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Recent Trends in Splitting, Adaptive and Hybrid Numerical Methods for Differential Equations

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Abstract: *Splitting, or decomposition, methods, associated with adaptive strategies, hybrid multi-scale settings, have been playing an important role in solving different differential equation problems in various applications. Latest developments in the area range from splitting for higher accuracy and flexibility in different parallel environments, splitting for nonlinear partial differential equations, splitting for singular differential equations and inverse problems, nonlinear stability and convergence of splitting schemes, iterative and adaptive splitting strategies, geometric integration and domain decomposition methods, to quantum splitting computations in modern bio-chemistry and life science applications. This survey will provide some key information on the most exciting recent achievements in the areas. Computer simulated illustrations will be given.*

Key words: Splitting and decomposition methods, adaptations, uniform and nonuniform meshes, time scales and hybrid methods, order of accuracy, numerical stability and convergence, large systems of equations.

1 Introduction

A splitting, or decomposition, method is a numerical method for the time integration of an ordinary or a partial differential equation. With a phase space M, differential equation

$$\dot{x} = X(x),\ x \in M, \tag{1.1}$$

and X a vector field on M, splitting methods involve three equally important steps:

1. choosing a set of vector fields X_k such that $X = \sum X_k$;
2. integrating either exactly or approximately each X_k; and
3. combining these solutions to yield an integrator for X.

For instance, writing the flow of (1.1) as

$$x(t) = \exp(tX)x(0),$$

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where $x(0)$ is an initial flow, we might use the composition method

$$\varphi_1(\tau) = \exp(\tau X_1)\exp(\tau X_2)\cdots\exp(\tau X_n), \tag{1.2}$$

where

$$\varphi_1(\tau) = \exp\left(\tau \sum X_k\right) + O(\tau^2). \tag{1.3}$$

Formula (1.2) is called a *first order exponential splitting.* The value of τ is refereed as the *time step,* while each $X_i,\ 1 \le i \le n$, is simpler than the original vector field X in the following two ways:

1. The types of X_i are simpler. For example, the Navier-Stokes equations contain advection, diffusion, and pressure terms, each with distinct characteristic properties and appropriate numerical methods. red Example: a conservation law may contain fast and slow wave terms which can be treated separately.
2. The X_i are easier to treat numerically. For example, dimensional splitting for multidimensional diffusion equations. another example is the split-step Fourier method for the linear Schrödinger equation $iu = u_{xx} + V(x)u$, where each term is linear and Hamiltonian, but the first term can be integrated more quickly if a splitting (1.2) is utilized.

Splitting methods are developed for the motivations of computational speed, accuracy, and stability. The methods have been playing a significant role in numerical analysis, or more precisely, in computational mathematics [9, 17, 24, 33-36, 40-44, 56-59].

2 Splitting preliminaries

Let us consider a more general form of the splitting:

$$\varphi(\tau) = \sum_{k=1}^{K} \gamma_k E_k(\tau), \tag{2.1}$$

where $E_k(\tau)$ is a finite product of the exponentials $\exp(\alpha\tau X_n),\ 1 \le n \le N$, and $\alpha > 0$ depends on k and n. Consider the spectral norm $\|\cdot\|$. We have

Definition 1. The splitting formula φ is *stable* if

$$\|\varphi\| < 1.$$

Definition 2. The splitting formula φ is an *order ρ approximation* of $\exp(\tau X)$ if

$$\|\varphi(\tau) - \exp(\tau X)\| = O\left(\tau^{\rho+1}\right).$$

It is not difficult to show that (1.2) is indeed a first order splitting. In addition to φ_1, the most frequently used splitting formulas including

$$\begin{aligned}
\varphi_2(\tau) &= [\exp(\tau X_1)\exp(\tau X_2)\cdots\exp(\tau X_n) \\
&\quad + \exp(\tau X_n)\exp(\tau X_{n-1})\cdots\exp(\tau X_1)]/2, \\
\varphi_3(\tau) &= \exp(\tau X_1/2)\exp(\tau X_2/2)\cdots\exp(\tau X_{n-1}/2) \\
&\quad \times \exp(\tau X_n)\exp(\tau X_{n-1}/2)\cdots\exp(\tau X_1/2).
\end{aligned}$$

Both φ_2 and φ_2 are second order in accuracy.

Conjecture 1 (Burstein and Mirin [6]). *There exist third and higher order stable splitting formulas* φ.

For the convexity and stability, we may assume that $\gamma_k \geq 0,\ 1 \leq k \leq K$.

Theorem 1 (Sheng [43], Suzuki [59]). *The highest order of a stable splitting is two.*

Surprisingly, the initial proof of the theorem was acquired via applications of the Lagrangian method of multipliers which is often used in optimizations. Several objective functions, such as

$$s = \sum_{k=1}^{K} \gamma_k h_k - \lambda \sum_{k=1}^{K} \gamma_k f_k - \mu \sum_{k=1}^{K} \gamma_k g_k,$$

where $\lambda,\ \mu$ are Lagrangian multipliers, and proper constrains are designed and used. The result was later refereed as the *Sheng-Suzuki Theorem* for the nonexistence of higher order stable splitting formulas [10, 56].

Different proofs of the above theorem can be found in later publications by McLachlan [32] and Schatzman [42] . Different strategies were used in the proofs. Extensions of the discussions can be also found in numerous outstanding papers and books by Strang, LeVeque, Hairer, Lubich and Wanner [20, 21, 28, 57, 58].

Another key question to the splitting is that, How accurate can be a splitting method in practical applications? Although Definition 2 offers a qualitative measure of the approximation errors, a quantitative error analysis is still necessary.

Traditionally, numerical error in approximations is estimated locally, that is, the time step $\tau > 0$ is sufficiently small. In 1993, Sheng and Iserles [44] introduced the concept of global error estimates which is particularly useful for splitting. The concept has been used by many researchers in the field since then.

Without loss of generality, assume that $X_1,\ X_2, \ldots, X_K,\ X \in \mathbb{C}^{N\times N}$. Consider the spectral norm.

Theorem 2 (Sheng [44]). *Let* $K = 2$. *For* $\tau > 0$ *we have*

$$\begin{aligned}
\|\varphi_1(\tau) - \exp(\tau X)\| &\leq \frac{\tau^2}{2}\|[X_1, X_2]\| \max\left\{e^{\tau\mu(X_1+X_2)}, e^{\tau(\mu(X_1)+\mu(X_2))}\right\};\\
\|\varphi_2(\tau) - \exp(\tau X)\| &\leq \frac{\tau^3}{6}\,\|X_1 - X_2\|\,\|[X_1, X_2]\|\\
&\quad \times \max\left\{e^{t\mu(X_1+X_2)}, e^{t(\mu(X_1)+\mu(X_2))}\right\};\\
\|\varphi_3(\tau) - \exp(\tau X)\| &\leq \frac{\tau^3}{6}\left\|\frac{1}{2}X_1 + X_2\right\|\|[X_1, X_2]\|\\
&\quad \times \max\left\{e^{t\mu(X_1+X_2)}, e^{t(\mu(X_1)/2+\mu(X_1/2+X_2))}\right\},
\end{aligned}$$

where $[X_1, X_2]$ *is the commutator of* $X_1,\ X_2$*, and* $\mu(Y)$ *is the logarithmic norm of* Y.

The proof of Theorem 2 is straightforward. To do so, say, for φ_3, we may consider the matrix function

$$Y(\tau) = [\exp(\tau X_1), \exp(\tau X_2)].$$

Different the above to yield

$$Y'(\tau) = (X_1 + X_2)Y(\tau) + \left[e^{\tau X_1}, X_2\right] e^{\tau X_2} + \left[X_1, e^{\tau X_2}\right] e^{\tau X_1}.$$

Therefore we have the solution

$$\begin{aligned} Y(\tau) &= \int_0^\tau e^{(\tau-s)(X_1+X_2)} \left(\left[e^{sX_1}, X_2\right] e^{sX_2} + \left[X_1, e^{sX_2}\right] e^{sX_1}\right) ds \\ &= \int_0^\tau e^{(\tau-s)(X_1+X_2)} \\ &\quad \times \int_0^s \left(e^{(s-\upsilon)X_1}[X_1, X_2]e^{\upsilon X_1}e^{sX_2} + e^{(s-\upsilon)X_2}[X_1, X_2]e^{\upsilon X_2}e^{sX_1}\right) d\upsilon ds. \end{aligned}$$

An estimate of the above via the spectral norm yields our result.

General global error analysis for $K > 2$ were obtained by several researchers. Commutator based sensitivity function,

$$\nu(X, Y, \tau) = \left\| \int_0^\tau e^{(1-s)X}[X, Y]e^{\tau X} ds \right\|,$$

has been introduced in the analysis. Effects of the linear and nonlinear perturbations to numerical errors were also introduced and studied. Matrix exponential condition number was introduced and studied by Sheng et al. [44, 45].

Definition 3 (Sheng [45])**.** A asymptotic splitting is defined as

$$\Phi_{k,m}(\tau) = \left[\prod_{j=1}^m \varphi_{\ell(j)}\left(\frac{\tau}{mk}\right)\right]^k, \quad 1 \le r(j) \le M,\ \tau > 0,$$

where

$$\varphi_\ell(\tau) = \sum_{k=1}^{K_\ell} \gamma_k(\ell)E_k(\ell)(\tau), \quad \ell = 1, 2, \ldots, M,$$

are stable splitting operators.

Theorem 3 (Sheng [45]). *The order of accuracy of a consistent asymptotic splitting is higher than the least order of* $\varphi_\ell,\ \ell = 1, 2, \ldots, M$.

Theorem 4 (Sheng [9, 45]). *The global error coefficient of a consistent asymptotic splitting is less than that of any* $\varphi_\ell,\ \ell = 1, 2, \ldots, M$*, when* k *is sufficiently large.*

Many interesting discussions are followed with important applications in computational mathematics, quantum physics, engineering research. A particularly interesting case is the splitting for solving regular and singular perturbed differential equation problems. For this, let us consider the approximation of the flow operator:

$$P_\epsilon(\tau) = \exp\left[\tau(X_1 + \epsilon X_2)\right], \quad \tau,\ \epsilon > 0.$$

Definition 4 (Sheng [45])**.** We say that the splitting operator φ is of order $(p; q_p, q_{p+1}, \ldots)$ if

$$\varphi(\tau) - P_\epsilon(\tau) = \sum_{k=p}^{\infty} \alpha_k \tau^{k+1} \epsilon^{q_k}, \quad \tau,\, \epsilon > 0.$$

Theorem 5 (Sheng [45, 50])**.** *The splitting operators* $\varphi_1,\ \varphi_2$ *and* φ_3 *are of order* $(1; 1, 1, \ldots),\ (2; 1, 1, \ldots)$ *and* $(2; 1, 1, \ldots)$*, respectively.*

Needless to say, we have been discussing the approximation of the following flow function

$$\exp(\tau X) = \exp\left(\tau \sum X_k\right), \quad \tau > 0,$$

especially when $X,\ X_1,\ X_2, \ldots, X_K$ are matrices due to the large ordinary differential systems anticipated, many of them are consequences of the popular semi-discretization method, or method of lines for solving partial differential equations in scientific and engineering applications.

That is the reason why splitting is often referred as *exponential splitting.* An exponential splitting formula can further approximated by a proper Padé or rational approximation. A final introduction of descritization yields an appropriate numerical method implementation, including the well-known Peaceman-Rachford, ADI and LOD methods [9, 18, 43].

As for the matrix exponential function computations involved, Moler and Van Loan published a paper in 1978 [35]. Interestingly, the same titled article, with a slight modification, was published again in the same journal in 2003 [36]. This indicates clearly that current matrix exponential function computation methods, especially those used in exponential splitting computations, are far from a satisfactory.

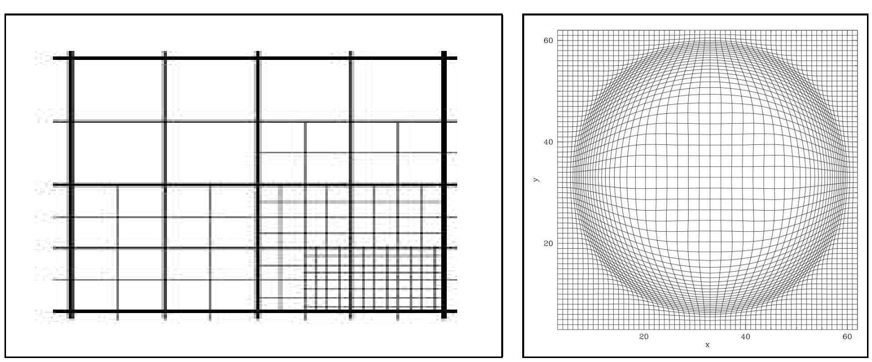

FIGURE 1. An illustration of the basic local grid refinement (left) and grid redistribution (right).

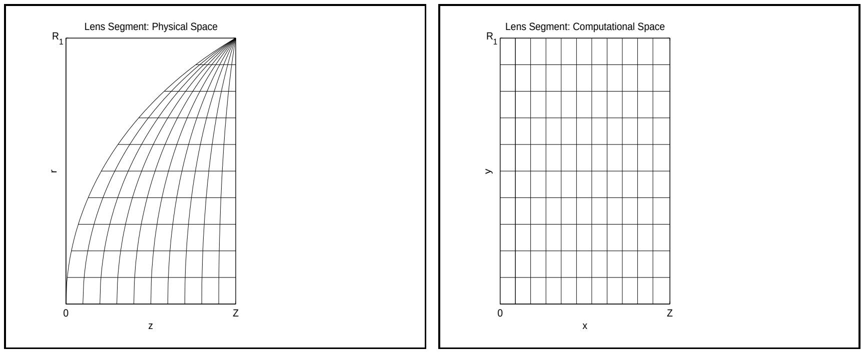

FIGURE 2. An illustration of the stretching adaptive transformation of a cylindrically symmetric lens domain (from the left to right). A dimensionless measurement is used.

3 A connection between adaptation and time scales

There are a variety of well-established techniques in adaptive computations. Among the most important methods, there are *local grid refinement,* and *grid redistribution.* For the former, interested readers may view recent publications by Berger, Liao, Ludwig, Oliger, and Flaherty [2, 30, 31, 37]. For the latter, references can be found in Cao, Huang, Budd, Russell, and Sheng [5, 7, 8, 15, 22, 48, 51, 52].

A different adaptation, called *interface method and domain transformation,* is introduced and developed by several researchers, including Guha, Li, LeVeque, Reinhart, Rogers and Sheng [18, 19, 29, 38].

No matter which adaptive method is used, the adaptation procedure involved is robotic and the grid movements are decided solely by the monitoring functions. For detailed discussions over different choices of the monitoring functions, their basic properties and restrictions, the reader is referred to recent publications by Budd, Huang, Russell, Van Vleck and Sheng [1, 5, 8, 9, 48].

A time scale can be viewed as a limit case when certain mesh steps in an adaptive mesh, which is nonuniform, tend to zero. Therefore a time scale may be viewed as a *hybrid grid* from computational point-of-view. In the case, an adaptive finite difference scheme may *reduce* to a dynamic equation.

Different dynamic derivatives are fundamental to the study of dynamic equations, since they provide necessary information about discrepancies between conventional derivatives and their discrete counterparts, that is, finite difference formulas. It is natural to conjecture that the most commonly used dynamic derivative formulas do offer reasonable approximations to the conventional derivatives in appropriate senses.

Theorem 6 (Sheng [46])**.** *Let f be sufficiently smooth in (a, b). Then the Δ, ∇ and $\diamondsuit_\alpha$ dynamic derivatives of f are consistent approximations to the conventional derivative f' in their domains of definitions. Further, their order of accuracy is one.*

Theorem 7 (Sheng [46]). *Let f be sufficiently smooth in (a, b). Then none of the existing second order dynamic derivatives is a consistent approximation to the conventional derivative f'' on appropriate time scales considered in general.*

Theorem 8 (Rogers and Sheng [39]). *There does not exist an anti-$\diamondsuit_\alpha$ dynamic derivative of a function defined on a time scales in general.*

Let us sketch the proof of Theorem 7 for the case involving $f^{\Delta\nabla}$ and $f^{\nabla\Delta}$. We only need to consider the case where $(f^\sigma(t))^\rho = (f^\rho(t))^\sigma = f(t)$ and $\mu^\rho(t) = \eta(t),\ \eta^\sigma(t) = \mu(t),\ t \in C \cap \mathbb{T}^\kappa_\kappa$. For this, we have

$$f^{\Delta\nabla}(t) = \frac{\eta(t)f^\sigma(t) - (\eta(t) + \mu(t))f(t) + \mu(t)f^\rho(t)}{\mu(t)\eta^2(t)}, \quad t \in C \cap \mathbb{T}^\kappa_\kappa.$$

On the other hand,

$$f^{\nabla\Delta}(t) = \frac{\eta(t)f^\sigma(t) - (\eta(t) + \mu(t))f(t) + \mu(t)f^\rho(t)}{\mu^2(t)\eta(t)}, \quad t \in C \cap \mathbb{T}^\kappa_\kappa.$$

Combining the two equations, we obtain

$$\eta(t)f^{\Delta\nabla}(t) = \mu(t)f^{\nabla\Delta}(t), \quad t \in C \cap \mathbb{T}^\kappa_\kappa.$$

Set $\lambda(t) = \mu(t)/\eta(t) > 0$. It follows immediately that

$$f^{\Delta\nabla}(t) = \lambda(t)f^{\nabla\Delta}(t), \quad t \in C \cap \mathbb{T}^\kappa_\kappa.$$

Since λ solely depends on the structures of $\mathbb{T}$, the theorem is clear via a contradiction.

Remark 1. Applications of the time scales theory and methods to adaptive computations may be limited. This is because, without incorporating the detailed structure of a time scale, a second order dynamic equation, say,

$$u^{\Delta\nabla}(t) = f(t), \quad t \in \mathbb{T}^\kappa_\kappa,$$

is irrelevant to a second order differential equation,

$$v''(t) = f(t), \quad t \in [a, b],$$

even though $\mathbb{T}$ is superimposed on $[a, b]$. On the other hand, an adaptive finite difference equation is independent to the nonuniform mesh used.

Remark 2. Since a second order dynamic derivative (so do higher dynamic derivatives) is irrelevant to a second order derivative, the time scales theory and methods provide a nonconventional way of approximation to practical problems. For instance, if the dynamic equation

$$u^{\Delta_t} = a^2 u^{\Delta_x\Delta_x}$$

does not model a heat diffusion, then what is the true physics behind it? On the other hand, what should be a correct dynamic equation for a head flow?

Remark 3. Suppose the above second order dynamic equation makes sense in certain applications. Then what should be a proper numerical algorithm for solving it?

Remark 4. More detailed investigations of finite differences on arbitrary grids may be needed.

The following interesting results were obtained during the study of derivative approximations on nonuniform meshes by Jain and Sheng.

Theorem 9 (Jain and Sheng [25]). *A higher order derivative cannot be approximated by a repeat application of the finite differences on an arbitrary grid* D.

Theorem 10 (Jain and Sheng [25]). *Approximations of a higher order derivative can always be obtained via proper combinations of the finite differences on an arbitrary grid* D.

Theorem 11 (Jain and Sheng [25]). *Detailed relative error estimates in terms of the grid sensitivity index of second order finite difference approximations.*

Most computational approaches are based on the theory and methods of time scales implemented by many researchers, including Bohner, Peterson and Hilger [3, 4, 16], Özkan, Sarikaya and Yildirim [23, 41], Eloe, Henderson, Ehrke, Kunkel and Sheng [11-14, 47, 49, 53, 55] and Thomas et al. [26, 60].

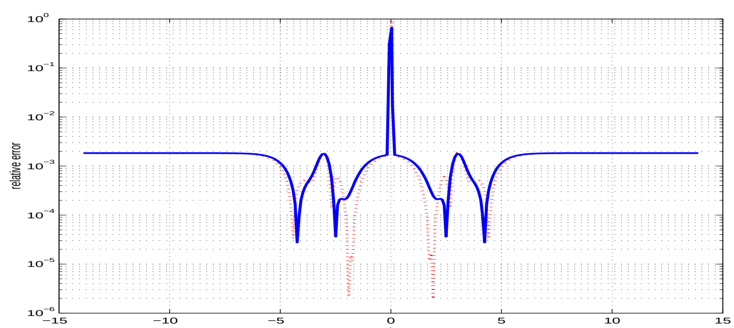

FIGURE 3. Numerical errors of the different approximations of u' on the discrete time scale $\mathbb{T}$. Relative errors of the $\diamondsuit_{1/2}$ (solid curve) and modified central difference formula (dotted curve) [39]. Logarithmic y-scale is used to show details of the error distributions.

4 Adaptive splitting

The latest developments in the area are associated with the quenching-combustion differential equations. Semi- and fully adaptive methods associated with splitting for solving multi-dimensional problems are implemented. Let

$$D = (0, a) \times (0, b), \quad a,\ b > 0, \quad \partial D \ \text{be its boundary,}$$
$$\Omega = D \times (0,\ T),\ S = \partial D \times (0,\ T), \quad 0 < T < \infty.$$

Consider the following degenerate quenching problem:

$$s(x,y)u_t = u_{xx} + u_{yy} + f(u), \quad (x,y,t) \in \Omega, \tag{4.1}$$

$$u(x,y,t) = 0,\ (x,y,t) \in S; \quad u(x,y,0) = u_0(x,y),\ (x,y) \in D, \tag{4.2}$$

where $s(x,y) = (x^2+y^2)^{q/2}$, $q \geq 0$, and $f(u)$ is strictly increasing for $0 \leq u < 1$ with

$$f(0) = f_0 > 0, \quad \lim_{u \to 1^-} f(u) = \infty.$$

It can be shown that, the positive solution of (4.1), (4.2) exists and is unique. Further, when certain environmental parameters exceed their limits, $\max\{u\} \to 1^-$ in a finite time. Quenching phenomena are distinguished for their important physical, engineering and industrial interpretations. They serve as an indicator of the steady and unsteady combustion processes, or burning and explosion of the rocket fuel. The solution of (4.1), (4.2) also plays a significant role in the theory of ecology and environmental studies, and in particular, in the prediction and control of pipeline decays.

Let $v(t)$ denote the numerical solution to (4.1), (4.2) through an uniform semidiscretization in space. Then

$$v_t(t) = Pv(t) + Rv(t) + g(v(t)), \quad 0 < t < T, \tag{4.3}$$

$$v(0) = v_0, \tag{4.4}$$

where P and R are matrices associated with discretizations in x and y directions, respectively. An application of the Peaceman-Rachford splitting to (4.3), (4.4) yields

$$\begin{aligned} v_{k+1} = & \left(I - \frac{\tau_k}{2}R\right)^{-1}\left(I - \frac{\tau_k}{2}P\right)^{-1}\left(I + \frac{\tau_k}{2}P\right)\left(I + \frac{\tau_k}{2}R\right)\left(v_k + \frac{\tau_k}{2}g(v_k)\right) \\ & + \frac{\tau_k}{2}g(w^{(k)}), \end{aligned} \tag{4.5}$$

where $w^{(k)} = v_k + \tau_k\left(Cv_k + g(v_k)\right)$ with $C = P + R$ and τ_k is the temporal adaptive step decided through the arc-length monitor function

$$m(v_t, t) = \sqrt{1 + v_{tt}^2}, \quad (x,y,t) \in \Omega. \tag{4.6}$$

Denote

$$\Psi = \left(\psi_{1,1}^{-1},\ \psi_{2,1}^{-1}, \ldots, \psi_{1,N}^{-1}, \psi_{2,1}^{-1}, \psi_{2,2}^{-1}, \ldots, \psi_{2,N}^{-1}, \ldots, \psi_{N,1}^{-1}, \psi_{N,2}^{-1}, \ldots, \psi_{N,N}^{-1}\right)^T,$$

where $\psi_{k,l} = (a^2k^2 + b^2l^2)^{q/2}$.

Theorem 12: Monotonicity (Sheng and Cheng [9])**.** *For any beginning step ℓ if*

(i) $\tau_k/(h^{q+2}\psi_{min}) < \min\{a^2, b^2\}/4$ *for all* $k \geq \ell$*,*

(ii) $Cv_\ell + g(v_\ell) > 0$*,* τ_k *is sufficiently small and* $h < 1/\sqrt{2f(0)\min\{a^2, b^2\}}$*,*
or $Cv_\ell + g(v_\ell) + \tau_\ell^2 PRg(v_\ell)/4 > 0$ *and* $\tau_k = \tau_\ell$ *for all* $k \geq \ell$*,*

then the sequence $\{v_k\}_{k\geq\ell}$ *produced by the semi-adaptive splitting scheme* (4.5) *increases monotonically until unity is exceeded by a component of* v_k *(i. e., until quenching occurs), or converges to the steady solution of the problem for both constant and variable* $\tau_k,\ k\geq\ell$*. In the latter case, we do not have a quenching solution.*

Theorem 13: Weak Stability (Sheng and Cheng [9]). *Let* $\tau_k/(h^{q+2}\psi_{min}) < \min\{a^2, b^2\}$*. Then the semi-adaptive splitting scheme* (4.5) *is stable in the weak von Neumann sense.*

Theorem 14: Stability (Sheng and Khaliq [27]). *Assume that* $\tau_i \max_j \left|\lambda_j^{(R)}\right| \leq 2$ *for all* $i\leq k$*. Then the semi-adaptive splitting scheme* (4.5) *is stable in the von Neumann sense under the* l_2 *norm, i.e.,*

$$\|z_{k+1}\|_2 \leq c_N \|z_0\|_2,$$

where $z_0 = v_0 - \tilde{v}_0$ *is an initial perturbation or error.* $z_{k+1} = v_{k+1} - \tilde{v}_{k+1}$ *is the perturbation arising from the initial perturbation* z_0*, and* c_N *is a positive constant independent of the number of time steps k and of adaptive time step* τ_k*.*

Let us sketch a brief proof. First, it can be shown that

$$P = B^{1/2}\left(B^{1/2}T_1B^{1/2}\right)B^{-1/2} \text{ and } R = B^{1/2}\left(B^{1/2}T_2B^{1/2}\right)B^{-1/2},$$

where B is diagonal and $T_1,\ T_2$ are block tridiagonal and symmetric. Note that $\psi_{i-[i/N]N,[i/N]+1} > 0$. Therefore, eigenvalues of P and R are real. Furthermore, T_1 and T_2 are symmetric negative definite according to Geršchgorin circle theorem or Bauer's theorem.

On the other hand, there exist orthogonal matrices $Q_1,\ Q_2$ such that

$$\begin{aligned} Q_1^T\left(B^{1/2}T_1B^{1/2}\right)Q_1 &= \Lambda_1 = \text{diag}\left(\lambda_i^{(P)}\right)_{i=1,2,\ldots,N^2}, \\ Q_2^T\left(B^{1/2}T_2B^{1/2}\right)Q_2 &= \Lambda_2 = \text{diag}\left(\lambda_i^{(R)}\right)_{i=1,2,\ldots,N^2}, \end{aligned}$$

where $\lambda_i^{(P)}$ and $\lambda_i^{(R)}$ are eigenvalues of P and R, respectively, and $\lambda_i^{(P)},\ \lambda_i^{(R)} < 0,\quad i = 1,2,\ldots,N^2$. Further,

$$\begin{aligned} z_{k+1} &= B^{1/2}\left(I - \frac{\tau_k}{2}B^{1/2}T_2B^{1/2}\right)^{-1}\left(I - \frac{\tau_k}{2}B^{1/2}T_1B^{1/2}\right)^{-1} \\ &\quad\times\left(I + \frac{\tau_k}{2}B^{1/2}T_1B^{1/2}\right) \\ &\quad\times\left(I + \frac{\tau_k}{2}B^{1/2}T_2B^{1/2}\right)\left(I - \frac{\tau_{k-1}}{2}B^{1/2}T_2B^{1/2}\right)^{-1}\cdots \\ &\quad\times\left(I - \frac{\tau_0}{2}B^{1/2}T_1B^{1/2}\right)^{-1} \\ &\quad\times\left(I + \frac{\tau_0}{2}B^{1/2}T_1B^{1/2}\right)\left(I + \frac{\tau_0}{2}B^{1/2}T_2B^{1/2}\right)B^{-1/2}z_0. \end{aligned} \tag{4.7}$$

The following estimates can be derived:

$$\begin{aligned}
&\left\|B^{1/2}\right\|_2 = \sqrt{\frac{1}{\psi_{min}}},\\
&\left\|\left(I - \frac{\tau_k}{2}B^{1/2}T_2B^{1/2}\right)^{-1}\right\|_2 \le \max_j\left(\left|1 - \frac{\tau_k}{2}\lambda_j^{(R)}\right|^{-1}\right),\\
&\left\|\left(I - \frac{\tau_\ell}{2}B^{1/2}T_1B^{1/2}\right)^{-1}\left(I + \frac{\tau_\ell}{2}B^{1/2}T_1B^{1/2}\right)\right\|_2\\
&\quad\le \max_j \frac{\left|1 + \frac{\tau_\ell}{2}\lambda_j^{(P)}\right|}{\left|1 - \frac{\tau_\ell}{2}\lambda_j^{(P)}\right|} \le 1, \ \ \ell = 0, 1, \dots, k,\\
&\left\|\left(I + \frac{\tau_\ell}{2}B^{1/2}T_2B^{1/2}\right)\left(I - \frac{\tau_{\ell-1}}{2}B^{1/2}T_2B^{1/2}\right)^{-1}\right\|_2\\
&\quad\le \max_j \frac{\left|1 + \frac{\tau_\ell}{2}\lambda_j^{(R)}\right|}{\left|1 - \frac{\tau_{\ell-1}}{2}\lambda_j^{(R)}\right|}, \ \ell = 1, 2, \dots, k,\\
&\left\|I + \frac{\tau_0}{2}B^{1/2}T_2B^{1/2}\right\|_2 = \left\|Q_2\left(I + \frac{\tau_0}{2}\Lambda_2\right)Q_2^T\right\|_2 \le \max_j\left|1 + \frac{\tau_0}{2}\lambda_j^{(R)}\right|,\\
&\left\|B^{-1/2}\right\|_2 \le \sqrt{\psi_{max}}\,.
\end{aligned}$$

Therefore,

$$\|z_{k+1}\|_2 \le \sqrt{\frac{\psi_{max}}{\psi_{min}}}\frac{\max_j\left|1 + \frac{\tau_0}{2}\lambda_j^{(R)}\right|}{\min_j\left|1 - \frac{\tau_k}{2}\lambda_j^{(R)}\right|}\prod_{\ell=1}^{k}\left(\max_j \frac{\left|1 + \frac{\tau_\ell}{2}\lambda_j^{(R)}\right|}{\left|1 - \frac{\tau_{\ell-1}}{2}\lambda_j^{(R)}\right|}\right)\|z_0\|_2.$$

To explore the above, we need the auxiliary function

$$\sigma(\tau_{\ell-1}, \tau_\ell) = \max_j \frac{\left|1 + \frac{\tau_\ell}{2}\lambda_j^{(R)}\right|}{\left|1 - \frac{\tau_{\ell-1}}{2}\lambda_j^{(R)}\right|}, \quad 1 \le \ell \le k.$$

It follows subsequently that

$$\begin{aligned}
\|z_{k+1}\|_2 &\le \sqrt{\frac{\psi_{max}}{\psi_{min}}}\frac{\max_j\left|1 + \frac{\tau_0}{2}\lambda_j^{(R)}\right|}{\min_j\left|1 - \frac{\tau_k}{2}\lambda_j^{(R)}\right|}\prod_{\ell=1}^{k}\sigma(\tau_{\ell-1}, \tau_\ell)\|z_0\|_2\\
&\le \sqrt{\frac{\psi_{max}}{\psi_{min}}}\frac{1 - \frac{\tau_0}{2}\min_j\left|\lambda_j^{(R)}\right|}{1 + \frac{\tau_k}{2}\min_j\left|\lambda_j^{(R)}\right|}\frac{1 - \frac{\tau_k}{2}\min_j\left|\lambda_j^{(R)}\right|}{1 + \frac{\tau_0}{2}\min_j\left|\lambda_j^{(R)}\right|}\|z_0\|_2 \ \le \ \sqrt{\frac{\psi_{max}}{\psi_{min}}}\|z_0\|_2.
\end{aligned}$$

The theorem is thus proved.

Remark 5. Set $\tau_\ell = \tau = \text{const.},\ \ell = 0, 1, \dots$. We have

$$\|z_{k+1}\|_2 \le \sqrt{\frac{\psi_{max}}{\psi_{min}}}\frac{\max_j\left|1 + \frac{\tau}{2}\lambda_j^{(R)}\right|}{\min_j\left|1 - \frac{\tau}{2}\lambda_j^{(R)}\right|}\|z_0\|_2 \le \sqrt{\frac{\psi_{max}}{\psi_{min}}}\frac{\max_j\left|\lambda_j^{(R)}\right|}{\min_j\left|\lambda_j^{(R)}\right|}\|z_0\|_2$$

without imposing any constraint on the step sizes τ and h.

Remark 6. Since

$$\max_j \left|\lambda_j^{(R)}\right| \le \frac{4}{b^2 h^{q+2}\psi_{min}}$$

by using the Geršchgorin circle theorem. Hence, the condition $\frac{\tau_i}{2}\max_j\left|\lambda_j^{(R)}\right| \le 1$ can be replaced by the following:

$$\frac{\tau_i}{h^{q+2}\psi_{min}} \le \frac{b^2}{2}.$$

The above may simplify the inequality in the theorem by suggesting a stronger constraint.

Remark 7. The time discretization is of trapezoidal type. It is A-stable but does not always damp local errors. A smaller step size is thus expected if there are local irregularities. However, such a step size restriction is in general not necessary in the smooth solution region.

Now, let us consider a full adaptation.

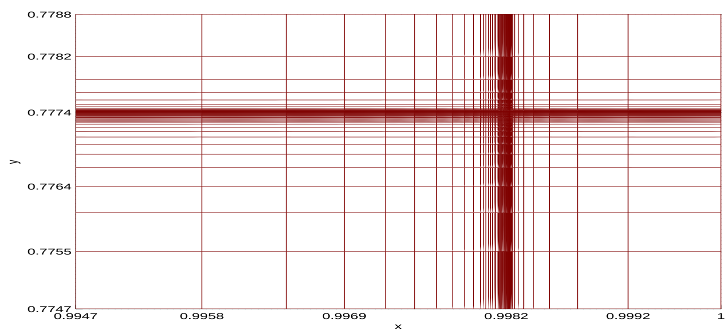

FIGURE 4. An illustration of the adaptation in space at $t = t_k$.

We adopt a nonuniform finite difference approximation,

$$\frac{f^{\Delta}(x) - f^{\nabla}(x)}{(h^+ + h^-)/2} \approx f''(x), \quad a < x < b, \tag{4.8}$$

where ∇ and Δ are the backward and forward difference operators, respectively.

Again, we may write a fully adaptive split scheme into the matrix form:

$$\begin{aligned} v_{k+1} &= \left(I - \frac{\tau_k}{2}R\right)^{-1}\left(I - \frac{\tau_k}{2}P\right)^{-1}\left(I + \frac{\tau_k}{2}P\right)\left(I + \frac{\tau_k}{2}R\right)\left(v_k + \frac{\tau_k}{2}g(v_k)\right) \\ &\quad + \frac{\tau_k}{2}g(w^{(k)}), \end{aligned} \tag{4.9}$$

where $w^{(k)}$ and C are in the same form as defined before.

Theorem 15: Monotonicity (Sheng and Khaliq [27]). *Let*

$$\hat{h} = \max(h_x^+,\ h_y^+, h_x^-,\ h_y^-),\ t = t_k.$$

For any beginning step ℓ if

(i) $\left(\tau_k/\alpha\hat{h}^2\right) < \frac{1}{4}\min\{a^2, b^2\}$ *for all $k \ge \ell$,*

(ii) $Cv_\ell + g(v_\ell) > 0$, *τ_k is sufficiently small and* $\hat{h} < 1/\sqrt{2f(0)\min\{a^2, b^2\}}$, *or* $Cv_\ell + g(v_\ell) + \tau_\ell^2 PRg(v_\ell)/4 > 0$ *and* $\tau_k = \tau_\ell$ *for all* $k \geq \ell$,

then the sequence $\{v_k\}_{k\geq\ell}$ *produced by the fully adaptive split scheme* (4.9) *based on* (4.8) *increases monotonically until unity is exceeded by a component of the solution vector, or converges to the steady solution of the problem for both constant and variable* $\tau_k,\ k \geq \ell$. *In the latter case, we do not have a quenching solution.*

Remark 8. Stabilities of the fully adaptive splitting scheme remain to be proved.

Adaptive splitting can also be used for solving multidimensional solitary wave equations, such as the Schrödinger equation,

$$iu_t + u_{xx} + u_{yy} + f(|u|^2)u = 0, \quad -\infty < x < \infty,\ t \geq t_0,$$

dispersive KdV equation,

$$u_t + u_{xxx} + u_{yyy} + \kappa_1 u u_x + \kappa_2 u u_y = 0, \quad -\infty < x < \infty,\ t \geq t_0,$$

and the sine-Gordon equation,

$$u_{tt} = u_{xx} + u_{yy} - \phi(x,y)\sin u, \quad -a < x < a,\ -b < y < b,\ t > t_0, \tag{4.10}$$

where the function ϕ can be determined through a Josephson current density. Spline collocations may be used for achieving a better long time stability.

Let us concentrate on the split solution of (4.10). A spacial semi-discretization of (4.10) yields

$$u_k'' = \left(h_x^{-2}B_1 + h_y^{-2}B_2\right)u_k + r(u_k) = Bu_k + r(u_k).$$

It further leads to the *nonlinear cosine scheme*

$$u_{k+1} - 2u_k + u_{k-1} = \tau^2\psi(\tau^2 A)(Bu_k + r(u_k)), \quad k = 1, 2, \ldots, \tag{4.11}$$

where

$$\begin{aligned} A &= \frac{\partial}{\partial u}(Bu + r(u))\bigg|_{u=u_k} = B + r_u(u_k), \\ \psi(z) &= \frac{\cos\sqrt{-z} - 1}{z/2}, \\ r_u(u_k) &= \mathrm{diag}\,(\phi_{1,1}\cos u_{1,1,k},\ \phi_{1,2}\cos u_{1,2,k},\ \ldots, \\ &\quad \phi_{1,n}\cos u_{1,n,k},\ \phi_{2,1}\cos u_{2,1,k},\ \ldots, \phi_{m,n}\cos u_{m,n,k}) \end{aligned}$$

and τ can be selected adaptively. Note that (4.11) can be written as

$$u_{k+1} - 2\cosh(\tau\sqrt{A})u_k + u_{k-1} = \tau^2\psi(\tau^2 A)\left[r(u_k) - r_u(u_k)u_k\right] \tag{4.12}$$

and

$$\cosh(\tau\sqrt{A}) = e^{\frac{\tau^2}{2}A} + O(\tau^4)$$

when the real parts of the eigenvalues of A are negative.

Thus, (4.12) can be approximated by

$$u_{k+1} - 2e^{\frac{\tau^2}{2}A}u_k + u_{k-1} = \tau^2\left(r(u_k) - r_u(u_k)u_k\right) \tag{4.13}$$

incurring a local error $O(\tau^4)$. Set

$$A_1 = \frac{1}{h_x^2}B_1 - \frac{1}{2}r_u(u_k), \quad A_2 = \frac{1}{h_y^2}B_2 - \frac{1}{2}r_u(u_k).$$

Recall the Strang's splitting φ_3. We have

$$u_{k+1} - 2e^{\frac{\tau^2}{4}A_1}e^{\frac{\tau^2}{2}A_2}e^{\frac{\tau^2}{4}A_1}u_k + u_{k-1} = \tau^2\left(r(u_k) - r_u(u_k)u_k\right).$$

Now, replace the matrix exponential functions in the above equation by $[0/1]$, $[1/1]$ and $[1/0]$ Padé formulas, respectively. We acquire the two-stage linearly implicit ADI cosine scheme:

$$\left(I - \frac{\tau^2}{4}A_1\right)v_k = \left(I + \frac{\tau^2}{4}A_2\right)\left(I - \frac{\tau^2}{4}A_2\right)^{-1}\left(I + \frac{\tau^2}{4}A_1\right)u_k, \tag{4.14}$$

$$u_{k+1} = 2v_k + \tau^2(r(u_k) - r_u(u_k)u_k) - u_{k-1}, \quad k = 1, 2, \ldots \tag{4.15}$$

Set

$$\sigma_1 = \max_i \left|\frac{2 + \tau^2\lambda_i^{(A_1)}}{2 - \tau^2\lambda_i^{(A_1)}}\right| \text{ and } \sigma_2 = \max_i \left|\frac{2 + \tau^2\lambda_i^{(A_2)}}{2 - \tau^2\lambda_i^{(A_2)}}\right|.$$

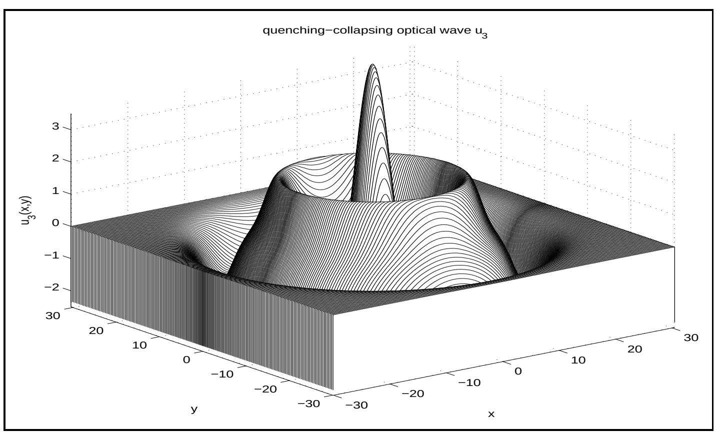

FIGURE 5. Simulation of the solution of (4.14), (4.15). The solution corresponds to the optical collapse of instability status of R_3 [54].

Theorem 16: Stability (Sheng [54])**.** *If*

$$2\sigma_1\sigma_2 \leq 1, \tag{4.16}$$

then the two-stage split cosine scheme (4.14)*,* (4.15) *is stable in the von Neumann sense.*

The proof of the theorem can be implemented through a throughout matrix analysis of the split matrices involved. A spectral norm is again utilized.

Adaptive splitting methods have also be extended for solving the Maxwell's field equations as well as Helmholtz equation for light,

$$\nabla_T^2 u - 2i\kappa u_z + u_{zz} = 0,$$

where ∇_T^2 is the *transverse Laplacian operator* and $\kappa(x, y, z) > 0$ is discontinuous over the given physical domain. For detailed results and discussions the reader is refereed to recent publications of Gonzelez, Guha, Haus, Rogers and Sheng [18, 19, 54].

5 Conclusions

It has been evident that, as being pointed out by many researchers in the fields, splitting, adaptive and hybrid computational methods have been providing incredibly powerful and reliable computational tools for solving different ordinary and partial differential equations. New splitting schemes are highly popular in real applications because of their outstanding simplicity in structures, great flexibility in working together with other numerical components, such as iteration, adaptation and hybridizartion, and their exceptionally high efficiency in solution procedures. Many new concepts and splitting strategies have emerged, such as the asymptotic splitting and hybrid splitting, in recent years.

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