A diffusion–modified quadrature finite element method for nonlinear reaction–diffusion equations

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(Received 8 August 2003, revised 22 January 2004)

Abstract

In this work we propose, analyse and implement a fully discrete diffusion–modified H^1-Galerkin method with quadrature for solving nonlinear variable diffusion coefficient reaction–diffusion equations on a rectangular region. In our least square quadrature finite element method, the trial space consists of twice continuously differentiable cubic or higher degree splines and the test space is obtained by applying the second order diffusion operator to the trial space. At each discrete time step, our algorithm requires solution of only a constant diffusion coefficient fully discrete linear problem. We prove that for

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See http://anziamj.austms.org.au/V45/CTAC2003/Gane for this article, © Austral. Mathematical Soc. 2004. Published June 18, 2004. ISSN 1446-8735

sufficiently small time step-size, the scheme is stable and converges with optimal order accuracy in time and space (with H^1 or H^2 norm). Finally, we present numerical results demonstrating the accuracy of our scheme in L^2, H^1 and H^2 norms.

Contents

1 Introduction

We consider the nonlinear reaction–diffusion equation for the field $u(x, y, t)$:

$$\frac{\partial u}{\partial t} - a(x, y, u)\Delta u = f(x, y, t, u)\,, \quad (x, y, t) \in \Omega \times [0, T]\,, \tag{1}$$

$$u(x, y, 0) = g(x, y)\,, \quad (x, y) \in \bar{\Omega}\,, \tag{2}$$

$$u(x, y, t) = 0\,, \quad (x, y, t) \in \partial\Omega \times [0, T]\,, \tag{3}$$

where $\Omega = (0, 1) \times (0, 1)$. Here, f, representing the effect of nonlinear reaction, is defined on $\Omega \times [0, T] \times \mathbb{R}$; the diffusivity of the media a (depending nonlinearly on the unknown u, for example chemical concentration in biological applications) is defined on $\Omega \times \mathbb{R}$ and the initial data g is defined on $\bar{\Omega}$. As usual, we assume the positivity and boundedness of the diffusion coefficient: $0 < a_{\min} \leq a \leq a_{\max}$ for some constants $a_{\min}$ and $a_{\max}$.

In this paper, we seek *twice* continuously differentiable approximate solutions (that are fourth and higher–order accurate in space) of the *second order* nonlinear problem (1–3). In addition, we want to analyse the stability and convergence of a computer implementable (fully discrete) scheme to compute such approximate solutions, without the need to use any nonlinear algebraic solvers. Our scheme involves a central difference approximation for the first–order time derivative and a diffusion–modified H^1-Galerkin method, also known as the least square finite element method (FEM) with quadrature for spatial discretization. The standard H^1-Galerkin method (without introducing diffusion–modification and quadrature in the scheme) with a trial space consisting of C^2 splines of degree $r \geq 3$ and the test space obtained by applying the Laplace operator to the trial space, was analysed only for linear parabolic problems on *smooth* domains in $\mathbb{R}^2$ (see [2] and references therein). In comparison to the standard C^0 FEMs, the method of [2] has the advantage of obtaining smoother approximate solutions with less degrees of freedom.

Our present fully discrete algorithm is motivated by the fully discrete Laplace–modified C^1 *orthogonal spline collocation* (OSC) method considered and analysed for linear parabolic problems on rectangles by many authors (see [1] and references therein). According to the survey paper [1, p.76], there is a growing interest in developing and analysing C^2 spline collocation methods. However, C^2 *nodal spline collocation* (NSC) method is yet to be explored for linear parabolic problems in two space dimensions. Even for elliptic problems on rectangles, analysis and applicability of NSC are restricted to cubic splines on uniform partitions [1]. In contrast our C^2 spline least square quadrature FEM and its analysis for (1–3) have the generality and properties in OSC and has the marked advantage of obtaining smoother approximate solutions with fewer unknowns compared to OSC.

The outline of this paper is as follows. In the next section, we introduce a fully discrete H^1-Galerkin diffusion–modified scheme with quadrature to solve (1–3). In section 3, we specify assumptions and recall from [3, 4] some preliminary results required for analysis. In section 4, we prove optimal order accuracy (in time and in H^1, H^2 normed spaces) of our fully discrete scheme. Numerical experiments in section 5 confirm our theoretical results and demonstrate optimal order convergence in the L^2, H^1 and H^2 norms of our scheme for a nonlinear reaction–diffusion model problem.

2 The fully discrete diffusion–modified FEM

For chosen integers $N^x, N^y \geq 2$, let $\Pi^x = \{x_k\}_{k=0}^{N^x}$ and $\Pi^y = \{y_l\}_{l=0}^{N^y}$ be partitions of $[0,1]$ in the x- and y-directions. Let $h^{x,k} = x_k - x_{k-1}$, $k = 1,\ldots,N^x$, $h^{y,l} = y_l - y_{l-1}$, $l = 1,\ldots,N^y$, $h^x = \max_{1\leq k\leq N^x} h^{x,k}$, $h^y = \max_{1\leq l\leq N^y} h^{y,l}$, $h = \max(h^x, h^y)$.

Let $S^x, S^y \subseteq H_0^1(0,1)\cap C^2[0,1]$ denote subspaces consisting of all splines of degree at most $r \geq 3$ defined on the fixed partitions. The trial and test spaces for the H^1-Galerkin method are respectively chosen to be $S_h = S^x \otimes S^y$, $T_h = \Delta S_h$.

For discretization of the Galerkin integrals on Ω, we choose the $J = \max\{3, r-1\}$-point Gauss quadrature on $(0,1)$ with weights and nodes respectively denoted by $\{w_j\}_{j=1}^J$ and $\{\xi_j\}_{j=1}^J$. (Our numerical experiments suggest that for $r = 3$, $J = r - 1$ is sufficient; but for analysis, we need J as specified.) We approximate the standard L^2 inner product and norm on Ω by

$$(v,z)_h = \sum_{k=1}^{N^x}\sum_{l=1}^{N^y} h^{x,k}h^{y,l}\sum_{m=1}^{J}\sum_{n=1}^{J} w_m w_n (vz)(x_{k,m}, y_{l,n}), \quad \|v\|_h^2 = (v,v)_h. \tag{4}$$

where $x_{k,m} = x_{k-1} + h^{x,k}\xi_m$ and $y_{l,n} = y_{l-1} + h^{y,l}\xi_n$.

For a positive integer N^t, let $\Pi^t = \{t_n\}_{n=0}^{N^t}$ be a partition of $[0,T]$ such that $t_n = n\tau$, where $\tau = T/N^t$. For a function ϕ defined on Π^t, let

$$\phi^n = \phi(t_n)\,, \quad \partial_t\phi^n = \frac{\phi^{n+1}-\phi^n}{\tau}\,, \quad \tilde\partial_t\phi^n = \frac{\phi^{n+1}-\phi^{n-1}}{2\tau}\,,$$
$$\partial_t^2\phi^n = \frac{\phi^{n+1}-2\phi^n+\phi^{n-1}}{\tau^2}\,.$$

Our fully discrete diffusion–modified H^1 Galerkin scheme with quadrature for solving (1–3) is to compute $U^{n+1} \in S_h$, $n = 1, \ldots, N^t - 1$ (approximating the exact solution $u(t_{n+1})$ of nonlinear reaction–diffusion equation) by solving the following *linear* algebraic system:

$$(\tilde\partial_t U^n, v)_h - \lambda\tau^2(\partial_t^2 \Delta U^n, v)_h = (\mathcal{F}(t_n)U^n, v)_h + (\mathcal{A}U^n\Delta U^n, v)_h\,, \quad v \in T_h\,, \tag{5}$$

where $\lambda > a_{\max}/4$ is an arbitrary constant and the superposition operators $\mathcal{A}$ and $\mathcal{F}(t)$ (for each fixed $t \in [0, T]$) representing the nonlinear diffusivity and reaction kinetics are defined by

$$[\mathcal{A}\psi](x,y) = a(x,y,\psi(x,y))\,, \quad [\mathcal{F}(t)\psi](x,y) = f(x,y,t,\psi(x,y))\,,$$
$$\psi \in C^0(\bar\Omega)\,, \quad (x,y) \in \bar\Omega\,. \tag{6}$$

It is useful to note that the matrix, say $\mathcal{M}_h$, in the diffusion–modified scheme (5) is independent of the discrete time variable and that $-\mathcal{M}_h$ is symmetric and positive–definite. Hence we may, for example, first obtain the Cholesky factorisation of $-\mathcal{M}_h$ and then (for all $n = 1, \ldots, N^t - 1$) solve the linear systems for different RHS terms in (5) by simple forward and backward eliminations.

The linearised scheme (5) requires selection of $U^0, U^1 \in S_h$. We select U^0 and U^1 (using the given initial data u^0 in (2) and u_t^0 from (1) and (2)) by solving the following fully discrete linear systems:

$$(\mathcal{A}u^0\Delta U^0, v)_h = (\mathcal{A}u^0\Delta u^0, v)_h\,, \quad v \in T_h\,, \tag{7}$$
$$(\mathcal{A}(u^0+\tau u_t^0)\Delta U^1, v)_h = (\mathcal{A}(u^0+\tau u_t^0)\Delta(u^0+\tau u_t^0), v)_h\,, \quad v \in T_h\,. \tag{8}$$

Remark 1 If $a = a(x, y, t)$, (that is, the diffusion coefficient a depends on t and is independent of u) then the diffusion–modified scheme for (1–3) is defined by (5), for $n = 1, \ldots, N_t - 1$, with $\mathcal{A}U^n$ be replaced by a^n. and we select $U^0, U^1 \in S_h$ as follows:

$$(a^0 \Delta U^0, v)_h = (\mathcal{A}u^0 \Delta u^0, v)_h\,, \quad (a^1 \Delta U^1, v)_h = (a^1 \Delta(u^0 + \tau u_t^0), v)_h\,, \quad v \in T_h\,.$$

In such cases, the analysis in the next section is simplified substantially. We restrict the choice of a in our analysis to depend on only three variables, instead of all the four variables x, y, t, u mainly to avoid lengthy technical details. If $a = a(x, y, t, u)$, in our scheme, we need to replace $\mathcal{A}U^n$, by $\mathcal{A}(t_n)U^n$, with $\mathcal{A}(t)$ defined similar to $\mathcal{F}(t)$. In this very general case, we again obtain optimal order convergence, as we demonstrate in section 5. Our numerical experiments suggest that for some class of fully nonlinear diffusion coefficients, in order to compute U^0, U^1, it may be sufficient to solve the linear system

$$(\Delta U^0, v)_h = (\Delta u^0, v)_h\,, \quad (\Delta U^1, v)_h = (\Delta(u^0 + \tau u_t^0), v)_h\,, \quad v \in T_h\,. \tag{9}$$

In fact, one may choose $U^0, U^1 \in S_h$ in any other way, as long as the assumption in Theorem 8 is satisfied. However, currently we could prove that the assumption of Theorem 8 hold only if $U^0, U^1 \in S_h$ satisfy (7) and (8) respectively.

3 Assumptions and preliminary results

For a nonnegative integer k, the standard norms in the Sobolev spaces H^k and k-times continuously differentiable function spaces C^k are denoted by $\|\cdot\|_k$ and $\|\cdot\|_{k,\infty}$ respectively. For a function $\psi \in \mathcal{C}^2(\Omega \times \mathbb{R})$, we define

$$v_{x^i y^j z^k} = \frac{\partial^{i+j+k} \psi}{\partial x^i \partial y^j \partial z^k}\,, \quad 0 \le i, j, k \le 2\,, \quad i + j + k \le 2\,.$$

Throughout the paper, we assume that the diffusion coefficient $a \in C^5(\bar{\Omega}\times \mathbb{R})$ and for each fixed $t \in [0,T]$, the nonlinear reaction term $f \in C^2(\bar{\Omega}\times\mathbb{R})$. Further, we assume that for $i,j,k = 0,1,2$ with $0 \le i+j+k \le 2$, $f_{x^iy^jz^k}(.,.,.,0) \in \mathcal{C}(\Omega\times[0,T])$ and that a, f satisfy the following Lipschitz conditions:

$$\left|a_{x^iy^jz^k}(x,y,z_1) - a_{x^iy^jz^k}(x,y,z_2)\right| \le C\,|z_1 - z_2|\,, \quad (x,y)\in\Omega,\ z_1,z_2\in\mathbb{R}\,, \tag{10}$$

$$\begin{aligned}&\left|f_{x^iy^jz^k}(x,y,t,z_1) - f_{x^iy^jz^k}(x,y,t,z_2)\right| \le C\,|z_1 - z_2|\,,\\ &(x,y)\in\Omega,\ z_1,z_2\in\mathbb{R}\,,\quad t\in[0,T]\,.\end{aligned} \tag{11}$$

For numerical experiments (and in analysis), we require only local Lipschitz continuity of a, f around a neighbourhood of the exact solution u of (1–3) that satisfy

$$u \in C^6(\bar{\Omega}\times[0,T])\,,\quad u,\, u_t,\, u_{tt} \in C(H^{r+3}(\Omega),[0,T])\,,\quad r \ge 3\,.$$

As usual, we assume that (5) is solved on a quasi-uniform collection of partitions $\Pi^x\times\Pi^y$ corresponding to a sequence of values (N^x,N^y). Hence, throughout the paper, C is a generic positive constant which may depend on r, but which is independent of h and τ. Finally, in order prove the optimal order $\mathcal{O}(\tau^2+h^{r+1-k})$ convergence in the $H^k(\Omega)$ norm for $k=1,2$, we assume that $Ch^{2r-2}\le\tau^2\le Ch^r$. (We observed in numerical experiments only sub-optimal order convergence in the H^2 norm for the choice $\tau^2 = h^{r-1}$.)

We recall the following results from our work [3, 4]:

Lemma 2 *[3] For any spline v, $\|v\|_h \le C\|v\|_0$.*

Lemma 3 *[3] If $v\in S_h$, then $\|\Delta v\|_0 \le C\|\Delta v\|_h$ and $\|v\|_1^2 \le -C(v,\Delta v)_h$.*

Lemma 4 *[4] If $z \in H^2(\Omega)\cap H_0^1(\Omega)$, then*

$$|(z,\Delta v)_h| \le C(h\,\|z\|_2 + \|z\|_1)\|v\|_1\,,\quad v\in S_h\,.$$

Let $W : [0,T] \to S_h$ be the comparison function defined by

$$(\mathcal{A}u\Delta W, v)_h = (\mathcal{A}u\Delta u, v)_h \,, \quad v \in T_h \,, \quad t \in [0,T] \,. \tag{12}$$

Throughout the paper we use the notation $\eta = u - W$.

Lemma 5 *[3, 4] For each $t \in [0,T]$,*

$$\begin{aligned} &\|W_t\|_{1,\infty} \le C \,, \quad \|\eta\|_\ell + \|\eta_t\|_\ell \le Ch^{r+1-\ell} \,, \\ &\|\Delta\eta\|_h + \|\Delta\eta_{tt}\|_h \le Ch^{r-1} \,, \quad \ell = 1, 2 \,. \end{aligned}$$

4 Convergence analysis

In this section, we assume that $\xi^n = U^n - W^n$, $n = 0, \ldots, N^t$, where $\{U^n\}_{n=2}^{N^t}$ and W are defined by (5) and (12) respectively. The following two lemmas can be proved following arguments used for similar results in [4].

Lemma 6 *Let U^0 and U^1 be defined as in (7) and (8). Then $\|\xi^0\|_2^2 + \|\xi^1\|_2^2 \le C\tau^4$.*

Lemma 7 *For $n = 1, \ldots, N^t - 1$, we have for any $v \in T_h$*

$$\begin{aligned} &-(\tilde\partial_t \xi^n, v)_h + (\mathcal{A}U^n\Delta\xi^n, v)_h + \lambda\tau^2(\Delta\partial_t^2\xi^n, v)_h \\ &= (\mathcal{F}(t_n)u^n - \mathcal{F}(t_n)U^n, v)_h - (u_t^n - \tilde\partial_t u^n, v)_h - (\tilde\partial_t\eta^n, v)_h \\ &\quad + ([\mathcal{A}u^n - \mathcal{A}U^n]\Delta W^n, v)_h - \lambda\tau^2(\Delta\partial_t^2 u^n, v)_h + \lambda\tau^2(\Delta\partial_t^2\eta^n, v)_h \,. \end{aligned} \tag{13}$$

Theorem 8 *Assume that $\|\xi^0\|_2^2 + \|\xi^1\|_2^2 \le C\tau^4$. If h and τ are sufficiently small, then*

$$\max_{0 \le n \le N^t} \|\Delta\xi^n\|_0^2 \le C\left\{\tau^4 + h^{2r}\right\} .$$

Proof: Taking $v=\tilde\partial_t\Delta\xi^n$ in (13), we get

$$\begin{aligned}-(\tilde\partial_t\xi^n\,,\tilde\partial_t\Delta\xi^n)_h+([\mathcal{A}U^n-2\lambda]\Delta\xi^n,\tilde\partial_t\Delta\xi^n)_h\\ +\lambda(\Delta\xi^{n+1}+\Delta\xi^{n-1},\tilde\partial_t\Delta\xi^n)_h=\textstyle\sum_{i=1}^6 I_i^n\,,\end{aligned}\tag{14}$$

where

$$\begin{aligned}I_1^n&=-(u_t^n-\tilde\partial_t u^n,\tilde\partial_t\Delta\xi^n)_h\,, & I_2^n&=-(\tilde\partial_t\eta^n\,,\tilde\partial_t\Delta\xi^n)_h,\\ I_3^n&=([\mathcal{A}u^n-\mathcal{A}U^n]\Delta W^n,\tilde\partial_t\Delta\xi^n)_h\,, & I_4^n&=-\lambda\tau^2(\Delta\partial_t^2u^n,\tilde\partial_t\Delta\xi^n)_h\,,\\ I_5^n&=\lambda\tau^2(\Delta\partial_t^2\eta^n,\tilde\partial_t\Delta\xi^n)_h\,, & I_6^n&=(\mathcal{F}(t_n)u^n-\mathcal{F}(t_n)U^n,\tilde\partial_t\Delta\xi^n)_h\,.\end{aligned}$$

For the first and third terms on the left-hand side of (14), we use Lemma 3 to obtain

$$\begin{aligned}-(\tilde\partial_t\xi^n,\tilde\partial_t\Delta\xi^n)_h+\lambda\left(\Delta\xi^{n+1}+\Delta\xi^{n-1},\tilde\partial_t\Delta\xi^n\right)_h\\ \geq C\|\tilde\partial_t\xi^n\|_1^2+\tfrac{\lambda}{2\tau}[\|\Delta\xi^{n+1}\|_h^2-\|\Delta\xi^{n-1}\|_h^2]\,.\end{aligned}\tag{15}$$

Next we bound terms on the right-hand side of (14). Since

$$u_t^n-\tilde\partial_t u^n=-\frac{1}{4\tau}\left[\int_{t_{n-1}}^{t_n}(s-t_{n-1})^2u_{ttt}\,ds+\int_{t_n}^{t_{n+1}}(s-t_{n+1})^2u_{ttt}\,ds\right]\,,$$

Lemma 4 and the ϵ inequality yield

$$\begin{aligned}I_1^n&\leq C\|u_t^n-\tilde\partial_t u^n\|_2\|\tilde\partial_t\xi^n\|_1\\ &\leq C\tau\int_{t_{n-1}}^{t_{n+1}}\|u_{ttt}\|_2\,ds\|\tilde\partial_t\xi^n\|_1\\ &\leq C\tau^2\|\tilde\partial_t\xi^n\|_1\leq\epsilon_1\|\tilde\partial_t\xi^n\|_1^2+C(\epsilon_1)\tau^4\,.\end{aligned}\tag{16}$$

Next we bound I_2^n. Using Lemma 4, the relation $\tilde\partial_t\eta^n=\frac{1}{2\tau}\int_{t_{n-1}}^{t_{n+1}}\eta_t\,ds$, Lemma 5, and the ϵ inequality we obtain

$$\begin{aligned}I_2^n&\leq C\left(h\|\tilde\partial_t\eta^n\|_2+\|\tilde\partial_t\eta^n\|_1\right)\|\tilde\partial_t\xi^n\|_1\\ &\leq C\tau^{-1}\int_{t_{n-1}}^{t_{n+1}}\left(h\|\eta_t\|_2+\|\eta_t\|_1\right)\,ds\|\tilde\partial_t\xi^n\|_1\\ &\leq Ch^r\|\tilde\partial_t\xi^n\|_1\leq\epsilon_2\|\tilde\partial_t\xi^n\|_1^2+C(\epsilon_2)h^{2r}\,.\end{aligned}\tag{17}$$

The bounds I_3^n and I_6^n follow from the bounds of similar terms in the main results of [4] obtained using the assumptions (10–11) and the ϵ inequality:

$$I_3^n + I_6^n \leq \epsilon_3 \|\tilde{\partial}_t \xi^n\|_1^2 + C(\epsilon_3)(1 + \|u^n\|_{2,\infty} + \|U^n\|_{1,\infty})^4 (h^{2r} + \|\Delta\xi^n\|_0^2)\,. \quad (18)$$

To bound I_4^n we use Lemma 3.2 [4], the ϵ inequality and the assumption $\|\xi^0\|_2^2 + \|\xi^1\|_2^2 \leq C\tau^4$ to get

$$I_4^n \leq \epsilon_4 \|\tilde{\partial}_t \xi^n\|_1^2 + C(\epsilon_4)\tau^4 + J_n\,, \quad (19)$$

and where for $2 \leq j \leq N^t$,

$$\tau \sum_{n=1}^{j-1} J_n \leq C\tau^2 \left[\tau \sum_{n=2}^{j-2} \|\Delta\xi^n\|_0 + \sum_{i=j-1}^{j} \left\|\Delta\xi^i\right\|_0 \right] + C\tau^4\,. \quad (20)$$

Since $\tau^2 \Delta \partial_t^2 \eta^n = \int_{t_{n-1}}^{t_{n+1}} (\tau - |s - t_n|) \Delta\eta_{tt}\, ds$, the Cauchy-Schwarz inequality, Lemmas 2 and 5, the inverse and ϵ inequalities yield

$$\begin{aligned} I_5^n &\leq C\|\tau^2 \Delta \partial_t^2 \eta^n\|_h \|\tilde{\partial}_t \Delta\xi^n\|_h \\ &\leq C\tau \int_{t_{n-1}}^{t_{n+1}} \|\Delta\eta_{tt}\|_h\, ds \|\tilde{\partial}_t \Delta\xi^n\|_0 \\ &\leq Ch^{r-2}\tau^2 \|\tilde{\partial}_t \xi^n\|_1 \leq \epsilon_5 \|\tilde{\partial}_t \xi^n\|_1^2 + C(\epsilon_5)\tau^4\,. \end{aligned} \quad (21)$$

Using (14–19), (21), taking ϵ_i, $i = 1, 2, 3, 4, 5$, sufficiently small, and multiplying through by 2τ, we obtain

$$\begin{aligned} &2\tau \|\tilde{\partial}_t \xi^n\|_1^2 + 2\tau \left([\mathcal{A}U^n - 2\lambda]\Delta\xi^n, \tilde{\partial}_t \Delta\xi^n \right)_h + \lambda \left[\|\Delta\xi^{n+1}\|_h^2 - \|\Delta\xi^{n-1}\|_h^2 \right] \\ &\leq C[1 + \|u^n\|_{2,\infty} + \|U^n\|_{1,\infty}]^4 \left[\tau J_n + \tau \|\Delta\xi^n\|_0^2 + \tau^5 + \tau h^{2r} \right]\,. \end{aligned} \quad (22)$$

Summing both sides of (22) for $n = 1, \ldots, k-1$, where $2 \le k \le N^t$, using Lemma 2 and that $\|\Delta\xi^0\|_h^2 + \|\Delta\xi^1\|_h^2 \le C\,[\|\xi^0\|_2^2 + \|\xi^1\|_2^2] \le C\tau^4$, we obtain

$$\tau\sum_{n=1}^{k-1}\|\tilde{\partial}_t\xi^n\|_1^2 + \tau\sum_{n=1}^{k-1}\Big([\mathcal{A}U^n - 2\lambda]\Delta\xi^n, \tilde{\partial}_t\Delta\xi^n\Big)_h + \lambda[\|\Delta\xi^k\|_h^2 + \|\Delta\xi^{k-1}\|_h^2]$$
$$\le C\max_{1\le n\le k-1}[1 + \|u^n\|_{2,\infty} + \|U^n\|_{1,\infty}]^4\left[\tau^4 + h^{2r} + \tau\sum_{n=1}^{k-1}J_n + \tau\sum_{n=1}^{k-1}\|\Delta\xi^n\|_0^2\right]. \tag{23}$$

The second term on the left hand side of (23) can be written as follows:

$$\begin{aligned}
&2\tau\sum_{n=1}^{k-1}\Big([\mathcal{A}U^n - 2\lambda]\Delta\xi^n, \tilde{\partial}_t\Delta\xi^n\Big)_h \\
&= \sum_{n=1}^{k-1}\big([\mathcal{A}U^n - 2\lambda]\Delta\xi^{n+1}, \Delta\xi^n\big)_h - \sum_{n=1}^{k-1}\big([\mathcal{A}U^n - 2\lambda]\Delta\xi^n, \Delta\xi^{n-1}\big)_h \\
&= \sum_{n=1}^{k-1}\big([\mathcal{A}U^n - 2\lambda]\Delta\xi^{n+1}, \Delta\xi^n\big)_h - \sum_{n=0}^{k-2}\big([\mathcal{A}U^{n+1} - 2\lambda]\Delta\xi^{n+1}, \Delta\xi^n\big)_h \\
&= \mathcal{J}^k + \big([\mathcal{A}U^{k-1} - 2\lambda]\Delta\xi^k, \Delta\xi^{k-1}\big)_h - \big([\mathcal{A}U^1 - 2\lambda]\Delta\xi^1, \Delta\xi^0\big)_h\,,
\end{aligned} \tag{24}$$

where

$$\mathcal{J}^k = \begin{cases} 0\,, & k = 2\,,\\ \sum_{n=1}^{k-2}\big([\mathcal{A}U^n - \mathcal{A}U^{n+1}]\Delta\xi^{n+1}, \Delta\xi^n\big)_h\,, & k = 3, \ldots, N^t\,. \end{cases} \tag{25}$$

Using (20), the Cauchy-Schwarz and ϵ inequalities, we obtain

$$\tau\sum_{n=1}^{k-1}J_n \le C\left[C(\epsilon)\tau^4 + \epsilon\left(\tau\sum_{n=1}^{k-1}\|\Delta\xi^n\|_0^2 + \sum_{i=k-1}^{k}\|\Delta\xi^i\|_0^2\right) + \tau^4\right]. \tag{26}$$

Hence, using (23), (24) and (26), we obtain for $k = 2, \dots, N^t - 1$,

$$2\tau \sum_{n=1}^{k-1} \|\tilde{\partial}_t \xi^n\|_1^2 + \left([\mathcal{A}(U^{k-1}) - 2\lambda]\Delta\xi^k, \Delta\xi^{k-1}\right)_h + \lambda[\|\Delta\xi^k\|_h^2 + \|\Delta\xi^{k-1}\|_h^2]$$
$$\leq \left|\mathcal{J}^k\right| + \left([\mathcal{A}(U^1) - 2\lambda]\Delta\xi^1, \Delta\xi^0\right)_h + C[1 + \max_{0 \leq n \leq k-1} \|U^n\|_{1,\infty}]^4$$
$$\times \left[(C(\epsilon)+1)\tau^4 + h^{2r} + \epsilon \sum_{i=k-1}^{k} \|\Delta\xi^i\|_0^2 + (\epsilon+1)\tau \sum_{n=1}^{k-1} \|\Delta\xi^n\|_0^2\right],$$

thus, using Lemma 3.3 in [4], Cauchy-Schwarz inequality, Lemma 2, the assumption $\|\xi^0\|_2 + \|\xi^1\|_2 \leq C\tau^2$, and taking ϵ sufficiently small, we obtain for $k = 2, \dots, N^t - 1$,

$$\tau \sum_{n=1}^{k-1} \|\tilde{\partial}_t \xi^n\|_1^2 + \sum_{i=k-1}^{k} \|\Delta\xi^i\|_0^2$$
$$\leq C[1 + \max_{0 \leq n \leq k-1} \|U^n\|_{1,\infty}]^4 \left[\tau^4 + h^{2r} + \tau \sum_{n=1}^{k-1} \|\Delta\xi^n\|_0^2\right] + \left|\mathcal{J}^k\right|. \tag{27}$$

For later use we bound $\|U^0\|_{1,\infty}$. Using $U^0 = W^0 + \xi^0$, the triangle inequality, Lemma 3.5 in [3], the inverse inequality, and the assumption that $\|\xi^0\|_2 \leq C\tau^2 \leq Ch^r$, we obtain

$$\|U^0\|_{1,\infty} \leq \|W^0\|_{1,\infty} + \|\xi^0\|_{1,\infty} \leq C + h^{-1}\|\xi^0\|_1 \leq C. \tag{28}$$

Next we show the following bounds

$$|\mathcal{J}^k| \leq C\tau \sum_{n=0}^{k} \|\Delta\xi^n\|_h^2, \quad \|U^{k-1}\|_{1,\infty} \leq C, \quad k = 2, \dots, N^t. \tag{29}$$

Using the Cauchy-Schwarz inequality (10), the Sobolev embedding theorem, Lemma 2, $U^n = W^n + \xi^n$, and the triangle inequality, we obtain for $n =$

$0, \ldots, N^t - 1$,

$$\begin{aligned}
&\big([\mathcal{A}U^n - \mathcal{A}U^{n+1}]\Delta\xi^{n+1}, \Delta\xi^n\big)_h \\
&\leq C\|\mathcal{A}U^n - \mathcal{A}U^{n+1}\|_{0,\infty}\|\Delta\xi^{n+1}\|_h\|\Delta\xi^n\|_h \\
&\leq C\|U^n - U^{n+1}\|_2\|\Delta\xi^{n+1}\|_0\|\Delta\xi^n\|_0 \\
&\leq C\tau(\|\partial_t W^n\|_{0,\infty} + \|\partial_t\xi^n\|_{0,\infty})\|\Delta\xi^{n+1}\|_0\|\Delta\xi^n\|_0 \,. \qquad (30)
\end{aligned}$$

Using the relation $\partial_t W^n = \tau^{-1}\int_{t_{n-1}}^{t_n} W_t\, ds$ and Lemma 5, we obtain

$$\|\partial_t W^n\|_{1,\infty} \leq \max_{0\leq t\leq T}\|W_t\|_{1,\infty} \leq C\,, \quad n = 0, \ldots, N^t - 1\,. \qquad (31)$$

Now, by induction we prove

$$\|\partial_t\xi^n\|_{1,\infty} \leq C_0\,, \quad n = 0, \ldots, N^t - 1\,, \qquad (32)$$

where C_0 is a fixed constant independent of τ and h.

For $n = 0$, using the inverse inequality, and the assumption that $\|\xi^0\|_2 + \|\xi^1\|_2 \leq C\tau^2 \leq Ch^r$,

$$\|\partial_t\xi^0\|_{1,\infty} \leq Ch^{-1}\|\partial_t\xi^0\|_1 \leq Ch^{-1}\tau^{-1}\sum_{i=0}^{1}\|\xi^i\|_1 \leq C_0\,,$$

for some suitable positive constant C_0, and hence (32) follows for $n = 0$. Let (32) be true for $n = 0, \ldots, \ell$ for some $0 \leq \ell \leq N^t - 2$. We show that (32) is true with $n = \ell + 1$.

Using (25), (30), (31) and the induction hypothesis, we get for $k = 2, \ldots, \ell + 2$,

$$|\mathcal{J}^k| \leq C\tau\sum_{n=1}^{k-2}\|\Delta\xi^n\|_0\|\Delta\xi^{n+1}\|_0 \leq C\tau\sum_{n=1}^{k-1}\|\Delta\xi^n\|_0^2\,. \qquad (33)$$

The triangle inequality, $U^n = \xi^n + W^n$, (28), (31), the induction hypothesis, yield for $n = 1, \ldots, \ell + 1$,

$$\begin{aligned} \|U^n\|_{1,\infty} &\le C\tau \sum_{i=0}^{n-1} \|\partial_t U^i\|_{1,\infty} + \|U^0\|_{1,\infty} \\ &\le C\tau \sum_{i=0}^{n-1} \left[\|\partial_t W^i\|_{1,\infty} + \|\partial_t \xi^i\|_{1,\infty}\right] + C \le C \,. \end{aligned} \tag{34}$$

Using (33) and (34) in (27), we obtain

$$\tau \sum_{n=1}^{k-1} \|\tilde{\partial}_t \xi^n\|_1^2 + \|\Delta \xi^k\|_0^2 \le C \left[\tau^4 + h^{2r} + \tau \sum_{n=0}^{k} \|\Delta \xi^n\|_0^2\right] , \quad k = 0, \ldots, \ell + 2 \,. \tag{35}$$

Hence, for τ sufficiently small, the discrete analogue of Gronwall's inequality gives

$$\tau \sum_{n=1}^{\ell+1} \|\tilde{\partial}_t \xi^n\|_1^2 + \|\Delta \xi^{\ell+2}\|_0^2 \le C \left\{\tau^4 + h^{2r}\right\} . \tag{36}$$

Further, using the triangle and Cauchy-Schwarz inequalities, (36), and the assumption that $\|\xi^0\|_2 + \|\xi^1\|_2 \le C\tau^2 \le Ch^r$,

$$\begin{aligned} \|\partial_t \xi^{\ell+1}\|_1 &\le C \sum_{i=1}^{\ell+1} \|\tilde{\partial}_t \xi^n\|_1 + \|\partial_t \xi^0\|_1 \\ &\le C\tau^{-1} \left(\sum_{i=1}^{\ell+1} \|\tilde{\partial}_t \xi^k\|_1^2 + \sum_{i=0}^{1} \|\xi^i\|_2 \right) \\ &\le Ch^{3/2} \,. \end{aligned} \tag{37}$$

The inverse inequality, (37), and h sufficiently small yield

$$\|\partial_t \xi^{\ell+1}\|_{1,\infty} \le Ch^{-1} \|\partial_t \xi^{\ell+1}\|_1 \le Ch^{1/2} \le C_0 \,. \tag{38}$$

Hence (32) holds for $n = 0, \ldots, N^t - 1$, and hence from (28) and (34), we obtain

$$\|U^n\|_{1,\infty} \le C\,, \quad n = 1, \ldots, N^t - 1\,. \tag{39}$$

Hence, using (25), (30–32), and (39), we obtain (29).

Finally, using (27) and (29) for $k = 2, \ldots, N^t$, we obtain

$$\|\Delta\xi^k\|_0^2 \le C\left[\tau^4 + h^{2r} + \tau\sum_{n=1}^{k}\|\Delta\xi^n\|_0^2\right]. \tag{40}$$

Clearly, (40) holds for $k = 0, \ldots, N^t$. Hence, for τ sufficiently small, the discrete analogue of Gronwall's inequality gives

$$\|\Delta\xi^n\|_0^2 \le C\left\{\tau^4 + h^{2r}\right\}, \quad n = 0, \ldots, N^t\,. \tag{41}$$

♠

The optimal order convergence of our fully discrete diffusion–modified quadrature FEM solutions follows now as a corollary to results in this section.

Corollary 9 *Let U^0 and U^1 be defined as in (7) and (8). If h and τ are sufficiently small, then*

$$\max_{0\le n\le N^t}\|u^n - U^n\|_\ell \le C\left\{\tau^2 + h^{r+1-\ell}\right\}, \quad \ell = 1, 2\,.$$

Proof: Since $u^n - U^n = \eta^n - \xi^n$, the desired inequalities follows from the triangle inequality, Lemma 5, $\|\xi^n\|_2 \le C\|\Delta\xi^n\|_0$, and Theorem 8. ♠

5 Numerical experiments

In this section, we apply our diffusion–modified least square quadrature H^1-Galerkin method to compute smoothest cubic spline ($r = 3$) approximate solutions U of the nonlinear reaction–diffusion model problem

$$\frac{\partial u}{\partial t} - t^4 \sin^2(u)\Delta u = f(x,y,t,u)\,, \quad (x,y,t) \in \Omega \times [0,1]\,, \tag{42}$$

$$u(x,y,0) = \sin(\pi x)\sin(\pi y)\,, \quad (x,y) \in \bar{\Omega}\,, \tag{43}$$

$$u(x,y,t) = 0\,, \quad (x,y,t) \in \partial\Omega \times [0,1]\,, \tag{44}$$

and the nonlinear reaction kinetics is chosen to be of the Fisher–Kolmogorov type:

$$f(x,y,t,u) = t^3 u(1-u) + f_1(x,y,t)\,,$$

where $f_1(x,y,t)$ is chosen so that $u(x,y,t) = (\sin(t)+\cos(t))\sin(\pi x)\sin(\pi y)$ is the exact solution of (42–44).

In our numerical experiments, for several values of $N^x = N^y = N$, we used uniform partitions in the x and y directions, with $h = 1/N$. We chose uniform partitions of the time–interval $[0,1]$ of equal widths τ so that $\tau^2 = h^{r+1}$ to check the L^2 rate of convergence $(R(H^0))$ and $\tau^2 = h^r$ to compute $(R(H^k))$ in the H^k norm, for $k = 1,2$. We calculated the errors $\|u-U\|_{k,\infty} = \max_{0\le n\le N_t} \|u^n - U^n\|_k$, for $k = 0,1,2$, using 25 translated Gauss quadrature points on each cell of the 49×49 uniform partition of Ω.

For a fixed h, we computed U^0 and U^1 by solving (9). Then, we computed the sparse Cholesky factorization of the time-independent symmetric matrix $\mathcal{M}_h$ resulting from our fully discrete scheme diffusion–modified scheme (5). We used the sparse factorization to compute U^{n+1} for all $n = 1,\ldots,N^t - 1$ by solving (5) with simple forward and backward substitutions. (We observed similar computational time if we instead used the preconditioned conjugate gradient method to solve the linear system in (5) for $n = 1,\ldots,N^t - 1$, with preconditioner at each time given by the matrix in (9).)

Numerical results in Table 1 confirm the optimal order $\mathcal{O}(h^{4-k})$ convergence of our efficient fully discrete scheme for the nonlinear model problem (without using any nonlinear algebraic solvers), proved in this paper for $k = 1,2$ and expected from our scheme for $k = 0$.

Table 1: Optimal order L^2, H^1 and H^2 convergence of quadrature FEM solutions

N	$\|u-U\|_{0,\infty}$	$R(H^0)$	$\|u-U\|_{1,\infty}$	$R(H^1)$	$\|u-U\|_{2,\infty}$	$R(H^2)$
4	2.0497e-02		3.1454e-01		1.4258e+00	
9	8.1110e-04	3.9827	3.2724e-02	2.7906	1.8124e-01	2.5435
16	8.1268e-05	3.9986	5.8807e-03	2.9832	5.1875e-02	2.1743
25	1.3636e-05	3.9997	1.5488e-03	2.9896	1.8938e-02	2.2579
36	3.1715e-06	3.9999	5.1961e-04	2.9951	8.2064e-03	2.2933
49	9.2405e-07	4.0000	2.0621e-04	2.9977	3.9978e-03	2.3327

Acknowledgements: the support of Australian Research Council is gratefully acknowledged.

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