Explicit- Implicit Runge-Kutta Methods to Solve the System of Nonlinear PPDEs in Two Dimensions

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ABSTRACT

In this paper, we will find the numerical solution of Gray-Scott model in two dimensions space, this method is a system of non-linear parabolic partial differential equations. Then transforming the original model (system of non-linear PPDEs), by using the method of lines to a system of ODEs. Therefore we used Runge-Kutta methods (Explicit RK method and Implicit RK method) to find the numerical solutions of the new systems, and we compared between these methods, we saw that the numerical results of IRK methods is more accurate than the numerical results of ERK method.

Keywords: Gray-Scott model in two dimensions, finite difference methods, Method of lines, Explicit Runge Kutta method , Implicit Runge Kutta method.

طرائق رانج–كوتا الصريحة والضمنية لحل نظام من المعادلات التفاضلية الجزئية غير الخطية من نوع القطع المكافيء في بعدين

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الملخص

في هذا البحث تم إيجاد الحلول العددية لنموذج **Gray-Scott** في فضاء البعد الثاني، هذا النموذج هو نظام من المعادلات التفاضلية الجزئية من نوع القطع المكافئ الغير خطي حيث تم تحويل النموذج الأصلي إلى نظم من المعادلات التفاضلية الاعتيادية باستخدام شبه التقطيعات **(MOLs)**. ثم استعملنا طرائق رانج–كوتا (طريقة رانج–كوتا الصريحة وطريقة رانج–كوتا الضمنية) لإيجاد الحلول العددية للنظم الجديدة وقارنا بين الطريقتين. لاحظنا أن النتائج العددية للطريقة الضمنية هي أكثر دقة من النتائج العددية للطريقة الصريحة.

الكلمات المفتاحية: أنموذج گراي-سكوت, طرائق الفروقات المنتهية, طريقة شبه التقطيعات, طريقة رانج–كوتا الصريحة, طريقة رانج–كوتا الضمنية.

1. Introduction:

Many physical, chemical and engineering problems, mathematically, can be modeled in the form of system of partial differential equations or system of ordinary differential equations. Parabolic PDEs (partial differential equations) describe practically useful phenomena such as transport-chemistry problems of the advection-diffusion-reaction type and problem of this type play an important role in the modeling of pollution of the atmosphere, ground water and surface water [9].

Khaddaj and Liddell [6] discussed the numerical solution of time-dependent partial differential equations (PDEs) by the numerical method of lines (NMOL) transporter based systems. Parallel methods for the solution of systems of ordinary differential equations (ODEs) are considered. Algorithms based on the NMOL are parallel ODEs solver are presented.

Celi, R [4] used the method of lines to apply on the equations of helicopter rotor vortex wakes, and converts the governing PDEs into a system of ODEs. These ODEs can then be coupled to other ODEs modeling helicopter dynamics, for time-marching simulations are to extract linearized models. The MOLs is applied to a simplified set of

wake equations that has an analytical solution. Because these simplified equations neglect key wake physics, the study is only a first step toward applying MOLs to realistic models. Therefore, the conclusions only apply to the simplified problem considered. He shows that the results of the MOLs are a suitable method to formulate vortex wake models in state-space form. The solutions are accurate and numerically stable. Refining the space discretization increases the stiffness of the ODEs, but explicit solvers can still be used.

Asher et. al. [1] show that the implicit- explicit Range-Kutta schemes are strictly related which provides a framework for the derivation of more general, accurate and efficient schemes.

Minion [10] used method of Lines on PDEs, and then semi- implicit formulation of the method of spectral deferred corrections for ODEs with both stiff and non-stiff terms.

Butcher [3] has developed many types of implicit Rung-Kutta method to reduce storage space and getting more accurate solution.

In this paper we find the numerical solution of system of non-linear PPDEs by transforming the non-linear PPDE to a system of non-linear ordinary differential equation and then using Explicit and implicit Rung-Kutta methods. We use the NMOLs to transform the system of parabolic partial differential equations (PPDEs) into a systems of ODEs, ([6], [7]), and then we study the properties of the numerical solution of IVPs in ODEs. Also we recall the basic definitions and theories that concern numerical solution of IVPs in ODEs.

2. The Gray-Scott Model Problem in Two Dimensions

Reaction-diffusion models of chemical species can produce a variety of patterns, reminiscent of those often seen in nature. The Gray-Scott equations model can be consider as reaction. Numerical simulations of this model were performed in an attempt to find stationary lamellar patterns like those observed in earlier laboratory experiments on ferrocyanideiodate-sulphite reactions [13]. The chemical reactions for this situation are described by

$$\mathrm{U+2V} \rightarrow \mathrm{3V},$$
$$\mathrm{V} \rightarrow \mathrm{P},$$

where U, V and P are chemical species. The system of reaction-diffusion equations for this situation is given by

$$u_t = \alpha_1\left(\frac{\partial^2 u}{\partial x^2}+\frac{\partial^2 u}{\partial y^2}\right) - uv^2 + f\left(1-u\right),$$
$$v_t = \alpha_2\left(\frac{\partial^2 v}{\partial x^2}+\frac{\partial^2 v}{\partial y^2}\right) + uv^2 - \left(f+g\right)v.$$

where u and v are concentrations of two reactions, α_1 and α_2 are the diffusion rates in the process, g represents the rate of conversion of V to P, and f the rate of the process that feeds U and drains U, V and P ([14], [12]).

We choose the model parameters as $\alpha_1 = 8\times10^{-5}$, $\alpha_2 = 4\times10^{-5}$, f = 0.02 and g = 0.066 to get the model showed in equations (1) and (2)

From pattern formation the following reaction diffusion system ([15], [5]) exhibits complicated Solution behavior:

$$\frac{\partial u}{\partial t}=\alpha_1\left(\frac{\partial^2 u}{\partial x^2}+\frac{\partial^2 u}{\partial y^2}\right)-uv^2+0.02(1-u)\,, \qquad \ldots(1)$$

$$\frac{\partial v}{\partial t}=\alpha_2\left(\frac{\partial^2 v}{\partial x^2}+\frac{\partial^2 v}{\partial y^2}\right)+uv^2-0.086\,v. \qquad \ldots(2)$$

where $\alpha_1=8\times10^{-5}$ and $\alpha_2=4\times10^{-5}$
The initial conditions are

$u(x,y,0)=1 \quad , \ 0\le x\ ,y\le 1,$

$v(x,y,0)=1 \quad , \ 0\le x\ ,y\le 1,$

on the spatial domain [0,1]×[0,1].

In this model self-replicating spots have been observed. These are regions in which the (chemical) concentrations of some of the species exhibit large amplitude perturbations from a surrounding homogenous state.

3. Runge-Kutta Methods Solution for ODEs

The general form of s-stage Runge-Kutta method [3] can be written as

$$u_{n+1}=u_n+h\,\phi(t_n,u_n,h),\ \ n\ge 0 \qquad \ldots(3)$$

where

$$\phi(t_n,u_n,h)=\sum_{i=1}^{s} b_i\ \mathrm{k_i} \qquad \ldots(4)$$

$$k_i=f\left(t_n+c_i h,u_n+h\sum_{j=1}^{s} a_{ij}\ \mathrm{k_j}\right),\mathrm{j}=1,2,\ldots,\mathrm{s} \qquad \ldots(5)$$

where s represents the number of stage for the method c_i, a_{ij}, b_i, i,j=,2,…,s are parameters.

The windows form of the method is

$$\begin{array}{c|ccccc} c_1 & a_{11} & a_{12} & \cdots & a_{1s} \\ c_2 & a_{21} & a_{22} & \cdots & a_{2s} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ c_n & a_{s1} & a_{s2} & \cdots & a_{ss} \\ \hline & b_1 & b_2 & \cdots & b_s \end{array} \equiv \begin{array}{c|c} \mathrm{C} & \mathrm{A} \\ \hline & \mathrm{b^T} \end{array} \qquad \ldots(6)$$

where $c_i=\sum_{j=1}^{s} a_{ij}$, $\sum_{i=1}^{s}\mathrm{b_i}=1$ [3].

If the coefficients a_{ij} are equal to zero for $j\ge i$ then each k_j can be explicitly computed in term of the (i-1) coefficients k_1, …, k_{j-1} and in this case the explicit RK method equation (5) becomes:

$$k_i=f\,(t_n+c_i h,u_n+h\sum_{j=1}^{i-1} a_{ij}\ \mathrm{k_j}),\ \mathrm{i}=1,2,...,\mathrm{s} \qquad \ldots(7)$$

If $k_i = hf(t_n + c_i h, u_n + h\sum_{j=1}^{s} a_{ij}\ \mathrm{k_j}), \mathrm{i} = 1,2,..., \mathrm{s}$ …(8)

and the function k_j are defined by a set of simplicity equations then RK method is said to be full IRK method ([2],[3]).

4. The Method of Lines:

The method of Lines (MOLs) is a convenient technique for solving time-dependent partial differential equations. Replace all spatial derivatives with finite differences, but leave the time derivatives intact, and use an ordinary differential equation solver on the resulting system. In effect, this is an implicit time-stepping finite difference algorithm with the time step determined automatically adaptively by the ODEs solver along a line in time (see figure (1)) [11].

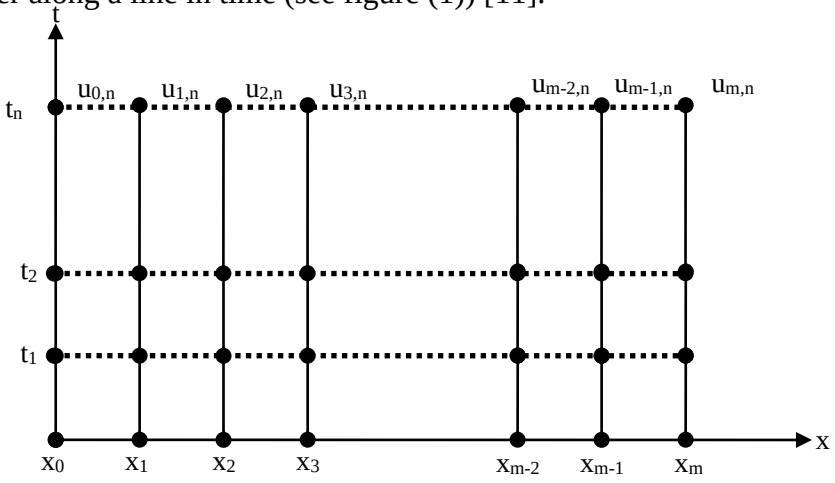

Figure (1). The method of lines

Example: Given a general parabolic equation of the form

$$u_t(x,t) = Lu(x,t) + f(x,t), \quad \ldots(9)$$

where L is an elliptic operator. Let L_n be a finite difference operator on a grid x_i=a+ih.

We can form a semi-discrete system [11] of ordinary differential of the following form

$$\frac{\partial U_i}{\partial t} = L_n U_i(t) + \mathrm{f}_i(t) \quad \ldots(10)$$

In other words, we only discretize the spatial variable. For the heat equation with a source $u_t = \alpha\, \mathrm{u_{xx}} + f$. We have $L = \frac{\partial^2}{\partial x^2}$, $L_h = \delta_{xx}^2$, the discretize system of ODE [11] is:

$$\frac{d\mathrm{U_i(t)}}{d\mathrm{t}} = \alpha \frac{U_{i-1}(t) - 2U_i(t) + U_{i+1}(t)}{h^2} + f(x_i, t), \quad \ldots(11)$$

i=1,2,...,m-1

The initial condition is $U_i(0)=u_0(x_i,0)$, i=1,2,...,m-1

The ODE system can be written as a vector form

$$\frac{\mathrm{d}\underline{\mathrm{y}}}{\mathrm{dt}} = \underline{\mathrm{f}}(\underline{\mathrm{y}}, \mathrm{t}),\ \underline{\mathrm{y}}(0) = \underline{\mathrm{y}}_0 \quad \ldots(12)$$

5. Numerical Methods

5.1. Explicit RK method

The form of ERK method of order four is [8]

$$u_{n+1} - u_n = \frac{h}{6}(k_1 + 2k_2 + 2k_3 + k_4) \quad \ldots(13a)$$

$$k_1 = f(t_n, u_n), \quad \ldots(13b)$$

$$k_2 = f(t_n + \frac{1}{2}h, u_n + \frac{1}{2}h\,k_1), \quad \ldots(13c)$$

$$k_3 = f(t_n + \frac{1}{2}h, u_n + \frac{1}{2}h\,k_2), \quad \ldots(13d)$$

$$k_4 = f(t_n + h, u_n + h\,k_3), \quad \ldots(13e)$$

5.2. Implicit Runge-Kutta Method

The general R-stage Implicit RK method is defined by [8]

$$u_{n+1} - u_n = h\,\phi(t_n, u_n, h), \quad \ldots(14a)$$

$$\phi(t, u, h) = \sum_{r=1}^{R} b_r k_r, \quad \ldots(14b)$$

$$k_r = f(t + h\,c_r, u + h\sum_{s=1}^{R} a_{rs}\,k_s), \ r = 1, 2, \ldots, R \quad \ldots(14c)$$

$$c_r = \sum_{s=1}^{R} a_{rs}, \ r = 1, 2, \ldots, R \quad \ldots(14d)$$

Then two-stage implicit Runge-Kutta method of order four is defined by

$$u_{n+1} - u_n = \frac{h}{2}(k_1 + k_2), \quad \ldots(15a)$$

$$k_1 = f\left(t_n + \left(\frac{1}{2} + \frac{\sqrt{3}}{6}\right)h, u_n + \frac{1}{4}h\,k_1 + \left(\frac{1}{4} + \frac{\sqrt{3}}{6}\right)h\,k_2\right), \quad \ldots(15b)$$

$$k_2 = f\left(t_n + \left(\frac{1}{2} - \frac{\sqrt{3}}{6}\right)h, u_n + \left(\frac{1}{4} - \frac{\sqrt{3}}{6}\right)h\,k_1 + \frac{1}{4}h\,k_2\right), \quad \ldots(15c)$$

6. Numerical Solution of the Model

We find the numerical solution to PPDEs, system (1) and (2) by two numerical methods ERK method and IRK method using MOLs to transform (4.1) and (4.2) to a system of ODEs which can be written when h=k in the form

$$\frac{du(t)}{dt} = \frac{\alpha_1}{h^2}\left[u_{i+1,j,n+1} - 2u_{i,j,n+1} + u_{i-1,j,n+1}\right] + \frac{\alpha_1}{h^2}\left[u_{i,j+1,n+1} - 2u_{i,j,n+1} + u_{i,j-1,n+1}\right] \quad \ldots(16)$$
$$- u_{i,j,n}v_{i,j,n}^2 + 0.02(1 - u_{i,j,n})$$

and

$$\frac{dv(t)}{dt} = \frac{\alpha_2}{h^2}\left[v_{i+1,j,n+1} - 2v_{i,j,n+1} + v_{i-1,j,n+1}\right] + \frac{\alpha_2}{h^2}\left[v_{i,j+1,n+1} - 2v_{i,j,n+1} + v_{i,j-1,n+1}\right] \quad \ldots(17)$$
$$+ u_{i,j,n}v_{i,j,n}^2 - 0.086\,v_{i,j,n}$$

where $x_i=ih$, $y_i=jh$ and i, j, n=1,2,…,N.

Then the above systems (16) and (17) can be written as

$$\frac{du(t)}{dt} = Au + Bu - uv^2 + 0.02(1-u)$$

$$\frac{dv(t)}{dt} = Cv + Dv + uv^2 - 0.086\,\mathrm{v}$$

where the tri-diagonal matrix A, B, C and D, and the concentration u and v have the form

$$A=\frac{\alpha_1}{h^2}\begin{bmatrix} -2 & 1 & 0 & \cdots & \cdots & \cdots & 0 \\ 1 & -2 & 1 & 0 & \cdots & \cdots & 0 \\ 0 & 1 & -2 & 1 & 0 & \cdots & 0 \\ \vdots & \ddots & & & & \ddots & \vdots \\ \vdots & & \ddots & & & & 0 \\ \vdots & & & \ddots & 1 & -2 & 1 \\ 0 & 0 & \cdots & \cdots & 0 & 1 & -2 \end{bmatrix}, \mathrm{u}=\begin{bmatrix} \mathrm{u}_{1,j,n+1} \\ \mathrm{u}_{2,j,n+1} \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ \mathrm{u}_{i+1,j,n+1} \end{bmatrix}$$

$$B=\frac{\alpha_1}{h^2}\begin{bmatrix} -2 & 1 & 0 & \cdots & \cdots & \cdots & 0 \\ 1 & -2 & 1 & 0 & \cdots & \cdots & 0 \\ 0 & 1 & -2 & 1 & 0 & \cdots & 0 \\ \vdots & \ddots & & & & \ddots & \vdots \\ \vdots & & \ddots & & & & 0 \\ \vdots & & & 0 & 1 & -2 & 1 \\ 0 & 0 & \cdots & \cdots & 0 & 1 & -2 \end{bmatrix}, \mathrm{u}=\begin{bmatrix} \mathrm{u}_{i,1,n+1} \\ \mathrm{u}_{i,2,n+1} \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ \mathrm{u}_{i,j+1,n+1} \end{bmatrix}$$

$$C=\frac{\alpha_2}{h^2}\begin{bmatrix} -2 & 1 & 0 & \cdots & \cdots & \cdots & 0 \\ 1 & -2 & 1 & 0 & \cdots & \cdots & 0 \\ 0 & 1 & -2 & 1 & 0 & \cdots & 0 \\ \vdots & \ddots & & & & \ddots & \vdots \\ \vdots & & \ddots & & & & 0 \\ \vdots & & & 0 & 1 & -2 & 1 \\ 0 & 0 & \cdots & \cdots & 0 & 1 & -2 \end{bmatrix}, \mathrm{v}=\begin{bmatrix} \mathrm{v}_{1,j,n+1} \\ \mathrm{v}_{2,j,n+1} \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ \mathrm{v}_{i+1,j,n+1} \end{bmatrix}$$

$$D=\frac{\alpha_2}{h^2}\begin{bmatrix} -2 & 1 & 0 & \cdots & \cdots & \cdots & 0 \\ 1 & -2 & 1 & 0 & \cdots & \cdots & 0 \\ 0 & 1 & -2 & 1 & 0 & \cdots & 0 \\ \vdots & \ddots & & & & \ddots & \vdots \\ \vdots & & \ddots & & & & 0 \\ \vdots & & & & 0 & -2 & 1 \\ 0 & \cdots & \cdots & \cdots & 0 & 1 & -2 \end{bmatrix}, \mathrm{v}=\begin{bmatrix} \mathrm{v}_{i,1,n+1} \\ \mathrm{v}_{i,2,n+1} \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ \mathrm{v}_{i,j+1,n+1} \end{bmatrix}$$

In table (1), we show that the comparison between the above two methods for finding numerical solution for the Gray-Scott model in two dimensions that represent in system of equations (1) and (2). Where ERK and IRK methods have been used.

Table (1). comparison between ERK method and IRK method for the values of concentrations u and v that computed at time step size δt=0.1 and space step size h=k=0.1.

Point (i,j,n)	ERK method	IRK method	Error Estimate
	Concentration u		
(6,8,1)	1	1	0
(9,4,2)	0.89622764746864	0.89941375892612	0.00318611145748
(5,3,3)	0.78639547711517	0.80766821506889	0.02127273795372
(4,9,4)	0.67368366462782	0.70659225379597	0.03290858916815
(10,7,5)	0.56235078311363	0.60062674328733	0.03827596017370
(2,5,6)	0.45712135947325	0.49309946585418	0.03597810638093
(3,2,7)	0.36225626706226	0.38910367142062	0.02684740435836
(10,5,8)	0.28067391221563	0.29434498857433	0.01367107635870
(7,10,9)	0.21351475439768	0.21375275330471	0.00023799890703
(8,6,10)	0.16028013846879	0.14994306532769	0.01033707314110
(10,10,11)	0.11935892378226	0.10262015433508	0.01673876944718
Point (i,j,n)	ERK method	IRK method	Error Estimate
	Concentration v		
(6,8,1)	1	1	0
(9,4,2)	1.09487172033376	1.09088683603301	0.00398488430075
(5,3,3)	1.19517617642356	1.20310722057464	0.00793104415108
(4,9,4)	1.29770852626288	1.32853728176919	0.03082875550631
(10,7,5)	1.39821040273145	1.46447592246093	0.06626551972948
(2,5,6)	1.49198744794097	1.60701967468687	0.11503222674590
(3,2,7)	1.57483857665302	1.74994874886784	0.17511017221482
(10,5,8)	1.64392934956359	1.88516728112346	0.24123793155987
(7,10,9)	1.69821488835099	2.00424085233369	0.30602596398270
(8,6,10)	1.73829122153923	2.10063687940548	0.32345657866318
(10,10,11)	1.76585857761869	2.17152569069154	0.40566711307285

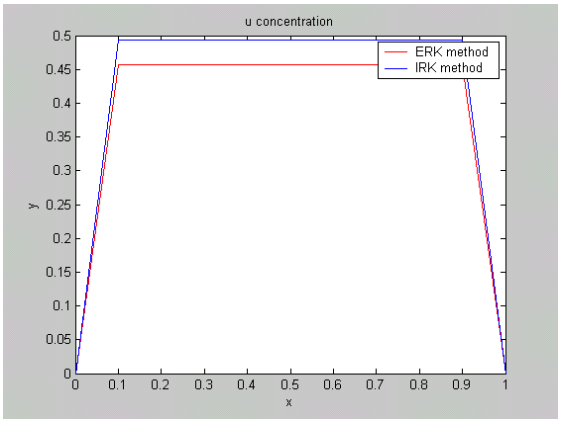

Figure (2). shows that the comparison between ERK and IRK methods for finding the concentration values u(6,:,6) at level n=6, row i=6 and for all columns j When $\alpha_1 = 8\times10^{-5}$, $\alpha_2 = 4\times10^{-5}$, and h=k=δt=0.1.

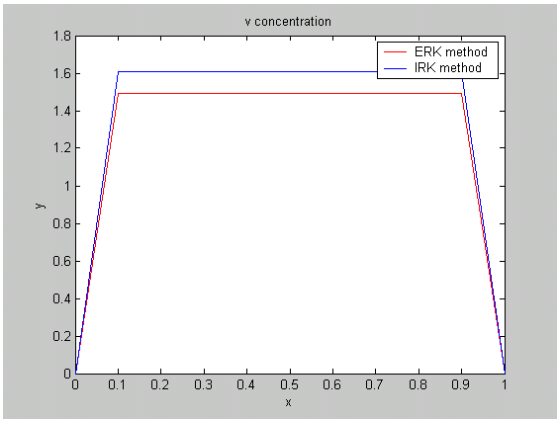

Figure (3). shows that the comparison between ERK and IRK methods for finding the concentration values v(6,:,6) at level n=6, row i=6 and for all columns j. When $\alpha_1 = 8\times10^{-5}$, $\alpha_2 = 4\times10^{-5}$, and h=k=δt=0.1.

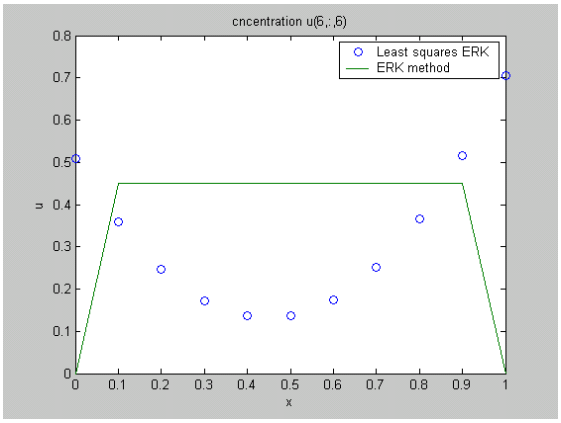

Figure (4). Least squares error of ERK methods for finding the concentration values u(6,:,6) at level n=6, row i=6 and for all columns j. When $\alpha_1 = 8\times10^{-5}, \alpha_2 = 4\times10^{-5}$, and h=k=δt=0.1.

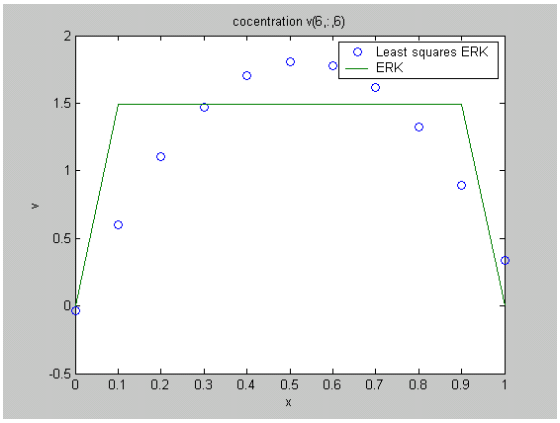

Figure (5) Least squares error of ERK methods for finding the concentration values v(6,:,6) at level n=6, row i=6 and for all columns j. When $\alpha_1 = 8\times10^{-5}$, $\alpha_2 = 4\times10^{-5}$, and h=k=δt=0.1.

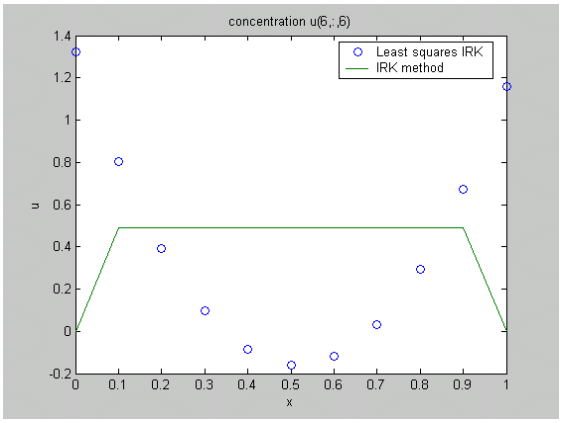

Figure (6). Least squares error of IRK methods for finding the concentration values u(6,:,6) at level n=6, row i=6 and for all columns j. When $\alpha_1 = 8\times10^{-5}$, $\alpha_2 = 4\times10^{-5}$, and h=k=δt=0.1.

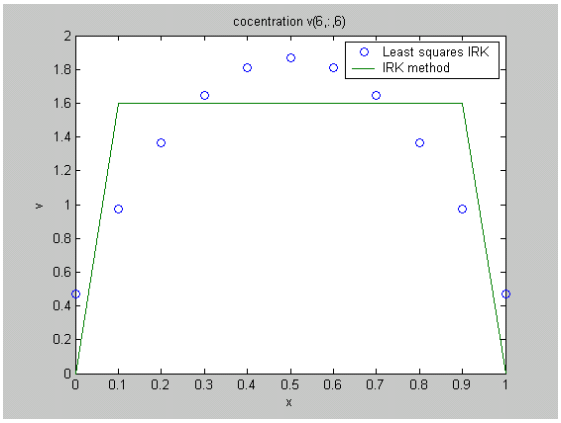

Figure (7) Least squares error of IRK methods for finding the concentration values v(6,:,6) at level n=6, row i=6 and for all columns j. When $\alpha_1 = 8\times10^{-5}$, $\alpha_2 = 4\times10^{-5}$, and h=k=δt=0.1.

7. Conclusion

The method of lines is convenient technique to transform the system of non-linear parabolic partial differential equations into the systems of ordinary differential equations and thus the new systems require special treatment. When we use ERK method to solve the system of ODEs, we notice that the region of stability is very small but when we used IRK method the stability region is big. Thus from table (1) we conclude that the numerical results of IRK method is more accurate than the results of ERK method, and we found least squares of each method.

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