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Partitioned Runge-Kutta methods for partial differential equations

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Abstract

We consider implicit-explicit Runge-Kutta (IMEX RK) schemes for time-dependent semi-linear partial differential equations. We show that the error of a scheme is of $\mathcal{O}(\Delta t^2)$ in time under some conditions, where Δt is the stepsize. This result is, in a sence, optimal. The so-called order reduction phenomena occur, i.e., the error of a scheme based on a partitioned RK method whose order ≥ 3 behaves as $\mathcal{O}(\Delta t^2)$, which is shown numerically.

1. Introduction

We consider initial-boundary value problems of the form

$$\frac{\partial u}{\partial t} = Lu + g(t,\, x,\, u),\ 0 \leq t \leq T,\ x \in \Omega, \tag{1.1}$$

$$\Phi_b u(t,\, x) = \varphi(t,\, x),\ 0 \leq t \leq T,\ x \in \partial\Omega, \tag{1.2}$$

$$u(0,\, x) = u^0(x),\quad x \in \Omega. \tag{1.3}$$

Here, $u = u(t,x)$ is an $\mathbb{R}^m$-valued unknown function, Ω is a bounded domain in $\mathbb{R}^d$ with the boundary $\partial\Omega$, L is a linear partial differential operator with constant coefficients with respect to x, Φ_b is a boundary operator. Various reaction-diffusion equations and nonlinear Schrödinger equations such as the Gross-Pitaevskii equation (see, e.g., [4]) are typical examples of (1.1).

Many numerical schemes for evolutional problems in partial differential equations (PDEs) are derived and implemented along the idea of the method of lines (MOL). In this approach a PDE is first discretized in space by finite difference or finite element techniques to be converted into a system of ordinary differential equations (ODEs). We consider the grid Ω_h defined by $\Omega_h = \Omega \cap hZ^d$ for $h > 0$, and MOL approximations of (1.1)–(1.2) in the form

$$\frac{\mathrm{d}U_h}{\mathrm{d}t} = L_h U_h + \varphi_h(t) + g_h(t,\, U_h). \tag{1.4}$$

Here, U_h is an approximate function of u on Ω_h, L_h is a difference approximation of L, g_h is the restriction of g onto Ω_h, and $\varphi_h(t)$ is a function determined from the boundary condition (1.2).

The ODE (1.4) is usually a stiff equation, not easily treated with the standard explicit methods. In some cases (e.g., [11]), the equation (1.4) is solved by a scheme of the form

$$U_h^{n+1} = U_h^n + \Delta t\Big(L_h U_h^{n+1} + \varphi_h(t_{n+1})\Big) + \Delta t\, g_h(t_n,\, U_h^n), \tag{1.5}$$

where Δt is the stepsize, given by $\Delta t = T/N$ for some integer $N \geq 1$, $t_n = n\Delta t$, and U_h^n is an approximate value of $U_h(t_n)$. The scheme (1.5) is obtained by applying the backward Euler formula to the linear part of (1.4) and the forward Euler formula to the nonlinear part. This type of scheme is called implicit-explicit (IMEX) scheme, or semi-implicit scheme.

The scheme (1.5) is of first order in the sense of order of convergence. There are two ways of improving (1.5) in accuracy: one is along the idea of linear multistep methods [1, 3, 12]; the other is along the idea of Runge-Kutta (RK) methods [2, 6, 8]. We follow the latter approach.

Let us consider a pair of two RK methods defined by the arrays

$$\begin{array}{c|cccccc} 0 & 0 & 0 & & \cdots & 0 \\ c_2 & a_{21} & a_{22} & 0 & \cdots & 0 \\ c_3 & a_{31} & a_{32} & a_{33} & & \vdots \\ \vdots & \vdots & & & \ddots & 0 \\ c_s & a_{s1} & a_{s2} & \cdots & a_{s,s-1} & a_{ss} \\ \hline & b_1 & b_2 & \cdots & b_{s-1} & b_s \end{array}\,, \qquad \begin{array}{c|cccccc} 0 & 0 & 0 & & \cdots & 0 \\ c_2 & \widehat{a}_{21} & 0 & & \cdots & 0 \\ c_3 & \widehat{a}_{31} & \widehat{a}_{32} & 0 & & \vdots \\ \vdots & \vdots & & & \ddots & 0 \\ c_s & \widehat{a}_{s1} & \widehat{a}_{s2} & \cdots & \widehat{a}_{s,s-1} & 0 \\ \hline & \widehat{b}_1 & \widehat{b}_2 & \cdots & \widehat{b}_{s-1} & \widehat{b}_s \end{array}\,. \tag{1.6}$$

The left formula determines a diagonally implicit (semi-implicit) RK method, the right formula an explicit RK method. As usual, we assume that

$$c_i = \sum_{j=1}^{i} a_{ij} = \sum_{j=1}^{i-1} \widehat{a}_{ij}\,, \quad 0 \leq c_i \leq 1, \quad i = 2,\ 3,\ \ldots\ ,\ s. \tag{1.7}$$

By applying the left formula to the linear part of (1.4) and the right formula to the nonlinear part, we obtain the following scheme for the initial-boundary value problem (1.1)–(1.2):

$$\begin{aligned} U_{h,n}^{(i)} &= U_h^n + \Delta t \sum_{j=1}^{i} a_{ij}\Big(L_h U_{h,n}^{(j)} + \varphi_h(t_n + c_j\Delta t)\Big) \\ &\qquad + \Delta t \sum_{j=1}^{i-1} \widehat{a}_{ij}\, g_h\Big(t_n + c_j\Delta t, U_{h,n}^{(j)}\Big), \quad i = 1,\ 2,\ \ldots\ ,\ s, \end{aligned} \tag{1.8}$$

$$\begin{aligned} U_h^{n+1} &= U_h^n + \Delta t \sum_{i=1}^{s} b_i\Big(L_h U_{h,n}^{(i)} + \varphi_h(t_n + c_i\Delta t)\Big) \\ &\qquad + \Delta t \sum_{i=1}^{s} \widehat{b}_i\, g_h\Big(t_n + c_i\Delta t, U_{h,n}^{(i)}\Big). \end{aligned} \tag{1.9}$$

Here, U_h^0 is given by $U_h^0 = [\, u^0(x)\,]_{x\in\Omega_h}$.

The main purpose of the present paper is to clarify the convergence property of the scheme (1.8)–(1.9), especially from a viewpoint of the B-convergence theory [7]. The concept of B-convergence is closely related to the so-called order reduction phenomena, which were first pointed out and studied by Verwer [15] in the PDE context (see also [13, 14]).

2. Main theorem

For $\mathbb{C}^m$-valued functions on Ω_h we define an inner product by

$$\langle U,\, V\rangle_h = h^d \sum_{x\in\Omega_h} \overline{U}(x)^T V(x), \tag{2.1}$$

and let $\|\cdot\|_h$ denote the corresponding norm. We also put

$$\alpha_h(t) = u_h'(t) - L_h u_h - \varphi_h(t) - g_h(t,\, u_h), \tag{2.2}$$

where $u_h(t) = [\, u(t,x)\,]_{x\in\Omega_h}$, and consider the following conditions concerning the problem (1.1)–(1.3) and the MOL approximation (1.4)

(A_1) The exact solution $u(t,x)$ is of class C^3 with respect to t; $g(t,x,u)$ is of class C^2 with respect to t, u and the functions

$$g,\quad \frac{\partial g}{\partial t},\quad \frac{\partial g}{\partial u_i},\quad \frac{\partial^2 g}{\partial t^2},\quad \frac{\partial^2 g}{\partial t\partial u_i},\quad \frac{\partial^2 g}{\partial u_i\partial u_j}$$

are bounded for $(t,x,u)\in[0,T]\times\Omega\times\mathbb{R}^m$.

(A_2) For any $\mathbb{C}^m$-valued function U on Ω_h, $\mathrm{Re}\langle U, L_h U\rangle_h \le 0$.

(A_3) $\|\,\alpha_h(t)\,\|_h \to 0$ as $h\to 0$.

Moreover, we write

$$A = (a_{ij})_{1\le i,j\le s},\quad b = [b_1,\ b_2,\ \dots,\ b_s]^T,$$
$$\widehat{A} = (\widehat{a}_{ij})_{1\le i,j\le s},\quad \widehat{b} = [\widehat{b}_1,\ \widehat{b}_2,\ \dots,\ \widehat{b}_s]^T,$$

and consider the following conditions concerning the RK pair (1.6).

(B_1) The partitioned RK method (1.6) is of second order, i.e., the parameters b_i, $\widehat{b}_i$, c_i satisfy

$$\sum_{i=1}^s b_i = 1,\quad \sum_{i=1}^s b_i\, c_i = 1/2,\quad \sum_{i=1}^s \widehat{b}_i = 1,\quad \sum_{i=1}^s \widehat{b}_i\, c_i = 1/2.$$

(B_2) The diagonally implicit RK method is A-stable, ASI-stable, and AS-stable, i.e., the stability function $r(z) = 1 + zb^T(I_s - zA)^{-1}\mathbf{1}$, $\mathbf{1} = [1, 1, \ldots, 1]^T$, satisfies

$$|r(z)| \leq 1 \quad \text{for any } z \in \mathbb{C}_-,$$

and each component of $(I_s - zA)^{-1}$ and $zb^T(I_s - zA)^{-1}$ is bounded on $\mathbb{C}_-$, where $\mathbb{C}_- = \{z \in \mathbb{C} : \operatorname{Re} z < 0\}$.

(B_3) The rational functions

$$\phi(z) = \frac{b^T(I_s - zA)^{-1}\gamma}{b^T(I_s - zA)^{-1}\mathbf{1}}, \quad \widehat{\phi}(z) = \frac{b^T(I_s - zA)^{-1}\widehat{\gamma}}{b^T(I_s - zA)^{-1}\mathbf{1}} \tag{2.3}$$

are bounded on $\mathbb{C}_-$, where

$$\gamma = [\gamma_1, \gamma_2, \ldots, \gamma_s]^T, \quad \widehat{\gamma} = [\widehat{\gamma}_1, \widehat{\gamma}_2, \ldots, \widehat{\gamma}_s]^T,$$
$$\gamma_i = c_i^2/2 - \sum_{j=1}^{i} a_{ij}c_j, \quad \widehat{\gamma}_i = \sum_{j=1}^{i} a_{ij}c_j - \sum_{j=1}^{i-1} \widehat{a}_{ij}c_j.$$

Theorem 2.1 *Assume that* (A_1)–(A_3) *and* (B_1)–(B_3) *are satisfied. Then, there are positive numbers* h_0, Δt_0, C *such that*

$$\max_{1 \leq n \leq N} \| U_h^n - u_h(t_n) \|_h \leq C\Big(\Delta t^2 + \max_{0 \leq t \leq T} \| \alpha_h(t) \|_h\Big) \tag{2.4}$$

holds for any $h \leq h_0$ *and* $\Delta t \leq \Delta t_0$.

The proof is carried out by a simular argument as in the proof of Theorem 3.3 [5], on the based of the following lemma (see, e.g., [10], IV.11).

Lemma 2.2 (Theorem of von Neumann) *Let* $\psi(z)$ *be a rational function which has no pole in* $\mathbb{C}_-$, *and assume that* L_h *satisfies* (A_2). *Then, we have*

$$\| \psi(\Delta t L_h) \|_h \leq \sup_{\operatorname{Re} z \leq 0} |\psi(z)|. \tag{2.5}$$

Proof of Theorem 2.1. Put $t_{n,i} = t_n + c_i \Delta t$ and define $r_{h,n}^{(i)}$, $\rho_{h,n}$ by

$$\begin{aligned} u_h(t_{n,i}) &= u_h(t_n) + \Delta t \sum_{j=1}^{i} a_{ij}\Big(L_h u_h(t_{n,j}) + \varphi_h(t_{n,j})\Big) \\ &\qquad + \Delta t \sum_{j=1}^{i-1} \widehat{a}_{ij}\, g_h\Big(t_{n,j},\ u_h(t_{n,j})\Big) + r_{h,n}^{(i)}, \end{aligned} \tag{2.6}$$

$$\begin{aligned} u_h(t_{n+1}) &= u_h(t_n) + \Delta t \sum_{i=1}^{s} b_i\Big(L_h u_h(t_{n,i}) + \varphi_h(t_{n,i})\Big) \\ &\qquad + \Delta t \sum_{i=1}^{s} \widehat{b}_i\, g_h\Big(t_{n,i}, u_h(t_{n,i})\Big) + \rho_{h,n}. \end{aligned} \tag{2.7}$$

Then, it follows from (2.2) and (1.7) that

$$r_{h,n}^{(i)} = u_h(t_{n,i}) - u_h(t_n) - \Delta t \sum_{j=1}^{i} a_{ij} \left[u_h'(t_{n,j}) - g_h\Big(t_{n,j}, u_h(t_{n,j})\Big) - \alpha_h(t_{n,j}) \right]$$
$$- \Delta t \sum_{j=1}^{i-1} \widehat{a}_{ij}\, g_h\Big(t_{n,j}, u_h(t_{n,j})\Big)$$
$$= \Delta t^2\, \gamma_i\, u_h''(t_n) + \Delta t^2\, \widehat{\gamma}_i\, g_h^{(1)}\Big(t_n, u_h(t_n)\Big) + \Delta t \sum_{j=1}^{i} a_{ij}\, \alpha_h(t_{n,j}) + \mathcal{O}(\Delta t^3), \quad (2.8)$$

where

$$g_h^{(1)}\Big(t, u_h(t)\Big) = \frac{\partial g_h}{\partial t}\Big(t, u_h(t)\Big) + \frac{\partial g_h}{\partial U}\Big(t, u_h(t)\Big) u_h'(t)$$

Similarly, it follows from (2.2) and (B_1) that

$$\rho_{h,n} \;=\; \Delta t \sum_{i=1}^{s} b_i\, \alpha_h(t_{n,i}) + \mathcal{O}(\Delta t^3). \quad (2.9)$$

On the other hand, (2.6), (2.7), (1.8), (1.9) imply

$$\delta_{h,n}^{(i)} \;=\; \varepsilon_h^n + \Delta t \sum_{j=1}^{i} a_{ij}\, L_h\, \delta_{h,n}^{(j)} + \Delta t \sum_{j=1}^{i-1} \widehat{a}_{ij}\, J_{h,n}^{(j)}\, \delta_{h,n}^{(j)} + r_{h,n}^{(i)},$$
$$\varepsilon_h^{n+1} \;=\; \varepsilon_h^n + \Delta t \sum_{i=1}^{s} b_i\, L_h\, \delta_{h,n}^{(i)} + \Delta t \sum_{i=1}^{s} \widehat{b}_i\; J_{h,n}^{(i)}\, \delta_{h,n}^{(i)} + \rho_{h,n},$$

where

$$\delta_{h,n}^{(i)} = u_h(t_{n,i}) - U_{h,n}^{(i)}, \quad \varepsilon_h^n = u_h(t_n) - U_h^n,$$
$$J_{h,n}^{(i)} = \int_0^1 \frac{\partial g_h}{\partial U}\Big(t_{n,i}, (1-\theta) U_{h,n}^{(i)} + \theta u_h(t_{n,i})\Big) \mathrm{d}\theta.$$

Eliminating $\delta_{h,n}^{(i)}$, we get

$$\varepsilon_h^{n+1} = \left[I + (\boldsymbol{b}^T \boldsymbol{Z} + \widehat{\boldsymbol{b}}^T \boldsymbol{W}_n)(\boldsymbol{I} - \boldsymbol{A}\boldsymbol{Z} - \widehat{\boldsymbol{A}}\boldsymbol{W}_n)^{-1}(\mathbf{1} \otimes I) \right] \varepsilon_h^n$$
$$+ (\boldsymbol{b}^T \boldsymbol{Z} + \widehat{\boldsymbol{b}}^T \boldsymbol{W}_n)(\boldsymbol{I} - \boldsymbol{A}\boldsymbol{Z} - \widehat{\boldsymbol{A}}\boldsymbol{W}_n)^{-1} \boldsymbol{r}_{h,n} + \rho_{h,n}, \quad (2.10)$$

where $\boldsymbol{A} = A \otimes I$, $\widehat{\boldsymbol{A}} = \widehat{A} \otimes I$, $\boldsymbol{b} = b \otimes I$, $\widehat{\boldsymbol{b}} = \widehat{b} \otimes I$, $\boldsymbol{I} = I_s \otimes I$,

$$\boldsymbol{Z} = \Delta t\Big(\mathbf{1} \otimes L_h\Big), \;\; \boldsymbol{W}_n = \Delta t\Big[(J_{h,n}^{(1)})^T,\; (J_{h,n}^{(2)})^T,\; \dots,\; (J_{h,n}^{(s)})^T\Big]^T,$$
$$\boldsymbol{r}_{h,n} = \Big[(r_{h,n}^{(1)})^T,\; (r_{h,n}^{(2)})^T,\; \dots,\; (r_{h,n}^{(s)})^T\Big]^T.$$

Moreover, letting

$$\widehat{\varepsilon}_h^n = \varepsilon_h^n + \Delta t^2 v_h^n, \quad v_h^n = \phi(\Delta t L_h)\, u_h''(t_n) + \widehat{\phi}(\Delta t L_h)\, g_h^{(1)}\Big(t_n, u_h(t_n)\Big),$$

we can rewrite (2.10) as

$$\begin{aligned}\widehat{\varepsilon}_h^{n+1} &= \Big[I + (\boldsymbol{b}^T\boldsymbol{Z} + \widehat{\boldsymbol{b}}^T\boldsymbol{W}_n)(\boldsymbol{I} - \boldsymbol{A}\boldsymbol{Z} - \widehat{\boldsymbol{A}}\boldsymbol{W}_n)^{-1}(\boldsymbol{1}\otimes I)\Big]\,\widehat{\varepsilon}_h^n \\ &\quad + (\boldsymbol{b}^T\boldsymbol{Z} + \widehat{\boldsymbol{b}}^T\boldsymbol{W}_n)(\boldsymbol{I} - \boldsymbol{A}\boldsymbol{Z} - \widehat{\boldsymbol{A}}\boldsymbol{W}_n)^{-1}\,\widehat{\boldsymbol{r}}_{h,n} + \widehat{\rho}_{h,n}, \qquad (2.11)\end{aligned}$$

where

$$\begin{aligned}\widehat{\boldsymbol{r}}_{h,n} &= \boldsymbol{r}_{h,n} - \Delta t^2\gamma\otimes u_h''(t_n) - \Delta t^2\widehat{\gamma}\otimes g_h^{(1)}\Big(t_n, u_h(t_n)\Big), \\ \widehat{\rho}_{h,n} &= \rho_{h,n} + \Delta t^2\Big(v_h^{n+1} - v_h^n\Big) \\ &\quad + \Delta t^2(\boldsymbol{b}^T\boldsymbol{Z} + \widehat{\boldsymbol{b}}^T\boldsymbol{W}_n)(\boldsymbol{I} - \boldsymbol{A}\boldsymbol{Z} - \widehat{\boldsymbol{A}}\boldsymbol{W}_n)^{-1}\boldsymbol{w}_{h,n}, \\ \boldsymbol{w}_{h,n} &= \gamma\otimes u_h''(t_n) + \widehat{\gamma}\otimes g_h^{(1)}\Big(t_n, u_h(t_n)\Big) - \boldsymbol{1}\otimes v_h^n.\end{aligned}$$

By (2.9), we have

$$\widehat{r}_{h,n}^{(i)} = \Delta t\sum_{j=1}^{i} a_{ij}\,\alpha_h(t_{n,j}) + \mathcal{O}(\Delta t^3). \qquad (2.12)$$

Moreover, $\boldsymbol{b}^T\boldsymbol{Z}(\boldsymbol{I} - \boldsymbol{A}\boldsymbol{Z})^{-1}\boldsymbol{w}_{h,n} = 0$, by the definitions of v_h^n and $\boldsymbol{w}_{h,n}$. Hence, it follows from

$$(\boldsymbol{I}-\boldsymbol{A}\boldsymbol{Z}-\widehat{\boldsymbol{A}}\boldsymbol{W}_n)^{-1} = (\boldsymbol{I}-\boldsymbol{A}\boldsymbol{Z})^{-1} + (\boldsymbol{I}-\boldsymbol{A}\boldsymbol{Z})^{-1}\widehat{\boldsymbol{A}}\boldsymbol{W}_n(\boldsymbol{I}-\boldsymbol{A}\boldsymbol{Z}-\widehat{\boldsymbol{A}}\boldsymbol{W}_n)^{-1} \qquad (2.13)$$

that

$$\begin{aligned}(\boldsymbol{b}^T\boldsymbol{Z} + \widehat{\boldsymbol{b}}^T\boldsymbol{W}_n)(\boldsymbol{I} - \boldsymbol{A}\boldsymbol{Z} - \widehat{\boldsymbol{A}}\boldsymbol{W}_n)^{-1}\boldsymbol{w}_{h,n} &= \widehat{\boldsymbol{b}}^T\boldsymbol{W}_n(\boldsymbol{I} - \boldsymbol{A}\boldsymbol{Z})^{-1}\boldsymbol{w}_{h,n} \\ &\quad + (\boldsymbol{b}^T\boldsymbol{Z} + \widehat{\boldsymbol{b}}^T\boldsymbol{W}_n)(\boldsymbol{I} - \boldsymbol{A}\boldsymbol{Z})^{-1}\widehat{\boldsymbol{A}}\boldsymbol{W}_n(\boldsymbol{I} - \boldsymbol{A}\boldsymbol{Z} - \widehat{\boldsymbol{A}}\boldsymbol{W}_n)^{-1}\boldsymbol{w}_{h,n}.\end{aligned}$$

By making use of Lemma 2.2 it is shown that this value is of $\mathcal{O}(\Delta t)$ by *ASI*-stability and *AS*-stability of the implicit RK method, which, together with, $v_h^{n+1} - v_h^n = \mathcal{O}(\Delta t)$, implies

$$\widehat{\rho}_{h,n} = \Delta t\sum_{i=1}^{s} b_i\,\alpha_h(t_{n,i}) + \mathcal{O}(\Delta t^3). \qquad (2.14)$$

It follows from (2.11), (2.12), (2.14) that there exists $\widehat{C}$ such that

$$\|\,\varepsilon_h^n\,\|_h \le \widehat{C}\Big(\Delta t^2 + \max_{0\le t\le T}\|\,\alpha_h(t)\,\|_h\Big) \qquad (2.15)$$

holds for sufficiently small h and Δt. This is also verified on the basis of Lemma 2.2. Therefore, (2.4) holds. □

3. Numerical examples

Consider the simple model problem

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + g(t,x,u), \quad t \geq 0,\ 0 \leq x \leq 1, \tag{3.1}$$

$$g(t,x,u) = \frac{\pi^2}{2} u - u^2 + \mathrm{e}^{-\pi^2 t} \cos^2(\pi x),$$

$$u(t,0) = \mathrm{e}^{-\pi^2 t/2}, \quad u(t,1) = -\,\mathrm{e}^{-\pi^2 t/2}, \quad t \geq 0, \tag{3.2}$$

$$u(0,x) = \cos(\pi x), \quad 0 \leq x \leq 1, \tag{3.3}$$

whose exact solution is

$$u(t,x) = \mathrm{e}^{-\pi^2 t} \cos(\pi x).$$

Moreover, consider the grid

$$0 = x_0 < \cdots < x_j = jh < \cdots < x_M = 1, \quad h = 1/M,$$

and an MOL approximation determined by

$$\begin{aligned} \frac{u'_{j-1} + 10\,u'_j + u'_{j+1}}{12} &= \frac{u_{j-1} - 2u_j + u_{j+1}}{h^2} \\ &\quad + \frac{g(t,x_{j-1},u_{j-1}) + 10\,g(t,x_j,u_j) + g(t,x_{j+1},u_{j+1})}{12}, \\ j &= 1,\ 2,\ \dots,\ M-1, \end{aligned} \tag{3.4}$$

where M is a positive integer and $u_j(t)$ is an approximation of $u(t,x_j)$. The functions $u_0(t)$ and $u_M(t)$ are given by

$$u_0(t) = \mathrm{e}^{-\pi^2 t/2}, \quad u_M(t) = -\,\mathrm{e}^{-\pi^2 t/2},$$

corresponding to (3.2). Simple computation shows that

$$\alpha_h(t) = \mathcal{O}(h^4) \tag{3.5}$$

holds for (3.4).

One of the simplest RK pairs which satisfy (B_1)–(B_3) is the pair of the trapezoidal rule and Heun's method (a modification of the Crank-Nicolson scheme),

$$\begin{array}{c|cc} 0 & 0 & 0 \\ 1 & 1/2 & 1/2 \\ \hline & 1/2 & 1/2 \end{array}\ , \qquad \begin{array}{c|cc} 0 & 0 & 0 \\ 1 & 1 & 0 \\ \hline & 1/2 & 1/2 \end{array}\ . \tag{3.6}$$

Clearly, (B_1) is satisfied, and it follows from

$$(I_2 - zA)^{-1} = \frac{1}{1-z/2} \begin{bmatrix} 1-z/2 & 0 \\ z/2 & 1 \end{bmatrix}, \quad zb^T(I_2 - zA)^{-1} = \frac{z}{1-z/2} \begin{bmatrix} 1/2, & 1/2 \end{bmatrix},$$

$$r(z) = 1 + zb^T(I_2 - zA)^{-1}\mathbf{1} = \frac{1+z/2}{1-z/2},$$

that the implicit method satisfies (B_2). In addition, $\gamma = [0,\ 0]^T$ and $\widehat{\gamma} = [0,\ 1/2]^T$. Hence,

$$\phi(z) = \frac{b^T(I_2 - zA)^{-1}\gamma}{b^T(I_2 - zA)^{-1}\mathbf{1}} = 0, \quad \widehat{\phi}(z) = \frac{b^T(I_2 - zA)^{-1}\widehat{\gamma}}{b^T(I_2 - zA)^{-1}\mathbf{1}} = 1/4,$$

and (B_3) is satisfied.

The RK pair

$$\begin{array}{c|ccc} 0 & 0 & 0 & 0 \\ \alpha & 0 & \alpha & 0 \\ 1-\alpha & 0 & 1-2\alpha & \alpha \\ \hline & 0 & 1/2 & 1/2 \end{array}, \quad \begin{array}{|ccc} 0 & 0 & 0 \\ \alpha & 0 & 0 \\ \alpha-1 & 2(1-\alpha) & 0 \\ \hline 0 & 1/2 & 1/2 \end{array} \quad \left(\alpha = \frac{3+\sqrt{3}}{6}\right) \tag{3.7}$$

also satisfies (B_1)–(B_3). This pair, which was proposed by Ascher, Ruuth and Spiteri [2], determines a third order partitioned RK method for ODEs. In particular, (B_1) is satisfied. The conditions (B_2) and (B_3) follow from

$$(I_3 - zA)^{-1} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \dfrac{1}{1-\alpha z} & 0 \\ 0 & -\dfrac{(2\alpha-1)z}{(1-\alpha z)^2} & \dfrac{1}{1-\alpha z} \end{bmatrix},$$

$$zb^T(I_3 - zA)^{-1} = \frac{z}{2}\left[\ 0,\ \frac{1-(3\alpha-1)z}{(1-\alpha z)^2},\ \frac{1}{1-\alpha z}\ \right],$$

$$r(z) = \frac{1-(2\alpha-1)z-(\alpha-1/3)z^2}{(1-\alpha z)^2},$$

$$\phi(z) = \left(\frac{\alpha^2}{2}\right)\frac{(2\alpha-1)z}{2+(1-4\alpha)z}, \quad \widehat{\phi}(z) = -\frac{\alpha^2(2\alpha-1)z}{2+(1-4\alpha)z}.$$

We apply the RK pairs (3.6) and (3.7) to the MOL approximation (3.4), and integrate it from $t = 0$ to $t = 1$, with various gridsizes and stepsizes of the form

$$\Delta t = h = \frac{1}{M}. \tag{3.8}$$

Table 1 shows the values

$$-\log_2 \varepsilon_M, \quad \varepsilon_M = \max_{1\le n\le M}\left(\max_{1\le j\le M} |\ u(t_n, x_j) - u_j^n\ |\right).$$

It is observed that ε_M is of $\mathcal{O}(\Delta t^2)$ for each method. Noting (3.5) and (3.8), we can consider the result for (3.7) presents an order reduction phenomenon, i.e., the error of a "third order" method behaves as $\mathcal{O}(\Delta t^2)$.

Table 1. Numerical results for the model problem (3.1)–(3.3)

M	20	40	80	160	320	640
Method (3.6)	3.63	5.09	6.79	8.64	10.56	12.52
Method (3.7)	5.60	7.42	9.32	11.25	13.19	15.16

Fig. 1 shows a numerical result concerning the "soliton solution"

$$w(t,x) = \sqrt{2\alpha}\,\exp\Big[\mathrm{i}\Big\{\frac{c}{2}x - \Big(\frac{c^2}{4} - \alpha\Big)t\Big\}\Big]\,\mathrm{sech}\big[\alpha(x-ct)\big] \tag{3.9}$$

to the simple nonlinear Schrödinger equation

$$\frac{\partial w}{\partial t} = \mathrm{i}\frac{\partial^2 w}{\partial x^2} + \mathrm{i}\mid w\mid^2 w. \tag{3.10}$$

The "1st order scheme" indicates the method (1.5), and the "2nd order scheme" indicates the method (3.6). The values $\alpha = 0.5$, $c = 1$, $\Delta x = 0.2$, $\Delta t = 0.005$ are used for the computation.

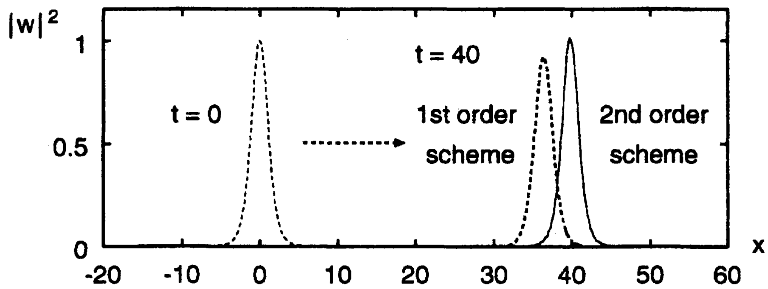

Fig. 1. Numerical solutions of the nonlinear Schrödinger equation (3.10).

Fig. 2 shows a stationary solution to the equation (Brusselator)

$$\begin{cases} \dfrac{\partial u}{\partial t} = D_U\Big(\dfrac{\partial^2 u}{\partial x^2} + \dfrac{\partial^2 u}{\partial y^2}\Big) + \alpha - (\beta+1)u + u^2 v \\ \dfrac{\partial v}{\partial t} = D_V\Big(\dfrac{\partial^2 v}{\partial x^2} + \dfrac{\partial^2 v}{\partial y^2}\Big) + \beta u - u^2 v \end{cases} \tag{3.11}$$

$$0 \le x \le 4,\ 0 \le y \le 4,\ D_U = 0.02,\ D_V = 1,\ \alpha = 1,\ \beta = 1.8,$$

under the Neumann boundary condition, obtained by the method (3.6). These figures suggest that the method (3.6) is useful for some problems.

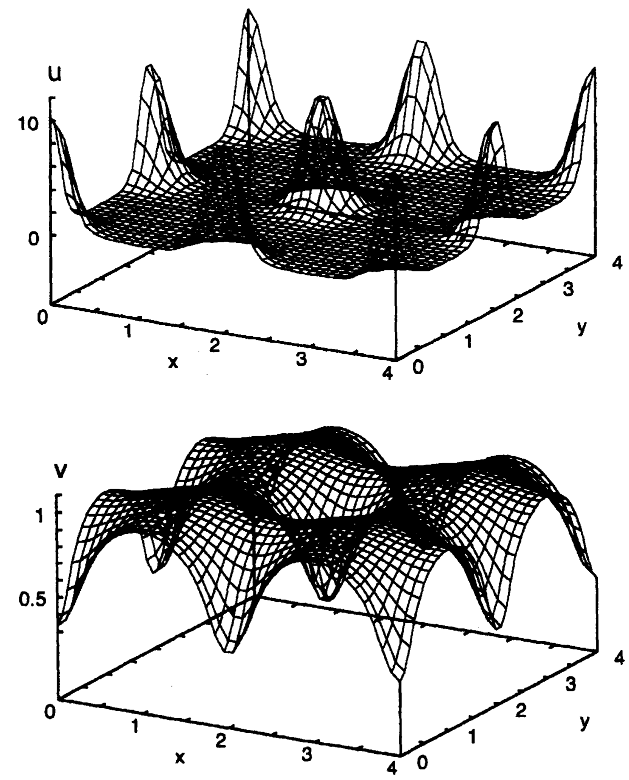

Fig. 2. Stationary solution to the equation (3.11).

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