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AN OPERATOR SPLITTING APPROACH FOR TWO–DIMENSIONAL KAWARADA PROBLEMS

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Abstract. The authors study a second order operator splitting formula for computing numerical solutions of singular and nonlinear Kawarada partial differential equation initial-boundary value problems. Their investigations particularly focus at the global numerical error, algorithmic realization, and stability of the decomposed schemes. Computational experiments are presented to validate and illustrate their results. The simulation demonstrates the viability and capability of the new splitting methods for solving nonlinear and singular problems with potential industrial applications.

1. Introduction

Splitting methods, with popular configurations such as ADI (alternating-direction implicit) and LOD (local one-dimensional) decompositions [3, 7, 12, 13], have been playing a significant role in approximations of ordinary and partial differential equations. The theoretical background of solutions of splitting methods can be traced back to Baker-Campbell-Hausdorff, Zassenhaus and Trotter formulas [2, 13, 14].

Needless to mention, classical splitting strategies have met a tremendous amount of new challenges in recent years, especially for newly emerged singular and high-dimensional models due to increasing simulation demands from biomedical, financial and energy industrial applications.

This paper is interested in an operator splitting approximations for solving a two-dimensional nonlinear Kawarada partial differential equation which is frequently used in solid fuel thermal combustion simulations and oil tanker corrosion preventions [10, 11]. To this end, we let $\mathscr{D}_a = (0,a)\times(0,a)$, where $a>0$, be a spacial domain and $\partial\mathscr{D}_a$ its boundary. We further let $\Omega_a = \mathscr{D}_a\times(t_0,T)$, $\mathscr{S}_a = \partial\mathscr{D}_a\times(t_0,T)$, where $T\in(t_0,\infty)$, $t_0\geqslant 0$. Consider the following semi-linear Kawarada initial-boundary value problem [6, 8],

$$u_t = u_{xx}+u_{yy}+f(u),\quad (x,y,t)\in\Omega_a, \tag{1.1}$$

$$u(x,y,t) = \phi(x,y,t),\quad (x,y,t)\in\mathscr{S}_a, \tag{1.2}$$

$$u(x,y,t_0) = \psi(x,y),\quad (x,y)\in\mathscr{D}_a, \tag{1.3}$$

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where $0 \leqslant \phi, \psi \ll 1$ and the nonlinear source function, $f(u)$, is strictly increasing for $0 \leqslant u < \sigma$ with

$$f(0) = f_0 > 0, \ \lim_{u \to \sigma^-} f(u) = \infty.$$

In the context of thermal combustion, the function $u(x,y,t)$ represents the temperature in an idealized combustor, and x and y are coordinates in the perpendicular and parallel directions to its walls, respectively. The value of σ is often referred to as the fuel ignition point in combustion, or the critical point for a massive corrosion to occur in a container [10]. Typical source functions include

$$f_1(u) = \frac{1}{\sigma - u}, \ f_2(u) = \exp\left\{\frac{u}{\sigma - u}\right\}, \quad 0 \leqslant u < \sigma.$$

The solution of (1.1)–(1.3) is said to *quench* if there exists a finite time T_c such that

$$\sup\{\, u_t(x,y,t) : (x,y) \in \mathscr{D}_a \,\} \to \infty, \text{ as } t \to T_c^-. \tag{1.4}$$

The value of T_c is referred as the *quenching time.* A necessary condition for this to occur is

$$\max\left\{\, u(x,y,t) : (x,y) \in \bar{\mathscr{D}}_a \,\right\} \to \sigma^-, \text{ as } t \to T_c^-. \tag{1.5}$$

A non-quenching solution of (1.1)–(1.3) tends to a steady state solution $\hat{u}(x,y)$, $(x,y) \in \bar{\mathscr{D}}_a$ as $t \to \infty$. In the circumstance we have $0 \leqslant \max\left\{\hat{u}(x,y) : (x,y) \in \bar{\mathscr{D}}_a\right\} < \sigma$. We are not interested in such solutions.

It is known that if f and f_u are nonnegative, then there exists a unique $a^* > 0$ and the solution of (1.1)–(1.3) quenches whenever $a \geqslant a^*$ in finite time T_a. Such a $\mathscr{D}_{a^*}$ is called a *critical domain,* and $\mathscr{D}_a$, $a > a^*$ are *quenching domains* [8, 9].

Considerable efforts have been devoted to the theory and computations of the Kawarada problem (1.1)–(1.3) and beyond in recent years [1, 6, 9, 11]. Once a critical domain is identified, quenching times corresponding to particular $a \geqslant a^*$ can be determined together with quenching solutions. The computational tasks turn out to be challenging due to the strong quenching singularities involved. The singularity will cause rapid changes in the gradient and temporal derivatives as quenching time is approached. This demands extremely fine resolution in the spatial and temporal grids. Temporal and/or spacial mesh adaptation is often necessary for capturing a quenching phenomenon. However, nonconstant mesh adaptations often become difficult in multi-dimensional settings [4]. Consequently, large amounts of computations need to be invested which may lead to undesirable numerical errors. Splitting techniques have been suggested as they offer efficient and effective means of advancing the solution. This motivates our present discussion.

This paper is organized as follows. In Section 2, semi- and fully discretized finite difference approximations are implemented for solving the Kawarada problem (1.1)–(1.3) on a uniform spatial grid. The temporal step is variable based on adaptation procedures via any suitable arc-length monitor function [1, 4, 11]. An analysis is carried out about properties of the coefficient matrices utilized. In Section 3, rigorous global error analysis and estimates are conducted for the schemes derived. It is shown that the errors are closely related to the commutativity of the coefficient matrices from operator splitting. The order of accuracy is shown to be consistent with that is anticipated in the theory. Section 4 is devoted to a study of the numerical stability of the semi-adaptive operator splitting schemes. Computational realization is completed with an [1/1] Padé approximation strategy. Section 5 provides a sequence of numerical experiments for algorithmic validations and illustrations of the quenching phenomena. It can be seen that our results match existing calculations and theoretical predictions satisfactorily. Finally, brief acknowledgments and appreciations are given in Section 6.

2. Semi- and fully discretized approximations

Let $N \in \mathbb{N}^+$ be sufficiently large and $h = a/(N+1)$. We define an uniform spatial mesh region $\mathscr{D}_h = \{(x_i, y_j) \mid x_i = ih, y_j = jh,\ 1 \leqslant i, j \leqslant N\} \subset \mathscr{D}$, with $\partial\mathscr{D}_h = \{(x_i, y_j) \mid x_i = ih, y_j = jh,\ i, j \in \{0, N+1\}\} \subset \partial\mathscr{D}$ as its boundary. Letting $v_{i,j} = v(x_i, y_j, t),\ (x_i, y_j) \in \bar{\mathscr{D}}_h,\ t > 0$, be an approximation of the solution $u(x_i, y_j, t)$ based upon standard central finite difference approximations of the derivatives, we obtain the following semi-discretized system from (1.1):

$$v'_{i,j} = \frac{1}{h^2}\left(v_{i-1,j} + v_{i+1,j} + v_{i,j-1} + v_{i,j+1} - 4v_{i,j}\right) + f(v_{i,j}),\ \ 1 \leqslant i, j \leqslant N.$$

Denote $v = [v_{1,1}, v_{2,1}, \ldots, v_{N,1}, v_{1,2}, v_{2.2} \ldots, v_{N,2}, v_{1,3}, \ldots, v_{N,N}]^\intercal \in \mathbb{R}^{N^2}$. Then the semi-discretized system can be compressed together with (1.2), (1.3) to yield a large system

$$v' = (A+B)v + g(v), \quad t > t_0, \tag{2.1}$$

$$v(t_0) = \psi, \tag{2.2}$$

where $A \in \mathbb{R}^{N^2 \times N^2}$ is a block diagonal matrix and $B \in \mathbb{R}^{N^2 \times N^2}$ is a block tridiagonal matrix of the forms $A = I_N \otimes A_0,\ B = A_0 \otimes I_N$, where $A_0 = \mathrm{tridiag}\,(1, -2,\ 1) \in \mathbb{R}^{N \times N}$, $I_N \in \mathbb{R}^{N \times N}$ is the identity matrix, $\otimes$ stands for the Kronecker product, and $g(v),\ \psi \in \mathbb{R}^{N^2}$. We notice that $A,\ B$ do not commute, that is, $[A, B] \neq \Phi$, where $[\cdot, \cdot]$ is the conventional Lie bracket and $\Phi \in \mathbb{R}^{N \times N}$ is an empty matrix. It can be readily shown that the truncation errors of (2.1), (2.2) are of $\mathscr{O}(h^2)$ [1, 5, 7].

LEMMA 1. *Matrices* A, B *are*
(i) *symmetric;*
(ii) *nonsingular and negative definite;*
(iii) *there exists a permutation matrix* $P \in \mathbb{R}^{N^2 \times N^2}$ *such that* $B = PAP^{-1}$.

Proof. The first two properties are true for A since eigenvalues of the tridiagonal and Toeplitz matrix A_0 are

$$\lambda_k = -2 - 2\cos\left(\frac{k\pi}{N+1}\right) < 0 \quad \text{for } k = 1, \ldots, N.$$

Now, we look at property 3. To this end, we denote $P \in \mathbb{R}^{N^2 \times N^2}$ as a permutation matrix with rows $e_i, e_{i+N}, e_{i+2N}, \ldots, e_{i+(N-1)N}$, for $i = 1, \ldots, N$, where e_k is the k^{th} standard basis vector for $\mathbb{R}^{N^2}$. We denote

$$P_i = \begin{pmatrix} e_{i+0}^{\mathsf{T}} \\ e_{i+N}^{\mathsf{T}} \\ e_{i+2N}^{\mathsf{T}} \\ \vdots \\ e_{i+(N-1)N}^{\mathsf{T}} \end{pmatrix} \in \mathbb{R}^{N \times N^2}, \quad i = 1, 2, \ldots, N.$$

We further define

$$P = \begin{pmatrix} P_1^{\mathsf{T}} \\ P_2^{\mathsf{T}} \\ P_3^{\mathsf{T}} \\ \vdots \\ P_N^{\mathsf{T}} \end{pmatrix} \in \mathbb{R}^{N^2 \times N^2}.$$

It follows therefore $P^{-1} = P^{\mathsf{T}}$. Furthermore, we may express B by rows, that is,

$$B = \begin{pmatrix} B_1^{\mathsf{T}} \\ B_2^{\mathsf{T}} \\ B_3^{\mathsf{T}} \\ \vdots \\ B_{N^2}^{\mathsf{T}} \end{pmatrix} \in \mathbb{R}^{N^2 \times N^2}.$$

Thus, we have

$$PB = P \begin{pmatrix} B_1^{\mathsf{T}} \\ B_2^{\mathsf{T}} \\ B_3^{\mathsf{T}} \\ \vdots \\ B_{N^2}^{\mathsf{T}} \end{pmatrix} = \begin{pmatrix} B_1^{\mathsf{T}} \\ B_{1+N}^{\mathsf{T}} \\ \vdots \\ B_{1+N(N-1)}^{\mathsf{T}} \\ B_2^{\mathsf{T}} \\ B_{2+N}^{\mathsf{T}} \\ \vdots \\ B_{2+N(N-1)}^{\mathsf{T}} \\ \vdots \\ B_N^{\mathsf{T}} \\ \vdots \\ B_{N^2}^{\mathsf{T}} \end{pmatrix} = \begin{pmatrix} C_1 \\ C_{1+N} \\ \vdots \\ C_{1+N(N-1)} \\ C_2 \\ C_{2+N} \\ \vdots \\ C_{2+N(N-1)} \\ \vdots \\ C_N \\ \vdots \\ C_{N^2} \end{pmatrix} \in \mathbb{R}^{N^2 \times N^2},$$

where the row vectors $C_i = B_i^{\mathsf{T}}$, $i = 1, 2, \ldots, N$.

Note that $P^T = P$. Thus,

$$PBP^{-1} = \begin{pmatrix} C_1 \cdot e_1 & C_1 \cdot e_{1+N} & \cdots & C_1 \cdot e_{N^2} \\ C_{1+N} \cdot e_1 & C_{1+N} \cdot e_{1+N} & \cdots & C_{1+N} \cdot e_{N^2} \\ \vdots & \ddots & \ddots & \\ C_{N^2} \cdot e_1 & C_{N^2} \cdot e_{1+N} & \cdots & C_{N^2} \cdot e_{N^2} \end{pmatrix},$$

where

$$C_i \cdot e_j = \begin{cases} -2 \text{ if } i = j, \\ \;\;1 \text{ if } |i-j| = N, \\ \;\;0 \text{ otherwise.} \end{cases}$$

Therefore $PBP^{-1} = A$, and thus B is symmetric, nonsingular, and negative definite. □

An integration of (2.1), (2.2) generates the following formal solution:

$$\begin{aligned} v &= e^{(t-t_0)(A+B)} v_0 + \int_{t_0}^{t} e^{(t-\xi)(A+B)} g(v(\xi))d\xi \\ &= e^{(t-t_0)(A+P^{-1}AP)} v_0 + \int_{t_0}^{t} e^{(t-\xi)(A+P^{-1}AP)} g(v(\xi))d\xi, \quad t \geqslant t_0. \end{aligned} \tag{2.3}$$

Let $0 < \tau = t - t_0 \ll 1.$ An application of the trapezoidal rule for (2.3) leads to

$$\begin{aligned} v(t) &= e^{\tau(A+P^{-1}AP)} \psi + \frac{\tau}{2}\left[g(v(t)) + e^{\tau(A+P^{-1}AP)} g(\psi)\right] + \mathscr{O}(\tau^3) \\ &= e^{\tau(A+P^{-1}AP)} \left(\psi + \frac{\tau}{2} g(\psi)\right) + \frac{\tau}{2} g(v(t)) + \mathscr{O}(\tau^3). \end{aligned}$$

Or, we have

$$v(t) - \frac{\tau}{2} g(v(t)) = e^{\tau(A+P^{-1}AP)} \left(\psi + \frac{\tau}{2} g(\psi)\right) + \mathscr{O}(\tau^3).$$

Let v_{k+1} be an approximation of $v(t_{k+1})$, where $t_{k+1} = t_k + \tau_k$ and $\tau_k,\ k = 0, 1, 2, \ldots, K,$ are variable temporal steps to be determined through a proper adaptation procedure [1, 4, 11]. Drop the truncation error. Then, (2.3) can be extended to following second order semi-adaptive implicit finite difference method,

$$v_{k+1} = e^{\tau_k(A+P^{-1}AP)} \left(v_k + \frac{\tau_k}{2} g(v_k)\right) + \frac{\tau_k}{2} g(v_{k+1}), \quad k = 0, 1, 2, \ldots, K. \tag{2.4}$$

Note that the size of A and B involved in (2.4) is large if $N \gg 1$ is large. However, the matrices are sparse and therefore, to decompose the matrix exponential operator properly becomes an effective and a sensitive approach to reduce the computational complexity and cost involved.

3. Operator splitting and errors incurred

Let us consider a second order sequential operator splitting, that is, the Strang's splitting [3],

$$e^{\tau_k(A+P^{-1}AP)} = e^{(\tau_k/2)A}e^{\tau_k P^{-1}AP}e^{(\tau_k/2)A} + E(\tau_k), \quad 0 < \tau_k \ll 1. \tag{3.1}$$

We first show the following lemma.

LEMMA 2. *For any $A \in \mathbb{R}^{N^2\times N^2}$, we have*

$$\left[A, e^{\tau_k P^{-1}AP}\right] = \int_0^\tau e^{(\tau-\xi)P^{-1}AP}\left[A, P^{-1}AP\right]e^{\xi P^{-1}AP}d\xi,$$
$$\left[P^{-1}AP, e^{(\tau/2)A}\right] = \frac{1}{2}\int_0^\tau e^{((\tau-\xi)/2)A}\left[P^{-1}AP, A\right]e^{(\xi/2)A}d\xi, \quad \tau \geqslant 0.$$

Proof. Apparently, we only need to show the first identity. To this end, we set $D(\tau) = \left[A, e^{\tau P^{-1}AP}\right]$, $\tau \geqslant 0$. Clearly, $D(0) = \Phi$. It follows that,

$$\begin{aligned}
D'(\tau) &= \left(Ae^{\tau P^{-1}AP}\right)' - \left(e^{\tau P^{-1}AP}A\right)' = Ae^{\tau P^{-1}AP}P^{-1}AP - P^{-1}APe^{\tau P^{-1}AP}A \\
&= P^{-1}APAe^{\tau P^{-1}AP} - P^{-1}APe^{\tau P^{-1}AP}A + Ae^{\tau P^{-1}AP}P^{-1}AP - P^{-1}APAe^{\tau P^{-1}AP} \\
&= P^{-1}AP\left(Ae^{\tau P^{-1}AP} - e^{\tau P^{-1}AP}A\right) + \left(AP^{-1}AP - P^{-1}APA\right)e^{\tau P^{-1}AP} \\
&= P^{-1}AP\left[A, e^{\tau P^{-1}AP}\right] + \left[A, P^{-1}AP\right]e^{\tau P^{-1}AP} \\
&= P^{-1}APD(\tau) + \left[A, P^{-1}AP\right]e^{\tau P^{-1}AP}.
\end{aligned}$$

Solving the initial value problem

$$D' - P^{-1}APD = \left[A, P^{-1}AP\right]e^{\tau P^{-1}AP}, \ D(0) = \Phi,$$

gives

$$D(\tau) = \int_0^\tau e^{(\tau-\xi)P^{-1}AP}\left[A, P^{-1}AP\right]e^{\xi P^{-1}AP}d\xi, \quad \tau \geqslant 0,$$

which confirms our result. □

This lemma offers a direct connection between the commutativity between the matrix exponentials and matrices, and the commutativity between the matrices involved. We further consider

$$\begin{aligned}
E(\tau_k) &= e^{\tau_k(A+P^{-1}AP)} - e^{(\tau_k/2)A}e^{\tau_k P^{-1}AP}e^{(\tau_k/2)A} \\
&= e^{\tau_k(A+P^{-1}AP)}\left[I - e^{-\tau_k(A+P^{-1}AP)}e^{(\tau_k/2)A}e^{\tau_k P^{-1}AP}e^{(\tau_k/2)A}\right] \\
&= e^{\tau_k(A+P^{-1}AP)}\left[I - F(\tau_k)\right], \quad 0 < \tau_k \ll 1,
\end{aligned}$$

where $F(\tau_k) = e^{-\tau_k(A+P^{-1}AP)}e^{(\tau_k/2)A}e^{\tau_k P^{-1}AP}e^{(\tau_k/2)A}$.

THEOREM 1. *We have*

$$
\begin{aligned}
E(\tau_k) = \frac{1}{2}\int_0^{\tau_k} & e^{(\tau_k-\xi)(A+P^{-1}AP)}\int_0^{\xi} e^{(\xi-\zeta)((1/2)A+P^{-1}AP)} \\
& \times \left[\frac{1}{2}A+P^{-1}AP, \int_0^{\zeta} e^{(\zeta-\eta)P^{-1}AP}\left[A,P^{-1}AP\right]e^{\eta P^{-1}AP}e^{(\zeta/2)A}d\eta\right]e^{(\xi/2)A}d\zeta d\xi.
\end{aligned}
$$

Proof. Consider the function

$$
F(\tau) = e^{-\tau(A+P^{-1}AP)}e^{(\tau/2)A}e^{\tau P^{-1}AP}e^{(\tau/2)A}, \quad \tau > 0. \tag{3.2}
$$

A differentiation of the above leads to

$$
\begin{aligned}
F'(\tau) &= -(A+P^{-1}AP)e^{-\tau(A+P^{-1}AP)}e^{(\tau/2)A}e^{\tau P^{-1}AP}e^{(\tau/2)A} \\
&\quad +\frac{1}{2}e^{-\tau(A+P^{-1}AP)}Ae^{(\tau/2)A}e^{\tau P^{-1}AP}e^{(\tau/2)A} \\
&\quad +e^{-\tau(A+P^{-1}AP)}e^{(\tau/2)A}P^{-1}APe^{\tau P^{-1}AP}e^{(\tau/2)A} \\
&\quad +\frac{1}{2}e^{-\tau(A+P^{-1}AP)}e^{(\tau/2)A}e^{\tau P^{-1}AP}Ae^{(\tau/2)A} \\
&= e^{-\tau(A+P^{-1}AP)}G(\tau)e^{(\tau/2)A}, \quad \tau > 0,
\end{aligned}
$$

where

$$
\begin{aligned}
G(\tau) &= -(A+P^{-1}AP)e^{(\tau/2)A}e^{\tau P^{-1}AP}+\frac{1}{2}Ae^{(\tau/2)A}e^{\tau P^{-1}AP} \\
&\quad +e^{(\tau/2)A}P^{-1}APe^{\tau P^{-1}AP}+\frac{1}{2}e^{(\tau/2)A}e^{\tau P^{-1}AP}A \\
&= -Ae^{(\tau/2)A}e^{\tau P^{-1}AP}-P^{-1}APe^{(\tau/2)A}e^{\tau P^{-1}AP}+\frac{1}{2}Ae^{(\tau/2)A}e^{\tau P^{-1}AP} \\
&\quad +e^{(\tau/2)A}P^{-1}APe^{\tau P^{-1}AP}+\frac{1}{2}e^{(\tau/2)A}e^{\tau P^{-1}AP}A \\
&= \frac{1}{2}e^{(\tau/2)A}e^{\tau P^{-1}AP}A-\frac{1}{2}Ae^{(\tau/2)A}e^{\tau P^{-1}AP} \\
&\quad +e^{(\tau/2)A}e^{\tau P^{-1}AP}P^{-1}AP-P^{-1}APe^{(\tau/2)A}e^{\tau P^{-1}AP} \\
&= \frac{1}{2}\left[e^{(\tau/2)A}e^{\tau P^{-1}AP},A\right]+\left[e^{(\tau/2)A}e^{\tau P^{-1}AP},P^{-1}AP\right] \\
&= \left[e^{(\tau/2)A}e^{\tau P^{-1}AP},\frac{1}{2}A+P^{-1}AP\right], \quad \tau > 0.
\end{aligned}
$$

Note that $F(0) = I$. Thus, an integration gives the equality

$$
F(\tau) = I+\int_0^{\tau} e^{-\xi(A+P^{-1}AP)}\left[e^{(\xi/2)A}e^{\xi P^{-1}AP},\frac{1}{2}A+P^{-1}AP\right]e^{(\xi/2)A}d\xi, \quad \tau \geqslant 0. \tag{3.3}
$$

We wish to explore further the Lie bracket

$$
\begin{aligned}
H(\xi) &= \left[e^{(\xi/2)A}e^{\xi P^{-1}AP}, \frac{1}{2}A + P^{-1}AP\right] \\
&= e^{(\xi/2)A}e^{\xi P^{-1}AP}\left(\frac{1}{2}A + P^{-1}AP\right) - \left(\frac{1}{2}A + P^{-1}AP\right)e^{(\xi/2)A}e^{\xi P^{-1}AP}, \quad \xi > 0,
\end{aligned}
$$

with $H(0) = \Phi$. It follows that

$$
\begin{aligned}
H'(\xi) &= \left(\frac{1}{2}Ae^{(\xi/2)A}e^{\xi P^{-1}AP} + e^{(\xi/2)A}e^{\xi P^{-1}AP}P^{-1}AP\right)\left(\frac{1}{2}A + P^{-1}AP\right) \\
&\quad - \left(\frac{1}{2}A + P^{-1}AP\right)\left(\frac{1}{2}Ae^{(\xi/2)A}e^{\xi P^{-1}AP} + e^{(\xi/2)A}e^{\xi P^{-1}AP}P^{-1}AP\right) \\
&= -\left(\frac{1}{2}A + P^{-1}AP\right)H(\xi) + \left(\frac{1}{2}A + P^{-1}AP\right)H(\xi) \\
&\quad + \frac{1}{2}Ae^{(\xi/2)A}e^{\xi P^{-1}AP}\left(\frac{1}{2}A + P^{-1}AP\right) + e^{(\xi/2)A}e^{\xi P^{-1}AP}P^{-1}AP\left(\frac{1}{2}A + P^{-1}AP\right) \\
&\quad - \left(\frac{1}{2}A + P^{-1}AP\right)\frac{1}{2}Ae^{(\xi/2)A}e^{\xi P^{-1}AP} - \left(\frac{1}{2}A + P^{-1}AP\right)e^{(\xi/2)A}e^{\xi P^{-1}AP}P^{-1}AP \\
&= -\left(\frac{1}{2}A + P^{-1}AP\right)H(\xi) - \left(\frac{1}{2}A + P^{-1}AP\right)\left[e^{\xi P^{-1}AP}, \frac{1}{2}A\right]e^{(\xi/2)A} \\
&\quad + \left[\frac{1}{2}A, e^{\xi P^{-1}AP}\right]e^{(\xi/2)A}\left(\frac{1}{2}A + P^{-1}AP\right), \quad \xi > 0.
\end{aligned}
$$

Recall (2.3). We obtain immediately the former solution

$$
\begin{aligned}
H(\xi) &= -\frac{1}{2}\int_0^\tau e^{(\tau-\xi)((1/2)A+P^{-1}AP)}\left\{\left(\frac{1}{2}A + P^{-1}AP\right)\left[e^{\xi P^{-1}AP}, A\right]e^{(\xi/2)A}\right. \\
&\quad \left. + \left[A, e^{\xi P^{-1}AP}\right]e^{(\xi/2)A}\left(\frac{1}{2}A + P^{-1}AP\right)\right\}d\xi \\
&= -\frac{1}{2}\int_0^\tau e^{(\tau-\xi)((1/2)A+P^{-1}AP)}\left[\frac{1}{2}A + P^{-1}AP, \left[e^{\xi P^{-1}AP}, A\right]e^{(\xi/2)A}\right]d\xi, \quad \tau \geqslant 0.
\end{aligned}
$$

Utilizing the above for (3.2), we obtain that

$$
\begin{aligned}
F(\tau) &= I - \frac{1}{2}\int_0^\tau e^{-\xi(A+P^{-1}AP)}\int_0^\xi e^{(\xi-\zeta)((1/2)A+P^{-1}AP)} \\
&\quad \times \left[\frac{1}{2}A + P^{-1}AP, \left[e^{\xi P^{-1}AP}, A\right]e^{(\zeta/2)A}\right]e^{(\xi/2)A}d\zeta d\xi, \quad \tau \geqslant 0.
\end{aligned}
$$

Subsequently,

$$
\begin{aligned}
E(\tau_k) &= e^{\tau_k(A+P^{-1}AP)}\left(I-F(\tau_k)\right)\\
&= \frac{1}{2}e^{\tau_k(A+P^{-1}AP)}\int_0^{\tau_k} e^{-\xi(A+P^{-1}AP)}\int_0^{\xi} e^{(\xi-\zeta)((1/2)A+P^{-1}AP)}\\
&\quad\times\left[\frac{1}{2}A+P^{-1}AP,\left[A,e^{\zeta P^{-1}AP}\right]e^{(\zeta/2)A}\right]e^{(\xi/2)A}d\zeta d\xi.
\end{aligned}
$$

In view of Lemma 2, the above ensures our result. $\square$

COROLLARY 1. *We have*

$$
\|E(\tau_k)\|_2 \leqslant \left\|\frac{1}{2}A+P^{-1}AP\right\|_2 \left\|\left[A,P^{-1}AP\right]\right\|_2 \tau_k^3, \quad 0<\tau_k\ll 1.
$$

Proof. We note that the matrices $e^{\kappa A}$, $e^{\kappa P^{-1}AP}$ and $e^{\kappa(A+P^{-1}AP)}$ are symmetric as far as $\kappa\geqslant 0$, since A and $P^{-1}AP$ are symmetric. Furthermore, we have

$$
\left\|e^{\kappa A}\right\|_2,\ \left\|e^{\kappa P^{-1}AP}\right\|_2,\ \left\|e^{\kappa(A+P^{-1}AP)}\right\|_2 \leqslant 1
$$

for $\kappa\geqslant 0$ since A and $P^{-1}AP$ are negative definite.

It follows from Theorem 1 that

$$
\begin{aligned}
\|E(\tau_k)\|_2 &= \frac{1}{2}\left\|\int_0^{\tau_k} e^{(\tau_k-\xi)(A+P^{-1}AP)}\int_0^{\xi} e^{(\xi-\zeta)((1/2)A+P^{-1}AP)}\right.\\
&\quad\times\left.\left[\frac{1}{2}A+P^{-1}AP,\int_0^{\zeta} e^{(\zeta-\eta)P^{-1}AP}\left[A,P^{-1}AP\right]e^{\eta P^{-1}AP}e^{(\zeta/2)A}d\eta\right]e^{(\xi/2)A}d\zeta d\xi\right\|_2\\
&\leqslant \frac{1}{2}\int_0^{\tau_k}\left\|e^{(\tau_k-\xi)(A+P^{-1}AP)}\right\|\int_0^{\xi}\left\|e^{(\xi-\zeta)((1/2)A+P^{-1}AP)}\right\|\\
&\quad\times\left\|\left[\frac{1}{2}A+P^{-1}AP,\int_0^{\zeta} e^{(\zeta-\eta)P^{-1}AP}\left[A,P^{-1}AP\right]e^{\eta P^{-1}AP}e^{(\zeta/2)A}d\eta\right]\right\|_2\left\|e^{(\xi/2)A}\right\|_2 d\zeta d\xi\\
&\leqslant \frac{1}{2}\int_0^{\tau_k}\int_0^{\xi}\left\|\left[\frac{1}{2}A+P^{-1}AP,\int_0^{\zeta} e^{(\zeta-\eta)P^{-1}AP}\left[A,P^{-1}AP\right]e^{\eta P^{-1}AP}e^{(\zeta/2)A}d\eta\right]\right\|_2 d\zeta d\xi\\
&\leqslant \frac{1}{2}\int_0^{\tau_k}\int_0^{\xi}\left(2\left\|\frac{1}{2}A+P^{-1}AP\right\|_2\left\|\int_0^{\zeta} e^{(\zeta-\eta)P^{-1}AP}\left[A,P^{-1}AP\right]e^{\eta P^{-1}AP}d\eta\right\|_2\right)d\zeta d\xi\\
&\leqslant \left\|\frac{1}{2}A+P^{-1}AP\right\|_2\int_0^{\tau_k}\int_0^{\xi}\int_0^{\zeta}\left\|e^{(\zeta-\eta)P^{-1}AP}\right\|_2\left\|\left[A,P^{-1}AP\right]\right\|_2\left\|e^{\eta P^{-1}AP}\right\|_2 d\eta d\zeta d\xi\\
&\leqslant \left\|\frac{1}{2}A+P^{-1}AP\right\|_2\left\|\left[A,P^{-1}AP\right]\right\|_2\tau_k\tau_k\tau_k.
\end{aligned}
$$

This completes our proof. $\square$

Needless to say, the result stated in Corollary 1 demonstrates that the absolute error of Strang's splitting can be dominated by the distance between A and $B=P^{-1}AP$ in the sense of commutative levels.

4. Splitting algorithm and realization

Recalling (2.4) and (3.1), we obtain that

$$\begin{aligned} v_{k+1} &= \left(e^{(\tau_k/2)A}e^{\tau_k P^{-1}AP}e^{(\tau_k/2)A}+E(\tau_k)\right)\left(v_k+\frac{\tau_k}{2}g(v_k)\right)+\frac{\tau_k}{2}g(v_{k+1}) \\ &= e^{(\tau_k/2)A}e^{\tau_k P^{-1}AP}e^{(\tau_k/2)A}\left(v_k+\frac{\tau_k}{2}g(v_k)\right)+\frac{\tau_k}{2}g(v_{k+1})+\hat{E}(\tau_k), \qquad (4.1) \\ &\qquad k=0,1,2,\ldots,K, \end{aligned}$$

where

$$\hat{E}(\tau_k)=E(\tau_k)\left(v_k+\frac{\tau_k}{2}g(v_k)\right)=\mathscr{O}(\tau_k^3).$$

Dropping the truncation error $\hat{E}$, we acquire an essential splitting algorithm for solving (1.1)–(1.3), namely,

$$w_{k+1}=e^{(\tau_k/2)A}e^{\tau_k P^{-1}AP}e^{(\tau_k/2)A}\left(w_k+\frac{\tau_k}{2}g(w_k)\right)+\frac{\tau_k}{2}g(w_{k+1}),\ k=0,1,2,\ldots,K,$$

or

$$w_{k+1}-\frac{\tau_k}{2}g(w_{k+1})=e^{(\tau_k/2)A}e^{\tau_k P^{-1}AP}e^{(\tau_k/2)A}\left(w_k+\frac{\tau_k}{2}g(w_k)\right),\ k=0,1,2,\ldots,K, \qquad (4.2)$$

where w_ℓ is a third order approximation of v_ℓ, $\ell=0,1,2,\ldots,K$.

THEOREM 2. *Let J_ℓ be the Jacobian matrix corresponding to the vector function $g(w_\ell)$ and $I-\frac{\tau_\ell}{2}J_{\ell+1}$ be invertible for sufficiently small τ_ℓ, $\ell=0,1,2,\ldots,K$. If*

$$\left\|\left(I-\frac{\tau_\ell}{2}J_{\ell+1}\right)^{-1}\right\|_2\left\|I+\frac{\tau_\ell}{2}J_\ell\right\|_2\leqslant 1,\ \ \ell=0,1,2,\ldots,K.$$

then the nonlinear implicit scheme (4.2) is asymptotically stable in the von Neumann sense.

Proof. We consider perturbed equations

$$\tilde{w}_{k+1}-\frac{\tau_k}{2}g(\tilde{w}_{k+1})=e^{(\tau_k/2)A}e^{\tau_k P^{-1}AP}e^{(\tau_k/2)A}\left(\tilde{w}_k+\frac{\tau_k}{2}g(\tilde{w}_k)\right),\ k=0,1,2,\ldots,K.$$

A subtraction between the above and (4.2) yields

$$\begin{aligned}\varepsilon_{k+1}-\frac{\tau_k}{2}\left(g(w_{k+1})-g(\tilde{w}_{k+1})\right)&=e^{(\tau_k/2)A}e^{\tau_k P^{-1}AP}e^{(\tau_k/2)A}\left[\varepsilon_k+\frac{\tau_k}{2}\left(g(w_k)-g(\tilde{w}_k)\right)\right],\\ &\qquad k=0,1,2,\ldots,K,\end{aligned}$$

where $\varepsilon_\ell=w_\ell-\tilde{w}_\ell$, $\ell=0,1,2,\ldots,K$. It follows that

$$\varepsilon_{k+1}-\frac{\tau_k}{2}J_{k+1}\varepsilon_{k+1}\approx e^{(\tau_k/2)A}e^{\tau_k P^{-1}AP}e^{(\tau_k/2)A}\left[\varepsilon_k+\frac{\tau_k}{2}J_k\varepsilon_k\right],\ \ k=0,1,2,\ldots,K,$$

where J_ℓ is the Jacobian matrices. Considering that the perturbation ε is sufficiently small, we may assume an asymptotic formula [6, 14],

$$\left(I-\frac{\tau_k}{2}J_{k+1}\right)\varepsilon_{k+1}=e^{(\tau_k/2)A}e^{\tau_k P^{-1}AP}e^{(\tau_k/2)A}\left(I+\frac{\tau_k}{2}J_k\right)\varepsilon_k,\ \ k=0,1,2,\ldots,K,$$

which is equivalent to

$$\varepsilon_{k+1}=\left(I-\frac{\tau_k}{2}J_{k+1}\right)^{-1}e^{(\tau_k/2)A}e^{\tau_k P^{-1}AP}e^{(\tau_k/2)A}\left(I+\frac{\tau_k}{2}J_k\right)\varepsilon_k,\ \ k=0,1,2,\ldots,K,$$

if $I-\frac{\tau_k}{2}J_{k+1}$ is invertible when $0<\tau_k\ll 1$ is sufficiently small.

Now, we have

$$\begin{aligned}\|\varepsilon_{k+1}\|_2&=\left\|\left(I-\frac{\tau_k}{2}J_{k+1}\right)^{-1}e^{(\tau_k/2)A}e^{\tau_k P^{-1}AP}e^{(\tau_k/2)A}\left(I+\frac{\tau_k}{2}J_k\right)\varepsilon_k\right\|_2\\&\leqslant\left\|\left(I-\frac{\tau_k}{2}J_{k+1}\right)^{-1}e^{(\tau_k/2)A}e^{\tau_k P^{-1}AP}e^{(\tau_k/2)A}\left(I+\frac{\tau_k}{2}J_k\right)\right\|_2\|\varepsilon_k\|_2\\&\leqslant\left\|\left(I-\frac{\tau_k}{2}J_{k+1}\right)^{-1}\right\|_2\left\|I+\frac{\tau_k}{2}J_k\right\|_2\|\varepsilon_k\|_2\ \leqslant\ \|\varepsilon_k\|_2.\end{aligned}$$

Therefore, the splitting algorithm (4.2) is asymptotically stable in the von Neumann sense [7]. □

COROLLARY 2. *Let matrices* $e^{(\tau_k/2)A}e^{\tau_k P^{-1}AP}e^{(\tau_k/2)A}$, $I+\frac{\tau_k}{2}J_k$, $0\leqslant\tau_k\ll 1$, *commute. If*

$$\left\|\left(I-\frac{\tau_k}{2}J_{k+1}\right)^{-1}\left(I+\frac{\tau_k}{2}J_k\right)\right\|_2\leqslant 1,\ \ k=0,1,2,\ldots,K,$$

then the nonlinear implicit scheme (4.2) *is asymptotically stable in the von Neumann sense.*

Proof. The result is straightforward and can be seen from

$$\begin{aligned}\|\varepsilon_{k+1}\|_2&=\left\|\left(I-\frac{\tau_k}{2}J_{k+1}\right)^{-1}e^{(\tau_k/2)A}e^{\tau_k P^{-1}AP}e^{(\tau_k/2)A}\left(I+\frac{\tau_k}{2}J_k\right)\varepsilon_k\right\|_2\\&\leqslant\left\|\left(I-\frac{\tau_k}{2}J_{k+1}\right)^{-1}\left(I+\frac{\tau_k}{2}J_k\right)e^{(\tau_k/2)A}e^{\tau_k P^{-1}AP}e^{(\tau_k/2)A}\right\|_2\|\varepsilon_k\|_2\\&\leqslant\left\|\left(I-\frac{\tau_k}{2}J_{k+1}\right)^{-1}\left(I+\frac{\tau_k}{2}J_k\right)\right\|_2\|\varepsilon_k\|_2\ \leqslant\ \|\varepsilon_k\|_2.\quad\square\end{aligned}$$

In realistic computations, often we may assume that $J_{k+1}=\sigma_k J_k$, $k=0,1,2,\ldots,K$, where the parameters σ_k, $0<\sigma_k<1$, are either given by a particular computational procedure or determined stochastically. Furthermore, we may assume that

$$\left\|\left(I-\frac{\tau}{2}J_k\right)^{-1}\left(I+\frac{\tau}{2}J_k\right)\right\|_2\leqslant M_0\left\|e^{\tau J_k}\right\|_2\leqslant M_1,\tag{4.3}$$

where $0<\tau\ll 1$, and M_0 and M_1 are positive constants. In this circumstance, we have the following result.

COROLLARY 3. *Let matrices* $e^{(\tau_k/2)A}e^{\tau_k P^{-1}AP}e^{(\tau_k/2)A}$, $I+\frac{\tau_k}{2}J_k$, $0\leqslant\tau_k\ll 1$, *commute,* (4.3) *be true, and*

$$\left\|\left(I+\frac{\tau}{2}J_k\right)\left(I+\frac{\tau}{2}J_k\right)^{-1}\right\|_2\leqslant M_2,$$

where $0<\tau\ll 1$ *and* M *is a positive constant. If* $M_1M_2\leqslant 1$, *then the nonlinear implicit scheme* (4.2) *is asymptotically stable in the von Neumann sense.*

Proof. We have

$$\begin{aligned}
\|\varepsilon_{k+1}\|_2 &\leqslant \left\|\left(I-\frac{\tau_k}{2}J_{k+1}\right)^{-1}\left(I+\frac{\tau_k}{2}J_k\right)e^{(\tau_k/2)A}e^{\tau_k P^{-1}AP}e^{(\tau_k/2)A}\right\|_2\|\varepsilon_k\|_2\\
&\leqslant \left\|\left(I-\frac{\tau_k}{2}J_{k+1}\right)^{-1}\left(I+\frac{\tau_k}{2}J_k\right)\right\|_2\|\varepsilon_k\|_2\\
&= \left\|\left(I-\frac{\tau_k\sigma_k}{2}J_k\right)^{-1}\left(I+\frac{\tau_k\sigma_k}{2}J_k\right)\left(I+\frac{\tau_k\sigma_k}{2}J_k\right)^{-1}\left(I+\frac{\tau_k}{2}J_k\right)\right\|_2\|\varepsilon_k\|_2\\
&\leqslant \left\|\left(I-\frac{\tau_k\sigma_k}{2}J_k\right)^{-1}\left(I+\frac{\tau_k\sigma_k}{2}J_k\right)\right\|_2\left\|\left(I+\frac{\tau_k\sigma_k}{2}J_k\right)^{-1}\left(I+\frac{\tau_k}{2}J_k\right)\right\|_2\|\varepsilon_k\|_2\\
&\leqslant M_1M_2\|\varepsilon_k\|_2 \;\leqslant\; \|\varepsilon_k\|_2 .
\end{aligned}$$

Therefore the corollary is clear. □

To utilize scheme (4.2) in practical computations, we may avoid evaluations of the matrix exponential functions by an introduction of proper Padé approximants. For preserving our second order approximation to the Kawarada problem, we may consider [1/1] Padé formulas. They lead to the following implicit split Crank-Nicolson method:

$$\begin{aligned}
w_{k+1}-\frac{\tau_k}{2}g(w_{k+1}) &= E\left(A,\frac{\tau_k}{2}\right)E\left(P^{-1}AP,\tau_k\right)E\left(A,\frac{\tau_k}{2}\right)\\
&\quad\times\left(w_k+\frac{\tau_k}{2}g(w_k)\right),\quad k=0,1,2,\ldots,K,
\end{aligned}\tag{4.4}$$

where

$$\begin{aligned}
E\left(A,\frac{\tau_k}{2}\right) &= \left(I+\frac{\tau_k}{4}A\right)\left(I-\frac{\tau_k}{4}A\right)^{-1},\\
E\left(P^{-1}AP,\tau_k\right) &= \left(I+\frac{\tau_k}{2}P^{-1}AP\right)\left(I-\frac{\tau_k}{2}P^{-1}AP\right)^{-1}.
\end{aligned}$$

REMARK 1. The implicit split Crank-Nicolson method (4.4) is different from any traditional Peachman-Rachford splitting methods [7, 13].

REMARK 2. The nonlinear implicit scheme (4.4) can be treated conveniently via either an application of iterative procedures, or a suitable linearization (for instance, see [1, 2, 3, 5, 12] and references therein).

5. Numerical experiments and concluding remarks

As an illustration of the theoretical discussions, we consider the following two-dimensional testing Kawarada reaction-diffusion initial-boundary value problem:

$$\begin{aligned} a^2 u_t &= u_{xx} + u_{yy} + \frac{a^2}{(1-u)^\theta}, \quad a, \theta > 0,\ (x,y,t) \in \mathscr{D}_1, \\ u(x,y,t) &= 0, \quad (x,y,t) \in \mathscr{S}_1, \\ u(x,y,0) &= \alpha \sin^2(\pi x)\sin^2(\pi y), \quad (x,y) \in \mathscr{D}_1, \end{aligned}$$

where $0 < \alpha \ll 1$ is a constant. Herewith we only consider the case of $\theta = 1$ since discussions with $\theta \neq 1$ are similar [7, 9]. The implicit split Crank-Nicolson realization (4.4) is employed. Nonuniformly adjusted and exponentially graded temporal grids are used as quenching time is approached [1, 4].

To achieve a sufficient resolution, we set the spatial grid graininess to be $h = aN^{-2}$, $N \geqslant 100$ [5]. This leads to $\mathscr{O}\left(N^2\right)$ internal mesh points in the two-dimensional spatial domain. In this circumstance, all coefficient matrices would be of $\mathscr{O}\left(N^2 \times N^2\right)$ in size. However, the computational tasks utilizing (4.4) are significantly simpler and more straightforward due to the split of A and $B = P^{-1}AP$, as compared with most non-splitting schemes. A fixed Courant number $\kappa = \tau/h^2 = 1/10$ is observed throughout experiments.

To show the amazing dynamics of a quenching solution, and to demonstrate the accuracy and stability of the splitting method developed, we adopt $a = \sqrt{4.75}$ which is slightly greater than the well-known critical domain parameter $a^* \approx \sqrt{4.49576}$ [7].

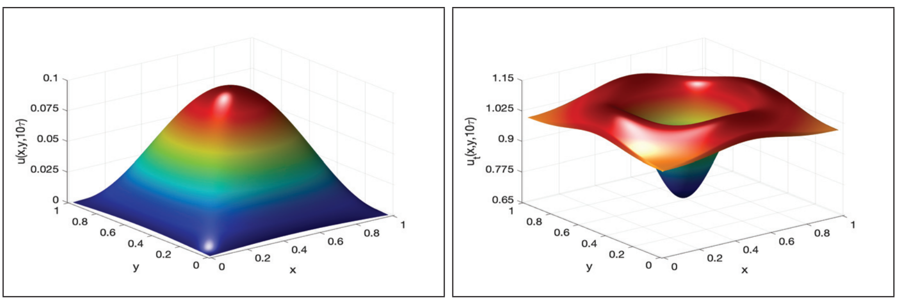

Figure 1: *Numerical solution $u(x,y,t)$ (LEFT) and $u_t(x,y,t)$ (RIGHT) at $t = 10\tau \approx 6.83013455 \times 10^{-5}$, respectively. Functions u and u_t are positive with their maximal values being approximately 0.10003070 and 1.11395428, respectively.*

The numerical solution u and its temporal derivative u_t are shown at time steps $M = 10, 1000, 10000, 65000, 66700, 66721, 66722, 66723$, respectively. Among them, the first five pairs of figures showing a steady growth of the solution profile. It can be observed that the solution u increases monotonically. Its maximal value increases from 0.10493003 to 0.98076123. The corresponding temporal derivative peak grows much faster from 1.11395428 to 47.71582321.

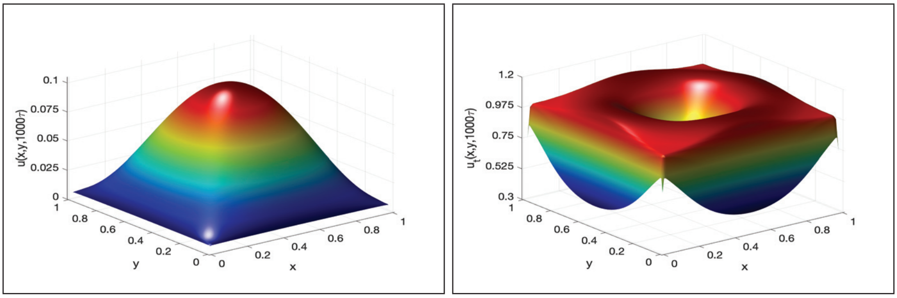

Figure 2: *Numerical solution* $u(x,y,t)$ *(LEFT) and* $u_t(x,y,t)$ *(RIGHT) at* $t = 1000\tau \approx$ 0.00683013, *respectively. Functions* u *and* u_t *are positive with their maximal values being approximately 0.10493003 and 1.11808111, respectively.*

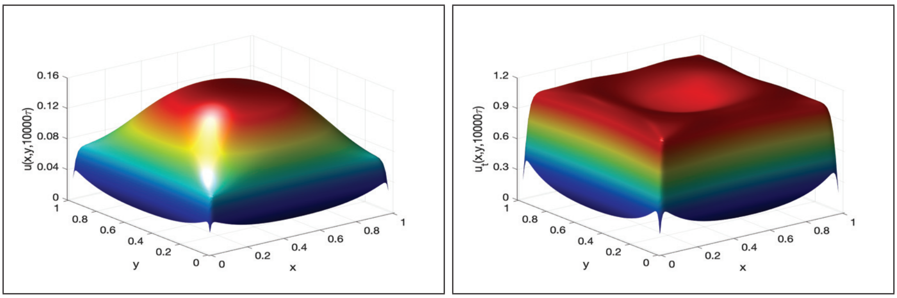

Figure 3: *Numerical solution* $u(x,y,t)$ *(LEFT) and* $u_t(x,y,t)$ *(RIGHT) at* $t = 10000\tau \approx$ 0.06830134, *respectively. Functions* u *and* u_t *are positive with their maximal values being approximately 0.15986359 and 1.15740322, respectively.*

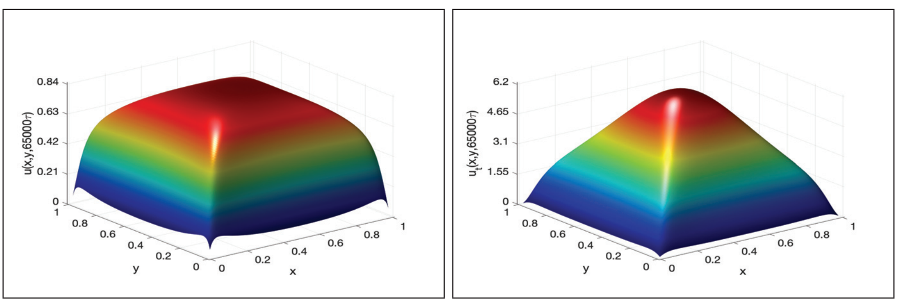

Figure 4: *Numerical solution* $u(x,y,t)$ *(LEFT) and* $u_t(x,y,t)$ *(RIGHT) at* $t = 65000\tau \approx$ 0.44395874, *respectively. Functions* u *and* u_t *are positive with their maximal values being approximately 0.85280375 and 6.21388153, respectively.*

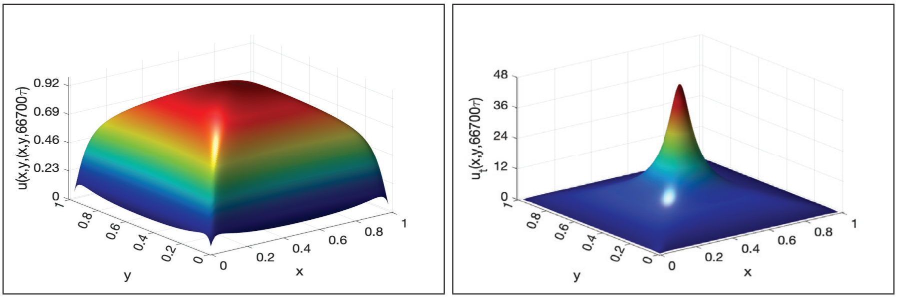

Figure 5: *Numerical solution* $u(x,y,t)$ *(LEFT) and* $u_t(x,y,t)$ *(RIGHT) at* $t = 66700\tau \approx 0.45556997$, *respectively. Functions* u *and* u_t *are positive with their maximal values being approximately 0.98076123 and 47.71582321, respectively.*

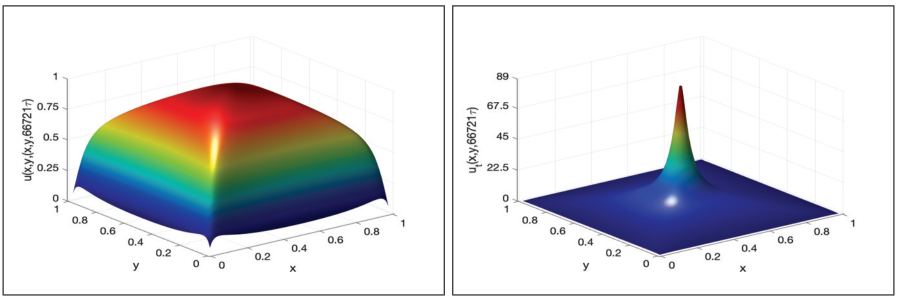

Figure 6: *Numerical solution* $u(x,y,t)$ *(LEFT) and* $u_t(x,y,t)$ *(RIGHT) at* $t = 66721\tau \approx 0.45571340$, *respectively. Functions* u *and* u_t *are positive with their maximal values being approximately 0.98980046 and 88.59740079, respectively.*

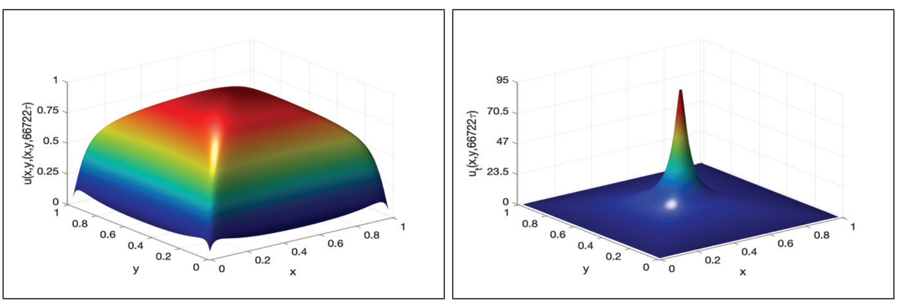

Figure 7: *Numerical solution* $u(x,y,t)$ *(LEFT) and* $u_t(x,y,t)$ *(RIGHT) at* $t = 66722\tau \approx 0.45572023$, *respectively. Functions* u *and* u_t *are positive with their maximal values being approximately 0.99044426 and 94.25843114, respectively.*

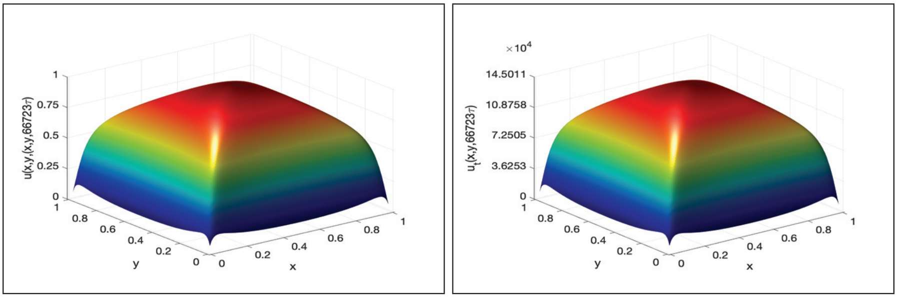

Figure 8: *Numerical solution* $u(x,y,t)$ *(LEFT) and* $u_t(x,y,t)$ *(RIGHT) at* $t = 66723\tau \approx 0.45572706$, *respectively. Functions* u *and* u_t *are positive with their maximal values being approximately 0.99394420 and* 1.45010945×10^5, *respectively.*

The final three figures are taken immediately before the quench of u. It can be observed that the increments of u_t are tremendous as compared that of u. The derivative blows up in the last step of calculations with a maximal reaches 1.45010945×10^5.

The shape changes, in particularly the derivative function u_t, are fascinating. We may observe that while the temperature field function u grows steadily, the derivative function is relatively violent. In a combustion process, the later represents the rate of changes of the temperature field. It is accelerated initially at the center of the domain, and then extended to the entire combustion chamber in the end. The split algorithm shows a satisfactory numerical stability throughout the 66,723 temporal step excursions for solving the nonlinear partial differential equation.

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