ is

$$P(\tau) = e^{-c\Delta t} f(u_{n+1})\left[\varphi(\varepsilon_{-1)}) + \varphi[\varepsilon_{-1}, \varepsilon_0](\tau - \varepsilon_{-1})\right] + f(u_n)\varphi(\varepsilon_{-1})$$

$$0 \le \tau \le \Delta t \quad .$$

2. Given $g(-\Delta t) = e^{c\Delta t} f(u_{n-1})$, $g(0) = f(u_n)$, $g(\Delta t) = e^{-c\Delta t} f(u_{n+1})$,the third approximation to $g(\tau)$ is

$$P(\tau) = e^{-c\Delta t} f(u_{n+1})[\varphi(\varepsilon_{-1}) + \varphi[\varepsilon_{-1}, \varepsilon_0](\tau - \varepsilon_{-1}) + \varphi[\varepsilon_{-1}, \varepsilon_0, \varepsilon_1](\tau - \varepsilon_{-1})(\tau - \varepsilon_0)] + f(u_n)[\varphi(\varepsilon_{-1}) + \varphi[\varepsilon_{-1}, \varepsilon_0, \varepsilon_1](\tau - \varepsilon_{-1})(\tau - \varepsilon_0)] + e^{c\Delta t} f(u_{n-1})[\varphi(\varepsilon_{-1}) + \varphi[\varepsilon_{-1}, \varepsilon_0](\tau - \varepsilon_{-1})]$$

$$0 \le \tau \le \Delta t \quad .$$

3. Given $g(-2\Delta t) = e^{2c\Delta t} f(u_{n-2})$, $g(-\Delta t) = e^{c\Delta t} f(u_{n-1})$, $g(0) = f(u_n)$, $g(\Delta t) = e^{-c\Delta t} f(u_{n+1})$, the fourth order approximation to $g(\tau)$ is

$$P(\tau) = e^{-c\Delta t} f(u_{n+1})[\varphi(\varepsilon_{-1}) + \varphi[\varepsilon_{-1}, \varepsilon_0](\tau - \varepsilon_{-1}) + \varphi[\varepsilon_{-1}, \varepsilon_0, \varepsilon_1](\tau - \varepsilon_{-1})(\tau - \varepsilon_0) + \varphi[\varepsilon_{-1}, \varepsilon_0, \varepsilon_1, \varepsilon_2](\tau - \varepsilon_{-1})(\tau - \varepsilon_0)(\tau - \varepsilon_1)] + f(u_n)[\varphi(\varepsilon_{-1}) + \varphi[\varepsilon_{-1}, \varepsilon_0, \varepsilon_1](\tau - \varepsilon_{-1})(\tau - \varepsilon_0) + \varphi[\varepsilon_{-1}, \varepsilon_0, \varepsilon_1, \varepsilon_2](\tau - \varepsilon_{-1})(\tau - \varepsilon_0)(\tau - \varepsilon_1)] + e^{c\Delta t} f(u_{n-1})[\varphi(\varepsilon_{-1}) + \varphi[\varepsilon_{-1}, \varepsilon_0](\tau - \varepsilon_{-1}) + \varphi[\varepsilon_{-1}, \varepsilon_0, \varepsilon_1, \varepsilon_2](\tau - \varepsilon_{-1})(\tau - \varepsilon_0)(\tau - \varepsilon_1)] + e^{2c\Delta t} f(u_{n-2})[\varphi(\varepsilon_{-1}) + \varphi[\varepsilon_{-1}, \varepsilon_0](\tau - \varepsilon_{-1}) + \varphi[\varepsilon_{-1}, \varepsilon_0, \varepsilon_1](\tau - \varepsilon_{-1})(\tau - \varepsilon_0)] .$$

3. Stability analysis of IIF

The steady condition is achieved from a dynamic evolution by using standard integration factor methods, which has an error of order (Δt^p). In addition, discretization errors are also related to the space [3]. Since the fixed points of the numerical scheme are not preserved, consequently the following decoupled linear problem cannot be used directly,

$$u_t = -qu + du, \qquad q > 0 . \tag{12}$$

For the IIF methods, the steady state of ODE system and the stability regions are examined with respect to the diffusion and the reaction [9, 10]. The boundaries of the stability region, which consist of a family of curves for different values of $q\Delta t$ are shown, based on the test problem (12) for the second and third-order IIF methods.

The second order IIF (11) is applied to equation (12), and then substituting $u_n = e^{in\theta}$ into the resulting equation, the following equation is derived

$$e^{i\theta} = e^{-q\Delta t}\left(1 - \tfrac{1}{2}\lambda\right) - \tfrac{1}{2}\lambda e^{i\theta}, \tag{13}$$

where $\lambda = d\Delta t$ has a real part λ_r and imaginary part λ_i . Thus the equation for λ_r and λ_i are considered as follows

$$\lambda_r = \frac{2(e^{-2q\Delta t} - 1)}{(1 - e^{-q\Delta t})^2 + 2(1 + \cos\theta)e^{-q\Delta t}} ,$$

$$\lambda_i = \frac{-4(sin\theta)e^{-q\Delta t}}{(1 - e^{-q\Delta t})^2 + 2(1 + \cos\theta)e^{-q\Delta t}} . \tag{14}$$

Since $q > 0$, then $\lambda_r < 0$, which resulted for $0 \le \theta \le 2\pi$. Then, the second order IIF is *A*-stable because the stability region has been included in the complex plane for λ with $\lambda_r < 0$.

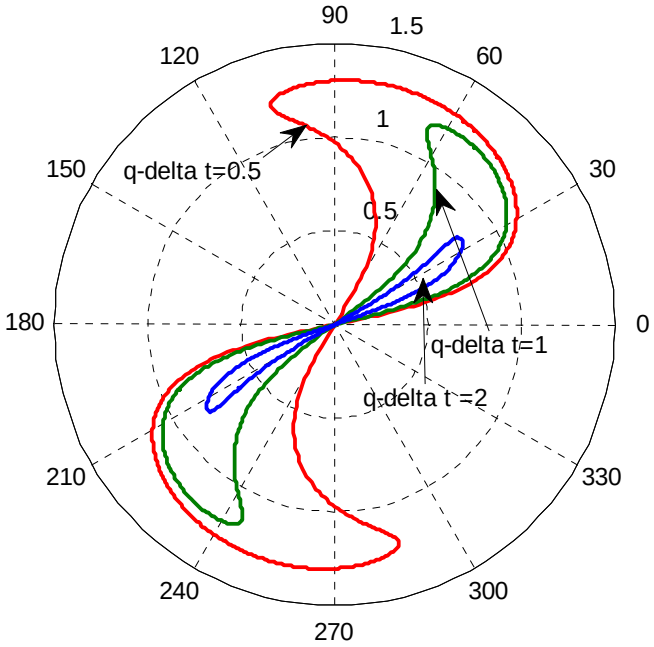

Fig. 1: Stability regions (exterior of the closed curves) for the second order with $q\Delta t = 0.5, 1, 2$.

In Figure.1 , the stability region is designed as such that the exterior of the closed curves are located on the complex plane with $\lambda_r < 0$, for $q\Delta t = 0.5, 1, 2$.

Note that in (14), in the limit $q \to 0$, the stability region agrees with the domain $\lambda_r < 0$, while in the limit $q \to \infty$, the stability region approaches the whole complex plane excluding the point $(-2,0)$.

The third- order IIF (or IIF3) scheme is considered

$$u_{n+1} = e^{c\Delta t}u_n + \Delta t(-\frac{1}{2}\, f(u_{n+1}) - \frac{1}{2}e^{c\Delta t}f(\, u_n) - \frac{1}{2}\, e^{2c\Delta t}f(u_{n-1}))\ . \tag{15}$$

The same approach is applied, so that the equation for λ is found to be

$$\lambda = \frac{e^{i\theta} - e^{-q\Delta t}}{-\frac{1}{2}e^{i\theta} - \frac{1}{2}e^{-q\Delta t} - \frac{1}{2}e^{-2q\Delta t - i\theta}}\ . \tag{16}$$

The following complex planes show the step by step stability region for λ in (16) for different values of $q\Delta t$.

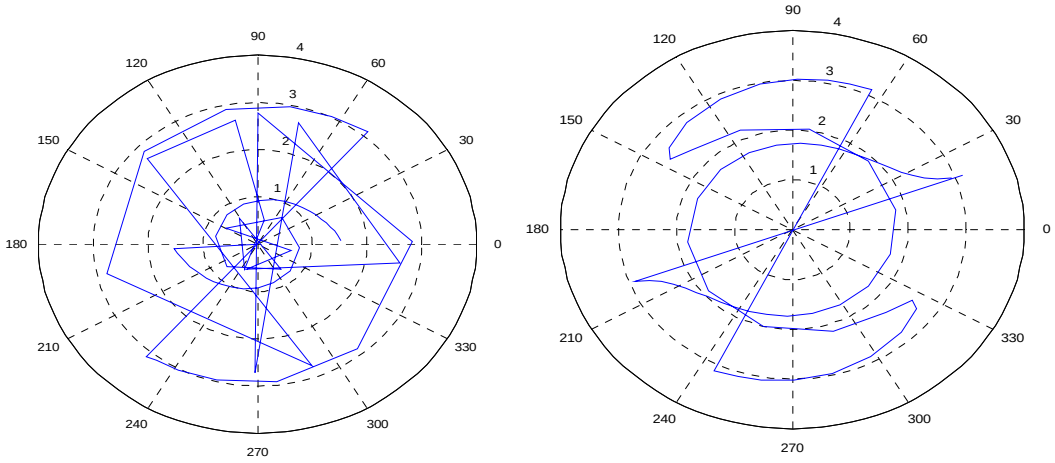

Fig. 2: Stability regions for the third- order IIF scheme with $q\Delta t = 0, 0.45$.

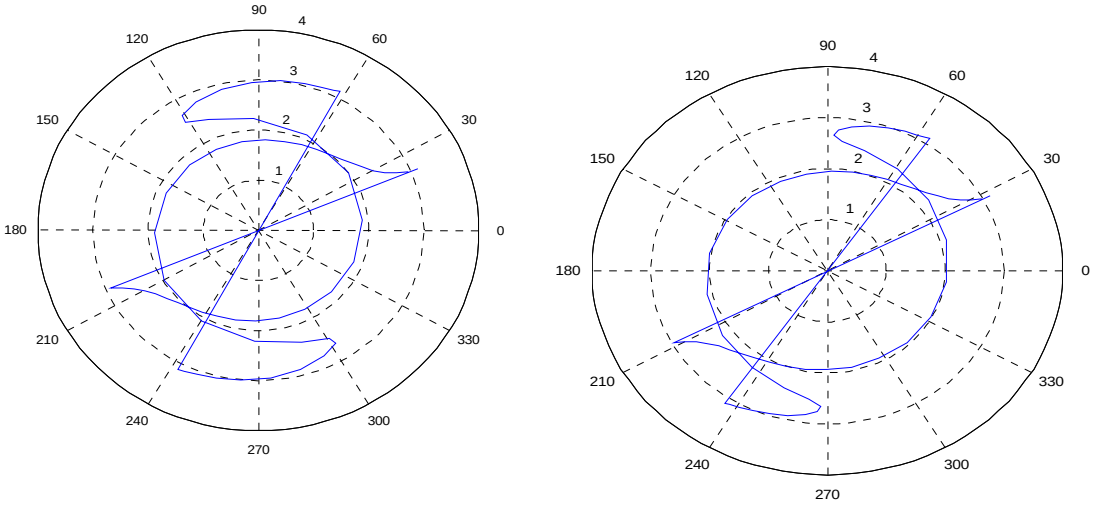

Fig. 3: Stability regions for the third- order IIF scheme with $\Delta t = 0.5, 0.6$.

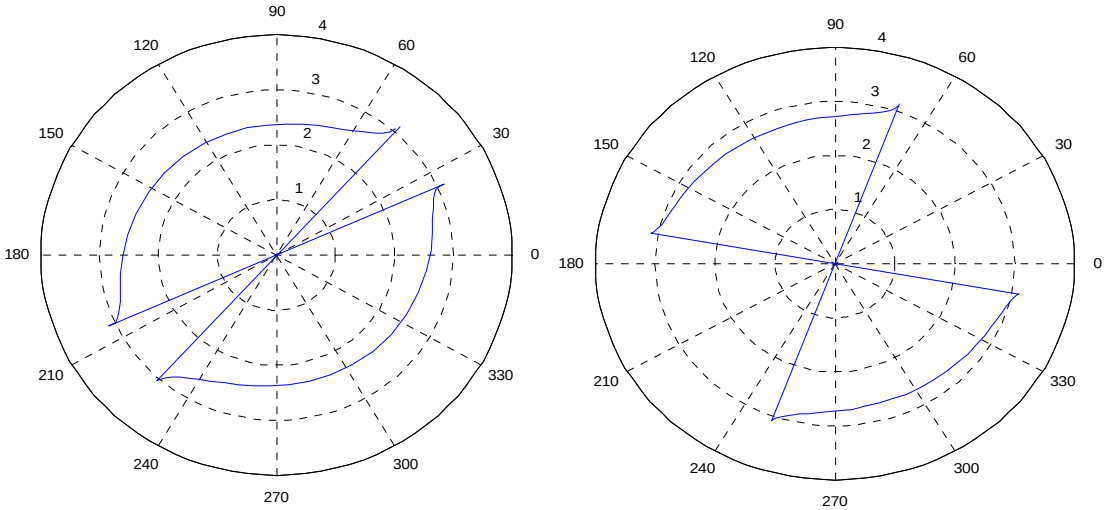

Fig. 4: Stability regions for the third -order IIF scheme with $q\Delta t = 1, 1.5$.

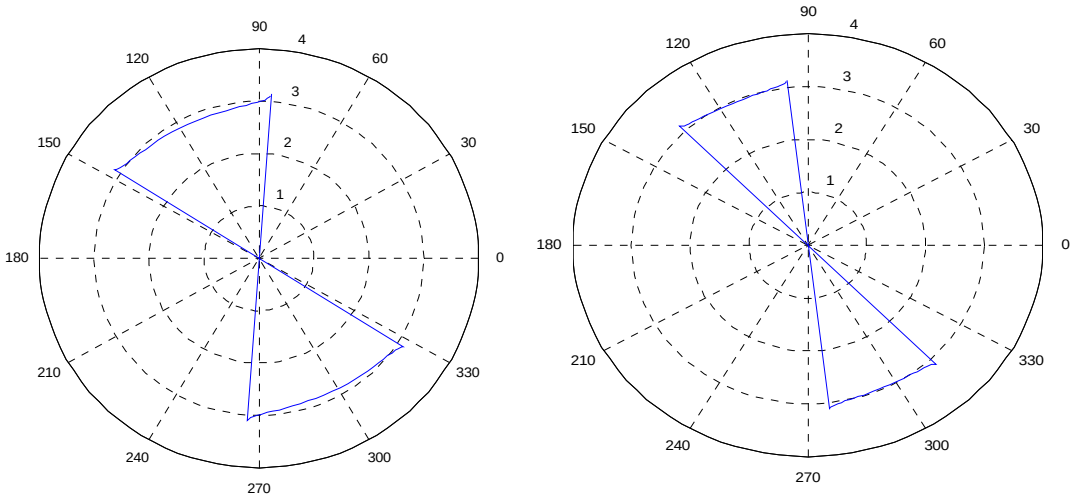

Fig. 5: Stability regions for the third - order IIF scheme with $q\Delta t = 2, 2.5$.

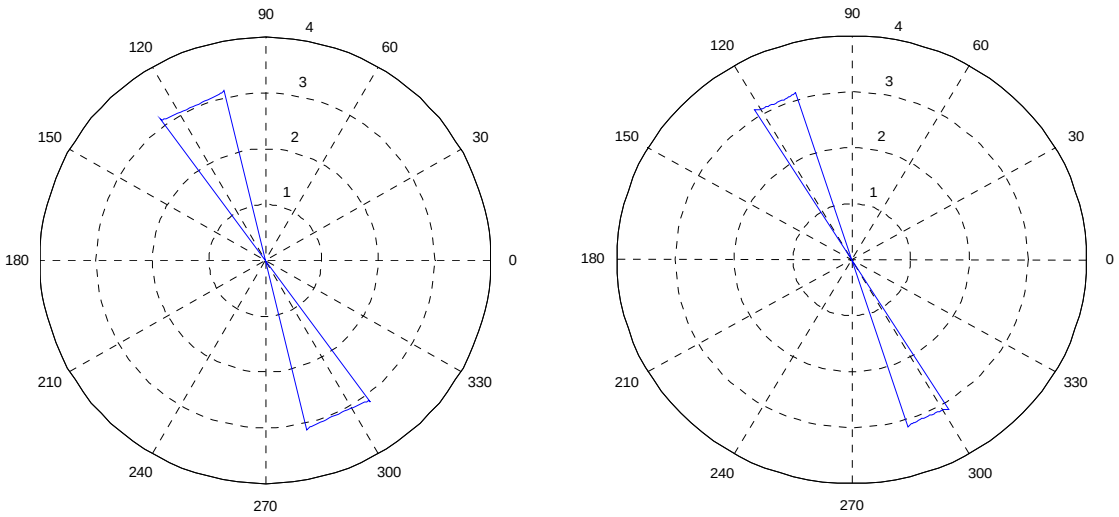

Fig. 6: Stability regions for the third order IIF scheme with $q\Delta t = 3, 3.5$.

In IIF3, all the Figures above show the step by step stability region for the third-order scheme, which finally becomes A-stable. Clearly, the size of the stability region is considered very sensitive to the value of $q\Delta t$, since it depends on the values of $q\Delta t$. It is found that the stability region is maintained by increasing $q\Delta t$. Thus when $q \to \infty$, the stability region in the complex plane approaches a point in the real axis.

As a result, the IIF method gives rise to the good stability properties as compared to the explicit integration factor methods and other exponential time difference schemes.

4. Conclusion

Even though, there have been attempts to treat the nonlinear reaction equations implicitly using implicit–explicit Runge–Kutta schemes [15, 16, 17], the diffusion term in these methods is still treated explicitly.

In this paper, we have presented a class of methods, which eliminates both restrictions on the setting of a linear stability theory. Moreover, in the new techniques, as a result of the implicit treatment of the nonlinear reaction equation, the nonlinear system has the same size as the number of original differential equations. Likewise, for systems in higher spatial dimensions or systems involving high-order derivatives, the new methods would be more advantageous than the studied one-dimensional system with diffusions. In addition, a fully implicit method is required for solving very large nonlinear systems, which depend on two- or three-dimensional spatial discretizations.

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