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Non-normal stability of embedded boundary methods through pseudospectra

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Abstract

We present non-normal linear stability of embedded boundary (EB) methods employing pseudospectra and resolvent norms. We analyze the stability of the linear wave equation in a domain with an embedded boundary in one and two dimensions. In particular, we characterize the stability in terms of the normalized distance of the EB to the nearest ghost node (α). An important objective is that the CFL condition remains unaffected by the EB which is taken to be that of the underlying grid (as if the EB is absent or aligned with the regular grid). We consider various spatial and temporal discretization methods including both central and upwind-biased schemes. Stability is guaranteed when $\alpha \leq \alpha_{\max}$ where $\alpha_{\max}$ ranges between 0.5 and 0.77 depending on the discretization scheme. The stability analysis is also briefly examined for the one-dimensional advection-diffusion equation. Sharper limits on the sufficient conditions for stability are obtained based on the pseudospectral radius (the Kreiss constant) than the restrictive limits based on the usual singular value decomposition analysis. A resulting sufficient condition for stability is that the intersection of the EB with the surface normal passing through a ghost node ($\vec{x}_g$) must lie within the ghost cell ($0.5\Delta x$ distance from $\vec{x}_g$). This condition leads us to propose a simple and robust reclassification scheme for the ghost cells (dubbed “hybrid ghost cells”) to ensure Lax stability of the discrete system. This has been tested successfully for both low and high order discretization schemes with transient growth of at most $\mathcal{O}(1)$. Moreover, we present a fourth order EB reconstruction scheme taking into account both accuracy and stability.

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Keywords: embedded boundary method, non-normal stability, pseudospectra, ghost cell

1. Introduction

For the past two decades, embedded boundary (EB) methods, also referred as immersed boundary (IB) methods by some authors, have emerged as an attractive alternative to body fitted grid methods for flow simulations involving complex geometry. These methods have unique advantages in terms of grid generation, higher accuracy and efficient solution techniques compared with their counterparts. Refer to Mittal and Iaccarino (2005) for a review on EB methods. Here, we focus on a specific class of EB methods known as sharp interface methods that are particularly

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attractive when the near boundary physics is crucial for accurate flow simulation. Stability of these methods is essential for successful and reliable simulation of variety of flows particularly high Reynolds number turbulent flows that are ubiquitous in both industrial and environmental applications. Yet, very few studies focus on *a priori* stability of the EB method. Here, for the first time, we employ pseudospectra to characterize the effect of the EB on the Lax-stability of discrete linear systems. In contrast, stability bounds in existing studies (Brehm and Fasel, 2013; Brehm et al., 2015) are not sharp, because they are based on spectral radius or the largest singular value of the full discretization.

Sharp interface methods reconstruct solution near an EB by using boundary/jump conditions at the EB and solution from the near-boundary cells. Furthermore, there are a few variants with regard to the reconstruction procedure. Mainly, the reconstruction is employed at cells immediately adjacent to the EB with their center lying exclusively in either the fluid region (IB cell method, Roman et al. (2009); Kang et al. (2009)) or the solid region (ghost cell method, Mittal et al. (2008); Tseng and Ferziger (2003)). The immersed interface method (IIM), another variant, uses modified discrete operators near an EB/interface which satisfy jump conditions across the EB/interface (Brehm and Fasel, 2013; Brehm et al., 2015). Notably, IB/ghost cell methods have the advantage that one need not develop a separate reconstruction formula for each discrete operator. Cut-cell methods mimic finite volume treatment near an EB and enforce boundary conditions at an EB without resorting to reconstruction (Ye et al., 1999; Tucker and Pan, 2000; Colella et al., 2006; Crockett et al., 2011; Devendran et al., 2017). An alternative to cut cells is a level set based approach which combines PDE reconstruction with inverse distance weightage method to enforce boundary conditions on the EB (Al-Marouf and Samtaney, 2017).

Cells cut by an EB lead to arbitrarily small sizes in the interior/fluid region and impose severe restrictions on the time step, known as the small cell issue. This issue is manifested differently in the aforementioned methods but has equivalent effect on the time step in all of them. For example, cut-cell finite volume methods discretize the governing equations over the small cells and the time step restriction emerges from the CFL condition. In IIM, a singularity appears in the boundary stencils as the EB approaches an interior node which may lead to arbitrarily small time steps. In ghost cell methods, a polynomial reconstruction may lead to large weightage coefficients and inherently restricts the time step. This can be recast as an issue of stability if the CFL condition for the cut-cells is computed based on regular cell width. The IB cell method bypasses this issue by excluding the small cells from the discretization stencils. But, the reconstruction stencils extend far into the interior and the local errors in the solution and the mass leakage across an EB could be larger than those with the ghost cell methods. A narrow stencil is desired for large scale computations on a parallel machine where both accuracy and communication cost play an important role.

Consider the 1D example shown in Fig. 2a where an EB is located at x_s , between the ghost node x_0 and the interior node x_1 , such that the normalized distance from x_0 is $\alpha \equiv \frac{x_s - x_0}{x_1 - x_0}$. Here, $\alpha = 0$ corresponds to the ideal case when EB coincides with the ghost node x_0 . The Courant-Friedrichs-Lewy (CFL) criterion for stability of the first order upwind scheme (UWS) requires that the Courant/convection number $C \equiv \frac{U\Delta t}{\Delta x} \leq C_{\max}$ (Courant et al., 1928). Here, U is the advection velocity, Δt is the time step, and Δx is the spatial grid size and $C_{\max}$ depends on both the spatial and temporal discretization methods. However, the effective mesh size between EB and node 1 becomes $(1 - \alpha)\Delta x$ and the CFL

criteria becomes $C \leq (1 - \alpha)C_{\max}$. The time step becomes arbitrarily small as $\alpha \rightarrow 1$ and renders the computation practically infeasible. The CFL constraint may be expressed in a general form as $C \leq \beta C_{\max}$, where β depends on the spatial discretization scheme. The UWS spatial discretization scheme has spectral radius $\frac{C}{1-\alpha}$ leading to $\beta = 1 - \alpha$. Note that the CFL criterion, based on the eigenvalue analysis, is merely a necessary but not sufficient condition for stability.

In practice, a majority of the EB methods do not account for β in determining Δt . In such cases, the above idea can be expressed in a different light. If Δt is determined based on the regular grid with $C = C_{\max}$, then the discrete system becomes unstable as the EB approaches a fluid node/moves away from a ghost node. Mathematically, at some value of $\alpha \geq \alpha_{\max}$ depending upon the discretization scheme the system becomes unstable. In other words, the range of proximity of an EB to a fluid cell resulting in an unstable situation is not well known. Tseng and Ferziger (2003) suggested an empirical value of 10% of the cell size, but a systematic stability investigation has not yet been carried out. Indeed, such an investigation also depends on both the spatial and temporal discretization schemes. The present work seeks to characterize the numerical stability of EB schemes in terms of the distance between the EB and the nearest fluid/solid node.

Various strategies are adopted as a remedy to the small cell issue ($\alpha \rightarrow 1$). Cut-cell finite volume methods adopt a technique that merges the small cells with the neighbour fluid cells and removes the constraint on the time step (Ye et al., 1999; Colella et al., 2006). They conserve mass up to desired order of accuracy. However, their implementation in three dimensions is non-trivial and are extensions to moving boundaries. Notably, Crockett et al. (2011); Devendran et al. (2017) adopt a cut-cell approach in solving Poisson equation for stationary boundaries.

A popular remedy among the ghost cell methods is to use an image of the ghost cell in the fluid region in a two stage reconstruction procedure (Tseng and Ferziger, 2003; Mittal et al., 2008). However, image point technique leads to multiple geometric configurations during the reconstruction. We aim to develop analytical expressions for the ghost cell reconstruction which requires similar stencil configuration for all the ghost cells (Rapaka et al., 2018). These analytical expressions could be utilized to reduce the computational cost of the reconstruction procedure significantly, and are especially desirable for moving boundary problems. Stability of this approach is essential for convergence of the numerical solution and is investigated in this article.

A majority of reconstruction methods in the literature are based solely on accuracy considerations. Stability is typically assessed *a posteriori* rather than *a priori*. An exception is the method of Brehm and Fasel (2013) which includes an additional point in the reconstruction stencil thereby introducing a free parameter. This parameter is tuned by minimizing the largest singular value of the discrete system to obtain better stability properties in the limit $\alpha \rightarrow 1$. Rapaka and Sarkar (2016) proposed an alternative approach wherein some of the fluid cells that are closer to the EB relative to their neighbors in the solid are reclassified as ghost cells where reconstruction is employed. This yields ghost cells on both sides of the EB. They applied this novel approach to successfully simulate stratified turbulent flows over complex bodies in the framework of direct numerical simulations and large eddy simulations. Though intuitively appealing, the reasons for improved stability properties were not apparent: the present work sheds light on this.

Although the present analysis is focused on scalar equations, its implications are relevant to systems of equations. Particularly, when the boundary treatment is applied on the characteristic variables, the stability of the system follows from that of a scalar equation (Gottlieb et al., 1982). However, a correction term is needed when the boundary treatment is applied on the natural/primitive variables.

In this paper, we systematically analyze the dependence of stability on the distance of EB to the nearest fluid/solid node. Also, we propose a simple alternative method by introducing hybrid ghost cells that yields stable reconstruction for discretizations that are stable when the EB is absent or ideally aligned with the regular grid ($\alpha = 0$). The attractive features of the proposed method include the usage of the most narrow and unique (depends only on the boundary normal orientation) reconstruction stencils for all possible geometrical configurations, ease of implementation, and no additional computational expense. Also, it facilitates determination of unique analytical expressions for reconstruction at the near boundary cells that are useful for moving boundary problems: these ideas will be explored in a future article Rapaka et al. (2018).

The paper is summarized as follows: Sec. 2 reviews non-normal stability of discrete linear systems and the bounds on transient growth in terms of pseudospectra, numerical range and singular value decomposition. Stability of the discrete wave equation is analysed for various spatio-temporal schemes in Sec. 3 and 4. In Sec. 5, stability of discrete advection-diffusion equation is briefly discussed. In Sec. 6, the viability of hybrid ghost cells (HGC) for stable discretizations in the presence of complex EB is demonstrated.

2. Lax-stability of linear discrete systems

In this section, we briefly review the stability of linear systems in the context of pseudospectra that aids the discussion in the subsequent sections. The information presented below may be obtained by an examination of the relevant literature. However, we believe the review presented below, as a condensed and somewhat abbreviated presentation of several concepts, is important for the sake of completeness.

2.1. Method of lines semi-discretization

Let $\mathbf{A} \in \mathbb{R}^{N \times N}$ be the discrete representation of a bounded linear operator $\mathcal{L}$. The method of lines semi-discretization of $\frac{\partial \phi}{\partial t} = \mathcal{L}\phi$ leads to the following linear system of ordinary differential equations,

$$\frac{d\phi_i}{dt} = A_{ij}\phi_j, \quad i = 1, 2, \dots, N; \quad j = 1, 2, \dots, N. \quad (1)$$

The exact solution to the above linear system of equations is

$$\phi(t) = e^{\mathbf{A}t}\phi(0) = \mathbf{P}e^{\mathbf{J}t}\mathbf{P}^{-1}\phi(0), \quad (2)$$

where, $\mathbf{P}$ is an invertible matrix whose columns are comprised of the generalized eigenvectors of $\mathbf{A}$, and $\mathbf{J}$ is the Jordan normal form of $\mathbf{A}$. Here, $\mathbf{P}$ represents similarity transformation between $\mathbf{A}$ and $\mathbf{J}$ which, in general, need not

be unitary except for normal matrices. Despite having the same algebraic and geometric multiplicities, $\mathbf{A}$ and $\mathbf{J}$ need not have the same basis of eigenvectors which determines the degree of non-normality and hence their pseudospectra (introduced later in this section) may differ. The discrete solution after n time steps ϕ^n , with step size Δt , is given by

$$\phi^n = f^n(\Delta t \mathbf{A}) \phi^0 = \mathbf{P} f^n(\Delta t \mathbf{J}) \mathbf{P}^{-1} \phi^0, \quad 0 \leq n \Delta t \leq T. \quad (3)$$

where, $f(\mathbf{A}) = e^{\mathbf{A}}$, and $t = n \Delta t$. In numerical integration, f is approximated using polynomials, rational functions, etc. For example,

$$f(\mathbf{A}) = \begin{cases} \mathbf{I} + \mathbf{A}, & \text{explicit Euler method,} \\ \mathbf{I} + \mathbf{A} + \mathbf{A}^2/2 + \mathbf{A}^3/6, & \text{explicit RK3 method.} \end{cases}$$

2.2. Lax stability and equivalence theorem

Lax equivalence theorem states that consistency and stability of a discrete linear system implies convergence of the numerical solution to the exact solution as the spatial and the temporal resolutions are increased. According to Lax and Richtmyer (1956), the discrete approximation $f(\Delta t \mathbf{A})$ in Eq. 3 is (Lax-)stable if the set of operators $f^n(\Delta t \mathbf{A})$ are uniformly bounded for all $n, \Delta t, N$, i.e.,

$$\|f^n(\Delta t \mathbf{A})\| \leq C(t), \quad 0 \leq n \Delta t \leq T, \quad (4)$$

2.3. Non-normality and pseudospectra

In a finite domain, boundary conditions and/or the presence of the embedded boundary typically render the semi-discretization matrix ($\mathbf{A}$) to be non-normal. Non-normal systems do not have an orthogonal basis of eigenfunctions. They usually exhibit transient growth with arbitrary magnitude which depends upon the non-normality/eigenfunctions of the system. In such cases, eigenvalue analysis provides merely a necessary condition for stability whereas the analysis of the ε -pseudospectra provides a sufficient condition for stability (Reddy and Trefethen, 1992).

$\lambda_\varepsilon \in \mathbb{C}$ is an ε -pseudo-eigenvalue of $\mathbf{A}$ if the resolvent norm $\|(\lambda_\varepsilon \mathbf{I} - \mathbf{A})^{-1}\| \geq \varepsilon^{-1}$. Alternatively, ε -pseudospectrum, denoted by $\sigma_\varepsilon(\mathbf{A})$, is the set of all eigenvalues of $(\mathbf{A} + \mathbf{E})$ where $\mathbf{E}$ is some random, complex perturbation matrix with $\|\mathbf{E}\| \leq \varepsilon$. Another definition useful from a computational standpoint is that $\sigma_\varepsilon(\mathbf{A})$ is the set of $z \in \mathbb{C}$ such that

$$s_{\min}(z\mathbf{I} - \mathbf{A}) \leq \varepsilon. \quad (5)$$

where, $s_{\min}(z\mathbf{I} - \mathbf{A})$ is the smallest singular value of $(z\mathbf{I} - \mathbf{A})$. This definition is valid only if $\|\cdot\| = \|\cdot\|_2$ and follows from the fact that $\|(z\mathbf{I} - \mathbf{A})^{-1}\|_2 = [s_{\min}(z\mathbf{I} - \mathbf{A})]^{-1}$. We refer to Reddy and Trefethen (1992), and Trefethen and Embree (2005) for alternative definitions.

2.4. Stability of semi-discretizations

For algebraic stability of the semidiscretizations, Theorem 5.1 of Reddy and Trefethen (1992) states that for some constants K and ω , if the ε -pseudo-eigenvalues λ_ε of A satisfy

$$\operatorname{Re}(\lambda_\varepsilon) \leq \omega + K\varepsilon \quad \forall \varepsilon \geq 0 \quad \implies \|e^{At}\| \leq eKN e^{\omega t} \quad \forall t \geq 0 \quad (6)$$

This implies that the pseudospectra should vary at most linearly with respect to ε ($K = \mathcal{O}(1)$) for algebraic stability of the system. Here, $K > 1$ implies transient growth of $\|e^{At}\|$. For normal matrices, $K = 1$ and $\|e^{At}\| = e^{\omega t}$ for all $t \geq 0$. For non-normal matrices, K may be much larger than 1 and obtained as the slope of the $|\operatorname{Re}(\lambda_\varepsilon)_{\max} - \operatorname{Re}(\lambda_0)|$ vs. ε curve plotted on a log-log scale. Note that $\omega = \operatorname{Re}(\lambda_0)$ is equal to $\operatorname{Re}(\lambda_\varepsilon)$ in the limit $\varepsilon \rightarrow 0$ and need not be equal to $\operatorname{Re}(\lambda)$, typically for systems that are physically unstable to perturbations. See examples 1 and 2 of Trefethen (1997) for an illustration of such cases. Here, we consider transient growth of $\mathcal{O}(1)$ to be practically stable and, therefore, require $K = \mathcal{O}(1)$ or, say, $K < 10$ for stability.

2.5. Stability of full discretizations

For Lax-stability of full discretizations, Theorem 8.2 of Reddy and Trefethen (1992) states that the ε -pseudo-eigenvalues $\{\lambda_\varepsilon\}$ of $\Delta t A$ must lie within a distance $\mathcal{O}(\varepsilon) + \mathcal{O}(\Delta t)$ of the stability region of the time stepping scheme (S) as $\varepsilon, \Delta t \rightarrow 0$. Mathematically, if

$$\|f^n(\Delta t A)\| \leq C_1, \quad 0 \leq n\Delta t \leq T, \quad (7)$$

then the ε -pseudospectra of $\Delta t A$ satisfy

$$\operatorname{dist}(\lambda_\varepsilon, S) \leq C_2\varepsilon + C_3\Delta t. \quad (8)$$

Conversely, Eq. 8 implies

$$\|f^n(\Delta t A)\| \leq C_4 \min\{N, n\}, \quad 0 \leq n\Delta t \leq T, \quad (9)$$

where S is the stability region of the time stepping method, C_1, C_2, C_3, C_4 are constants and $\operatorname{dist}(\cdot, \cdot)$ is the distance from a point to a set/region. This implies that outside S , the pseudospectra must vary at most linearly with respect to ε and Δt for stability.

Note that Eq. 9 implies only algebraic stability due to the possible dependence on N, n . In later sections, we test the Lax-stability of linear discrete systems in two steps. In the first step, we verify Eq. 8 which guarantees at least algebraic stability (Eq. 9). In the second step, we check the explicit dependence of the supremum of $\|f^n(\Delta t A)\|$ on the spatial grid size N to verify Lax-stability (Eq. 7). Also, based on numerical observations, we suggest an alternative procedure to verify Lax-stability through pseudospectra alone, without computing $\|f^n(\Delta t A)\|$ in Sec. 2.7.

2.6. Estimates of transient growth through pseudospectra

We note that $\|e^{At}\|$ is a measure of the size of the growth/decay of the solution of Eq. 1. For finite t , the transient growth is estimated by the bounds,

$$e^{t\alpha(A)} \leq \|e^{At}\| \leq \kappa(V)e^{t\alpha(A)} \quad (10)$$

where, $\alpha(A)$ is the spectral abscissa, and $\kappa(V) = \|V\| \|V^{-1}\|$ is the condition number of the eigenvector matrix (V). For highly non-normal matrices ($\kappa(V) \gg 1$) and defective or non-diagonalizable matrices ($\kappa(V) = \infty$), the upper bound is not of much practical use. For sharper estimates, bounds on the supremum of $\|e^{At}\|$ are expressed, up to an algebraic constant, in terms of the distance to the stability region and the resolvent norm by using the Kreiss matrix theorem (KMT) (LeVeque and Trefethen, 1984; Trefethen and Embree, 2005).

$$\mathcal{K}(A) \leq \sup_{t \geq 0} \|e^{At}\| \leq eN\mathcal{K}(A), \quad (11)$$

where, the Kreiss constant $\mathcal{K}(A)$ of the semi-discretization matrix A is defined with respect to the left half of the complex plane as,

$$\mathcal{K}(A) \equiv \sup_{\varepsilon > 0} \alpha_\varepsilon(A)/\varepsilon = \sup_{\operatorname{Re} z > 0} (\operatorname{Re} z) \|(zI - A)^{-1}\|, \quad (12)$$

where, $\alpha_\varepsilon(A)$ is the pseudospectral abscissa. Note that the upper bound of the supremum in Eq. 11 is a sharper version derived by LeVeque and Trefethen (1984); Spijker (1991).

The Lax-stability of full discretizations (Eq. 4) requires powers of $B \equiv f(\Delta t A) \in \mathbb{R}^{N \times N}$ to be bounded. Upper bounds on $\|B^n\|$ are expressed by the KMT in terms of the Kreiss constant $\mathcal{K}(B)$ of the full discretization matrix B with respect to the unit disk given by, (Kreiss, 1962; Spijker, 1991; Trefethen and Embree, 2005),

$$\mathcal{K}(B) \leq \sup_{n \geq 0} \|B^n\| \leq eN\mathcal{K}(B), \quad (13)$$

$$\|B^n\| \leq e(n+1)\mathcal{K}(B), \quad (14)$$

$$\mathcal{K}(B) \equiv \sup_{\varepsilon > 0} (\rho_\varepsilon(B) - 1)/\varepsilon = \sup_{|z| > 1} (|z| - 1) \|(zI - B)^{-1}\|. \quad (15)$$

Here, $\rho_\varepsilon(B)$ is the pseudospectral radius of B . Note that Eq. 14 is a variant of the KMT which is particularly useful as $N \rightarrow \infty$ (Toh and Trefethen, 1999; Trefethen and Embree, 2005). Let us define a point in the complex plane outside the unit disk $z \equiv (1+d)e^{i\theta}$, where $d \equiv |z| - 1 \geq 0$ is the distance to the unit disk and θ is the polar angle. Also, define the Kreiss variable at z , $\tilde{\mathcal{K}}(z) \equiv (|z| - 1) \|(zI - B)^{-1}\|$ whose polar form is $\tilde{\mathcal{K}}(d, \theta) = d \|((1+d)e^{i\theta}I - B)^{-1}\|$. Note that the Kreiss constant $\mathcal{K}(B)$ in Eq. 15 is the supremum of $\tilde{\mathcal{K}}(d, \theta)$ which occurs at, say, $d = d^*$ and $\theta = \theta^*$. Our numerical observations show that θ^* is independent of N , but d^* may depend on N . So, we denote the radial variation $\tilde{\mathcal{K}}(d, \theta^*)$, for notational simplicity, as $\hat{\mathcal{K}}(d)$ so that

$$\hat{\mathcal{K}}(d) \equiv \tilde{\mathcal{K}}(d, \theta^*) = d \|((1+d)e^{i\theta^*}I - B)^{-1}\| = \frac{d}{\varepsilon(d, \theta^*)}, \quad (16)$$

$$\mathcal{K}(B) = \sup_{d > 0, 0 \leq \theta \leq 2\pi} \tilde{\mathcal{K}}(d, \theta) = \tilde{\mathcal{K}}(d^*, \theta^*) = \sup_{d > 0} \tilde{\mathcal{K}}(d, \theta^*) = \sup_{d > 0} \hat{\mathcal{K}}(d) = \hat{\mathcal{K}}(d^*). \quad (17)$$

If the pseudospectra protrude significantly outside the unit disk in the sense that $\rho_\varepsilon(\mathbf{B}) > 1 + \varepsilon$ or $\hat{\mathcal{K}}(d) > 1$ for some ε or d , then there must be transient growth. Furthermore, for finite time $t \leq \tau$ and some $\text{Re } z = a$ with $K_a \equiv a \|(z\mathbf{I} - \mathbf{A})^{-1}\| > 1$, growth in solution through the semi-discretization is given by (Trefethen and Embree, 2005),

$$\sup_{0 < t \leq \tau} \|e^{\mathbf{A}t}\| \geq e^{a\tau} / \left(1 + \frac{e^{a\tau} - 1}{K_a}\right). \quad (18)$$

This indicates that, for small $\tau \ni e^{a\tau} \ll K_a$, z behaves like an eigenvalue near $t = 0$ on a time scale a^{-1} and $\|e^{\mathbf{A}t}\|$ is at least as large as $e^{a\tau}$ for some t over an interval $[0, \tau]$. Larger values of K_a imply a longer duration during which z behaves like an eigenvalue. Similarly, for finite number of time steps $n \leq m$ and some $|z| = \gamma = 1 + d > 1$ with $\hat{\mathcal{K}}(d, \theta) > 1$, growth in solution through the full discretization is given by (see p.160 of Trefethen and Embree (2005)),

$$\sup_{0 < n \leq m} \|\mathbf{B}^n\| \geq \gamma^m / \left(1 + \frac{\gamma^m - 1}{\gamma \hat{\mathcal{K}}(d, \theta) - \gamma + 1}\right). \quad (19)$$

This implies that $\|\mathbf{B}^n\|$ must be at least as large as $\hat{\mathcal{K}}(d, \theta)$ with $n = \mathcal{O}(d^{-1})$.

2.7. Algebraic vs. Lax-stability based on ε -pseudospectra

The KMT (Eq. 13) states that a family of $N \times N$ matrices has a uniform power bound ($\sup \|\mathbf{B}^n\|$ with fixed N and $n \geq 0$) if and only if it has a uniform Kreiss constant $\mathcal{K}(\mathbf{B})$ (Trefethen and Embree, 2005). However, Eq. 4 requires $\|\mathbf{B}^n\|$ to be uniformly bounded for all n and N because N/n is constant for a given t . Since Eq. 13 provides merely algebraic stability criteria, we consider Eq. 14 which guarantees Lax-stability if the following two conditions are met:

1. $\mathcal{K}(\mathbf{B})$ must be uniformly bounded for all N , and
2. $\sup \|\mathbf{B}^n\|$ must occur at finite $n \leq n^*$ for all N so that Eq. 14 yields $\|\mathbf{B}^n\| \leq e(n^* + 1)\mathcal{K}(\mathbf{B})$.

Condition (1) can be verified by computing $\sup \hat{\mathcal{K}}(d)$ (Eq. 16) for different N . If $\sup \hat{\mathcal{K}}(d)$ occurs at $d = d^*$, existing theory (Eq. 19) and our numerical observations in this work suggest that $n^* = \mathcal{O}(d^{*-1}) = \eta d^{*-1}$, where η is a constant of $\mathcal{O}(1)$. Therefore, uniform upper bounds on $\mathcal{K}(\mathbf{B})$ and d^{*-1} for all N are sufficient for Lax-stability, and Eq.14 yields,

$$\|\mathbf{B}^n\| \leq e(n^* + 1)\mathcal{K}(\mathbf{B}) = \underbrace{e(\eta d^{*-1} + 1)\mathcal{K}(\mathbf{B})}_{\text{constant}}. \quad (20)$$

In this work, the Lax-stable cases have uniform $\sup \hat{\mathcal{K}}(d), d^{*-1}, n^*$ (e.g., Fig. 4a,b) and algebraic stable cases exhibit dependency of $\sup \hat{\mathcal{K}}(d), d^*, n^*$ on N (e.g. Fig. 4c). For example, see Fig. 4 and the description in Sec. 3.1.

For example consider the following matrices exemplified in Trefethen (1992),

$$\mathbf{A}_1 = \begin{bmatrix} -1 & 1 \\ 0 & -1 \end{bmatrix}, \quad \mathbf{A}_2 = \begin{bmatrix} -1 & 5 \\ 0 & -2 \end{bmatrix}. \quad (21)$$

The norms of the exponentials of $\mathbf{A}_1$ and $\mathbf{A}_2$ are shown in Fig. 1(a). Let us denote the inverse of the resolvent norm with $r \equiv \|(z\mathbf{I} - \Delta t \mathbf{A})^{-1}\|^{-1}$ and the direction of increasing r with the unit vector $\hat{n} \equiv \nabla r / |\nabla r|$. Note that $r = 0$ when $z \in \sigma(\mathbf{A})$ where $\sigma(\mathbf{A})$ represents the spectrum of $\mathbf{A}$. Then, by definition $\frac{\partial r}{\partial n} > 0$, and for normal systems it follows

Figure 1: (a) Transient behaviour of the exponentials of matrices A_1, A_2 as measured by their 2-norm. Boundaries of the ε -pseudospectra marked by the iso-contours of $\|(zI - \Delta t A)^{-1}\|^{-1} = \varepsilon$ for matrices (b) A_1 and (c) A_2 .

that $r = \text{dist}(z, \sigma(A))$, $\frac{\partial r}{\partial n} = 1$, and $\frac{\partial^2 r}{\partial n^2} = 0$ for all ε , whereas for non-normal systems $\frac{\partial^2 r}{\partial n^2} \neq 0$ for at least a range of ε which, if it occurs outside the stability region, determines the transient behaviour of e^{At} or $f^n(\Delta t A)$. If $\frac{\partial^2 r}{\partial n^2} \leq 0$, the maximum Δr occurs as $\varepsilon \rightarrow 0$ and the pseudospectra indicates only a finite transient growth near $t = 0$. This can be graphically interpreted as, see Fig. 1(b) and (c) for the above example, the spacing between isocontours of r with equal intervals (Δr) decreases or remains constant along the direction of n . On the other hand if $\frac{\partial^2 r}{\partial n^2} > 0$, Δr increases with ε (more than linear growth) and indicates exponential growth for a time period $\mathcal{O}(d^{-1})\Delta t$.

In the following sections, we consider bounded growth to be (Lax-)stable. But, in practice, one must be cautious of the upper bound because this may be arbitrarily high. An estimate of this upper bound through the Kreiss constant (Eq. 13,14) provides us a more accurate picture of the transient growth and stability from a practical point of view.

2.8. Computation of pseudospectra and resolvent norm

To study the stability of the discrete linear system Eq. 1, ε -pseudospectra of $\Delta t A$ are computed with $\|E\| \leq \varepsilon$ for realizations of $\varepsilon = 10^{-6}, 10^{-4}, 10^{-2}$. Here, E is a matrix of random complex numbers chosen from the standard normal distribution, normalized by its two norm (largest singular value), i.e., $E = \varepsilon E / \|E\|_2$. The pseudospectra thus computed represents only a sample of the total set. In fact, the pseudospectra sample set becomes denser with more samples of E . Nonetheless, the sample set provides useful estimates about the stability of the linear system.

A better and inclusive method to compute ε -pseudospectra uses the resolvent norms. The total set of ε -pseudospectra is all possible values of $z \in \mathbb{C}$ bounded by the resolvent norm $\|(zI - \Delta t A)^{-1}\| \geq \varepsilon^{-1}$. In the following sections, boundaries of the ε -pseudospectra are shown by the iso-contours of $\|(zI - \Delta t A)^{-1}\|^{-1} = \varepsilon$ for $\varepsilon = \mathcal{O}(\Delta t) - \mathcal{O}(10\Delta t)$. Here, the resolvent norm $\|(zI - \Delta t A)^{-1}\|$ is computed using the lowest singular value of $zI - \Delta t A$ (Eq. 5) on a grid of $M \times M$ with M ranging between 50 and 100. In this work, $\|\cdot\|$ refers to 2-norm unless specified otherwise.

2.9. Stability bounds based on the numerical range or field of values

The numerical range (also field of values) of a matrix $\mathbf{A} \in \mathbb{C}^{N \times N}$ is defined as

$$W(\mathbf{A}) \equiv \{\mathbf{z}^* \mathbf{A} \mathbf{z} : \mathbf{z}^* \mathbf{z} = 1, \mathbf{z} \in \mathbb{C}^N\}. \quad (22)$$

The ε -pseudospectra lies between the spectrum and the numerical range and approaches the spectrum in the limit $\varepsilon \rightarrow 0$ and the numerical range in the limit $\varepsilon \rightarrow \infty$. Mathematically,

$$\sigma(\mathbf{A}) + \Delta_\varepsilon \subseteq \sigma_\varepsilon(\mathbf{A}) \subseteq W(\mathbf{A}) + \Delta_\varepsilon \quad (23)$$

where Δ_ε is the closed disk of radius ε in the complex plane centered at the origin. While the asymptotic ($t \rightarrow \infty$) behaviour of $\|f(\mathbf{A})\|$ is determined by its spectrum $\sigma(\mathbf{A})$, its early ($t \rightarrow 0$) and transient behaviour ($0 \leq t \leq T$) are determined by the numerical range $W(\mathbf{A})$ and the ε -pseudospectra $\sigma_\varepsilon(\mathbf{A})$, respectively.

The maximum real part of $W(\mathbf{A})$ is known as the numerical abscissa $\omega(\mathbf{A})$ and the maximum absolute value of $W(\mathbf{A})$ is known as the numerical radius $\mu(\mathbf{A})$. In the context of PDEs, these are useful quantities in the stability estimates of the semi and the full discretizations, respectively.

$$\omega(\mathbf{A}) = \max\{\Re(w) : w \in W(\mathbf{A})\} = \max\left\{\sigma\left(\frac{\mathbf{A} + \mathbf{A}^*}{2}\right)\right\}, \quad \mu(\mathbf{A}) = \max|w|, w \in W(\mathbf{A}) = \max_{\mathbf{z}^* \mathbf{z} = 1} |\mathbf{z}^* \mathbf{A} \mathbf{z}| \quad (24)$$

They can be efficiently computed due to the fact that $\omega(\mathbf{A})$ is the largest eigenvalue of $\mathbf{H} \equiv (\mathbf{A} + \mathbf{A}^*)/2$ and $\max |\mathbf{z}^* \mathbf{A} \mathbf{z}|$ occurs for the eigenvector $\mathbf{z}$ corresponding to the largest eigenvalue of $\mathbf{H}$. In this work, the boundary of the numerical range in the complex plane is traced by $\mu(\mathbf{A}e^{i\theta})$ with $\theta \in [0, 2\pi]$ (Mengi and Overton, 2005).

Recently, Crouzeix and Palencia (2017) have shown that “the numerical range of a linear operator on a Hilbert space is a (complete) $(1 + \sqrt{2})$ - spectral set” which implies the following upper bound on powers of the full discretizations,

$$\|\mathbf{B}^n\| \leq (1 + \sqrt{2}) \sup_{w \in W(\mathbf{B})} |w^n|, \quad \implies \quad \|\mathbf{B}^n\| \leq (1 + \sqrt{2}) \mu^n(\mathbf{B}). \quad (25)$$

2.10. Stability bounds based on the singular value

Following the fact that $\|\mathbf{B}^n\| \leq \|\mathbf{B}\|^n$, powers of the full discretization matrix $\mathbf{B}$ can be bound in terms of its spectral radius $\rho(\mathbf{B})$ and its largest singular value $s(\mathbf{B})$ which is equal to $\|\mathbf{B}\|_2$ as

$$\rho^n(\mathbf{B}) \leq \|\mathbf{B}^n\| \leq s^n(\mathbf{B}), \quad \frac{s(\mathbf{B})}{2} \leq \mu(\mathbf{B}) \leq s(\mathbf{B}), \quad (26)$$

where the second inequality relation above (Mengi and Overton, 2005; Ando, 2006) indicates that $s(\mathbf{B})$ is larger than the numerical radius $\mu(\mathbf{B})$ which can be significantly larger than the normalized pseudospectral radius $(\rho_\varepsilon(\mathbf{B}) - 1)/\varepsilon$ or $\mathcal{K}(\mathbf{B})$. Therefore, the upper bound of $\|\mathbf{B}^n\|$ based on $s(\mathbf{B})$ (Eq. 26) may not be sharp and can be significantly larger compared with the bounds (Eq. 14) based on the Kreiss constant (Eq. 15). Here, we emphasize that Brehm and

Figure 2: Schematic of the computational domain in (a) one and (b) two dimensions. The EB segments are located at x_s and y_s near the left and the bottom boundaries shown by the dashed lines.

Fasel (2013) used the spectral/singular value bounds (Eq. 26) to determine stable reconstruction schemes whereas we consider the pseudospectral bounds (Eq. 14) in this work. The former may yield highly conservative estimates of the sufficient conditions of stability, and thus severely restrict the CFL limit/time step, particularly for non-normal systems with the peak transient growth occurring at finite $t > 0$.

3. Stability of discrete wave equation

In this section, we analyze the stability of the discrete wave equation in the presence of an embedded boundary (EB) in one and two dimensions. We consider two qualitatively different spatial discretization schemes, viz., the first order upwind (UWS) and the second order central difference (CDS), and two temporal integration methods, viz., the explicit (forward) Euler method (EE) and an explicit third order Runge-Kutta method (RK3). A fourth order central discretization scheme (CDS4) and a fifth order upwind compact scheme (UCS5) are considered in Sec. 4.

Fig. 2a shows the discrete grid in one dimension with uniform spacing of Δx in a domain length of $L = 1$. The EB is located off the regular grid at x_s , expressed as a non-dimensional distance $\alpha \equiv \frac{x_s - x_0}{x_1 - x_0}$ from the ghost node x_0 . Here, $\alpha = 0$ corresponds to the ideal case when the EB is aligned with the regular grid. A two-dimensional unit square domain (Fig. 2b) is divided uniformly into N_x, N_y intervals along x, y directions with spacing $\Delta x, \Delta y$, respectively. In multi-dimensions, a general curved EB (Fig. 15, 16a) yields a range of α determined by the local slope of the EB and are considered in Sec. 6. Here, to study the effect of α in a two dimensional domain, we consider an idealized EB (Fig. 2b) comprised of two individual segments: one located vertically at $x = x_s$, and the other horizontally at $y = y_s$; with non-dimensional distances of $\alpha_x \equiv \frac{x_s - x_0}{x_1 - x_0}, \alpha_y \equiv \frac{y_s - y_0}{y_1 - y_0}$ from x_0, y_0 , respectively. Consequently, the

reconstruction depends only on the adjacent nodes along x, y - directions and not on the diagonal cell.

$$\frac{\partial \phi}{\partial t} + U_x \frac{\partial \phi}{\partial x} + U_y \frac{\partial \phi}{\partial y} = 0, \quad x_s, y_s \leq x, y \leq 1, \quad (27)$$

$$\phi(x_s, y, t) = 0, \quad \phi(x, y_s, t) = 0, \quad \phi(x, y, 0) = f(x, y). \quad (28)$$

The 2D wave equation (Eq. 27) is solved for the interior nodes (x_i, y_j) with $i = 1, 2, \dots, N_x$ and $j = 1, 2, \dots, N_y$. For the numerical examples considered here, we set $U_x = U \cos \theta$, $U_y = U \sin \theta$ with $U = 1$, and $\theta = 0$ (1D) or $\theta = \pi/4$ (2D). The initial condition $\phi(x, 0) = \sin[2\pi k(x - x_s)]$ in 1D and $\phi(x, y, 0) = \sin[2\pi k(x - x_s)] \sin[2\pi k(y - y_s)]$ in 2D (with $k = 2$), satisfies the boundary condition at the EB. The ghost nodes (x_0, y) and (x, y_0) use a bilinear reconstruction in a manner that satisfies the homogeneous Dirichlet boundary condition $\phi(x_s, y) = 0, \phi(x, y_s) = 0$ at the left and bottom boundaries. The discrete solution is denoted as $\phi_{ij} = \phi(x_i, y_j)$,

$$\phi_{0j} = -\frac{\alpha_x}{1 - \alpha_x} \phi_{1j}, \quad \phi_{i0} = -\frac{\alpha_y}{1 - \alpha_y} \phi_{i1}. \quad (29)$$

In one dimension, the 1D wave equation ($U_x = U$ and $U_y = 0$ in Eq. 27) is solved for the interior nodes $x_i, i = 1, 2, \dots, N$. The ghost node (x_0) uses a linear reconstruction scheme including the interior node x_1 and the boundary condition at the EB $\phi(x_s) = 0$ as follows,

$$\phi_0 = -\frac{\alpha}{1 - \alpha} \phi_1. \quad (30)$$

The time step Δt is computed based on the CFL criteria for stability: $\left| \frac{U \Delta t}{\Delta x} \right| \equiv C \leq C_{\max}$ in 1D and $|C_x| + |C_y| \equiv C \leq C_{\max}$ in 2D where, $C_x \equiv \frac{U_x \Delta t}{\Delta x}$, $C_y \equiv \frac{U_y \Delta t}{\Delta y}$, and $C'_x \equiv \frac{C_x}{1 - \alpha_x}$, $C'_y \equiv \frac{C_y}{1 - \alpha_y}$. Here, we consider $\alpha_x = \alpha_y = \alpha$ and $\Delta x = \Delta y$; consequently, $C_x = C_y$ and $C'_x = C'_y$.

The semi-discrete form of Eq. 27 combined with the boundary condition (Eq. 30) results in the spatial discretization matrix $A^{N \times N}$ for UWS and CDS as follows,

$$A = \frac{C}{\Delta t} \underbrace{\begin{bmatrix} -\frac{1}{1-\alpha} & & & & \\ 1 & -1 & & & \\ & 1 & -1 & & \\ & & \ddots & \ddots & \\ & & & 1 & -1 \end{bmatrix}}_{\text{UWS}}, \quad A = \frac{C}{2\Delta t} \underbrace{\begin{bmatrix} -\frac{\alpha}{1-\alpha} & -1 & & & \\ 1 & 0 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & 0 & -1 \\ & & 1 & -4 & 3 \end{bmatrix}}_{\text{CDS}} \quad (31)$$

In 2D, the solution vector $\phi_l = \{\phi_{1,1}, \phi_{2,1}, \dots, \phi_{N_x,1}, \phi_{1,2}, \phi_{2,2}, \dots, \phi_{N_x,2}, \dots, \phi_{1,N_y}, \phi_{2,N_y}, \dots, \phi_{N_x,N_y}\}^T$ has a size $N = N_x \times N_y$ and the spatial discretization matrix $A^{N \times N}$ for UWS is given by,

$$\mathbf{A} = \frac{1}{\Delta t} \begin{bmatrix} -C'_x - C'_y & & & & \\ C_x & -C_x - C'_y & & & \\ & \ddots & \ddots & & \\ C_y & \dots & 0 & -C'_x - C_y & \\ & C_y & \dots & C_x & -C_x - C_y \\ & & \ddots & & \ddots & \ddots \\ & & & C_y & \dots & 0 & -C'_x - C_y \\ & & & & C_y & \dots & C_x & -C_x - C_y \\ & & & & & \ddots & & \ddots & \ddots \\ & & & & & & C_y & \dots & C_x & -C_x - C_y \end{bmatrix}_{N \times N} \quad (32)$$

UWS_{2D}

For CDS, it has a similar structure with elements analogous to the 1D case and is not shown here.

Stability of the full discretization ($\mathbf{B} = f(\Delta t \mathbf{A})$) depends on both $\mathbf{C}$ and α . In the following discretizations, we first consider the ideal case ($\alpha = 0$) when the EB is aligned with the ghost node x_0 and find the maximum CFL limit $C_{\max}$ for stability. Then, we investigate $\alpha_{\max}$, the limiting value of α for stability, by fixing $\mathbf{C}$ at its ideal value $C_{\max}$.

Let S be the stability region of a temporal integration method. For $\alpha > \alpha_{\max}$, the discrete linear system is unstable if any of the eigenvalue lies outside S , which violates the necessary condition of stability. Furthermore, the system is stable for $\alpha \leq \alpha_{\max}$, if and only if the ε -pseudospectra lies within $\mathcal{O}(\varepsilon) + \mathcal{O}(\Delta t)$ distance of S as $\varepsilon, \Delta t \rightarrow 0$. This is visually verified by the boundaries of the ε -pseudospectra obtained through Eq. 5. Specifically, the inverse of the resolvent norm should vary at most linearly outside S which is quantified by the Kreiss constant $\mathcal{K}(\mathbf{B})$ of the full discretization (Eq. 15). Here, we choose ε greater than Δt by an order of magnitude.

3.1. Explicit Euler Upwind Scheme (EE-UWS)

3.1.1. One dimension

For the ideal case ($\alpha = 0$), the discrete operator ($\Delta t \mathbf{A}$) of UWS has a repeated eigenvalue $\lambda = -C$ with a deficit of $N - 1$. Corresponding ε -pseudospectra lies inside a disk of radius $C + \varepsilon$ centered at $-C$ which is within $\mathcal{O}(\varepsilon)$ distance of the stability region (S) of EE for $C \leq 1$; therefore, the ideal CFL limit of EE-UWS scheme is $C_{\max} = 1$. Now, for $\alpha \neq 0$, we examine conditions of stability such that the EB does not affect the CFL limit by fixing $C = C_{\max}$.

Theoretical estimates of $\alpha_{\max}$ are straightforward in the UWS case for which $\Delta t \mathbf{A}$ is upper triangular (Eq. 31) with real eigenvalues $\lambda_i = -C$ and $\lambda_b = -C/(1 - \alpha)$, corresponding to the interior and the boundary nodes, respectively. Since $|\lambda_b| \geq |\lambda_i|$, λ_b is the most unstable eigenvalue which lies outside the stability region of the time-stepping method S for $|\lambda_b| = \frac{C}{1-\alpha} > M$. Here, M is the abscissa of S along the negative real axis (2 for the EE method and 2.5 for the

Figure 3: EE-UWS discretization using $N = 100$ with $C = 1$: ε -pseudospectra of $\Delta t\mathbf{A}$ with $\varepsilon = 10^{-6}, 10^{-4}, 10^{-2}$ for (a) $\alpha = 0.4$, (b) $\alpha = 0.5$, (c) $\alpha = 0.6$; and the solution $\phi(x, t)$ at $t = 0.5$ for (d) $\alpha = 0.49$, (e) $\alpha = 0.50$, (f) $\alpha = 0.51$. The thick dashed line is boundary of the numerical range $W(\Delta t\mathbf{A})$ and the thin solid lines are boundaries of ε -pseudospectra $\sigma_\varepsilon(\Delta t\mathbf{A})$.

RK3 method). Therefore, for $C = C_{\max}$, the stability limit of α , subject to verification of the sufficient conditions, is

$$\alpha_{\max} = 1 - \frac{C_{\max}}{M}. \quad (33)$$

Fig. 3(a-c) shows the ε -pseudospectra $\sigma_\varepsilon(\Delta t\mathbf{A})$ of the spatial discretization matrix corresponding to the UWS (Eq. 31) for $\alpha = 0.4, 0.5, 0.6$, respectively. The stability region of the EE method (S) is marked by the shaded area. Boundaries of the ε -pseudospectra are shown for $\varepsilon = 0.01, 0.1, 0.2, 0.3$. Also, the samples of ε -pseudospectra are shown for $\varepsilon = 10^{-6}, 10^{-4}, 10^{-2}$ to visualize the sensitivity to minute perturbations. The dashed line is the boundary of the numerical range $W(\Delta t\mathbf{A})$. For the EE method, $W(\mathbf{B}) = 1 + W(\Delta t\mathbf{A})$ and $\sigma_\varepsilon(\mathbf{B}) = 1 + \sigma_\varepsilon(\Delta t\mathbf{A})$.

As α increases from zero, λ_b moves away from λ_i along the negative real axis (Fig. 3a), eventually approaches the boundary of S as $\alpha \rightarrow 0.5$ (Fig. 3b), and lies outside S for $\alpha > 0.5$ (Fig. 3c), consistent with Eq. 33. Clearly, for $\alpha > 0.5$, the necessary condition of stability is violated and hence the EE-UWS method is unstable.

To verify the sufficiency condition for stability for $\alpha \leq 0.5$, we examine the ε -pseudospectra. For $\alpha = 0.4$ (Fig. 3a), the boundaries of the $\sigma_\varepsilon(\Delta t\mathbf{A})$ vary almost linearly with respect to ε outside S (Kreiss constant $\mathcal{K}(\mathbf{B}) = 1.012$).

According to Eq. 8, this implies algebraic stability (Eq. 9) for a given mesh size N , which is a weaker form of stability. Further, Lax-stability (Eq. 7), a stronger criteria and applies uniformly for all N and n , is verified by a uniform upper bound on $\|f^n(\Delta t A)\| = 1.34$ for all n, N .

As $\alpha \rightarrow 0.5$, a bulge grows in $\sigma_\varepsilon(\Delta t A)$ near λ_b and becomes prominent for $\alpha = 0.5$ ($z = -2$ in Fig. 3b); and similarly, $\sigma_\varepsilon(\mathbf{B}) = 1 + \sigma_\varepsilon(\Delta t A)$ has a bulge near $z = -1$ (not shown). This bulge is examined by computing the Kreiss variable $\hat{\mathcal{K}}(d)$ (Eq. 16) of $\mathbf{B}$ along the negative real axis ($\theta^* = \pi$) for different N (Fig. 4a-c). The $\mathcal{K}(\mathbf{B}) = \sup \hat{\mathcal{K}}(d)$ and d^{*-1} are uniformly bounded and increase with α as shown in Fig. 4a,b for $\alpha = 0.49, 0.499$, respectively. In agreement with Sec. 2.7, $\|\mathbf{B}^n\|$ and n^* are uniformly bounded with $\sup \|\mathbf{B}^n\| = 3.61, 11.20$ for $\alpha = 0.49, 0.499$ (Fig. 4d,e), respectively. This shows Lax-stability for $\alpha < 0.5$. Notably, for $\alpha < 0.5$, $\|\mathbf{B}^n\|$ peaks at $n^* = \mathcal{O}(d^{*-1})$ and remains constant until $n = N$ and then decreases for $n > N$ (see Fig. 4d,e). As $\alpha \rightarrow 0.5$, the gap with constant $\|\mathbf{B}^n\|$ between n^* and N decreases (Fig. 4d,e), and $d^{*-1}, n^*, \mathcal{K}(\mathbf{B})$ and $\sup \|\mathbf{B}^n\|$ increase and eventually become functions of N for $\alpha = 0.5$: $d^{*-1} \sim \mathcal{O}(N), n^* = N, \mathcal{K}(\mathbf{B}) = N^{1/2}, \sup \|\mathbf{B}^n\| = N^{1/2}$ (Fig. 4c,f).

Figure 4: EE-UWS with $C = 1$: Kreiss variable $\hat{\mathcal{K}}(d)$ of $\mathbf{B}$ with $\theta^* = \pi$ for (a) $\alpha = 0.49$ ($d^* = 1/23$, $\sup \hat{\mathcal{K}}(d) = 1.91$), (b) $\alpha = 0.499$ ($d^* = 1/240$, $\sup \hat{\mathcal{K}}(d) = 5.63$), (c) $\alpha = 0.5$ ($d^* = \mathcal{O}(1/N)$, $\sup \hat{\mathcal{K}}(d) = N^{1/2}$); and $\|\mathbf{B}^n\|$ shown till $t = 1.5$ for (d) $\alpha = 0.49$ ($n^* = 97$, $\sup \|\mathbf{B}^n\| = 3.61$), (e) $\alpha = 0.499$ ($n^* = 823$, $\sup \|\mathbf{B}^n\| = 11.20$), (f) $\alpha = 0.5$ ($n^* = N$, $\sup \|\mathbf{B}^n\| = N^{1/2}$). Note $\mathbf{B} = f(\Delta t A)$, $\sup \hat{\mathcal{K}}(d)$ occurs at $d = d^*$ and $\sup \|\mathbf{B}^n\|$ occurs at $n = n^* = \mathcal{O}(d^{*-1})$.

For $\alpha = 0.5$ (Fig. 4c), $\hat{\mathcal{K}}(d)$ asymptotes to 1 for $d \gg 1$ (normal like behavior), but for $d \ll 1$, it grows approximately as $d^{-1/2}$ until it reaches the supremum while, from Eq. 15, the inverse of the resolvent norm $\|(zI - B)^{-1}\|^{-1}$ grows approximately as $d^{3/2}$, i.e., faster than linear growth. Further, $\sup \hat{\mathcal{K}}(d)$ varies as $N^{1/2}$ indicating algebraic dependence (Fig. 4c). Fig. 4f shows $\|f^n(\Delta t A)\|$ for different N which is bounded for a given mesh size N , but the $\sup \|f^n(\Delta t A)\|$ increases as $N^{1/2}$. This shows that for $\alpha = 0.5$, the system is algebraically stable but not Lax-stable. We also observed $C = 0.99, \alpha = 0.5$ to be Lax-stable with uniform $\sup \|B^n\| = 3.11$ (Table 4). This implies that the EE-UWS is Lax-stable for either $C \leq 1, \alpha < 0.5$ or $C < 1, \alpha \leq 0.5$ but only algebraically stable for $C = 1, \alpha = 0.5$.

In addition, we examine the usual vector p-norms ($\|\cdot\|_{\ell^p}$) and the integral p-norms ($\|\cdot\|_{L^p}$), appropriate for measurable quantities, of the numerical error e defined as below (LeVeque, 2002) to verify the dependence of the error growth on n, N for $C = 1, \alpha = 0.5$.

$$\|e\|_{L^p} = \left(\Delta x \sum_{i=1}^N |e_i|^p \right)^{1/p}, \quad \|e\|_{\ell^p} = \left(\sum_{i=1}^N |e_i|^p \right)^{1/p}, \quad \|\cdot\|_{\ell^p} = N^{1/p} \|\cdot\|_{L^p}. \quad (34)$$

For $x_i < t$, the sawtooth region in Fig. 3e, the amplitude of the error is uniform ($= \ell^\infty = L^\infty$) and for $x_i \geq t$, the error is zero (up to the machine precision) which gives $L^1 = tL^\infty, L^2 = t^{1/2}L^\infty$ for $t \leq 1$ and $L^1 = L^2 = L^\infty$ for $t \geq 1$. Somewhat surprisingly, we observe convergence of the solution with grid refinement: the max norm L^∞ decreases linearly with Δx ($L^\infty = 0.1266, 0.0631, 0.0315, 0.0157$ for $N = 50, 100, 200, 400$, respectively). Also, $L^1, L^2 = \mathcal{O}(\Delta x)$, ℓ^1 is nearly constant, $\ell^2 = \mathcal{O}(\Delta x^{1/2})$ in contrast to the $N^{1/2}$ increase in $\|f^n(\Delta t A)\|_2$ (Fig. 4f). The reason for convergence is explained as follows. Let us denote the right singular vector of B corresponding to the largest singular value as $v(B)$. For EE-UWS scheme with $C = 1, v(B^n) = v(B)$, given below,

$$v_i(B^n) = v_i(B) = \delta_{1i}, \quad \text{for } i = 1, 2, \dots, N. \quad (35)$$

The Lax-stability requires $\|B^n \phi\| \leq C(n\Delta t)\|\phi\|$. Since $\|B^n \phi\| \leq \|B^n\| \|\phi\|$ where the equality holds if $\phi = v(B^n)$, $\|B^n\| \leq C(n\Delta t)$ is both necessary and sufficient condition for $\|B^n \phi\| \leq C(n\Delta t)\|\phi\|$ for arbitrary initial conditions. However, for initial conditions other than $v(B)$, $\|B^n \phi\| \leq C(n\Delta t)\|\phi\|$ may still hold uniformly even though $\|B^n\| \leq C(n\Delta t)$ does not hold uniformly. For any initial condition that is locally smooth near the boundary and satisfies the boundary condition $\phi(x_s, t) = 0, \phi_1^0 \rightarrow 0$ as $N \rightarrow \infty$. Thus, the component of the initial condition associated with $v(B)$ goes to zero, $\phi^0 \cdot v(B) \rightarrow 0$, as $N \rightarrow \infty$. In such cases, $\|B^n \phi\|$ may have a uniform upper bound, even if $\|B^n\|$ has no uniform upper bound. This is also true for any ϕ orthogonal to v . Notably, Dahlquist (1954) studied convergence problem for analytic initial-values in situations that violate the standard CFL criteria. Although round-off errors may be amplified in his studies, their amplitude remains constant (neutrally stable) in case of EE-UWS with $C = 1, \alpha = 0.5$ and practically, this case has both stability and convergence.

The solution $\phi(x, t)$ at $t = 0.5$ is visualized in Fig. 3(d-f) for $\alpha = 0.49, 0.50, 0.51$, respectively. The numerical error due to the EB condition introduces a spurious mode of wavelength $2\Delta x$ for $\alpha \neq 0$, which is then advected into the domain. The amplitude of these numerical perturbations at x_0 varies as $(\frac{\alpha}{1-\alpha})^n$, i.e., decays with time as 0.9608^n

for $\alpha = 0.49$ (Fig. 3d), remains constant for $\alpha = 0.50$ (Fig. 3e), and grows as 1.0408^n for $\alpha = 0.51$ (Fig. 3f). This shows that the reconstruction scheme with EE-UWS method is stable for $\alpha \leq 0.5$ and unstable for $\alpha > 0.5$.

As shown in Table 1, for $C = C_{\max}$, the numerical radius $\mu(\mathbf{B}) > 1$ and yet, the solution has bounded transient growth. So, the numerical range $W(\mathbf{B})$ may lie outside the unit disk for stable systems (see the dashed line in Fig. 3a,b for $W(\Delta t \mathbf{A})$). However, for $C = C_{\mu}$, the numerical radius $\mu(\mathbf{B}) = 1$ and $W(\mathbf{B})$ lies inside the unit disk. Therefore, $\hat{\mathcal{K}}(d) \leq 1$ outside the unit disk and the discrete system behaves like a normal system with negligible transient growth ($\leq (1 + \sqrt{2})$ from Eq. 25).

3.1.2. Two dimensions

Here, we consider the EE-UWS discretization in 2D. Similar to the 1D case, we fix $C = C_{\max} = 1$ and obtain the stability limit $\alpha_{\max}$. Clearly, from Eq. 32, the eigenvalues of $\Delta t \mathbf{A}$ are $\lambda_i = -C_x - C_y$, $\lambda_b = -C_x - C'_y = -C'_x - C_y$, and $\lambda_c = -C'_x - C'_y$ corresponding to the interior nodes, the boundary nodes, and the corner node (x_0, y_0) , respectively. Since $|\lambda_c| \geq |\lambda_b| \geq |\lambda_i|$, λ_c is the most unstable eigenvalue which lies outside S for $\alpha > 0.5$ (from Eq. 33 with $C = 1$ and $M = 2$). Therefore, the stability limit of α , subject to verification of the sufficient conditions, is $\alpha_{\max} = 0.5$.

Figure 5: EE-UWS discretization in 2D with $C = 1$: ε -pseudospectra of $\Delta t \mathbf{A}$ with $\varepsilon = 10^{-6}, 10^{-4}, 10^{-2}$ for (a) $\alpha = 0.45$, (b) $\alpha = 0.50$, (c) $\alpha = 0.55$; and the solution $\phi(x, y, t)$ at $t = 0.25$ for (d) $\alpha = 0.45$, (e) $\alpha = 0.50$, (f) $\alpha = 0.55$. S is the stability region of the explicit Euler method. Here, $N_x = N_y = 20$ for (a-c) and $N_x = N_y = 50$ for (d-f).

Fig. 5(a-c) shows the $\sigma_\varepsilon(\Delta t \mathbf{A})$ of the UWS and the stability region (S) of the explicit Euler method for $\alpha = 0.45, 0.50, 0.55$, respectively. The ε -pseudospectra for $\varepsilon = 10^{-6}, 10^{-4}, 10^{-2}$ are distributed around a larger circle centered at $z = \lambda_i$, a smaller circle centered at $z = \lambda_b$, and at $z = \lambda_c$. Notably, λ_c lies inside S for $\alpha = 0.45$ (Fig. 5a), on the boundary of S for $\alpha = 0.50$ (Fig. 5b), and outside S for $\alpha = 0.55$ (Fig. 5c). This implies that $\alpha = 0.55$ yields unstable discretization while $\alpha = 0.45, 0.50$ satisfy the necessary condition of stability. Further, the discretization is Lax-stable for $\alpha < 0.5$ as the $\sigma_\varepsilon(\Delta t \mathbf{A})$ is within $\mathcal{O}(\varepsilon)$ distance of S (see Fig. 5a for $\alpha = 0.45$), quantified by $\mathcal{K}(\mathbf{B}) = 4.38, \|\mathbf{B}^n\| = 10.48$ for $\alpha = 0.49$ in Table 1. For $\alpha = 0.50$, the $\sigma_\varepsilon(\Delta t \mathbf{A})$ has a bulge near $z = -2.5$ (Fig. 5b) and $\sup \|\mathbf{B}^n\| = N^{1/2}$ (data not shown) similar to the 1D case, which is bounded for each N and indicates only algebraic but not Lax-stability. Table 1 shows that $d_{2D}^{*-1} \sim 2d_{1D}^{*-1}, \mathcal{K}(\mathbf{B})_{2D} \sim 2\mathcal{K}(\mathbf{B})_{1D}, \sup \|\mathbf{B}^n\|_{2D} \sim (\sup \|\mathbf{B}^n\|_{1D})^2$ where the subscripts 1D, 2D denote one and two dimensions, respectively. Therefore, EE-UWS in 2D is Lax-stable for $C = 1, \alpha < 0.5$ and algebraically stable for $C = 1, \alpha = 0.5$.

To verify the above results, Fig. 5(d-f) shows the solution at $t = 0.25$ for $\alpha = 0.45, 0.50, 0.55$, respectively. While Fig. 5(d-e) show the solution to be stable for $\alpha = 0.45, 0.50$, Fig. 5(f) shows growing perturbations originating at the corner node for $\alpha = 0.55$. Therefore, in accordance with the findings through the pseudospectra, the linear system is stable for $\alpha \leq 0.50$ and unstable for $\alpha > 0.50$.

3.2. Higher-order time integration: RK3-UWS and RK3-CDS

We now examine the RK3 method to exemplify the stability of higher order time stepping methods for both upwinding (UWS) and central (CDS) schemes. For $\alpha = 0$, stability of RK3-UWS discretization requires $C \leq 1.25$ (the ε -pseudospectra lies within a distance ε of the stability region of RK3 method); therefore, $C_{\max} = 1.25$. Now, we fix $C = C_{\max}$ and characterize the stability for $\alpha \neq 0$.

Fig. 6(a-c) shows $\sigma_\varepsilon(\Delta t \mathbf{A})$ for $\alpha = 0.4, 0.5, 0.6$, respectively. The shaded area indicates the stability region of the RK3 method (S). According to Eq. 33, with $M = 2.5$, the most unstable eigenvalue λ_b lies inside S for $\alpha = 0.4$ (Fig. 6a), on the boundary of S for $\alpha = 0.5$ (Fig. 6b), and outside S for $\alpha = 0.6$ (Fig. 6c) and the discrete system is unstable for $\alpha > 0.5$. For $\alpha = 0.4$, $\sigma_\varepsilon(\Delta t \mathbf{A})$ lies within $\mathcal{O}(\varepsilon)$ distance of S ($\mathcal{K}(\mathbf{B}) = 1$) and the discrete system satisfies Eq. 7 for $N = 50, 100, 200$ with $C_1 = 1.179$ (not shown here) and is therefore Lax-stable for $\alpha = 0.4$.

For $\alpha = 0.5$, the $\sigma_\varepsilon(\Delta t \mathbf{A})$ has a bulge near λ_b ($z = -2.5$ in Fig. 6b), and, similarly, $\sigma_\varepsilon(\mathbf{B})$ has a bulge near $z = -1$ (not shown). Near this bulge, the Kreiss variable $\hat{\mathcal{K}}(d)$ of $\mathbf{B}$ varies as $d^{-1/4}$ for $d \sim \mathcal{O}(0.1 - 1)$ along the negative real axis (Fig. 7a). Therefore, according to Eq. 15, $\|(zI - \mathbf{B})^{-1}\|^{-1}$ grows as $d^{5/4}$ which is slightly higher than linear growth. This implies transient growth, quantified by the Kreiss constant $\mathcal{K}(\mathbf{B}) \approx 2.8$ (Table 1) and $\|f^n(\Delta t \mathbf{A})\|$ for different N in Fig. 8a. Since $\|\mathbf{B}^n\|$ has a uniform upper bound of 4.25 (Table 1), the system is Lax-stable for $\alpha = 0.5$.

Fig. 6(d-f) shows the solution at $t = 0.5$ for $\alpha = 0.49, 0.50, 0.51$, respectively. The amplitude of the boundary generated perturbations decay for $\alpha = 0.49$, remains constant for $\alpha = 0.50$, and grows exponentially for $\alpha = 0.51$. Evidently, we conclude that the RK3-UWS is Lax-stable for $C = 1.25, \alpha \leq 0.5$ and unstable for $C = 1.25, \alpha > 0.5$.

Next we examine the CDS scheme because central schemes are fundamentally different from upwind schemes in

Figure 6: RK3 - UWS discretization with $C = 1.25$: ε -pseudospectra of $\Delta t A$ with $\varepsilon = 10^{-6}, 10^{-4}, 10^{-2}$ for (a) $\alpha = 0.4$, (b) $\alpha = 0.5$, (c) $\alpha = 0.6$; and the solution $\phi(x, t)$ at $t = 0.5$ for (d) $\alpha = 0.49$, (e) $\alpha = 0.50$, (f) $\alpha = 0.51$.

the sense that these exhibit dispersion error and generally have no dissipation. We analyze the stability characteristics of the RK3 combined with a second order CDS with EB reconstruction (Eq. 30). The spatial discretization matrix A of CDS with a second order one-sided stencil at the right boundary $x = 1$ is given by Eq. 31.

RK3-CDS has $C_{\max} \approx 1.7$ in the ideal case $\alpha = 0$; so we fix $C = 1.7$ for $\alpha \neq 0$. Fig. 9(a-c) shows boundaries of the $\sigma_\varepsilon(\Delta t A)$ for $\varepsilon = 0.01, 0.1, 0.2, 0.3$ for $\alpha = 0.75, 0.76, 0.77$, respectively. As α increases, the eigenvalue depending on the EB condition λ_{EB} moves to the left and lies outside S for $\alpha = 0.77$ (Fig. 9c). Therefore, the discrete system is unstable for $\alpha \geq 0.77$. But for $\alpha \leq 0.76$, λ_{EB} lies inside S and $\sigma_\varepsilon(\Delta t A)$ varies at most linearly outside S without any local bulges (Fig. 9a,b), with $\mathcal{K}(B) = 1.002$ for $\alpha = 0.76$. This shows that the RK3-CDS scheme is at least algebraically stable (Eq. 9) for $\alpha \leq 0.76$. Furthermore, Lax-stability is verified by a uniform upper bound 1.5 (Table 1) on $\|f^m(\Delta t A)\|$ for $N = 50, 100, 200$ and $\alpha = 0.76$.

Fig. 9(d-f) shows the solution $\phi(x, t)$ at $t = 0.5$ for $\alpha = 0.75, 0.76, 0.77$, respectively. Near the EB, boundary generated perturbations grow exponentially for $\alpha = 0.77$ (Fig. 9f) and decay for $\alpha = 0.75, 0.76$ (Fig. 9d,e). This confirms that the discrete system is Lax-stable for $\alpha \leq 0.76$ and unstable for $\alpha > 0.76$.

In 2D, similar to the 1D case, the RK3-UWS (RK3-CDS) method has $C_{\max} = 1.25(1.7)$ for $\alpha = 0$. Hence, we fix $C = 1.25$ and investigate the stability limit $\alpha_{\max}$. Fig. 10(a-c) shows $\sigma_\varepsilon(\Delta t A)$ of the RK3-UWS for $\alpha =$

Figure 7: Kreiss variable $\hat{\mathcal{K}}(d)$ near the bulge ($\theta = \theta^*$) in $\sigma_\varepsilon(\mathbf{B})$ for (a) RK3-UWS with $C = 1.25, \alpha = 0.5, d^* \approx 1/23, \theta^* = \pi$, (b) RK3-CDS4 with $C = 1.25, \alpha = 0.77, d^* \approx 1, \theta^* = 0$, (c) RK4-UCS5 with $C = 1.034, \alpha = 0.67, d^* \approx 1/25, \theta^* = 0$.

Figure 8: $\|f^n(\Delta t A)\|$ for (a) RK3-UWS, $C = 1.25, \alpha = 0.5, n^* = 23$, (b) RK3-CDS4, $C = 1.25, \alpha = 0.77, n^* = 1$, (c) RK4-UCS5, $C = 1.034, \alpha = 0.67, n^* = 20$. Each case has a uniform upper bound on $\|f^n(\Delta t A)\|$ for $N > \mathcal{O}(d^{n^*-1})$.

0.45, 0.50, 0.55, respectively. The most unstable eigenvalue λ_c lies inside S for $\alpha = 0.45$, on the boundary of S for $\alpha = 0.50$ and outside S for $\alpha = 0.55$ indicating instability for $\alpha = 0.55$ and possible stability for $\alpha \leq 0.50$. However, the $\sigma_\varepsilon(\Delta t A)$ has a slight bulge near λ_c ($z = -2.5$ in Fig. 10b) for $\alpha = 0.45, 0.50$, indicating transient growth. Further inspection of $\sup \|\mathbf{B}^n\|$ shows that the method is Lax-stable for $C \leq 1.22$ with a uniform bound $\sup \|\mathbf{B}^n\| = 3.09$ for $C = 1.22$ and $\alpha = 0.5$ (Table 1) and algebraically stable for $1.22 < C \leq 1.25$ and $\alpha = 0.5$. Fig. 10(d-f) shows the pseudospectra of the RK3-CDS method with $C = 1.7$ for $\alpha = 0.70, 0.76, 0.80$, respectively. The eigenvalues corresponding to the corner (λ_c), boundary (λ_b), and interior (λ_i) nodes are segregated. Particularly, λ_c, λ_b depend on α and move towards left as α increases. Here, λ_c is the most unstable mode which lies inside the stability region S for $\alpha = 0.70$, close to the boundary of S for $\alpha = 0.76$, and outside S for $\alpha \geq 0.77$. Clearly, the $\sigma_\varepsilon(\Delta t A)$ lies within a distance ε of S for $\alpha \leq 0.76$ and $\sup \|\mathbf{B}^n\| = 2.14$ is uniformly bounded for $\alpha = 0.76$ (see Table 1). Therefore, we

Figure 9: RK3 - CDS discretization with $C = 1.7$: ε -pseudospectra of $\Delta t \mathbf{A}$ with $\varepsilon = 10^{-6}, 10^{-4}, 10^{-2}$ for (a) $\alpha = 0.75$, (b) $\alpha = 0.76$, (c) $\alpha = 0.77$; and the solution $\phi(x, t)$ at $t = 0.5$ for (d) $\alpha = 0.75$, (e) $\alpha = 0.76$, (f) $\alpha = 0.77$.

conclude that the RK3-CDS method is Lax-stable for $\alpha \leq 0.76$ and unstable for $\alpha > 0.76$.

In summary, for $C = C_{\max}$, the UWS is stable for $\alpha \leq 0.5$ with both EE and RK3 temporal integration methods and the RK3-CDS is stable for $\alpha \leq 0.76$. Also, the stability of the discrete system depends somewhat in a similar fashion on α in both one and two dimensions.

Table 1 also shows, for $\alpha = \alpha_{\max}$, two different stability limits: C_{μ} based on the unit numerical radius ($\mu(\mathbf{B}) = 1$) and C_s based on the unit 2-norm (the largest singular value, $s_{\max}(\mathbf{B}) = \|\mathbf{B}\|_2 = 1$), which are obtained by reducing C (starting with $C_{\max}$) until $\mu(\mathbf{B}) = 1$, $s_{\max}(\mathbf{B}) = 1$ are observed, respectively. While C_{μ} results in a normal like behavior ($\|\mathbf{B}^n\| \leq 1 + \sqrt{2}$), C_s results in a contraction $\|\mathbf{B}^n\| \leq 1$. In contrast to $C_{\max}$ based on $\mathcal{K}(\mathbf{B})$, C_{μ} and C_s can be significantly smaller. In some cases such as CDS and CDS4 (higher-order is discussed in Section 4), $\|\mathbf{B}\| \leq 1$ is not possible at all for any $C_s > 0$ and one may opt for the infimum of $\|\mathbf{B}\|$ instead of $\|\mathbf{B}\| \leq 1$ as in Brehm and Fasel (2013), which, however, does not guarantee the stability. Also note that $\sup \|\mathbf{B}^n\|$ may be smaller compared with $\sup \|\mathbf{B}\|^n$ and may occur at different n or $t = n\Delta t$.

scheme	$\alpha_{\max}$	$C_{\max}$	d^{*-1}	$\mathcal{K}(\mathbf{B})$	$\mu(\mathbf{B})$	n^*	$\sup \ \mathbf{B}^n\ $	d^{*-1}	$\mathcal{K}(\mathbf{B})$	n^*	$\sup \ \mathbf{B}^n\ $	C_{μ}	$\sup_{\mu=1} \ \mathbf{B}^n\ $	C_s
description		$\alpha = 0$	1D	1D	1D	$\mathcal{O}(d^{*-1})$	1D	2D	2D	$\mathcal{O}(d^{*-1})$	2D	$\mu(\mathbf{B}) = 1, 1D$	$\ \mathbf{B}\ = 1$	
EE - UWS	0.49 [‡]	1.00	23	1.91	1.22	97	3.61	53	4.38	99	10.48	0.90	1.19	0.76
RK3-UWS	0.50	1.25	23	2.75	1.39	23	4.25	48	8.86	48	17.40	1.15	1.24	1.06
RK4-UWS	0.50	1.38	13	2.06	1.33	13	3.07	25	5.00	27	9.38	1.28	1.10	1.24
RK3-CDS	0.76	1.70	1	1.00	1.03	1	1.50	1	1.25	1	2.14	1.68	1.46	0.00
RK4-CDS	0.70	2.825	1	1.03	1.10	1	1.48	1	2.55	1	9.11	2.61	1.32	0.00
RK3-CDS4	0.77	1.25	1	1.20	1.62	1	2.81	–	–	–	–	0.81	1.40	0.00
RK4-CDS4	0.75	2.05	1	2.08	3.55	1	6.80	–	–	–	–	1.00	1.31	0.00
RK4-UCS5	0.67	1.034	25	4.43	1.78	20	6.44	–	–	–	–	0.88	1.26	0.00

Table 1: Lax-stability limit $\alpha_{\max}$ of various schemes corresponding to the ideal ($\alpha = 0$) CFL limit $C_{\max}$ in one and two dimensions and corresponding values of the Kreiss constant $\mathcal{K}(\mathbf{B})$, the numerical radius $\mu(\mathbf{B})$ and the $\sup \|\mathbf{B}^n\|$. Notably, $\sup \hat{\mathcal{K}}(d) = \mathcal{K}(\mathbf{B})$ occurs at $d = d^*$ and $\sup \|\mathbf{B}^n\|$ occurs at $n = n^* = \mathcal{O}(d^{*-1})$. All values are independent of the size of $\mathbf{B}$ for sufficiently large $N > \mathcal{O}(d^{*-1})$ in 1D and $N_x = N_y > \mathcal{O}(d^{*-1})$ in 2D. Also, for $\alpha = \alpha_{\max}$, the CFL limits C_{μ} and C_s based on unit numerical radius ($\mu(\mathbf{B}) = 1$) and unit 2-norm ($s_{\max}(\mathbf{B}) = \|\mathbf{B}\|_2 = 1$), respectively, are shown in 1D. The superscript [‡] indicates Lax-stability for any $\alpha < 0.5$ and algebraic stability for $\alpha = 0.5$. We also report results using RK4 time marching method with UWS, CDS, CDS4 but omit the discussion in the article.

4. Higher order spatial discretization

In this section, we examine the sufficient condition of stability for higher order spatial discretization of the 1D wave equation in the presence of EB. A fourth order central scheme and a fifth order upwind compact scheme are considered for example. Furthermore, higher order EB reconstruction schemes for arbitrary values of α are obtained and their stability limits are expressed in terms of $\alpha_{\max}$.

4.1. Fourth order central difference scheme (CDS4)

The following fourth order central discretization scheme (CDS4) is considered in this section.

$$\left. \frac{\partial \phi}{\partial x} \right|_i = \frac{\phi_{i-2} - 8\phi_{i-1} + 8\phi_{i+1} - \phi_{i+2}}{12\Delta x} + \mathcal{O}(\Delta x^4), \quad i = 1, 2, \dots, N. \quad (36)$$

The discretization stencil requires two ghost nodes each at the left boundary x_0, x_{-1} and the right boundary x_{N+1}, x_{N+2} , where $x_0 = x_1 - \Delta x$, $x_{-1} = x_1 - 2\Delta x$, $x_{N+1} = x_N + \Delta x$ and $x_{N+2} = x_N + 2\Delta x$.

4.1.1. EB reconstruction scheme

At the left boundary, the nodal values ϕ_0, ϕ_{-1} are expressed in terms of four regular interior nodes and a Dirichlet boundary condition at the EB (x_s) which is located at a distance of $\alpha\Delta x$ from x_0 and $(1 + \alpha)\Delta x$ from x_{-1} . Denote $\phi(x_s) = \phi_s$ and the fifth order schemes for the ghost nodes at the left boundary are given below, with the weightage coefficients $\omega_{0,i}, \omega_{-1,i}$ shown in Table 2.

$$\phi_0 = \sum_i \omega_{0,i} \phi_i, \quad \phi_{-1} = 5\phi_0 - 10\phi_1 + 10\phi_2 - 5\phi_3 + \phi_4 = \sum_i \omega_{-1,i} \phi_i, \quad i = 1, 2, 3, 4, s, \quad (37)$$

Figure 10: (a-c) RK3-UWS discretization in 2D with $C = 1.25$: ε -pseudospectra of $\Delta t \mathbf{A}$ with $\varepsilon = 10^{-6}, 10^{-4}, 10^{-2}$ for (a) $\alpha = 0.45$, (b) $\alpha = 0.50$, (c) $\alpha = 0.55$; (d-f) RK3-CDS discretization in 2D with $C = 1.7$: ε -pseudospectra of $\Delta t \mathbf{A}$ with $\varepsilon = 10^{-6}, 10^{-4}, 10^{-2}$ for (d) $\alpha = 0.70$, (e) $\alpha = 0.76$, (f) $\alpha = 0.80$. S is the stability region of the explicit RK3 method. Here, $N_x = N_y = 20$.

Since the right boundary has no physical boundary condition, one sided fifth order schemes with five regular interior nodes are given below for the ghost nodes $N + 1, N + 2$.

$$\phi_{N+1} = 5\phi_N - 10\phi_{N-1} + 10\phi_{N-2} - 5\phi_{N-3} + \phi_{N-4}, \quad \phi_{N+2} = 15\phi_N - 40\phi_{N-1} + 45\phi_{N-2} - 24\phi_{N-3} + 5\phi_{N-4}. \quad (38)$$

The order of accuracy is verified using an exact solution $\phi(x) = \sin\left(2\pi\frac{(x-x_s)}{(L-x_s)} + \pi/4\right) - \sin(\pi/4)$ which satisfies the EB condition $\phi(x_s) = 0$. The phase $\pi/4$ ensures all the higher derivatives at x_s are non-zero to estimate the order of error correctly. Numerical error in computing $-U\frac{\partial\phi_i}{\partial x}$ is quantified for $\alpha = 0.5$ by the integral p-norm (Eq. 34). Both the local (L^∞) and the global (L^1, L^2) norms of the error show (Fig. 11) fourth order accuracy $\mathcal{O}(\Delta x^4)$, as expected.

4.1.2. Stability

Now, we examine the stability of the RK3-CDS4 scheme to find $\alpha_{\max}$ corresponding to $C = C_{\max}$. Fig. 12(a-c) shows the ε -pseudospectra of the full discretization $\sigma_\varepsilon(\mathbf{B})$ for $\alpha = 0, 0.77, 0.78$, respectively. For $\alpha = 0$, the

Figure 11: Spatial accuracy test with $\alpha = 0.5$: numerical error in computing $-U \frac{\partial \phi}{\partial x}$ for $\phi(x) = \sin(2\pi \frac{(x-x_s)}{(L-x_s)} + \pi/4) - \sin(\pi/4)$ using CDS4 spatial discretization scheme. Ghost nodes are reconstructed using a fourth order polynomial fit.

i	1	2	3	4	s
$\omega_{0,i}$	$\frac{-4\alpha}{1-\alpha}$	$\frac{6\alpha}{2-\alpha}$	$\frac{-4\alpha}{3-\alpha}$	$\frac{\alpha}{4-\alpha}$	$\frac{24}{(1-\alpha)(2-\alpha)(3-\alpha)(4-\alpha)}$
$\omega_{-1,i}$	$\frac{-10(1+\alpha)}{1-\alpha}$	$\frac{20(1+\alpha)}{2-\alpha}$	$\frac{-15(1+\alpha)}{3-\alpha}$	$\frac{4(1+\alpha)}{4-\alpha}$	$\frac{120}{(1-\alpha)(2-\alpha)(3-\alpha)(4-\alpha)}$

Table 2: Weightage coefficients for the ghost nodes x_0, x_{-1} in a fifth order accurate EB reconstruction scheme.

eigenvalues lie outside the unit disk S for C slightly greater than 1.25. Moreover, for $C = 1.25$, $\sigma_\varepsilon(\mathbf{B})$ has a prominent bulge of size greater than ε outside S near $z = 1$ (Fig. 12a) and the Kreiss variable $\tilde{\mathcal{K}}(d, \theta^* = 0)$ indicates transient growth of at least 3-4 times on the order of 10 - 100 ($\mathcal{O}(d^{-1})$) time steps. In addition, the $\sup \|\mathbf{B}^n\|$ has a uniform bound of approximately 7. Therefore, $C_{\max} \approx 1.25$ and we fix $C = C_{\max}$ for $\alpha \neq 0$.

For $\alpha = 0.77$, all the eigenvalues lie inside S and the ε -pseudospectra is within $\mathcal{O}(\varepsilon)$ distance of S (Fig. 12b). The Kreiss constant $\mathcal{K}(\mathbf{B})$ indicates a mild transient growth of at least 1.2 (Table 1) in $\mathcal{O}(1)$ time steps. Agreeably, Fig. 8b shows $\sup \|\mathbf{B}^n\|$ to be approximately 3. However, for $\alpha = 0.78$, the boundary eigenvalue lies outside S (Fig. 12c) indicating that the method is linearly unstable. Therefore, the stability limit for RK3-CDS4 method is $\alpha_{\max} = 0.77$ with $C_{\max} = 1.25$.

Fig. 12(d-f) demonstrates the above limits by showing the solution at $t = 0.5$ for $\alpha = 0, 0.77, 0.78$, respectively. Clearly, no sign of instabilities appear when $\alpha \leq 0.77$ (Fig. 12d,e) while growing instabilities appear near EB when $\alpha = 0.78$ (Fig. 12f). In passing, we comment that the Kreiss constant $\mathcal{K}(\mathbf{B})$ decreases as α increases from 0 to 0.77 which implies that the EB reconstruction has stabilizing effect on the scheme.

Figure 12: RK3 - CDS4 discretization with $C = 1.25$: boundaries of the $\sigma_\varepsilon(\mathbf{B})$ with $\varepsilon = 0.01, 0.1, 0.2, 0.3$ for (a) $\alpha = 0$, (b) $\alpha = 0.77$, (c) $\alpha = 0.78$. The thick dashed line denotes boundary of the numerical range $W(\mathbf{B})$ of the full discretization; the solution $\phi(x, t)$ at $t = 0.5$ for (d) $\alpha = 0$, (e) $\alpha = 0.77$, (f) $\alpha = 0.78$; Here, $N = 100$.

4.2. Fifth order upwind compact scheme (UCS5) with conservative finite difference approach

Here, we consider EB reconstruction with a fifth order upwind compact scheme (UCS5) (Pirozzoli, 2002). Define $\tilde{\phi}$ such that $\phi_i \equiv \frac{1}{\Delta x} \int_{x_{i-1/2}}^{x_{i+1/2}} \tilde{\phi} \, dx$ or $\frac{\partial \phi}{\partial x} \Big|_i = \frac{\tilde{\phi}_{i+1/2} - \tilde{\phi}_{i-1/2}}{\Delta x}$. Now, the 1D wave equation is conservatively discretized as,

$$\frac{d\phi_i}{dt} = -U \frac{\tilde{\phi}_{i+1/2} - \tilde{\phi}_{i-1/2}}{\Delta x} = A_{il}\phi_l, \quad i = 1, 2, \dots, N, \quad (39)$$

where, $\tilde{\phi}_{i+1/2+l}$, $l \in [-L_1, L_2]$, are expressed in terms of ϕ_{i+m} , $m \in [-M_1, M_2]$, through a compact scheme of order $p = L_1 + L_2 + M_1 + M_2 + 1$. Here, UCS5 is obtained by choosing $L_1 = L_2 = M_1 = M_2 = 1$ (Pirozzoli, 2002),

$$3\tilde{\phi}_{i-1/2} + 6\tilde{\phi}_{i+1/2} + \tilde{\phi}_{i+3/2} = \frac{1}{3}\phi_{i-1} + \frac{19}{3}\phi_i + \frac{10}{3}\phi_{i+1}, \quad i = 1, 2, \dots, N. \quad (40)$$

Pirozzoli (2002) employed the following fourth order boundary schemes to accommodate a Dirichlet condition at the inflow boundary ($\tilde{\phi}_{1/2} = 0$) and a one-sided stencil at the outflow boundary,

$$\tilde{\phi}_{1/2} = \frac{1}{4}\phi_0 + \frac{13}{12}\phi_1 - \frac{5}{12}\phi_2 + \frac{1}{12}\phi_3, \quad \tilde{\phi}_{N+1/2} = \frac{25}{12}\phi_N - \frac{23}{12}\phi_{N-1} + \frac{13}{12}\phi_{N-2} - \frac{1}{4}\phi_{N-3}. \quad (41)$$

i	0	1	2	3
ω_i	$-\frac{1}{6}\alpha^3 + \alpha^2 - \frac{43}{24}\alpha + \frac{11}{12}$	$\frac{1}{2}\alpha^3 - \frac{5}{2}\alpha^2 + \frac{23}{8}\alpha + \frac{5}{24}$	$-\frac{1}{2}\alpha^3 + 2\alpha^2 - \frac{11}{8}\alpha - \frac{1}{6}$	$\frac{1}{6}\alpha^3 - \frac{1}{2}\alpha^2 + \frac{7}{24}\alpha + \frac{1}{24}$
$\omega_i(\alpha = 0.5)$	$\frac{1}{4}$	$\frac{13}{12}$	$-\frac{5}{12}$	$\frac{1}{12}$

Table 3: Weightage coefficients for the ghost cell x_0 in a fourth order accurate EB reconstruction scheme for $\tilde{\phi}_s$ on the EB.

4.2.1. Fourth order explicit EB closure

The following EB scheme yields the explicit boundary scheme of Pirozzoli (2002) when $\alpha = 0.5$. For general values of α , the EB condition is $\tilde{\phi}_s = 0$ which is identical to $\tilde{\phi}_{1/2} = 0$ when $\alpha = 0.5$. A k^{th} order EB scheme consistent with the formulation of Pirozzoli (2002) includes a Taylor expansion of ϕ_i w.r.t. $\tilde{\phi}(x_s)$,

$$\phi_i = \frac{1}{\Delta x} \int_{x_{i-1/2}}^{x_{i+1/2}} \tilde{\phi}(x) dx = \sum_{n=0}^{k-1} \left[\left(i + \frac{1}{2} - \alpha \right)^{(n+1)} - \left(i - \frac{1}{2} - \alpha \right)^{(n+1)} \right] \frac{\tilde{\phi}_s^{(n)}}{(n+1)!} \Delta x^n + \mathcal{O}(\Delta x^k) \quad (42)$$

Now, a k^{th} order explicit EB closure for $\tilde{\phi}_s$ is expressed in terms of k regular nodes. Using Eq. 42, we have,

$$\tilde{\phi}_s = \sum_{i=0}^{k-1} \omega_i \phi_i = \sum_{n=0}^{k-1} \left(\sum_{i=0}^{k-1} \omega_i \left[\left(i + \frac{1}{2} - \alpha \right)^{(n+1)} - \left(i - \frac{1}{2} - \alpha \right)^{(n+1)} \right] \right) \frac{\tilde{\phi}_s^{(n)}}{(n+1)!} \Delta x^n + \mathcal{O}(\Delta x^k) \quad (43)$$

where, the weights ω_i are obtained by solving a system of k linear equations obtained by equating the coefficients of $\tilde{\phi}_s^{(n)}$ on both sides for each n . For a fourth order EB scheme ($k = 4$), ω_i are shown in table 3. Finally, ϕ_0 is expressed in terms of ϕ_i , $i = 1, 2, 3$ from Eq. 43 by imposing the EB condition $\tilde{\phi}_s = 0$.

4.2.2. Stability of RK4-UCS5 with fourth order explicit EB scheme

Here, we analyse the stability of the full discretization ($\mathbf{B}$) for RK4-UCS5 method. The von Neumann analysis (assumes periodicity and requires spectral radius $\rho(\mathbf{B}) \leq 1$) gives a necessary condition for stability $C \leq 1.034$ (Pirozzoli, 2002). However, the discretization with the boundary conditions ($\alpha = 0.5$) in Eq. 41 is non-normal and $C = 1.034$ has negligible transient growth ($\mathcal{K}(\mathbf{B}) = 1.01$, $\mu(\mathbf{B}) = 1.11$, $s(\mathbf{B}) = 1.9$ and $\sup \|\mathbf{B}^n\| = 1.9$). We found $C_{\max} \approx 1.05$ not significantly different compared with the von Neumann limit and therefore, we fix $C = 1.034$.

Fig. 13(a-c) shows $\sigma_\varepsilon(\mathbf{B})$ for $C = 1.034$ and $\alpha = 0.5, 0.67, 0.68$, respectively. For $\alpha \geq 0.68$, the spectrum $\sigma(\mathbf{B})$ lies partly outside the unit disk S (Fig. 13c) and therefore, the EB scheme is unstable. For $\alpha = 0.5$, the $\sigma_\varepsilon(\mathbf{B})$ lies within $\mathcal{O}(\varepsilon)$ distance of S (Fig. 13a) with $\mathcal{K}(\mathbf{B}) = 1.01$, $\mu(\mathbf{B}) = 1.11$ and $\sup \|\mathbf{B}^n\| = 1.9$ (Table 4) and is therefore Lax-stable. For $\alpha = 0.67$, $\sigma_\varepsilon(\mathbf{B})$ lies within $\mathcal{O}(\varepsilon)$ distance of S (Fig. 13b) with a bulge near $z = 1$ ($\theta^* = 0$) quantified by $\mathcal{K}(\mathbf{B}) = 4.43$, $d^{*-1} = 25$ (Fig. 7c, Table 1). Further, $\mu(\mathbf{B}) = 1.78$, $\|\mathbf{B}\| = 2.44$ and the transient growth is acceptable with a uniform upper bound $\sup \|\mathbf{B}^n\| = 6.44$, $n^* = 20$ (Fig. 8c, Table 1). Therefore, the discretization is Lax-stable for $\alpha \leq 0.67$. Fig. 13(d-f) demonstrates that the solution at $t = 0.1$ is stable for $\alpha \leq 0.67$ and unstable for $\alpha \geq 0.68$.

Figure 13: Explicit RK4 - UCS5 discretization with $C = 1.034$: ε -pseudospectra of B with $\varepsilon = 10^{-6}, 10^{-4}, 10^{-2}$ when (a) $\alpha = 0.50$, (b) $\alpha = 0.67$, (c) $\alpha = 0.68$; and the solution $\phi(x, t)$ at $t = 0.1$ for (d) $\alpha = 0.50$, (e) $\alpha = 0.67$, (f) $\alpha = 0.68$. The thick dashed line denotes boundary of the numerical range $W(B)$ of the full discretization. Here, $N = 100$.

5. Advection-diffusion equation in 1D

Because the advection-diffusion equation serves as an important surrogate for the Navier-Stokes equations, we now briefly analyze the stability of the advection-diffusion in 1D in the presence of an embedded boundary (EB).

$$\frac{\partial \phi}{\partial t} + U \frac{\partial \phi}{\partial x} = \kappa \frac{\partial^2 \phi}{\partial x^2}, \quad x_s \leq x \leq x_N, \quad (44)$$

$$\phi(x_s, t) = 0, \quad \phi(x_{N+1}, t) = 0, \quad \phi(x, 0) = f(x). \quad (45)$$

An important non-dimensional parameter that indicates the relative importance of advection to diffusion is the cell Péclet number or the cell Reynolds number, $Re \equiv \frac{U \Delta x}{\kappa} = \frac{C}{D}$. Here, $D \equiv \frac{\kappa \Delta t}{\Delta x^2}$ is the Diffusion number. A method of lines semi-discretization leads to,

$$\frac{d\phi_i}{dt} = -U \frac{\delta \phi_i}{\delta x} + \kappa \frac{\delta}{\delta x} \frac{\delta \phi_i}{\delta x} = A_{ij} \phi_j, \quad i = 1, 2, \dots, N. \quad (46)$$

5.1. RK3-CDS scheme

We consider CDS for the spatial derivatives (both advection and diffusion terms) and RK3 method for temporal integration. The spectrum of the mixed advection-diffusion operator $\Delta t A$ with the CDS lies inside an ellipse

Figure 14: RK3 - CDS discretization of advection-diffusion equation (Eq. 44) in 1D with $C = 1.7$ and/or $D = 0.625$ and $\alpha = 0.5$: ε -pseudospectra of $\Delta t A$ with $\varepsilon = 10^{-6}, 10^{-4}, 10^{-2}$ for (a) $Re = 0.2$, (b) $Re = 1$, (c) $Re = 2$, (d) $Re = 10$, (e) $Re = 20$, (f) $Re = 2000$.

with semi-axes $2D$ and C . Necessary conditions of stability of the RK3-CDS scheme in case of the ideal domain ($\alpha = 0$ or no EB) require $C \leq C_{\max} = 1.7, D \leq D_{\max} = 0.625$. Therefore, the time step is determined as $\Delta t = \min\{C_{\max}\Delta x/U, D_{\max}\Delta x^2/\kappa\}$. At $Re = 2.72$, $C = C_{\max}$ and $D = D_{\max}$ which implies that $Re_c = 2.72$ is the crossover Reynolds number where, diffusion dominates with $\Delta t \propto \Delta x^2$ below Re_c and advection dominates with $\Delta t \propto \Delta x$ above Re_c .

Fig. 14 shows the ε -pseudospectra of RK3-CDS scheme with $\alpha = 0.5$, $N = 100$ and Re ranging from 0.2 to 2000 for $\varepsilon = 0.01, 0.1, 0.2, 0.3$ are shown. At low $Re = 0.2$, the eigenvalues lie on the negative real axis (Fig. 14a). The eigenvalue due to the EB (λ_{EB}) lies on the boundary of the stability region S at $z = -2.5$. The corresponding ε -pseudospectra lies within a distance ε of S . For $\alpha > 0.5$, the eigenspectrum lies outside S indicating instability. As the Re increases, D and, consequently, the minor axis of the ellipse (ordinate) increases as shown in Fig. 14(b) for $Re = 1$. At $Re = 2$, both the semi-axes are equal with $C = 2D = 1.25$ (Fig. 14c) and the λ_{EB} lies on the boundary of S when $\alpha = 0.5$.

Above $Re = 2.72$, advection dominates diffusion and the spectrum approaches that of the wave equation as

Figure 15: Schematic of the reconstruction stencil in 2D for (a) an exterior/solid ghost cell G and (b) an interior/fluid ghost cell G near an arbitrarily oriented EB. Ghost cell (G) is reconstructed using three regular nodes (P_1, P_2, P_3) and a boundary condition at the surface node $S(x_s, y_s)$. The stencil may include other ghost cells.

$Re \rightarrow \infty$. Fig. 14(d-f) shows the spectrum for $Re = 10, 20, 2000$, respectively, which is spread almost vertically and approaches the imaginary axis as the Re increases. As Re increases, the λ_{EB} with $\alpha = 0.5$ moves away from the left boundary and towards the right boundary of the stability region S . This is consistent with the inviscid case which has $\alpha_{\max} = 0.76$ for RK3-CDS as discussed in Sec. 3.

We note that Brehm and Fasel (2013) developed stable discretizations for advection-diffusion equation in the range $2.4 \leq Re < 1667$ for RK4 – CDS discretization with $C = 0.5, N = 60$ and $Re = 22 - 216$ for RK4 – CDS4 with $C = 1$. In their method, the stencil coefficients depend on the physical quantities such as the advection speed U and the diffusion coefficient κ . In contrast, our method is independent of the physical properties and is stable for inviscid and viscous problems over the entire range $0 \leq Re < \infty$.

6. Complex EB: hybrid ghost cells (HGC)

In this section, we consider the reconstruction procedure for general, complex EB which may have arbitrary curvature and, in general, not be aligned with the Cartesian grid. Based on the stability analysis in earlier sections, we reclassify conventional ghost cells to hybrid ghost cells (HGC) which are expected to yield stable discretizations. Furthermore, superior stability characteristics of HGC over conventional ghost cells are demonstrated. In the following sections, FLUID region refers to the interior of the domain and SOLID region refers to the exterior of the domain.

6.1. Reconstruction method for complex EB in 2D

For two dimensional boundaries embedded in a Cartesian grid, a direct bilinear reconstruction for ghost nodes (G), proposed in Rapaka et al. (2018) and shown below, is used. It includes three regular nodes and a Dirichlet boundary condition at the surface node S on EB (see Fig. 15).

$$\phi_G = \omega_1\phi_1 + \omega_2\phi_2 - \omega_1\omega_2\phi_3 + (1 - \omega_1)(1 - \omega_2)\phi_s, \quad \omega_1 = \frac{x_1 - x_s}{x_2 - x_s}, \quad \omega_2 = \frac{y_1 - y_s}{y_2 - y_s}, \quad (47)$$

where subscripts 1 and 2 represents the immediate neighbor nodes along the x, y -directions towards the interior/fluid region, as shown in Fig. 15. Subscript 3 indicates the diagonal node towards the interior/fluid region and subscript s indicates the surface node $S(x_s, y_s)$ located at the intersection of the EB with the surface normal passing through the ghost node. Here, $\phi_s = 0$ is imposed at the surface node S . Note that the stencil may include other ghost cells which usually requires a iterative solution procedure during the reconstruction. However, we propose a procedure that eliminates the need for iterative solution in Rapaka et al. (2018).

6.2. Hybrid ghost cells

Conventional ghost cell methods (Tseng and Ferziger, 2003; Mittal et al., 2008) restrict the ghost cells to the solid region by considering only those cells that satisfy $0 \leq \alpha_{x_i} < 1$. In contrast, other approaches (Roman et al., 2009; Kang et al., 2009) restrict the reconstruction to near boundary cells inside the fluid region that satisfies $-1 < \alpha_{x_i} \leq 0$. While the former approach suffers from possible numerical instabilities when combined with Eq. 47, the latter approach suffers from larger numerical error/mass leakage due to reconstruction stencils extending far into the interior/fluid region.

Ideally, the reconstruction method must be stable and should also have compact reconstruction stencils for better accuracy. To achieve this, consider the near boundary cells that satisfy the sufficient condition of stability: $\alpha \leq \alpha_{\max}$ when $C = C_{\max}$. This requires,

$$|\alpha_{x_i}| = \frac{|\psi_G n_{x_i}|}{\Delta x_i} \leq \alpha_{\max}. \quad (48)$$

Here, no summation is implied over the repeated index i ; n_{x_i} are components of the unit surface normal vector and $|\psi_G| = \|\vec{x}_G - \vec{x}_s\|$ is the distance between the ghost cell center (G) and the surface node (S) located at the intersection of the EB with the surface normal passing through G (see Fig. 15). Table 1 shows that $\alpha_{\max}$ ranges from 0.5 to 0.77 for the spatio-temporal discretizations considered in this work. Therefore, $\alpha_{\max} = 0.5$ is sufficient for the stability of all the discretizations considered in this work. In some cases, Eq. 48 may yield redundant ghost cells, for example, cells with $|\psi_G|$ ranging between $\Delta x/2 - \sqrt{3}\Delta x/2$ for isotropic grids in 3D. To remove these redundant cells from the method, and thus reduce the distance from the ghost cells to the EB, we consider only those ghost cells with the surface node S inside an ellipsoid centered at G with semi-axes $\alpha_{\max}(\Delta x, \Delta y, \Delta z)$. Mathematically, such ghost cells can be identified in three dimensions as

$$\|\vec{x}_G - \vec{x}_s\| = |\psi_G| \leq R, \quad \text{if } \vec{x}_G \in \text{SOLID}, \quad \|\vec{x}_G - \vec{x}_s\| = |\psi_G| < R, \quad \text{if } \vec{x}_G \in \text{FLUID}, \quad (49)$$

where R is the boundary normal radius of the ellipsoid given below,

$$R \equiv \alpha_{\max} \left[\left(\frac{n_x}{\Delta x} \right)^2 + \left(\frac{n_y}{\Delta y} \right)^2 + \left(\frac{n_z}{\Delta z} \right)^2 \right]^{-\frac{1}{2}}, \quad (50)$$

with the surface normal (n_x, n_y, n_z) pointing into the fluid region. For isotropic grids, $R = \alpha_{\max} \Delta x$. Henceforth, we set $\alpha_{\max} = 0.5$ so that Eqs. 49 and 50 ensure $|\alpha_{x_i}| \leq 0.5$ in multi-dimensions and minimize the distance from the ghost cells to EB. Consequently, the reconstruction method has compact stencil and is inherently stable. But, the ghost cells now lie on both sides of the EB and henceforth, we refer to these as “hybrid ghost cells” (HGC). For grids that are nearly isotropic around EB, the EB geometry does not pose problem in finding HGC (cells within distance R of EB). However, highly anisotropic grids near EB may yield situations where HGC can not be found. Though EB methods typically employ isotropic grids near EB, it may not be practically feasible in some applications with significantly different length scales in different directions (e.g., oceanic flows). In Rapaka et al. (2018), we propose a simple solution for such cases through anisotropic stencil width which allows Eq. 47 to satisfy the stability criteria.

6.3. Stability of hybrid ghost cells

We presently test whether the HGC yield stable reconstruction in case of a general, curved EB (Eq. 47) for which the neighboring cell along the diagonal may have a non-trivial contribution. We consider the 2D wave equation (Eq. 27) in a unit domain enclosing a quarter circle with radius 0.5 (Fig. 16a). The domain $0 \leq x, y \leq 1$ is discretized with $N_x = N_y = 20$. We use $U_x = U_y = 1$ and the following boundary and initial conditions for further analysis.

$$\phi(0, y, t) = 0, \quad \phi(x, 0, t) = 0, \quad \phi(x_s, y_s, t) = 0 \quad (51)$$

$$\phi(x, y, 0) = \begin{cases} \frac{(1 + \tanh x^*)}{2} \frac{(1 + \tanh y^*)}{2} \frac{(1 + \tanh \psi^*)}{2}, & x, y \in \text{FLUID} \\ 0, & x, y \in \text{SOLID} \end{cases} \quad (52)$$

where, $x^* = (x - x_c)/\sigma$, $y^* = (y - x_c)/\sigma$, $\psi^* = (-\psi - x_c)/\sigma$, and ψ is the signed distance function with $\psi < 0$ in the fluid region and $\psi > 0$ for the solid region. Here, we choose $x_c = 0.05$ and $\sigma = \Delta x = 0.05$ so that the tanh profile is spread over few Δx .

We consider bilinear reconstruction (Eq. 47) with both the conventional ghost cells (Fig. 16a) and the hybrid ghost cells (Fig. 16d). Fig. 16(a) shows the conventional ghost cells (tagged with +2) with their center lying inside the solid region so that $0 \leq \alpha_x, \alpha_y < 1$ (Mittal et al., 2008; Tseng and Ferziger, 2003). Fluid and solid cells are tagged with 0 and 1, respectively. The filled circles are the surface nodes $S(x_s, y_s)$ where the boundary condition is imposed. Similarly, Fig. 16(d) shows the hybrid ghost cells (HGC) with their centers lying on either side of the EB (tagged with +2 in solid and -2 in fluid), resulting in $-0.5 \leq \alpha_x, \alpha_y < 0.5$. Note that the EB intersects all the HGC (Fig. 16d), and all the surface nodes S lie inside the HGC which may not be true for the conventional ghost cells (Fig. 16a). Also, when $N = 20$, the HGC have $\max(\alpha_x) = \max(\alpha_y) = 0.486$ while the conventional ghost cells have $\max(\alpha_x) = \max(\alpha_y) = 0.747$.

Figure 16: RK3-UWS discretization with $C = 1.25$ and $N_x = N_y = 20$: (a) conventional ghost cells (Mittal et al., 2008; Tseng and Ferziger, 2003) are tagged with +2 and located in the solid region only, $0 \leq \alpha_x, \alpha_y < 1$, $\max(\alpha_{x,y}) = 0.747$, (b) the ε -pseudospectra of $\Delta t A$, (c) $\phi(x, y, t)$ at $t = 0.25$, (d) hybrid ghost cells (present) are tagged with ± 2 and located in both the solid (+2) and the fluid (-2) regions, $-0.5 \leq \alpha_x, \alpha_y < 0.5$, $\max(\alpha_{x,y}) = 0.486$, (e) the ε -pseudospectra of $\Delta t A$, (f) $\phi(x, y, t)$ at $t = 0.25$. Filled circles in (a) and (d) are the surface nodes $S(x_s, y_s)$.

6.3.1. RK3-UWS discretization

Fig. 16(b) shows the ε -pseudospectra of the RK3-UWS scheme with $C = C_{\max} = 1.25$ and reconstruction (Eq. 47) at the conventional ghost cells. Some of the eigenvalues lie outside the stability region S indicating the method to be linearly unstable. This is expected because $\max(\alpha_x) = \max(\alpha_y) = 0.747$ which is greater than $\alpha_{\max} = 0.5$ for the RK3-UWS method. The instability is evident from examining the solution at time $t = 0.25$, shown in Fig. 16(c), in which exponentially growing perturbations originate at the EB, around locations $(0.45, 0.2)$ and $(0.2, 0.45)$ where α_x, α_y are above the stability limit, respectively.

Similarly, Fig. 16(e) shows the ε -pseudospectra of the RK3-UWS scheme with $C = 1.25$ and reconstruction (Eq. 47) at the HGC. All the eigenvalues lie inside the stability region S and the ε -pseudospectra lies within $\mathcal{O}(\varepsilon)$ distance of the stability region S ($\mathcal{K}(\mathbf{B}) = 1.02$, $\sup \|\mathbf{B}''\| = 1.02$). Note that the eigenvalue at the origin corresponds to the solid cells where the solution remains constant at zero. Also, the bulge in the pseudospectra near the origin appears

merely due to the non-smooth union of the ε -disks at the origin with the ε -pseudospectra of the eigenvalues associated with the fluid region. Here, the solution is expected to be stable because $\max \alpha_x = \max \alpha_y = 0.486$ which is less than $\alpha_{\max} = 0.5$ for the RK3-UWS method. Furthermore, the stability of HGC is evident from the solution at time $t = 0.25$, shown in Fig. 16(f), which has no sign of growing perturbations in the entire domain.

6.3.2. RK3-CDS discretization

Figure 17: RK3-CDS discretization with $C = 1.7$ and $N_x = N_y = 24$: (a) conventional ghost cells (Mittal et al., 2008; Tseng and Ferziger, 2003) are tagged with +2 and located in the solid region only, $0 \leq \alpha_x, \alpha_y < 1$, $\max(\alpha_{x,y}) = 0.884$, (b) the ε -pseudospectra of $\Delta t A$, (c) $\phi(x, y, t)$ at $t = 0.2$; (d) hybrid ghost cells (present) are tagged with ± 2 and located in both the solid (+2) and the fluid (-2) regions, $-0.5 \leq \alpha_x, \alpha_y < 0.5$, $\max(\alpha_{x,y}) = 0.489$, (e) the ε -pseudospectra of $\Delta t A$, (f) $\phi(x, y, t)$ at $t = 0.2$. Filled circles in (a) and (d) are the surface nodes $S(x_s, y_s)$.

Here, we test the stability of the RK3-CDS scheme with $C = C_{\max} = 1.7$ applied over the same domain. According to Table 1, the RK3-CDS scheme must yield stable solution even with the conventional ghost cells because $\max(\alpha_x) = \max(\alpha_y) = 0.747$ while $\alpha_{\max} = 0.76$ for the RK3-CDS scheme. Indeed, we verified this to be true (not shown here). In order to demonstrate an unstable case, we adopt the spatial grid size to $N_x = N_y = 24$ so that the conventional ghost cells yield $\max(\alpha_x) = \max(\alpha_y) = 0.884$ (Fig. 17a) while the HGC yield $\max(\alpha_x) = \max(\alpha_y) = 0.489$ (Fig. 17d). Again, note that all the surface nodes lie within the HGC.

Fig. 17(b) shows the ε -pseudospectra of the RK3-CDS scheme with $C = 1.7$ and reconstruction (Eq. 47) at the conventional ghost cells. Some of the eigenvalues lie outside the stability region S and render the method linearly unstable, as expected. Evidently, the solution at time $t = 0.2$ (Fig. 17c) exhibits exponentially growing perturbations along the EB, particularly near the cells with the largest α_x, α_y .

On the other hand, for the HGC, Fig. 17(e) shows the ε -pseudospectra of the RK3-CDS scheme with $C = 1.7$ and reconstruction (Eq. 47) with all the eigenvalues within the stability region S and the ε -pseudospectra within $\mathcal{O}(\varepsilon)$ distance of the stability region S ($\mathcal{K}(\mathbf{B}) = 1.57, \sup \|\mathbf{B}^n\| = 2.14$). This implies that the method is stable according to Eq. 8 and is evident from the solution at time $t = 0.2$ (Fig. 17f) which has no sign of growing perturbations in the entire domain.

We demonstrated the superior stability properties of HGC over conventional ghost cells in the presence of 2D complex EB for RK3-UWS and RK3-CDS schemes. The same is expected for other schemes considered in this work and are not explored further here.

HGC yield maximum transient growth with $\alpha = 0.5$ for a fixed C because HGC satisfy $\alpha \leq 0.5$. Table 4 shows the spectral radius $\rho(\mathbf{B})$, the Kreiss constant $\mathcal{K}(\mathbf{B})$, numerical radius $\mu(\mathbf{B})$, the largest singular value $s_{\max}(\mathbf{B})$ and the supremum of $\|\mathbf{B}^n\|$ for $C = C_{\max}$ and $\alpha = 0.5$ in 1D to quantify the maximum possible growth for HGC. Both the $\mathcal{K}(\mathbf{B})$ and the $\mu(\mathbf{B})$ are $\mathcal{O}(1)$ and the expected growth of perturbations is negligible as indicated by $\sup \|\mathbf{B}^n\|$. Moreover, the transient growth peaks within few time steps ($\mathcal{O}(1)$ except for UWS) indicated by $n^* = \mathcal{O}(d^{*-1})$ in Table 4. In practical applications involving non-linear fluid flow, typically $C < 1 < C_{\max}$ is widely used and, therefore, the HGC are expected to yield negligible transient growth.

It is worthwhile to mention that the immersed interface method (IIM) of Brehm and Fasel (2013) uses an additional node in the reconstruction stencil than required by the order of accuracy, thereby introducing a free parameter. This parameter is then optimized to either yield $\rho(\mathbf{B}) \leq 1$ or minimize $\|\mathbf{B}\|_2$ (need not be $\|\mathbf{B}\|_2 \leq 1$) through localization assumption so that the stability is improved in the limit $\alpha \rightarrow 1$. Interestingly, they reported that the optimization problem needs to be solved only for $0.4 \leq \alpha \leq 1$ for the second interior node in an explicit fourth order scheme and it was sufficient to ignore the additional node for $\alpha < 0.4$. This implies that as α increases from 0.4 to 1, the magnitude of the weightage coefficient decreases for the interior node closest to EB and increases for the interior node farthest to EB (the additional node) in a continuous sense. Therefore, the optimized free parameter exerts a larger influence on the stability as α approaches 1. Notably, reconstruction methods involving least squares approach also make use of additional nodes to improve stability (Peller et al., 2006; Vanella and Balaras, 2009; Li et al., 2015).

In contrast, our method uses *a priori* stability criteria (table 1) and reclassifies conventional ghost cells to HGC which effectively moves the stencils closer to the interior/fluid region by one cell for $\alpha > \alpha_{\max}$ in a discrete sense. Consequently, our method has no additional computational expense while the method of Brehm and Fasel (2013) requires a runtime optimization of the stencil coefficients that depends on the specific problem parameters such as diffusivity/cell Reynolds number. For moving boundary problems, this step may be computationally expensive and complicated as the stencil coefficients need to be computed at every time step. Moreover, the optimization procedure

	$\rho(\mathbf{B})$	$\mathcal{K}(\mathbf{B})$	d^{*-1}	n^*	$\mu(\mathbf{B})$	$s_{\max}(\mathbf{B})$	$\sup \ \mathbf{B}^n\ $	C
description	$\max z , z \in \sigma(\mathbf{B})$	$\sup \frac{\rho(\mathbf{B})-1}{\varepsilon}$	$\sup \hat{\mathcal{K}}(d)$	$\mathcal{O}(d^{*-1})$	$\sup_{ z =1} z^* \mathbf{B} z $	$\ \mathbf{B}\ _2$	1D	CFL
EE - UWS	0.98	2.03	22.9	24	1.23	1.39	3.11	0.99
RK3-UWS	0.98	2.74	22.4	24	1.39	1.66	4.25	1.25
RK4-UWS	0.96	2.06	12.6	13	1.33	1.53	3.07	1.38
RK3-CDS	0.99*	1.00	0.0	1	1.00	1.24	1.24	1.70
RK4-CDS	0.99*	1.00	0.2	2	1.04	1.47	1.48	2.825
RK3-CDS4	0.99*	1.17	0.6	1	1.62	2.81	2.81	1.25
RK4-CDS4	0.94*	2.08	1.0	1	3.55	6.80	6.80	2.05
RK4-UCS5	0.66*	1.01	0.3	1	1.11	1.90	1.90	1.034

Table 4: Spectral radius ρ , Kreiss constant $\mathcal{K}$, numerical radius μ and the largest singular value $s_{\max}$ of the full discretization $\mathbf{B}$ for various schemes with $\alpha = 0.5$ in 1D. HGC ($\alpha \leq 0.5$) yield maximum transient growth for $\alpha = 0.5$. Here, $C = C_{\max}$ for all cases except $C = 0.99$ for EE-UWS as the scheme is Lax-stable for $C < 1, \alpha = 0.5$ and only algebraically stable for $C = C_{\max} = 1, \alpha = 0.5$). Notably, $\sup \hat{\mathcal{K}}(d) = \mathcal{K}(\mathbf{B})$ occurs at $d = d^*$, $\sup \|\mathbf{B}^n\|$ occurs at $n = n^* = \mathcal{O}(d^{*-1})$ and the solution grows by at least $\mathcal{K}(\mathbf{B})$ times in $n^* = \mathcal{O}(d^{*-1})$ time steps. We also report results using RK4 time marching method with UWS, CDS, CDS4 but omit the discussion in the article. $^*\rho(\mathbf{B})$ is shown for $N = 100$ and approaches unity as N increases. All other values are independent of N for $N > \mathcal{O}(d^{*-1})$.

of Brehm and Fasel (2013) does not account for non-normal stability/sufficient conditions of stability and uses localization approximation. Also, in multi-dimensions, their stencils follow Cartesian directions only in contrast to our method that includes the diagonal/boundary normal direction in addition to the Cartesian directions.

7. Conclusions

We employed pseudospectra to analyse the non-modal stability of embedded boundary methods (EBM) in the context of discrete linear initial boundary value problems. In particular, the scalar wave equation is extensively analysed in one and two dimensions. The method of lines approach is employed with spatial and temporal discretizations of varying accuracy ($2^{nd} - 5^{th}$) including both central and upwind biased schemes.

Stability of EBM is a function of the Courant number (C) and the distance of the embedded boundary (EB) to the ghost cell center normalized by the grid spacing (α). An objective of practical importance is that the CFL condition $C \leq C_{\max}$ remains unaffected by the EB. Then, the stability depends only on α . The boundary conditions and/or EB reconstruction method are potential sources of non-normality which may result in transient growth. Upper bounds on the transient growth are estimated in terms of the Kreiss constant $\mathcal{K}(\mathbf{B})$ and compared with the supremum of $\|\mathbf{B}^n\|$. These bounds provide only algebraic stability conditions (depends on the grid size N, n). Here, Lax-stability is verified by explicitly checking the dependency on the grid size.

Pseudospectra of various schemes revealed that the Lax-stability requires $\alpha \leq \alpha_{\max}$ which ranges from 0.5 to 0.77 for various schemes considered in one dimension. Moreover, $\alpha_{\max}$ for UWS and CDS schemes remain the same in two dimensions as well and the same is expected for other schemes also.

A fourth order EB reconstruction stencil is developed and is tested to be stable with fourth order central scheme (CDS4) and fifth order upwind biased compact scheme (UCS5). Furthermore, the analysis is briefly extended to the advection-diffusion equation in one dimension.

This stability analysis motivates reclassification of the ghost cells to “hybrid ghost cells” (HGC) which ensures $\alpha \leq \alpha_{\max}$, in particular $\alpha \leq 0.5$. Stability of HGC for general complex boundaries in 2D is demonstrated for RK3-UWS and RK3-CDS discretizations. HGC yield stable reconstruction even when the conventional ghost cells yield unstable reconstruction for the same spatial and temporal discretization. They also minimize the discretization error ($\alpha \leq 0.5$) and maintain the Courant number C at its ideal value $C_{\max}$.

In contrast to the approach of Brehm and Fasel (2013), HGC offer simple and robust reconstruction without any additional computational expense, do not require any localization approximations and the stability characteristics are independent of flow parameters such as Reynolds number. Moreover, Brehm and Fasel (2013); Brehm et al. (2015) employ an optimization procedure that minimizes the largest singular value of the full discretization matrix (need not be less than 1) to compute stable reconstruction stencils. As such the stencil coefficients are determined based on the localization assumption and depend on the flow properties. Also, their method is stable for cell Reynolds number $2.4 \leq Re_{\Delta x} \leq 1600$ while our method using HGC is stable in both the viscous and the inviscid regimes $0 \leq Re_{\Delta x} \leq \infty$.

Although Lax-stability allows transient growth of finite amplitude independent of the spatial and the temporal grid size, the magnitude itself must be small for practical stability of numerical simulations, preferably $\mathcal{O}(1)$. This ensures that the discretization and round-off errors remain at the same order of magnitude. Quantitative estimates are presented in terms of the Kreiss constant, spectral radius, numerical radius and the largest singular value of the full discretization matrix $\mathbf{B}$. These estimates are compared with the actual growth among which the Kreiss constant based on the pseudospectral radius provides the sharpest estimate. A key result is that reconstruction through HGC confines the transient growth to $\mathcal{O}(1)$ for all spatial and temporal discretizations considered in this work. This implies Lax-stability of the discretizations which is essential for reliable numerical simulations of flows involving complex EB.

We conclude that HGC offer simple, robust, parameter independent and inexpensive reconstruction for discretizations involving embedded boundaries and are an attractive alternative to the existing methods. Also, the stability estimates based on the pseudospectra provide sharper estimates compared with those based on the singular value decomposition.

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