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The Effect of Weighton Simi-ImplicitScheme

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Abstract: *In this paper, two types of methods are presented: the basic type, which can be considered as an implicit integration factor (IIF) method, and an advanced type, which combinesthe IIF method with standard explicit ETD method through appropriate weights to ensure the conservation offixed points of the numerical schemes. Moreover, we present the weighted IIF-ETD methods and discuss their stability properties.*

***Keywords**: Implicit schemes; Reaction-diffusion equations; Integration factor methods; Exponential time differencing methods.*

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I. Introduction

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

$$\frac{\partial u}{\partial t} = D\Delta u + F(u), \quad (1.1)$$

where$u \in R^m$ shows a group of biological or physical species, $D \in R^{m\times m}$ represents diffusion constraint matrix, Δu is the Laplacian which is related to the diffusion of species u, and $F(u)$ illustrates chemical or biological reactions. To solve the equation numerically, the method of lines is utilized; reaction-diffusion (1. 1) is decreased to a system of ODEs:

$$u_t = Lu + G(u), \quad (1.2)$$

whereLu is a finite difference approximation of $D\Delta u$. For the approximation of Laplacian Δu, Nshows an independence of number of spatial dimensions (the number of spatial grid points).Thus $u(t) \in R^{N\times m}$ and $L$are a $(N.m) \times (N.m)$ matrix instead of a spatial discretization of the diffusion. Tosolve (1.2), the range of the time-step is limited for a time integrator via the inverse of the eigenvalues of the diffusion matrix D with the stiffness of the nonlinear reaction term $G(u)$. As N increases, in the system (1.1), the diffusion constants become bigger or the spatial resolution get better and the stability restriction becomes very rigorous because of diffusion [1-3].

The part of the linear diffusion has been decreased to the estimation of an exponential function of the matrix$L$, after that an approximation of an integral relating the nonlinear term $G(u)$. Unlike approximations of the integral relating, nonlinear term $G(u)$ gives rise to either the exponential time differencing (ETD) or the IF (integration factor) method. For the ETD methods, particular treatments for a variety of operations on L (e.g., its inverse) are required to preserve a steady order of accuracy [4-6]. Leo *et al*. [7] studied the fixed points for the new systems which are not precisely preserved in the numerical scheme, and consequently, further terms have to be included into the standard methods called IF to protect such preservation. Cox and Matthews discussed in one direction of reforming the region of stability for a stiff reaction is to take in an RK kind estimate for the term relating$G(u)$ into the ETD scheme [8].

In general, the ETDRK method has a better region of stability than the standard ETD, while the multi-stage nature of RK methods needs additional function estimations[9]. On the other hand, for systems with extremely stiff reactions, it is still not effective enough, since generally it is the case for some applications of biological, for example, the morphogen gradient scheme in which the reaction rate constants in $F(u)$ can be different via four to five order of magnitude [10-13]. Other papers on this subject include [14 - 28].

The present paper is organized as follows: In section 1, we present the subject. In section 2, we demonstrate background of the study. In section 3, we consider the weighted IIF-ETD methods, and discuss their stability properties. In section 4, a brief conclusion is given.

II. Background Of The Study

2.1. Stability analysis of IIF

In this section, we intend to show the stability region for IIF2[24].For this purpose, the steady condition is achieved as a dynamic progress by applying standard IF methods, which has an error of order (Δt^p).

Moreover, discretization errors relate to space [3]. Since the fixed points of the numerical scheme are not preserved, the following decoupled linear problem cannot be used directly,

$$u_t = -qu + du \qquad q > 0 \,. \tag{2.1}$$

For the IIF methods, the steady state of ODE system, the stability regions are examined by means of the diffusion and the reaction [7].The boundaries of the region of stability, which consist of a class of curves for unusual values of $q\Delta t$ are shown, based on the analysis of problem (2.1) for IIF2 method. Thus,the IIF2 (second order) scheme is derived in the following form ,

$$u_{n+1} = e^{c\Delta t}\left(u_n - \frac{\Delta t}{2} f(u_n)\right) - \frac{\Delta t}{2} f(u_{n+1}) \,. \tag{2.2}$$

The second order IIF (2.2) to equation (2.1) is applied, and then substituting $u_n = e^{in\theta}$ into resulting equation (2.1), the following equation is derived

$$e^{i\theta} = e^{-q\Delta t}\left(1 - \frac{1}{2}\lambda\right) - \frac{1}{2}\lambda e^{i\theta}, \tag{2.3}$$

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

$$\lambda_r = \frac{2(e^{-2q\Delta t} - 1)}{(1 - e^{-q\Delta t})^2 + 2(1 + \cos\,\theta)e^{-q\Delta t}}\,, \tag{2.4}$$

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

Since $q > 0$, then $\lambda_r < 0$, which resultedfor $0 \le \theta \le 2\pi$. Subsequently, IIF2 is A-stable because the region of stability has been included in the complex plane for λ with $\lambda_r < 0$.

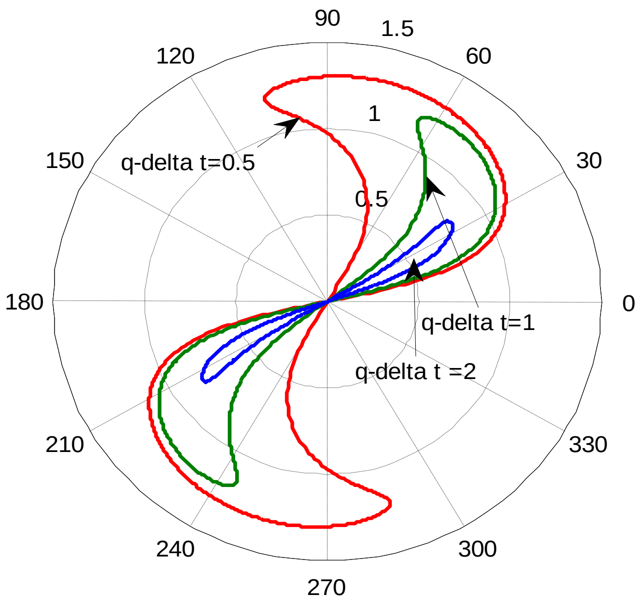

Figure1: The regions of stability (exterior of the closed curves) for IIF2 with $\boldsymbol{q\Delta t = 0.5, 1, 2}$.

III. Weighted IIF2 And ETD

In this section, we derive a weight formula from the second order IIF and ETD. For this purpose, we define two weights $w_1$and w_2IIF and ETD, respectively.

$$u(t_{n+1}) = u(t_n)e^{c\Delta t} + w_1\left(e^{c\Delta t}\int_0^{\Delta t} e^{-c\tau} f(u(t_n+\tau))d\tau\right) + w_2\left(e^{c\Delta t}\int_0^{\Delta t} e^{-c\tau} f(u(t_n+\tau))d\tau\right)$$

To estimate the integral in w_1 term applying the second order IIF (IIF2) approach and the integral in $w_2$term applying the second order ETD (ETD2) approach, we find

$$u_{n+1} = u_n e^{c\Delta t} + w_1\left[-\frac{\Delta t}{2} f(u_{n+1}) - \frac{e^{c\Delta t}\Delta t}{2} f(u_n)\right]$$
$$+ w_2\left[\frac{(1+c\Delta t)e^{c\Delta t} - 1 - 2c\Delta t}{c^2\Delta t} f(u_n) + \frac{-e^{c\Delta t} + 1 + c\Delta t}{c^2\Delta t} f(u_{n-1})\right] \tag{3.1}$$

To show$\tilde{u}$ as the fixed point of the above equation (setting$u_{n+1} = u_n = u_{n-1} = \tilde{u}$)and $\bar{u}$ as a fixed point of the equation (3.2) (setting c$\bar{u} = -f(\bar{u})$). If $\tilde{u} = \bar{u}$ yields

$$\frac{du}{dt} = cu + f(u), \qquad t > 0 \;, u(0) = u_o \tag{3.2}$$

$w_2 = 1 - \frac{c\Delta t}{2}\frac{1+e^{c\Delta t}}{1-e^{c\Delta t}}w_1$ (3.3)

The scheme (3.1) has the second order accuracy due to $w_1 + w_2 = 1 + O(\Delta t^2)$.

For the stability, $c = -q$ and $q > 0$ in the description of w_2, and$w_1$should satisfy

$0 \le w_1 \le \frac{2(1-e^{-q\Delta t})}{q\Delta t(1+e^{-q\Delta t})} = W(q\Delta t)$ (3.4)

for any fixed $q\Delta t$ in order to formulatew_1 and w_2 both positive .As a result, $0 \le w_2 \le 1$.$q\Delta t = \alpha$ischosen , then we have $W(\alpha) < 1$ for $\alpha > 0$. This can be verified by considering $f(\alpha) \equiv 2(1-e^{-\alpha}) - \alpha(1+e^{-\alpha})$ is a decreasing function for$\alpha \ge 0$.$W(\alpha) < 1$comesfrom $f(\alpha) < f(0) = 0$ for $\alpha > 0$ .Moreover, we have$W(\alpha) \to 1$ as $\alpha \to 0$ and $W(\alpha) \to 0$as $\to \infty$ .Applying those properties, we can illustrate $0 \le w_1 + w_2 \le 1$ for any $q\Delta t > 0$ given that$0 \le w_1 \le W(q\Delta t)$.

To apply the equation (3.1) to equation (2.1), in that case, substituting $u_n = e^{in\theta}$ into the resulting equation, the following equation is obtained

$e^{i\theta} = e^{-\alpha} + w_1\left(-\frac{\lambda}{2}e^{i\theta} - \frac{e^{-\alpha}\lambda}{2}\right) + \left(1 + \frac{\alpha(1+e^{-\alpha})}{2(1-e^{-\alpha})}\right)w_1\left[\frac{(1-\alpha)e^{-\alpha}-1+2\alpha}{\alpha^2}\lambda + \frac{-e^{-\alpha}+1-\alpha}{\alpha^2}\lambda e^{-i\theta}\right]$or,

(3.6)

$$\lambda = \frac{e^{i\theta} - e^{-\alpha}}{-\frac{w_1}{2}(e^{i\theta} + e^{-\alpha}) + \left(1 + \frac{\alpha(1+e^{-\alpha})}{2(1-e^{-\alpha})}\right)w_1\left[\frac{(1-\alpha)e^{-\alpha}-1+2\alpha}{\alpha^2} + \frac{1-\alpha-e^{-\alpha}}{\alpha^2}e^{-i\theta}\right]}$$

(3.7)

where$\lambda = d\Delta t$, $\alpha = q\Delta t$ and .

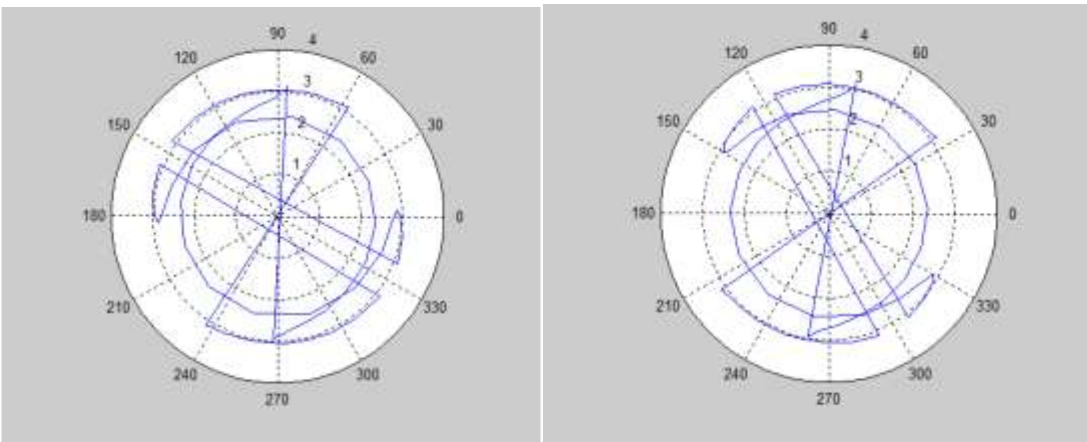

Figure 2: The regions of stability for IIF2 scheme with $\boldsymbol{w_1 = 0, 0.5}$

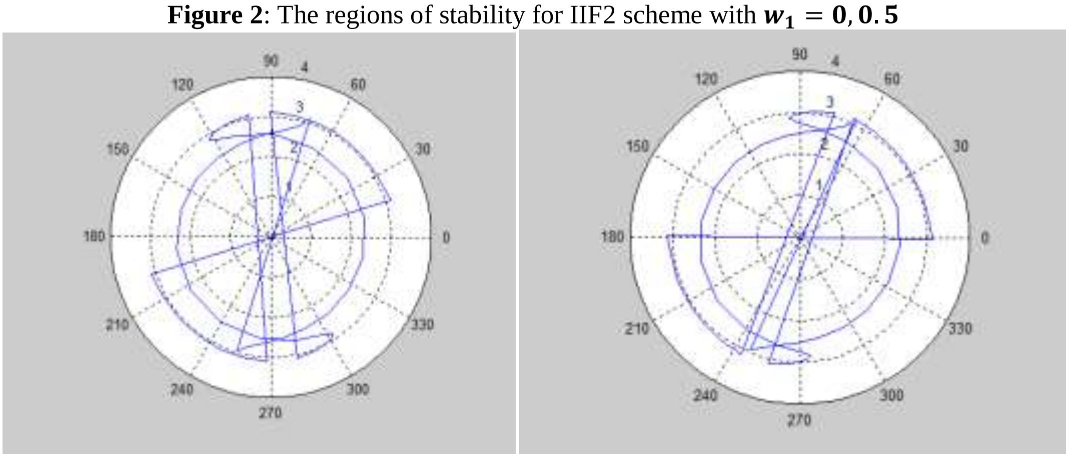

Figure 3: The regions of stability for IIF2 scheme with$\boldsymbol{w_1 = 0.55,\ 0.6}$

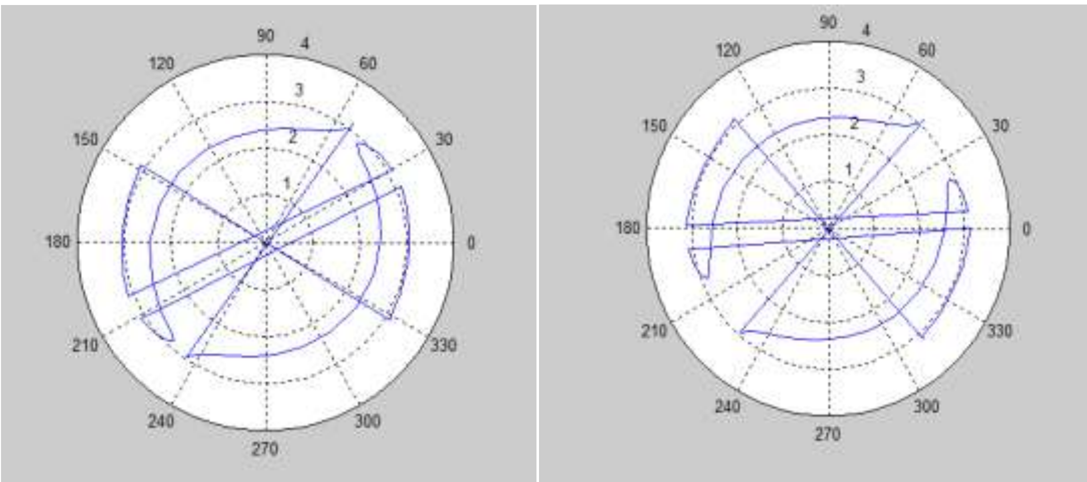

Figure 4: The regions of stability for IIF2 scheme with $\boldsymbol{w_1 = 0.66, 0.8}$

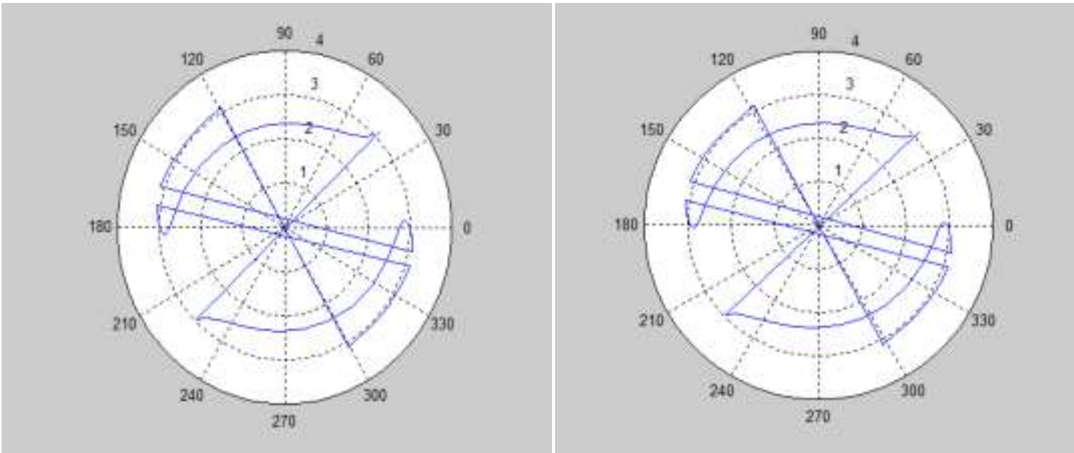

Figure 5: The regions of stability for IIF2 scheme with $\boldsymbol{w_1 = 0.88, 0.9}$

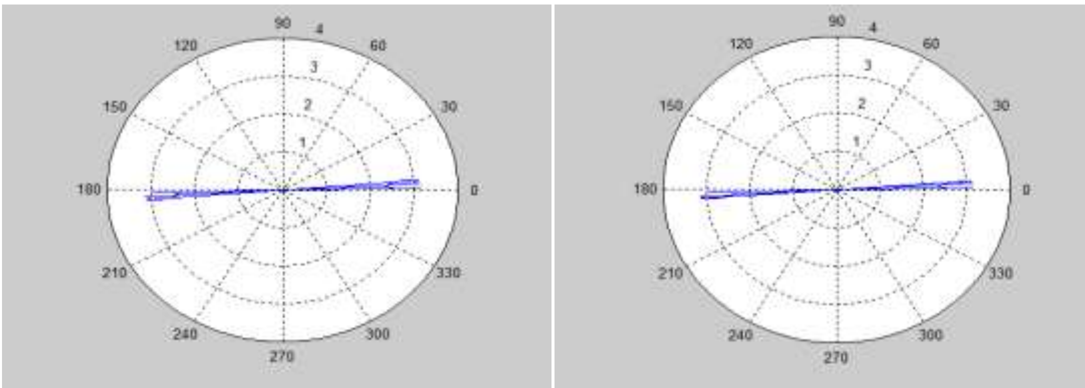

Figure6: The regions of stability for IIF2 scheme with$\boldsymbol{w_1 = 0.99, 1}$

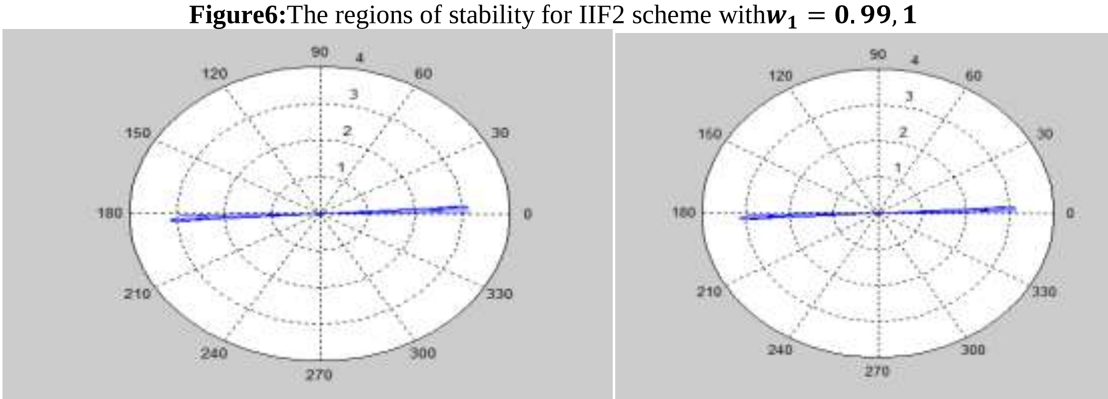

Figure 7: The regions of stability for IIF2 scheme with $\boldsymbol{w_1 = 35, 40}$

IV. Results and Discussion

In IIF2, Figures 2 and3 illustrate the regions of stability are chaos. However, Figures 4,5, 6 and 7 show the step by step stability region for the third-order scheme, which finally becomes A-stable. Clearly, the regions of stability are considered extremely 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 region of stability in the complex plane approaches a point in the real axis.

Acknowledgments

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Appendix A

```
clear
clc
closeall

qdelta=.5;
```

```
w1=[0 .5 .55 .6 .66 .8 .88 .9 .99 1 35 40];

for h=1:length(w1);
% k3=w1;
teta=0:0.1:2*pi;
alfa=qdelta;
num=exp(1i*teta)-exp(-alfa);
a1(h,:)=-0.5*w1(h)*(exp(1i*teta)+exp(-alfa));

% k=(exp(1i*teta)+exp(-alfa))
a2(h,:)=w1(h).*(1+alfa*(1+exp(-alfa))./2*(1-exp(-alfa));

% a3=((1-alfa)*exp(-alfa)-1+2*alfa)./(alfa)^2;
a4(h,:)=(((1-alfa)*exp(-alfa)-1+2*alfa)./(alfa)^2)+((1-alfa-exp(-
alfa))./(alfa).^2).*exp(-1i*teta);

% denm=-1/2*exp(1i*teta)-1/2*exp(-qd);elta)-1/2*exp(-2*qdelta-1i*teta);
denm(h,:)=a1(h,:)+a2(h,:).*(a4(h,:));

landa(h,:)=num./denm(h,:);
abs_complex(h,:)=abs(landa(h,:));
teta_complex(h,:)=angle(landa(h,:));
figure
polar(abs_complex(h,:),teta_complex(h,:));
end
```

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