

EIGENVALUE ANALYSIS FOR SUMMATION-BY-PARTS FINITE DIFFERENCE TIME DISCRETIZATIONS*

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Abstract. Diagonal norm finite difference based time integration methods in summation-by-parts form are investigated. The second, fourth, and sixth order accurate discretizations are proven to have eigenvalues with strictly positive real parts. This leads to provably invertible fully discrete approximations of initial boundary value problems. Our findings also allow us to conclude that the Runge–Kutta methods based on second, fourth, and sixth order summation-by-parts finite difference time discretizations automatically satisfy previously unreported stability properties. The procedure outlined in this article can be extended to even higher order summation-by-parts approximations with repeating stencil.

Key words. time integration, initial value problem, summation-by-parts operators, finite difference methods, eigenvalue problem

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1. Introduction. Implicit time integration methods can be used to reduce severe stability restrictions for stiff spatially discretized well-posed initial boundary value problems. Summation-by-parts (SBP) operators [12, 21], with simultaneous-approximation-terms (SAT) weakly imposing boundary and initial conditions, allow for energy-stable and high order accurate approximations [6, 17, 14, 3]. The solution of the resulting fully discrete problem is unique, provided that the eigenvalues of the time discretization operator have strictly positive real parts [17, 14, 18]. This assumption on the eigenvalues has been proved for pseudospectral collocation methods [19] and second order finite difference discretizations [17]. However, it does not hold for all types of SBP-SAT approximations [18, 13], and it has only been conjectured for higher order finite difference methods [17, 14].

The dual-consistent [2, 9] SBP-SAT time discretizations based on finite difference methods are also A -, L -, and B -stable [14]. However, the existence of eigenvalues with strictly positive real parts allows for the proof of various additional stability properties [13]. In this article, we prove that second, fourth, and sixth order accurate SBP-SAT time approximations based on diagonal-norm finite difference methods have eigenvalues with strictly positive real parts. We also provide a general procedure that can be used to show that this property also holds for higher order approximations with repeating stencil.

The paper is organized as follows. In section 2, the finite difference based SBP-SAT time discretizations are introduced for initial value problems. The invertibility of the resulting algebraic problem is reinterpreted in terms of the eigenvalues of the time operator. Section 3 deals with the eigenvalue analysis of second order approximations in SBP form. In this case, the eigenvalues can be computed in closed form by means

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of a necessary and sufficient condition for the existence of the eigenvectors. This condition outlines a general procedure for a proof that the fourth (section 4) and sixth order (section 5) accurate time approximations fulfill the eigenvalue assumption. In section 6, we demonstrate numerically that the theoretical results are correct. We also provide final remarks about our findings and relate these to Runge–Kutta methods. The conclusions are given in section 7.

2. Finite difference implicit methods for initial value problems. In this section we briefly introduce finite difference based SBP-SAT approximations for initial value problems [17] and discuss their invertibility [19].

2.1. SBP-SAT time discretizations. Let $\mathbf{t} = [t_0, t_1, \dots, t_N]^T$ be a set of $N+1$ equidistant nodes $t_j = \alpha + j\Delta t$, with $j = 0, \dots, N$, and $\Delta t = (\beta - \alpha)/N$. A finite difference based SBP operator discretizing the first derivative on \mathbf{t} can be defined as follows [21].

DEFINITION 2.1. A discrete operator $D = P^{-1}Q$ is a (p, q) -accurate approximation of the first derivative with the SBP property if (i) its truncation error is $\mathcal{O}(\Delta t^p)$ in the interior and $\mathcal{O}(\Delta t^q)$ at the boundaries, (ii) P is a symmetric positive definite matrix, and (iii) $Q + Q^T = B = \text{diag}(-1, 0, \dots, 0, 1)$.

Condition (ii) in Definition 2.1 defines a norm induced by P , which is a discrete counterpart to the one in $L^2(\alpha, \beta)$. In particular, by denoting with $\mathbf{v} = [v_0, \dots, v_N]$ the vector of the function evaluations of a real-valued function $v(t)$, $t \in [\alpha, \beta]$, onto the grid nodes \mathbf{t} , we can write

$$\|\mathbf{v}\|_P := \sqrt{\mathbf{v}^T P \mathbf{v}} \approx \sqrt{\int_{\alpha}^{\beta} v^2 dt}.$$

SBP operators based on centered finite differences and diagonal norms P are available for even orders $p = 2q$ in the interior, while the boundary closure is q th order accurate. We will for stability reasons [15, 7, 22] only consider operators with a diagonal P . Under this assumption, the global truncation error of first derivative SBP-SAT discretizations with diagonal norms and pointwise bounded solution is $\mathcal{O}(\Delta t^{q+1})$ [24]. However, dual consistent formulations exhibit a superconvergent behavior for the solution at the last time-step, with an accuracy of $\mathcal{O}(\Delta t^{2q})$ [2, 9]. For this reason we will refer to $(2q, q)$ -accurate approximations as $2q$ th order discretizations.

The restriction to diagonal norms makes the second and fourth order accurate SBP first derivative operators with minimal bandwidth unique [21]. For higher order approximations, the SBP operators D are usually given in terms of free parameters which can be tuned to fulfill additional constraints, such as, for example, minimizing the bandwidth [21], reducing the error constant, and minimizing the spectral radius [23].

2.2. The initial value problem and its discretization. Consider the initial value problem

$$(2.1) \quad \begin{aligned} u_t + \lambda u &= 0, & 0 < t < T, \\ u(0) &= f, \end{aligned}$$

where the complex constant λ represents the eigenvalue of a suitable spatial discretization of an initial boundary value problem. Assuming that the corresponding semidiscrete approximation is energy-stable, it is known that $\text{Re}(\lambda) \geq 0$ [17].

To obtain an estimate of the solution at $t = T$, we apply the energy method (multiplying by the complex conjugate of u , integrating in time, and using integration by parts) to (2.1) and get

$$(2.2) \quad |u(T)|^2 + 2\operatorname{Re}(\lambda)\|u\|^2 = |f|^2.$$

In (2.2), $\|u\|^2 = \int_0^T |u|^2 dt$ and the solution at the final time is bounded by the initial data.

A discrete approximation of the initial value problem (2.1) can be obtained by using the SBP operators in Definition 2.1. These allow for a perfect mimicking of the energy method used to get the continuous estimate (2.2). In particular, by considering the grid $\mathbf{t} = [t_0, \dots, t_N]^T \subset [0, T]$, the SBP discretization of (2.1) with a weakly imposed initial condition using SAT reads

$$(2.3) \quad P^{-1}Q\mathbf{u} + \lambda\mathbf{u} = \sigma P^{-1}E_0(\mathbf{u} - f\mathbf{e}_0),$$

where $\mathbf{e}_0 = [1, 0, \dots, 0]^T$. In (2.3), the vector $\mathbf{u} = [u_0, \dots, u_N]^T$ contains the numerical approximations of u at each t_i , $i = 0, \dots, N$, i.e., $u_i \approx u(t_i)$. Moreover, σ is a penalty parameter and $E_0 = \operatorname{diag}(1, 0, \dots, 0)^T$. If $\sigma = -1$, the approximation is dual consistent [2, 16], and it is also known to be A -, L -, and B -stable [14].

Remark 2.2. Although the approximation in (2.3) is based on equidistant grids, the results of this article can be easily extended to discretizations with nonconstant time-step by applying a nonlinear transformation to (2.1).

By applying the discrete energy method to (2.3) (multiplying by \mathbf{u}^*P , where $*$ denotes the conjugate transpose, and using the SBP property), we find [17]

$$(2.4) \quad |u_N|^2 + 2\operatorname{Re}(\lambda)\|\mathbf{u}\|_P^2 = (1 + 2\sigma)|u_0|^2 - \sigma(\overline{u_0}f + u_0\overline{f}).$$

In (2.4), the bar indicates complex conjugation. The dual consistent choice $\sigma = -1$ leads to

$$|u_N|^2 + 2\operatorname{Re}(\lambda)\|\mathbf{u}\|_P^2 = |f|^2 - |u_0 - f|^2,$$

which mimics the continuous estimate (2.2). The additional term on the right-hand side adds numerical dissipation, which vanishes as the number of nodes increases.

The estimate (2.4) indicates that the discretization (2.3) is energy-stable for $\sigma \leq -1/2$, which implies that the approximation of the solution at the final time is bounded by data. However, the invertibility of (2.3) for SBP-SAT discretizations based on centered finite differences with order higher than two is unclear [17, 3, 19]. To begin the analysis, we recast the problem (2.3) as

$$(2.5) \quad (\mathcal{D} + \lambda I)\mathbf{u} = \mathbf{F},$$

where $\mathcal{D} = P^{-1}(Q - \sigma E_0)$ and $\mathbf{F} = -\sigma f P^{-1}\mathbf{e}_0$. Under the assumption $\operatorname{Re}(\lambda) \geq 0$, we conclude that the following proposition holds.

PROPOSITION 2.3. *The discrete problem (2.5) leads to an invertible system if the operator \mathcal{D} has eigenvalues with strictly positive real parts.*

The eigenvalues of the discrete operator \mathcal{D} will henceforth be denoted by μ . These eigenvalues were proved to have strictly positive real parts for SBP-SAT approximations based on pseudospectral collocation methods [19]. On the other hand, $\operatorname{Re}(\mu) > 0$ is not fulfilled for all types of SBP operators [18, 13], and hence the invertibility of (2.5) is in general not guaranteed.

For dual-consistent finite difference approximations (i.e., for $\sigma = -1$), $\operatorname{Re}(\mu) > 0$ leads not only to the uniqueness of the solution of (2.5) but also to null-space consistency of the SBP operator $D = P^{-1}Q$ associated to \mathcal{D} [25]. The operator D is said to be null-space consistent when $D\mathbf{w} = \mathbf{0}$ if and only if $\mathbf{w} \in \operatorname{Span}\{\mathbf{1}\}$, where $\mathbf{1} = [1, \dots, 1]^T$. If this property holds, the problem (2.5) can be reinterpreted as a Runge–Kutta time integration method satisfying various stability properties [13]. In the following we will prove strict positivity of $\operatorname{Re}(\mu)$ for discretizations based on SBP operators with a repeating stencil, such as the second, fourth, and sixth order accurate finite difference formulations.

2.3. The eigenvalue problem for repeating stencil approximations. We recall the following theorem [19, 5, 4].

THEOREM 2.4. *Given a matrix $A \in \mathbb{R}^{n \times n}$, suppose that $H = \frac{1}{2}(GA + A^T G)$ and $S = \frac{1}{2}(GA - A^T G)$ for some positive definite matrix G and some positive semidefinite matrix H . Then A has eigenvalues with strictly positive real parts if and only if no eigenvector of $G^{-1}S$ lies in the null space of H .*

By applying Theorem 2.4 to $A = \mathcal{D} = P^{-1}(Q - \sigma E_0)$ with $G = P$, we get

$$H = \frac{1}{2} \left[(Q - \sigma E_0) + (Q - \sigma E_0)^T \right] = \frac{1}{2} \begin{bmatrix} -(1+2\sigma) & 0 & \dots & 0 \\ 0 & 0 & \dots & 0 \\ \vdots & \vdots & \dots & \vdots \\ 0 & 0 & \dots & 0 \\ 0 & 0 & \dots & 1 \end{bmatrix},$$

which is positive semidefinite for $\sigma \leq -1/2$, and

$$S = \frac{1}{2} \left[(Q - \sigma E_0) - [(Q - \sigma E_0)^T] \right] = Q - \frac{B}{2},$$

which is skew-symmetric.

Note that the matrix $P^{-1}S$ is similar to the skew-symmetric matrix $P^{-\frac{1}{2}}SP^{-\frac{1}{2}}$, and hence its eigenvalues lie on the imaginary axis. For this reason, the eigenvalue problem associated to $P^{-1}S$ can be rewritten as $P^{-1}S\mathbf{v} = i\xi\mathbf{v}$, with $\xi \in \mathbb{R}$. By limiting the analysis to $\sigma < -1/2$, the null-space of H is given by the set of vectors $\mathbf{v} = (v_0, v_1, \dots, v_N)^T$ with $v_0 = v_N = 0$, since $H\mathbf{v} = \mathbf{0}$ is fulfilled by all vectors with first and last components equal to zero. Therefore, the following lemma is a direct consequence of Theorem 2.4.

LEMMA 2.5. *Let $\sigma < -1/2$. For SBP operators of finite difference type, the matrix $\mathcal{D} = P^{-1}(Q - \sigma E_0)$ has eigenvalues with strictly positive real parts if and only if $P^{-1}S$ does not have imaginary eigenvalues with eigenvectors where the first and last components are equal to zero.*

Remark 2.6. A similar criterion was already introduced in [17]. The condition to check is independent of σ for $\sigma < -1/2$. However, since we are interested in dual-consistent formulations, we will henceforth only consider $\sigma = -1$.

Before the eigenvalue analysis, we mention that, due to the structure of Q , the matrix S is also skew-centrosymmetric; i.e., it is such that $JS = -SJ$, where

$$J = \begin{bmatrix} & & & 1 \\ & & \ddots & \\ & & & \\ 1 & & & \end{bmatrix}.$$

As a result, we can prove the following lemma.

LEMMA 2.7. *If $(i\xi, \mathbf{v})$ is an eigenpair of $P^{-1}S$, then $(-i\xi, J\mathbf{v})$ is also an eigenpair.*

Proof. The relation $P^{-1}S\mathbf{v} = i\xi\mathbf{v}$ can be multiplied from the left by the non-singular matrix J . Since P^{-1} is centrosymmetric, it commutes with J and we get $P^{-1}JS\mathbf{v} = i\xi J\mathbf{v}$. By the skew-centrosymmetry of S , we get $P^{-1}S(J\mathbf{v}) = -i\xi(J\mathbf{v})$, and the claim follows. \square

Remark 2.8. In the upcoming sections we will implicitly assume (unless otherwise stated) that $\Delta t = 1$, since $P^{-1}S\mathbf{v} = i\xi\mathbf{v}$ can be rewritten as $\bar{P}^{-1}S\mathbf{v} = i\xi\Delta t\mathbf{v}$, with $\bar{P} = P/\Delta t$ independent of Δt . This implies that the time-step acts only as a rescaling parameter for the eigenvalues of $P^{-1}S$ and does not modify its eigenvectors. In particular, the existence of eigenvectors \mathbf{v} with $v_0 = v_N = 0$ does not depend on Δt .

3. Spectral analysis for the second order approximation. In this section, we study the second order approximation of (2.1). Despite that the invertibility of this problem was already proved in [17], the second order case clarifies and identifies a sufficient and necessary condition for the existence of the eigenvectors to $P^{-1}S$. For second order approximations, this condition enables a complete eigenvalue analysis of the operator. For higher order approximations, it provides a clear path for excluding the existence of eigenvectors with first and last components equal to zero.

3.1. Condition for the existence of the eigenvectors. We start by considering the matrix $P^{-1}S$ for the standard second order centered finite difference approximations on SBP form:

$$(3.1) \quad P^{-1}S = \begin{bmatrix} 0 & 1 & & & & \\ -\frac{1}{2} & & \frac{1}{2} & & & \\ & -\frac{1}{2} & & \frac{1}{2} & & \\ & & \ddots & \ddots & \ddots & \\ & & & -\frac{1}{2} & & \frac{1}{2} \\ & & & & -1 & 0 \end{bmatrix}.$$

To find the spectrum of this operator, we solve the internal stencil relation

$$\frac{1}{2}v_{k+1} - \frac{1}{2}v_{k-1} = i\xi v_k, \quad k = 1, \dots, N-1.$$

The ansatz $v_k = r^k$ gives rise to the characteristic equation $r^2 - 2i\xi r - 1 = 0$, which is solved by $r_{1,2}(\xi) = i\xi \pm \sqrt{1 - \xi^2}$. As a consequence, assuming that $r_1 \neq r_2$, i.e., $\xi \neq \pm 1$, the general expression for the interior components of the eigenvectors is

$$(3.2) \quad v_k = c_1(\xi) r_1^k(\xi) + c_2(\xi) r_2^k(\xi), \quad k = 1, \dots, N-1,$$

where the coefficients $c_1(\xi)$, $c_2(\xi)$ must be determined by additional conditions.

Since v_0 and v_N are not given explicitly, we must derive a set of equations that relate the unknown coefficients $c_1(\xi)$, $c_2(\xi)$ to the boundary closure of $P^{-1}S$. In particular, by solving explicitly the first two equations of $P^{-1}S\mathbf{v} = i\xi\mathbf{v}$ with v_0 as a free parameter, we get $v_1 = i\xi v_0$ and $v_2 = (1 - 2\xi^2)v_0$. These two components should match the solution in (3.2), leading to the homogeneous linear rectangular system

$$\begin{bmatrix} r_1 & r_2 & -i\xi \\ r_1^2 & r_2^2 & 2\xi^2 - 1 \end{bmatrix} \begin{bmatrix} c_1(\xi) \\ c_2(\xi) \\ v_0 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}.$$

The 3×2 matrix has rank 2, since the determinant of the first 2×2 block is equal to $r_1 r_2 (r_1 - r_2) \neq 0$. By the rank-nullity theorem [10], the null-space of the matrix, which provides the solution to the problem, has dimension one and can be computed as the set of vectors

$$(3.3) \quad [c_1(\xi), c_2(\xi), v_0]^T = v_0 \left[\frac{1}{2}, \frac{1}{2}, 1 \right]^T.$$

We will henceforth denote the coefficients in (3.2) that fit with the left boundary equation by the vector $\mathbf{c}^L(\xi) = v_0 [c_1^L(\xi), c_2^L(\xi)]^T = v_0 [1/2, 1/2]^T$.

Remark 3.1. Solving explicitly the eigenvector problem also for v_3 would have led to a third equation, $c_1(\xi) r_1^3(\xi) + c_2(\xi) r_2^3(\xi) = i\xi(3 - 4\xi^2) v_0$, and to the square system

$$\begin{bmatrix} r_1 & r_2 & -i\xi \\ r_1^2 & r_2^2 & 2\xi^2 - 1 \\ r_1^3 & r_2^3 & i\xi(4\xi^2 - 3) \end{bmatrix} \begin{bmatrix} c_1(\xi) \\ c_2(\xi) \\ v_0 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}.$$

However, the additional equation is linearly dependent on the other two. It can be obtained by summing the first equation with $2i\xi$ times the second equation. Indeed, both r_1 and r_2 fulfill $r^3 = r + 2i\xi r^2$.

The candidate eigenvector with $v_k = (v_0/2) [r_1^k(\xi) + r_2^k(\xi)]$ for $k = 1, \dots, N-1$ should also match the equations at the right boundary. To guarantee that this is the case, one could substitute these components into the last two equations of $P^{-1}S\mathbf{v} = i\xi\mathbf{v}$, solving these separately for v_N and equating the two expressions. The ξ values fulfilling the resulting equation would determine the eigenvalues of $P^{-1}S$. However, this procedure would lead to a problem as difficult as finding the eigenvalues of the operator. To avoid the direct computation of the eigenvalues $i\xi$, we mimic the approach used for the left boundary nodes by explicitly solving the last two equations of $P^{-1}S\mathbf{v} = i\xi\mathbf{v}$ for v_{N-2} and v_{N-1} with v_N as free parameter. Thus, equating the formal stencil expressions of v_{N-2} and v_{N-1} as functions of $c_1(\xi)$, $c_2(\xi)$ with the explicit solutions in terms of v_N , we get the homogeneous system

$$\begin{bmatrix} r_1^{N-2} & r_2^{N-2} & 2\xi^2 - 1 \\ r_1^{N-1} & r_2^{N-1} & i\xi \end{bmatrix} \begin{bmatrix} c_1(\xi) \\ c_2(\xi) \\ v_N \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}.$$

Again, the null-space of the matrix has dimension one since the determinant of the first 2×2 block is $r_1^{N-2} r_2^{N-2} (r_1 - r_2) \neq 0$. The null-space of this matrix can be computed as

$$(3.4) \quad [c_1(\xi), c_2(\xi), v_N]^T = v_N [c_1^R(\xi), c_2^R(\xi), 1]^T$$

with

$$c_1^R(\xi) = -\frac{i\xi + r_2(1 - 2\xi^2)}{r_1^{N-2}(r_1 - r_2)}, \quad c_2^R(\xi) = \frac{i\xi + r_1(1 - 2\xi^2)}{r_2^{N-2}(r_1 - r_2)}.$$

The two resulting sets of coefficients, $\mathbf{c}^L(\xi) = [c_1^L(\xi), c_2^L(\xi)]^T$ and $\mathbf{c}^R(\xi) = [c_1^R(\xi), c_2^R(\xi)]^T$, lead to the same eigenvector \mathbf{v} in (3.2) if and only if $v_0 \mathbf{c}^L(\xi) = v_N \mathbf{c}^R(\xi) \neq \mathbf{0}$ for some $\xi \in \mathbb{R}$. This implies that the existence of the eigenvectors for

some fixed eigenvalue $i\xi$ is restricted by the linear dependence of the vectors $\mathbf{c}^L(\xi)$ and $\mathbf{c}^R(\xi)$, i.e.,

$$(3.5) \quad \det \begin{pmatrix} c_1^L(\xi) & c_1^R(\xi) \\ c_2^L(\xi) & c_2^R(\xi) \end{pmatrix} = 0 \quad \Leftrightarrow \quad 1 = - \left(\frac{r_2}{r_1} \right)^{N-2} \frac{i\xi + r_2(1 - 2\xi^2)}{i\xi + r_1(1 - 2\xi^2)}.$$

Vice versa, the linear independence of the coefficients can be used to exclude the existence of eigenvectors with $v_0 = v_N = 0$ for higher order approximations, thus proving $\operatorname{Re}(\mu) > 0$. However, before we move on to these problems, we complete the eigenvalue analysis of $P^{-1}S$ in (3.1) by further studying (3.5).

3.2. Computation of the spectrum. By substituting $r_1 = i\xi + \sqrt{1 - \xi^2}$, $r_2 = i\xi - \sqrt{1 - \xi^2}$ and recalling that $r_1 r_2 = -1$, we can rewrite the right-hand side of (3.5) as

$$\left(\frac{r_2}{r_1} \right)^{N-2} \frac{1 - 2\xi^2 - 2i\xi\sqrt{1 - \xi^2}}{1 - 2\xi^2 + 2i\xi\sqrt{1 - \xi^2}} = \left(\frac{r_2}{r_1} \right)^{N-2} \left(\frac{r_2}{r_1} \right)^2 = (-r_2^2)^N.$$

The equation $(-r_2^2)^N = 1$ can be solved by writing 1 in complex form as $e^{2i\pi m}$, with $m \in \mathbb{N}$. In particular, we can write $-r_2^2 = e^{2i\pi m/N}$, or equivalently $r_2^2 = e^{(2m/N+1)i\pi}$ for $m = 0, \dots, N$. Taking the square root of both sides yields

$$r_2 = e^{(\frac{m}{N} + \frac{1}{2})i\pi} = \cos \left(\left(\frac{m}{N} + \frac{1}{2} \right) \pi \right) + i \sin \left(\left(\frac{m}{N} + \frac{1}{2} \right) \pi \right), \quad m = 0, \dots, N.$$

This expression implies that r_2 must lie on the unit circle. On the other hand, the closed form expression for this complex number, $r_2 = i\xi - \sqrt{1 - \xi^2}$, indicates that r_2 has a modulus equal to one only if $-1 \leq \xi \leq 1$. Under this condition, we find that the imaginary part of r_2 is also equal to ξ , yielding

$$(3.6) \quad \xi = \sin \left(\left(\frac{m}{N} + \frac{1}{2} \right) \pi \right), \quad m = 0, \dots, N.$$

These $N + 1$ values of ξ uniquely determine the spectrum of $P^{-1}S$.

This conclusion seems to contradict the assumption of single roots for which $\xi \neq \pm 1$, since these values can be obtained from (3.6) for $m \in \{0, N\}$. However, repeating the argument above for the double-root case ($\xi = \pm 1$), which gives $v_k = (c_1(\xi) + c_2(\xi)k)r_1^k$ for $k = 1, \dots, N - 1$, leads to

$$c_1^L(\xi) = 1, \quad c_2^L(\xi) = 0, \quad c_1^R(\xi) = e^{\frac{i\pi N}{2}}, \quad c_2^R(\xi) = 0.$$

These coefficients are compatible with the single roots ansatz (since the term kr_1^k vanishes), and hence the double-root analysis leads to the same closed form of ξ as in (3.6).

Remark 3.2. The eigenvectors of $P^{-1}S$ in (3.1) do not satisfy $v_0 = v_N = 0$, since substituting $v_0 = 0$ into (3.3) and $v_N = 0$ into (3.4) gives $\mathbf{v} = \mathbf{0}$. Hence the operator \mathcal{D} has eigenvalues μ with positive real parts due to Lemma 2.5 (as previously proved in [17]).

In Figure 1, the spectrum of $P^{-1}S$ is shown for different N . Note that the closed form of the eigenvalues $i\xi$ agrees with the eigenvalues computed numerically. Moreover, all the values for ξ are bounded by the double-root conditions $\xi = \pm 1$.

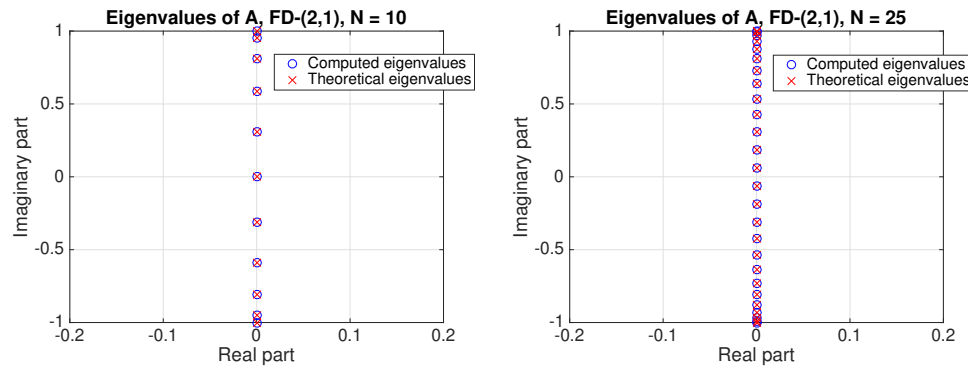


FIG. 1. Computed and theoretical eigenvalues of $P^{-1}S$ for the second order accurate finite difference approximation with $N = 10$ and $N = 25$.

3.3. Summarizing the proof procedure. The analysis in this section helps us to design a general procedure to prove the positivity of $\text{Re}(\mu)$ also for higher order discretizations. Rather than computing the eigenpairs of $P^{-1}S$ in closed form, we will focus on the coefficients $c_i(\xi)$ that define the interior components of the eigenvectors. By solving explicitly the first and last equations of $P^{-1}S\mathbf{v} = i\xi\mathbf{v}$, we can find two sets of coefficients $\mathbf{c}^L(\xi)$, $\mathbf{c}^R(\xi)$ that fit the left and right boundary equations, respectively. As shown for the second order case, the existence of the eigenvectors depends on the linear dependence of the vectors $\mathbf{c}^L(\xi)$, $\mathbf{c}^R(\xi)$ for all the eigenvalues $i\xi$.

Similarly, the existence of eigenvectors \mathbf{v} with first and last components equal to zero is restricted by the linear dependence of the vectors $\mathbf{c}^L(\xi)$, $\mathbf{c}^R(\xi)$ that are compatible with the constraints $v_0 = v_N = 0$. In particular, if these constraints give rise to $\mathbf{c}^L(\xi)$, $\mathbf{c}^R(\xi)$ that are provably linearly independent for every eigenvalue $i\xi$ and dimensions N , then $\text{Re}(\mu) > 0$ follows due to Theorem 2.4. Of course it is not feasible to check the linear dependence for all the eigenvalues of $P^{-1}S$, since it would require an a priori knowledge of the spectrum itself. However, that is not necessary since the Gershgorin theorem yields a bound on viable values of ξ .

Thus, to prove that no eigenvectors with $v_0 = v_N = 0$ exist for a discretization with a repeating stencil, the condition of linear dependence will be analyzed as a function of the ξ parameter, which is bounded in a closed interval I_ξ (given by the Gershgorin theorem). Forcing the linear dependence of the vectors $\mathbf{c}^L(\xi)$, $\mathbf{c}^R(\xi)$ yields an equation which may be solved for the dimension of the operator, N . If no $\xi \in I_\xi$ exists for which N is an integer, then no eigenvector of $P^{-1}S$ with first and last components equal to zero can exist, and we can conclude that $\text{Re}(\mu) > 0$ due to Theorem 2.4. When the constraint of linear dependence cannot be solved analytically for N , the condition will be checked numerically (see section 5).

Below, we summarize the procedure for the $2q$ th order discretization.

1. Determine the interval I_ξ in which ξ can be bounded by the Gershgorin theorem.
2. Solve, when possible, the characteristic equation obtained from the internal stencil relation for the roots $r_j(\xi)$, $j = 1, \dots, 2q$. Identify the condition for multiple roots in terms of ξ .
3. Assume that the characteristic equations have single roots $r_j(\xi)$, $j = 1, \dots, 2q$. Solve explicitly the first $3q$ equations of the eigenvalue problem for v_{2q}, \dots, v_{4q-1} by fixing $v_0 = 0$ and using v_1, \dots, v_{q-1} as free parameters. By equating

these components with

$$v_k = \sum_{j=1}^{2q} c_j(\xi) r_j^k(\xi), \quad k = 2q, \dots, 4q-1,$$

it is possible to write a $2q \times (3q-1)$ linear homogeneous system, which is solved by $q-1$ linearly independent vectors. The solution of this problem leads to the coefficients of the internal stencil relation, which can be written as a linear combination $\mathbf{c}^L(\xi) = \sum_{k=1}^{q-1} v_k \mathbf{c}^{L,k}(\xi)$.

4. Repeat the third step by solving the last $3q$ equations of the eigenvalue problem for $v_{N-2q}, \dots, v_{N-4q+1}$ by fixing $v_N = 0$ and using $v_{N-q+1}, \dots, v_{N-1}$ as free parameters. The coefficients of the internal stencil relation can be found as a linear combination $\mathbf{c}^R(\xi) = \sum_{k=1}^{q-1} v_{N-k} \mathbf{c}^{R,k}(\xi)$.
5. If an eigenvector with $v_0 = v_N = 0$ exists, the two vectors $\mathbf{c}^L(\xi)$ and $\mathbf{c}^R(\xi)$ must be equal for some $(v_1, \dots, v_{q-1}, v_{N-q+1}, \dots, v_{N-1}) \in \mathbb{R}^{2q-2}$. If the vectors $\mathbf{c}^{L,1}(\xi), \dots, \mathbf{c}^{L,q-1}(\xi), \mathbf{c}^{R,1}(\xi), \dots, \mathbf{c}^{R,q-1}(\xi)$ are linearly independent for every $(\xi, N) \in I_\xi \times \mathbb{N}$, then \mathcal{D} has eigenvalues with strictly positive real parts due to Lemma 2.5.
6. Repeat the third, fourth, and fifth steps for the double-root case.

4. The fourth order approximation. The matrix $P^{-1}S$ for the fourth order approximation is given by [8]

$$(4.1) \quad P^{-1}S = \begin{bmatrix} 0 & \frac{59}{34} & -\frac{4}{17} & -\frac{3}{34} & & & & \\ -\frac{1}{2} & 0 & \frac{1}{2} & 0 & & & & \\ \frac{4}{3} & -\frac{59}{86} & 0 & \frac{59}{86} & -\frac{4}{43} & & & \\ \frac{43}{98} & 0 & -\frac{59}{98} & 0 & -\frac{32}{49} & -\frac{4}{23} & & \\ & & \frac{1}{12} & -\frac{2}{3} & 0 & \frac{2}{3} & -\frac{1}{12} & \\ & & & \ddots & \ddots & \ddots & \ddots & \ddots \end{bmatrix}.$$

The eigenvalues $i\xi$ of this matrix satisfy $|\xi| \leq 35/17$, due to the Gershgorin theorem. Moreover, the stencil relation for the eigenvalue problem

$$-\frac{1}{12}v_{k+2} + \frac{2}{3}v_{k+1} - \frac{2}{3}v_{k-1} + \frac{1}{12}v_{k-2} = i\xi v_k, \quad k = 4, \dots, N-4,$$

yields the characteristic equation $r^4 - 8r^3 + 12i\xi r^2 + 8r - 1 = 0$, whose roots $r_j(\xi)$, $j = 1, \dots, 4$, can be found in closed form.

Since the roots of the characteristic equation are continuous functions of the parameter ξ , it is possible to uniquely identify them by an “initial” condition, i.e., the value that each $r_j(\xi)$ assumes for $\xi = 0$. With $r_1(\xi)$ we denote the root such that $r_1(0) = 4 - \sqrt{15}$. The other roots are $r_2(0) = -1$, $r_3(0) = 4 + \sqrt{15}$, and $r_4(0) = 1$ (see Figure 2). The explicit form of the functions $r_j(\xi)$ will not be provided here, since they are neither easy to write down nor particularly useful for the upcoming study. For further details on closed form solutions of quartic equations, see, for example, [20].

We split the analysis into two parts by considering the single- and double-root cases separately. In order to increase the readability of the upcoming proofs, we introduce the notation

$$(4.2) \quad \pi_k = \prod_{j=1, j \neq k}^4 (r_k - r_j), \quad \sigma_k^{(n)} = \sum_{\tau \in A_k^{(n)}} \prod_{j \in \tau} r_j,$$

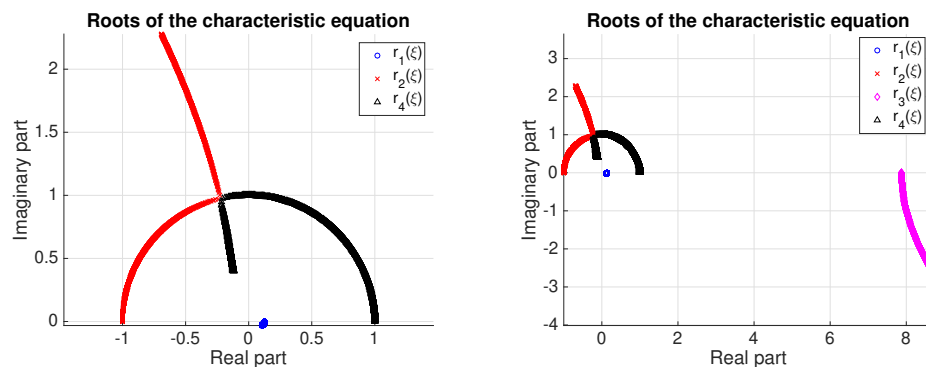


FIG. 2. The roots $r_j(\xi)$ of the characteristic equation $r^4 - 8r^3 + 12i\xi r^2 + 8r - 1 = 0$ are shown in the complex plane for $\xi \in I_\xi = [0, 35/17]$. The roots $r_j(\xi)$ are continuous functions of ξ labeled according to the conditions $r_1(0) = 4 - \sqrt{15}$, $r_2(0) = -1$, $r_3(0) = 4 + \sqrt{15}$, and $r_4(0) = 1$. The left figure is a magnification of the right figure.

where $A_k^{(n)}$ is the family of sets of n indices in $\{1, \dots, 4\}$ not containing k . For example, if $k = 3$ and $n = 2$, we get

$$\pi_3 = (r_3 - r_1)(r_3 - r_2)(r_3 - r_4), \quad A_3^{(2)} = \{\{1, 2\}, \{1, 4\}, \{2, 4\}\},$$

$$\sigma_3^{(2)} = r_1 r_2 + r_1 r_4 + r_2 r_4.$$

4.1. The single-root case. To start, we prove the following lemma.

LEMMA 4.1. *If $\xi \neq \pm \frac{1}{6}\sqrt{9 + 24\sqrt{6}}$, the eigenvalue problem for (4.1) is not solved by any eigenpair $(i\xi, \mathbf{v})$ with $v_0 = v_N = 0$.*

Proof. If the characteristic equation has single roots ($\xi \neq \pm \frac{1}{6}\sqrt{9 + 24\sqrt{6}}$), the general expression of the interior components of the eigenvectors \mathbf{v} of $P^{-1}S$ in (4.1) is

$$(4.3) \quad v_k = \sum_{j=1}^4 c_j(\xi) r_j^k(\xi), \quad k = 4, \dots, N-4.$$

The structure of $P^{-1}S$ in (4.1) enables the explicit computation of the first eigenvector components as linear functions of v_0 and v_1 , e.g.,

$$\begin{aligned} v_2 &= v_0 + 2i\xi v_1, \\ v_3 &= \frac{1}{3}[-(8 + 34i\xi)v_0 + (59 - 16i\xi)v_1]. \end{aligned}$$

The following eigenvector components v_4, v_5, \dots can be computed sequentially by substitution. In particular, the constraint $v_0 = 0$ leads to $v_j = w_j(\xi)v_1$, $j = 4, \dots, 7$, where

$$\begin{aligned} w_4(\xi) &= \frac{1}{6}(826 - 236i\xi + 129\xi^2), \\ w_5(\xi) &= \frac{1}{6}(3304 - 1711i\xi + 320\xi^2), \\ w_6(\xi) &= \frac{1}{3}(25960 - 18510i\xi + 1144\xi^2 - 774i\xi^3), \\ w_7(\xi) &= \frac{1}{3}(204435 - 186800i\xi - 11896\xi^2 - 10032i\xi^3). \end{aligned}$$

By equating these expressions of v_j with the stencil form (4.3), we get the rectangular

homogeneous system

$$\begin{bmatrix} r_1^4 & r_2^4 & r_3^4 & r_4^4 & -w_4(\xi) \\ r_1^5 & r_2^5 & r_3^5 & r_4^5 & -w_5(\xi) \\ r_1^6 & r_2^6 & r_3^6 & r_4^6 & -w_6(\xi) \\ r_1^7 & r_2^7 & r_3^7 & r_4^7 & -w_7(\xi) \end{bmatrix} \begin{bmatrix} c_1(\xi) \\ c_2(\xi) \\ c_3(\xi) \\ c_4(\xi) \\ v_1 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}.$$

The null-space of the matrix has dimension one, since the first 4×4 block has the determinant

$$\prod_{k=1}^4 r_k^4 \cdot \prod_{k < j} (r_k - r_j) \neq 0.$$

The general solution of the system is

$$[c_1(\xi), c_2(\xi), c_3(\xi), c_4(\xi), v_1]^T = v_1 [c_1^L(\xi), c_2^L(\xi), c_3^L(\xi), c_4^L(\xi), 1]^T,$$

where the closed form expression for the coefficients $c_j^L(\xi)$, $j = 1, \dots, 4$, can be computed by using the command `NullSpace` in MAPLE. In particular, with the notation in (4.2) we can write

$$(4.4) \quad c_j^L(\xi) = -\frac{w_4(\xi)\sigma_j^{(3)} - w_5(\xi)\sigma_j^{(2)} + w_6(\xi)\sigma_j^{(1)} - w_7(\xi)}{r_j^4\pi_j}, \quad j = 1, \dots, 4.$$

In a similar fashion, the last six equations of the eigenvalue problem can be used to find explicitly $v_j = w_j(\xi)v_{N-1}$, $j = N-7, \dots, N-4$. The coefficients of the stencil relation (4.3) that are compatible with these eigenvector components are given by $v_{N-1}\mathbf{c}^R(\xi)$, where

$$(4.5) \quad c_j^R(\xi) = -\frac{\bar{w}_7(\xi)\sigma_j^{(3)} - \bar{w}_6(\xi)\sigma_j^{(2)} + \bar{w}_5(\xi)\sigma_j^{(1)} - \bar{w}_4(\xi)}{r_j^{N-7}\pi_j}, \quad j = 1, \dots, 4.$$

Once again, the bar indicates the complex conjugation of the coefficients of the polynomials $w_i(\xi)$.

An eigenvector \mathbf{v} with $v_0 = v_N = 0$ exists if and only if it is possible to find $(v_1, v_{N-1}) \in \mathbb{R}^2$ and $\xi \in \mathbb{R}$ such that $v_1\mathbf{c}^L(\xi) = v_{N-1}\mathbf{c}^R(\xi)$. This implies that the existence of \mathbf{v} is guaranteed if the vectors $\mathbf{c}^L(\xi)$, $\mathbf{c}^R(\xi)$ are linearly dependent for some eigenvalue $i\xi$, i.e., if

$$(4.6) \quad \det \begin{pmatrix} c_i^L(\xi) & c_i^R(\xi) \\ c_j^L(\xi) & c_j^R(\xi) \end{pmatrix} = 0 \quad \forall i, j = 1, \dots, 4, \quad i \neq j.$$

It suffices to consider a couple of indices. The linear dependence constraint (4.6) for $i = 1, j = 3$ gives rise to the equation

$$(4.7) \quad \left(\frac{r_3(\xi)}{r_1(\xi)} \right)^{N-11} = g(\xi),$$

where

$$g(\xi) = \frac{(w_4\sigma_1^{(3)} - w_5\sigma_1^{(2)} + w_6\sigma_1^{(1)} - w_7)(\bar{w}_7\sigma_3^{(3)} - \bar{w}_6\sigma_3^{(2)} + \bar{w}_5\sigma_3^{(1)} - \bar{w}_4)}{(\bar{w}_7\sigma_1^{(3)} - \bar{w}_6\sigma_1^{(2)} + \bar{w}_5\sigma_1^{(1)} - \bar{w}_4)(w_4\sigma_3^{(3)} - w_5\sigma_3^{(2)} + w_6\sigma_3^{(1)} - w_7)}.$$

If (4.7) holds, then the same relation is fulfilled for the absolute values of the left- and right-hand sides. In particular, we find

$$(4.8) \quad N = \frac{\log(|g(\xi)|)}{\log(|r_3(\xi)/r_1(\xi)|)} + 11 =: G(\xi).$$

Since for the matrix in (4.1) the Gershgorin theorem states that $|\xi| \leq 35/17$, we can evaluate $G(\xi)$ in this interval and find the values ξ for which this function becomes an integer. As can be seen in Figure 3, the only integer value assumed by $G(\xi)$ is 3, which is not compatible with the dimension of a fourth order accurate SBP operator. \square

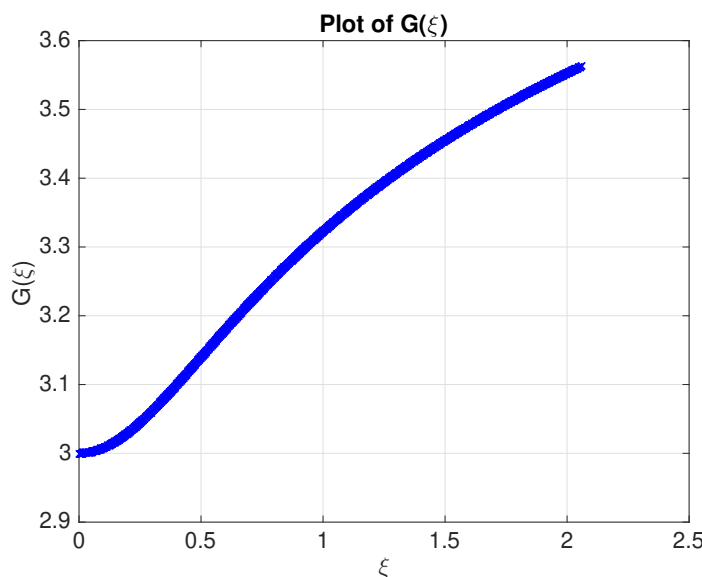


FIG. 3. Plot of $G(\xi)$ in (4.8) for $\xi \in [0, 35/17]$. The only integer value assumed by the function is $N = 3$, which is not compatible with the dimension of a fourth order accurate SBP operator.

Remark 4.2. Due to Lemma 2.7, it suffices to evaluate the function $G(\xi)$ for $\xi \in [0, 35/17]$, rather than for $\xi \in [-35/17, 35/17]$. Indeed, if an eigenvector with the property $v_0 = v_N = 0$ does exist for a fixed ξ , it exists for $-\xi$ as well.

4.2. The double-root case. To conclude the proof, we must repeat the analysis for the double-root case, i.e., for $\xi = \pm \frac{1}{6}\sqrt{9 + 24\sqrt{6}}$. We prove the following lemma.

LEMMA 4.3. *If $\xi = \pm \frac{1}{6}\sqrt{9 + 24\sqrt{6}}$, the eigenvalue problem for (4.1) is not solved by any eigenpair $(i\xi, \mathbf{v})$ with $v_0 = v_N = 0$.*

Proof. Due to Lemma 2.7, it suffices to consider $\xi = \frac{1}{6}\sqrt{9 + 24\sqrt{6}}$. For this ξ value $r_2(\xi) = r_4(\xi)$ (see Figure 2), and we must consider the double-root ansatz

$$(4.9) \quad v_k = c_1 r_1^k + (c_2 + c_4 k) r_2^k + c_3 r_3^k, \quad k = 4, \dots, N-4.$$

As for the single-root analysis, we can find the coefficients that are compatible with the left boundary closure of $P^{-1}S\mathbf{v} = i\xi\mathbf{v}$ by solving the rectangular homogeneous

system

$$\begin{bmatrix} r_1^4 & r_2^4 & r_3^4 & 4r_2^4 & -w_4 \\ r_1^5 & r_2^5 & r_3^5 & 5r_2^5 & -w_5 \\ r_1^6 & r_2^6 & r_3^6 & 6r_2^6 & -w_6 \\ r_1^7 & r_2^7 & r_3^7 & 7r_2^7 & -w_7 \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \\ v_1 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}.$$

Also in this case, the null-space of the matrix has dimension one, since the determinant of the first 4×4 block is

$$r_1^4 r_2^9 r_3^4 (r_1 - r_2)^2 (r_1 - r_3) (r_2 - r_3)^2 \neq 0.$$

In particular, the problem is solved by $v_1 \mathbf{c}^L$, where the closed form expression for the coefficients c_j^L , $j = 1, \dots, 4$, can be computed by using the command `NullSpace` in MAPLE. Similarly, it is possible to find the coefficients that fit the right boundary equations of the eigenvalue problem as $v_{N-1} \mathbf{c}^R$.

A necessary and sufficient condition for the existence of an eigenvector \mathbf{v} with $v_0 = v_N = 0$ is that the vectors \mathbf{c}^L , \mathbf{c}^R are linearly dependent, i.e., that (4.6) holds. However, the coefficients

$$\begin{aligned} c_1^L &= -\frac{w_4 r_2^2 r_3 - w_5 (r_2^2 + 2r_2 r_3) + w_6 (2r_2 + r_3) - w_7}{r_1^4 (r_1 - r_2)^2 (r_1 - r_3)}, \\ c_3^L &= -\frac{w_4 r_2^2 r_1 - w_5 (r_2^2 + 2r_2 r_1) + w_6 (2r_2 + r_1) - w_7}{r_3^4 (r_3 - r_2)^2 (r_3 - r_1)}, \\ c_1^R &= -\frac{\bar{w}_7 r_2^2 r_3 - \bar{w}_6 (r_2^2 + 2r_2 r_3) + \bar{w}_5 (2r_2 + r_3) - \bar{w}_4}{r_1^{N-7} (r_1 - r_2)^2 (r_1 - r_3)}, \\ c_3^R &= -\frac{\bar{w}_7 r_2^2 r_1 - \bar{w}_6 (r_2^2 + 2r_2 r_1) + \bar{w}_5 (2r_2 + r_1) - \bar{w}_4}{r_3^{N-7} (r_3 - r_2)^2 (r_3 - r_1)} \end{aligned}$$

have the same formal expression as for the single-root case, provided that $r_2 = r_4$. Thus, the linear independence of \mathbf{c}^L and \mathbf{c}^R can be checked by studying Figure 3 at $\xi = \frac{1}{6}\sqrt{9 + 24\sqrt{6}} \approx 1.3722$. Since $G\left(\frac{1}{6}\sqrt{9 + 24\sqrt{6}}\right) \notin \mathbb{N}$, the claim follows. \square

Remark 4.4. The linear dependence constraint (4.6) for $i = 1$, $j = 3$ takes into account only the coefficients associated to the nonrepeated roots. The purpose of Lemma 4.3 is to show that this condition varies continuously with respect to the values $\xi \in I_\xi = [0, 35/17]$, despite that two different ansatzes are considered. Note that the determinant in (4.6) for $i, j \in \{2, 4\}$ cannot be a continuous function of $\xi \in I_\xi$, because at $\xi = \frac{1}{6}\sqrt{9 + 24\sqrt{6}}$ the numerators of $c_i^{L,R}(\xi)$ in (4.4), (4.5) do not vanish, while $\pi_2 = \pi_4 = 0$.

For the sixth order approximations, we will verify and mention the continuity of the linear dependence constraint without stating a dedicated lemma.

Due to Lemma 2.5, Lemma 4.1 and Lemma 4.3 imply the following theorem.

THEOREM 4.5. *The fourth order diagonal-norm finite difference SBP-SAT operator \mathcal{D} has eigenvalues with strictly positive real parts.*

5. The sixth order approximations. The argument used for the fourth order approximation can be generalized to sixth order approximations with repeating stencil. Although the idea to prove the invertibility is the same, there are some additional technicalities one must take care of. To start with, the sixth order approximations with minimal stencil bandwidth are not unique and are defined in terms of a free parameter x [21]. In this case, the matrix S is given by

$$(5.1) \quad \begin{bmatrix} 0 & s_{0,1} & s_{0,2} & s_{0,3} & s_{0,4} & s_{0,5} & & & & \\ -s_{0,1} & 0 & s_{1,2} & s_{1,3} & s_{1,4} & s_{1,5} & & & & \\ -s_{0,2} & -s_{1,2} & 0 & s_{2,3} & s_{2,4} & s_{2,5} & & & & \\ -s_{0,3} & -s_{1,3} & -s_{2,3} & 0 & s_{3,4} & s_{3,5} & a_1 & & & \\ -s_{0,4} & -s_{1,4} & -s_{2,4} & -s_{3,4} & 0 & s_{4,5} & a_2 & a_1 & & \\ -s_{0,5} & -s_{1,5} & -s_{2,5} & -s_{3,5} & -s_{4,5} & 0 & a_3 & a_2 & a_1 & \\ & & & -a_1 & -a_2 & -a_3 & 0 & a_3 & a_2 & a_1 \\ & & & & & & \ddots & \ddots & \ddots & \ddots \end{bmatrix},$$

where the $s_{i,j}$'s are linear functions of x and $a_1 = 1/60$, $a_2 = -3/20$, $a_3 = 3/4$. Hence, for sixth order approximations the condition for the existence of the eigenvectors must be studied as a function of both ξ and x .

Remark 5.1. The coefficients $s_{i,j}$, as well as the matrix P and all the quantities that are not written explicitly in this section, can be found in the supplement in Appendix A.

Furthermore, the internal stencil relation for the eigenvalue problem

$$\frac{1}{60}v_{k+3} - \frac{3}{20}v_{k+2} + \frac{3}{4}v_{k+1} - \frac{3}{4}v_{k-1} + \frac{3}{20}v_{k-2} - \frac{1}{60}v_{k-3} = i\xi v_k, \quad k = 6, \dots, N-6,$$

leads to the sextic equation $r^6 - 9r^5 + 45r^4 - 60i\xi r^3 - 45r^2 + 9r - 1 = 0$, which cannot be solved in closed form due to the Abel–Ruffini theorem [11]. This implies that in order to prove the statement we must compute the roots numerically for every $\xi \in I_\xi$, where I_ξ is the closed interval in which ξ can be bounded by the Gershgorin theorem. On the other hand, the width of I_ξ may depend on x , making the proof more challenging. However, three common choices for the free parameter are $x_1 = 342523/518400$ [8], $x_2 = 89387/129600$ [21], and $x_3 = 0.70127127127\dots$ (the value for which the spectral radius of $P^{-1}Q$ is minimized [23, 1]), and for all three of these values the Gershgorin theorem leads to $I_\xi = [0, 4.21]$.

Remark 5.2. The parameter $x = x_3 = 0.70127127127\dots$ minimizes the spectral radius of $P^{-1}S$ for sixth order approximations on SBP form, but its value is yet unpublished [1].

Limiting the analysis to $x \in \{x_1, x_2, x_3\}$, the roots of the characteristic equations $r_j(\xi)$ are shown for $\xi \in I_\xi$ in Figure 4.

A further additional difficulty compared to the fourth order case is due to the polynomial

$$\psi_x = -1728 (64900362240000x^2 - 99055767153600x + 37572249231809),$$

which determines the form of the coefficients $c_j(\xi)$ in the single-root ansatz

$$(5.2) \quad v_k = \sum_{j=1}^6 c_j(\xi) r_j^k(\xi), \quad k = 6, \dots, N-6.$$

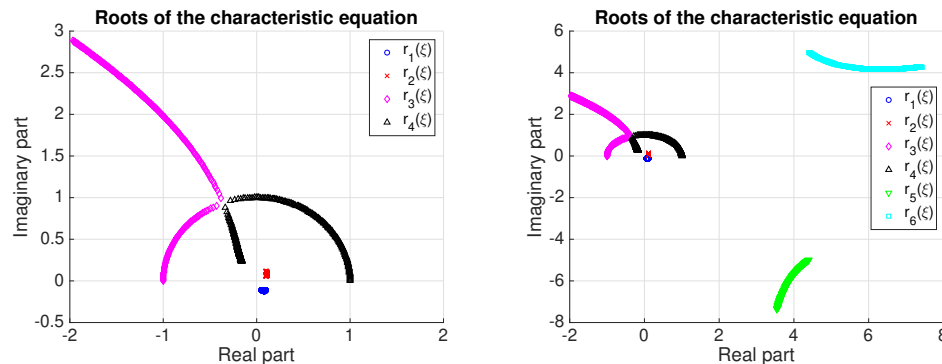


FIG. 4. The roots $r_j(\xi)$ of the characteristic equation $r^6 - 9r^5 + 45r^4 - 60i\xi r^3 - 45r^2 + 9r - 1 = 0$ are shown in the complex plane for $\xi \in I_\xi = [0, 4.21]$. The roots are ordered, for any fixed ξ , in ascending order by their modulus. If the moduli of two roots match, the roots are ordered in ascending order by their real part. With these criteria, $r_j(\xi)$ are continuous functions of ξ . For $\xi = 0$, we get $r_1(0) \approx 0.0950032 - 0.1127423i$, $r_2(0) \approx 0.0950032 + 0.1127423i$, $r_3(0) = -1$, $r_4(0) = 1$, $r_5(0) \approx 4.400500 - 4.986139i$, $r_6(0) \approx 4.400500 + 4.986139i$. The left figure is a magnification of the right figure.

In particular the candidate eigenvector may have a different form whether ψ_x is different or equal to zero, i.e., whether

$$x = x^* = 764319191/1001548800 \pm \sqrt{3467141604054577}/1001548800$$

is fulfilled or not. However, the critical values $x^* \notin \{x_1, x_2, x_3\}$, and as a result we will henceforth consider the case $\psi_x \neq 0$.

In order to increase the readability of the upcoming proofs, we generalize the notations (4.2) to six indices as

$$\pi_k = \prod_{j=1, j \neq k}^6 (r_k - r_j), \quad \sigma_k^{(n)} = \sum_{\tau \in A_k^{(n)}} \prod_{j \in \tau} r_j,$$

where $A_k^{(n)}$ is the family of sets of n indices in $\{1, \dots, 6\}$ not containing k . For example, if $k = 3$ and $n = 4$, we get

$$\pi_3 = (r_3 - r_1)(r_3 - r_2)(r_3 - r_4)(r_3 - r_5)(r_3 - r_6),$$

$$A_3^{(4)} = \{\{1, 2, 4, 5\}, \{1, 2, 4, 6\}, \{1, 2, 5, 6\}, \{1, 4, 5, 6\}, \{2, 4, 5, 6\}\},$$

$$\sigma_3^{(4)} = r_1 r_2 r_4 r_5 + r_1 r_2 r_4 r_6 + r_1 r_2 r_5 r_6 + r_1 r_4 r_5 r_6 + r_2 r_4 r_5 r_6.$$

5.1. The proof for sixth order approximations. Before discussing the invertibility of \mathcal{D} for $x \in \{x_1, x_2, x_3\}$, we first outline the argument for any $x \in \mathbb{R}$. Consider the eigenvalue problem $P^{-1}S\mathbf{v} = i\xi\mathbf{v}$ with S in (5.1) and $v_0 = v_N = 0$. We start by studying the case in which the characteristic equation has single roots; thus

$$\xi \neq \xi_\pm^* = \pm \sqrt{\frac{1}{9} + \frac{3}{2} \sqrt{\frac{5}{2}} + \frac{1}{\sqrt[3]{20}}}.$$

By solving sequentially the first nine equations of the eigenvalue problem with v_1 and v_2 as free parameters, we can obtain the eigenvector components v_3, \dots, v_{11} as linear functions of v_1, v_2 . In particular, equating

$$v_j = w_j(\xi, x) v_1 + z_j(\xi, x) v_2, \quad j = 6, \dots, 11,$$

with v_j in (5.2) yields the 6×8 homogeneous linear system

$$\begin{bmatrix} r_1^6 & r_2^6 & r_3^6 & r_4^6 & r_5^6 & r_6^6 & -w_6(\xi, x) & -z_6(\xi, x) \\ r_1^7 & r_2^7 & r_3^7 & r_4^7 & r_5^7 & r_6^7 & -w_7(\xi, x) & -z_7(\xi, x) \\ r_1^8 & r_2^8 & r_3^8 & r_4^8 & r_5^8 & r_6^8 & -w_8(\xi, x) & -z_8(\xi, x) \\ r_1^9 & r_2^9 & r_3^9 & r_4^9 & r_5^9 & r_6^9 & -w_9(\xi, x) & -z_9(\xi, x) \\ r_1^{10} & r_2^{10} & r_3^{10} & r_4^{10} & r_5^{10} & r_6^{10} & -w_{10}(\xi, x) & -z_{10}(\xi, x) \\ r_1^{11} & r_2^{11} & r_3^{11} & r_4^{11} & r_5^{11} & r_6^{11} & -w_{11}(\xi, x) & -z_{11}(\xi, x) \end{bmatrix} \begin{bmatrix} c_1(\xi) \\ c_2(\xi) \\ c_3(\xi) \\ c_4(\xi) \\ c_5(\xi) \\ c_6(\xi) \\ v_1 \\ v_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}.$$

The rank of the matrix above is 6 since the first 6×6 block has a nonzero determinant in the single-root case. As a consequence, the null-space of the matrix has dimension 2, and the solution of the system can be expressed as the linear combination

$$\mathbf{c}^L(\xi, x) = v_1 \mathbf{c}^{L,1}(\xi, x) + v_2 \mathbf{c}^{L,2}(\xi, x),$$

where the coefficients $c_k^{L,j}$ can be computed with MAPLE as

$$\begin{aligned} c_k^{L,1}(\xi, x) = & -\frac{1}{r_k^6 \pi_k} \left[w_6(\xi, x) \sigma_k^{(5)} - w_7(\xi, x) \sigma_k^{(4)} + w_8(\xi, x) \sigma_k^{(3)} \right. \\ & \left. - w_9(\xi, x) \sigma_k^{(2)} + w_{10}(\xi, x) \sigma_k^{(1)} - w_{11}(\xi, x) \right] = \frac{\kappa_k^{L,1}(\xi, x)}{\psi_x r_k^6 \pi_k}, \end{aligned}$$

and

$$\begin{aligned} c_k^{L,2}(\xi, x) = & -\frac{1}{r_k^6 \pi_k} \left[z_6(\xi, x) \sigma_k^{(5)} - z_7(\xi, x) \sigma_k^{(4)} + z_8(\xi, x) \sigma_k^{(3)} \right. \\ & \left. - z_9(\xi, x) \sigma_k^{(2)} + z_{10}(\xi, x) \sigma_k^{(1)} - z_{11}(\xi, x) \right] = \frac{\kappa_k^{L,2}(\xi, x)}{\psi_x r_k^6 \pi_k}. \end{aligned}$$

Similarly, by solving the last nine equations of the eigenvalue problem sequentially from the bottom with v_{N-2} and v_{N-1} as free parameters, we find the coefficients

$$\mathbf{c}^R(\xi, x) = v_{N-1} \mathbf{c}^{R,1}(\xi, x) + v_{N-2} \mathbf{c}^{R,2}(\xi, x),$$

where

$$\begin{aligned} c_k^{R,1}(\xi, x) = & -\frac{1}{r_k^{N-11} \pi_k} \left[\bar{w}_{11}(\xi, x) \sigma_k^{(5)} - \bar{w}_{10}(\xi, x) \sigma_k^{(4)} + \bar{w}_9(\xi, x) \sigma_k^{(3)} \right. \\ & \left. - \bar{w}_8(\xi, x) \sigma_k^{(2)} + \bar{w}_7(\xi, x) \sigma_k^{(1)} - \bar{w}_6(\xi, x) \right] = \frac{\kappa_k^{R,1}(\xi, x)}{\psi_x r_k^{N-11} \pi_k}, \end{aligned}$$

and

$$\begin{aligned} c_k^{R,2}(\xi, x) = & -\frac{1}{r_k^{N-11} \pi_k} \left[\bar{z}_{11}(\xi, x) \sigma_k^{(5)} - \bar{z}_{10}(\xi, x) \sigma_k^{(4)} + \bar{z}_9(\xi, x) \sigma_k^{(3)} \right. \\ & \left. - \bar{z}_8(\xi, x) \sigma_k^{(2)} + \bar{z}_7(\xi, x) \sigma_k^{(1)} - \bar{z}_6(\xi, x) \right] = \frac{\kappa_k^{R,2}(\xi, x)}{\psi_x r_k^{N-11} \pi_k}. \end{aligned}$$

Thus, there exists an eigenvector \mathbf{v} with $v_0 = v_N = 0$ if and only if it is possible to find $v_1, v_2, v_{N-2}, v_{N-1}$ such that

$$v_1 \mathbf{c}^{L,1}(\xi, x) + v_2 \mathbf{c}^{L,2}(\xi, x) = v_{N-1} \mathbf{c}^{R,1}(\xi, x) + v_{N-2} \mathbf{c}^{R,2}(\xi, x).$$

In other words, the existence of eigenvectors with first and last components equal to zero is subject to the linear dependence of the vectors $\mathbf{c}^{L,1}(\xi, x)$, $\mathbf{c}^{L,2}(\xi, x)$, $\mathbf{c}^{R,1}(\xi, x)$, and $\mathbf{c}^{R,2}(\xi, x)$ for some fixed ξ and x . For example, one can consider the indices $\{1, 2, 5, 6\}$ and study the determinant $D(\xi, x, N)$ of the matrix

$$\begin{bmatrix} c_1^{L,1}(\xi, x) & c_1^{L,2}(\xi, x) & c_1^{R,1}(\xi, x) & c_1^{R,2}(\xi, x) \\ c_2^{L,1}(\xi, x) & c_2^{L,2}(\xi, x) & c_2^{R,1}(\xi, x) & c_2^{R,2}(\xi, x) \\ c_5^{L,1}(\xi, x) & c_5^{L,2}(\xi, x) & c_5^{R,1}(\xi, x) & c_5^{R,2}(\xi, x) \\ c_6^{L,1}(\xi, x) & c_6^{L,2}(\xi, x) & c_6^{R,1}(\xi, x) & c_6^{R,2}(\xi, x) \end{bmatrix},$$

which is

$$\begin{aligned} \frac{1}{\psi_x^4 \pi_1 \pi_2 \pi_5 \pi_6 r_1^6 r_2^6 r_5^6 r_6^6} & \left[\frac{\left(\kappa_1^{R,2} \kappa_2^{R,1} - \kappa_2^{R,2} \kappa_1^{R,1} \right) \left(\kappa_5^{L,2} \kappa_6^{L,1} - \kappa_6^{L,2} \kappa_5^{L,1} \right)}{(r_1 r_2)^{N-17}} \right. \\ & - \frac{\left(\kappa_1^{R,2} \kappa_5^{R,1} - \kappa_5^{R,2} \kappa_1^{R,1} \right) \left(\kappa_2^{L,2} \kappa_6^{L,1} - \kappa_6^{L,2} \kappa_2^{L,1} \right)}{(r_1 r_5)^{N-17}} \\ & + \frac{\left(\kappa_1^{R,2} \kappa_6^{R,1} - \kappa_6^{R,2} \kappa_1^{R,1} \right) \left(\kappa_2^{L,2} \kappa_5^{L,1} - \kappa_5^{L,2} \kappa_2^{L,1} \right)}{(r_1 r_6)^{N-17}} \\ & + \frac{\left(\kappa_2^{R,2} \kappa_5^{R,1} - \kappa_5^{R,2} \kappa_2^{R,1} \right) \left(\kappa_1^{L,2} \kappa_6^{L,1} - \kappa_6^{L,2} \kappa_1^{L,1} \right)}{(r_2 r_5)^{N-17}} \\ & - \frac{\left(\kappa_2^{R,2} \kappa_6^{R,1} - \kappa_6^{R,2} \kappa_2^{R,1} \right) \left(\kappa_1^{L,2} \kappa_5^{L,1} - \kappa_5^{L,2} \kappa_1^{L,1} \right)}{(r_2 r_6)^{N-17}} \\ & \left. + \frac{\left(\kappa_5^{R,2} \kappa_6^{R,1} - \kappa_6^{R,2} \kappa_5^{R,1} \right) \left(\kappa_1^{L,2} \kappa_2^{L,1} - \kappa_2^{L,2} \kappa_1^{L,1} \right)}{(r_5 r_6)^{N-17}} \right] \end{aligned}$$

or, equivalently,

$$\begin{aligned} D(\xi, x, N) &= \frac{1}{\psi_x^4 \pi_1 \pi_2 \pi_5 \pi_6 r_1^6 r_2^6 r_5^6 r_6^6} \left[\frac{\tau_{1,2}(\xi, x)}{(r_1 r_2)^{N-17}} + \frac{\tau_{1,5}(\xi, x)}{(r_1 r_5)^{N-17}} \right. \\ (5.3) \quad & \left. + \frac{\tau_{1,6}(\xi, x)}{(r_1 r_6)^{N-17}} + \frac{\tau_{2,5}(\xi, x)}{(r_2 r_5)^{N-17}} + \frac{\tau_{2,6}(\xi, x)}{(r_2 r_6)^{N-17}} + \frac{\tau_{5,6}(\xi, x)}{(r_5 r_6)^{N-17}} \right]. \end{aligned}$$

If $D(\xi, x, N) = 0$ does not hold for any $(\xi, x, N) \in I_\xi \times \mathbb{R} \times \mathbb{N}$, then the eigenvalues of \mathcal{D} have strictly positive real parts due to Lemma 2.5.

In order to prove the result for the double-root case, it suffices to show that the coefficients $c_k^{L,1}(\xi, x)$, $c_k^{L,2}(\xi, x)$, $c_k^{R,1}(\xi, x)$, and $c_k^{R,2}(\xi, x)$ are the same as for the single-root analysis for $k \in \{1, 2, 5, 6\}$. According to the labeling of the roots in Figure 4, at $\xi = \xi_+^*$ we find $r_3(\xi_+^*) = r_4(\xi_+^*)$. Hence, the double-root ansatz is

$$v_k = c_1 r_1^k + c_2 r_2^k + (c_3 + c_4 k) r_3^k + c_5 r_5^k + c_6 r_6^k, \quad k = 6, \dots, N-6,$$

which leads to the following homogeneous system for the left boundary:

$$\begin{bmatrix} r_1^6 & r_2^6 & r_3^6 & 6r_3^6 & r_5^6 & r_6^6 & -w_6 & -z_6 \\ r_1^7 & r_2^7 & r_3^7 & 7r_3^7 & r_5^7 & r_6^7 & -w_7 & -z_7 \\ r_1^8 & r_2^8 & r_3^8 & 8r_3^8 & r_5^8 & r_6^8 & -w_8 & -z_8 \\ r_1^9 & r_2^9 & r_3^9 & 9r_3^9 & r_5^9 & r_6^9 & -w_9 & -z_9 \\ r_1^{10} & r_2^{10} & r_3^{10} & 10r_3^{10} & r_5^{10} & r_6^{10} & -w_{10} & -z_{10} \\ r_1^{11} & r_2^{11} & r_3^{11} & 11r_3^{11} & r_5^{11} & r_6^{11} & -w_{11} & -z_{11} \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \\ c_5 \\ c_6 \\ v_1 \\ v_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}.$$

One can verify that this problem is solved by the same $c_k^{L,1}(\xi, x)$, $c_k^{L,2}(\xi, x)$ as in the single-root case for $k \in \{1, 2, 5, 6\}$, which are the indices of the nonrepeated roots. Similarly, the coefficients $c_k^{R,1}(\xi, x)$ and $c_k^{R,2}(\xi, x)$ are unchanged for these indices. Thus, the solvability of $D(\xi, x, N) = 0$ determines the existence of the eigenvectors with $v_0 = v_N = 0$ for the double-root case as well.

5.2. Invertibility analysis for some parameter values. Since the problem $D(\xi, x, N) = 0$ is not explicitly solvable for N , it appears prohibitive to show the invertibility of \mathcal{D} for all the possible sixth order approximations with minimal bandwidth. In fact, one may even conjecture the existence of a parameter x such that the SBP-SAT operator is not invertible for some N . For this reason, we will limit our analysis to the values $x \in \{x_1, x_2, x_3\}$ that are, to the best of our knowledge, the only ones used in the literature so far.

Remark 5.3. We only consider sixth order approximations with at least one interior stencil relation; hence $N \geq 12$.

We show the following theorem.

THEOREM 5.4. *The sixth order diagonal-norm finite difference SBP-SAT operator \mathcal{D} with $x = x_1 = 342523/518400$ has eigenvalues with strictly positive real parts.*

Proof. We start by noticing that the expression of $D(\xi, x, N)$ in (5.3) depends on the products of the roots $r_1 r_2$, $r_1 r_5$, $r_1 r_6$, $r_2 r_5$, $r_2 r_6$, $r_5 r_6$. The moduli of their reciprocals are shown in Figure 5 as functions of $\xi \in I_\xi = [0, 4.21]$. For any fixed ξ , the magnitude of $1/(r_1 r_2)$ is significantly greater than the ones of the other reciprocals. In particular, by extracting the maximum and the minimum from the computed absolute values of the reciprocals, we can write

$$(5.4) \quad \begin{aligned} 44.228 &\lesssim \left| \frac{1}{r_1 r_2} \right| \lesssim 69.898, & 0.952 &\lesssim \left| \frac{1}{r_1 r_6} \right| \leq 1, \\ 1 &\leq \left| \frac{1}{r_2 r_5} \right| \lesssim 1.051, & 0.014 &\lesssim \left| \frac{1}{r_5 r_6} \right| \lesssim 0.023, \end{aligned}$$

while $r_1 r_5 = r_2 r_6 = 1 \forall \xi \in I_\xi$. As a consequence, for $N \geq 17$ the first term in (5.3) is significantly larger than the other contributions of $D(\xi, x, N)$, since

$$\begin{aligned} |\tau_{1,2}(\xi, x_1)| &\gtrsim 2.507 \cdot 10^{87}, & |\tau_{1,5}(\xi, x_1)| &\lesssim 3.050 \cdot 10^{75}, \\ |\tau_{1,6}(\xi, x_1)| &\lesssim 1.798 \cdot 10^{75}, & |\tau_{2,5}(\xi, x_1)| &\lesssim 3.737 \cdot 10^{75}, \\ |\tau_{2,6}(\xi, x_1)| &\lesssim 3.050 \cdot 10^{75}, & |\tau_{5,6}(\xi, x_1)| &\lesssim 5.935 \cdot 10^{55}, \end{aligned}$$

for $\xi \in I_\xi$.

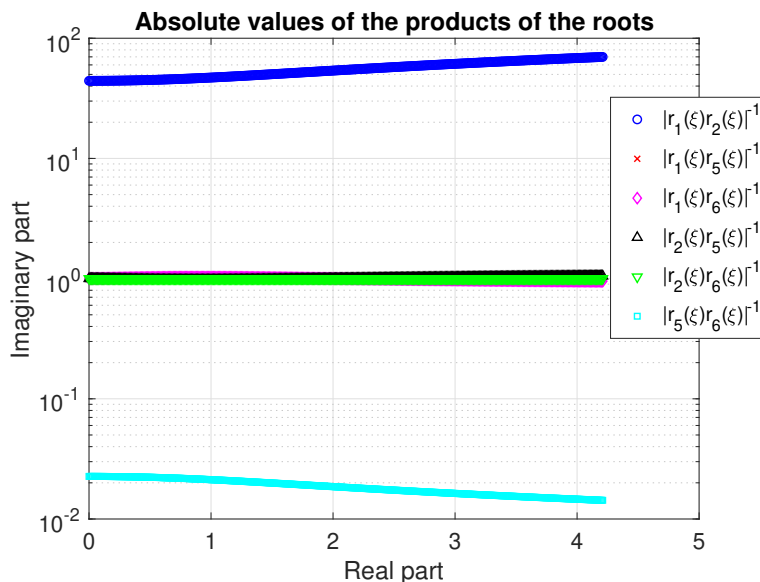


FIG. 5. The moduli of $(r_1 r_2)^{-1}$, $(r_1 r_5)^{-1}$, $(r_1 r_6)^{-1}$, $(r_2 r_5)^{-1}$, $(r_2 r_6)^{-1}$, $(r_5 r_6)^{-1}$ as functions of $\xi \in I_\xi$.

The term with $1/(r_1 r_2)^{N-17}$ has a reduced magnitude as N gets smaller, but it is still dominant for $N \geq 12$. Indeed, due to (5.4) for $N = 12$ we can write

$$\begin{aligned} \left| \frac{\tau_{1,2}(\xi, x_1)}{(r_1 r_2)^{-5}} \right| &\gtrapprox 1.502 \cdot 10^{78}, & \left| \frac{\tau_{1,5}(\xi, x_1)}{(r_1 r_5)^{-5}} \right| &\lesssim 3.050 \cdot 10^{75}, \\ \left| \frac{\tau_{1,6}(\xi, x_1)}{(r_1 r_6)^{-5}} \right| &\lesssim 2.299 \cdot 10^{75}, & \left| \frac{\tau_{2,5}(\xi, x_1)}{(r_2 r_5)^{-5}} \right| &\lesssim 3.737 \cdot 10^{75}, \\ \left| \frac{\tau_{2,6}(\xi, x_1)}{(r_2 r_6)^{-5}} \right| &\lesssim 3.050 \cdot 10^{75}, & \left| \frac{\tau_{5,6}(\xi, x_1)}{(r_5 r_6)^{-5}} \right| &\lesssim 1.104 \cdot 10^{65} \end{aligned}$$

for $\xi \in I_\xi$.

Hence, we proved that $D(\xi, x_1, N) \neq 0$ for any $\xi \in I_\xi$. This implies that it is not possible to have eigenvectors \mathbf{v} of $P^{-1}S$ with $v_0 = v_N = 0$ for $x = x_1 = 342523/518400$, and the claim follows due to Lemma 2.5. \square

In a similar fashion, we prove the following theorem.

THEOREM 5.5. *The sixth order diagonal-norm finite difference SBP-SAT operator \mathcal{D} with $x = x_2 = 89387/129600$ and $x = x_3 = 0.70127127127 \dots$ has eigenvalues with strictly positive real parts.*

Proof. See Appendix B and Appendix C in the supplement. \square

6. Final remarks on the strict positivity of the eigenvalues. The spectrum of \mathcal{D} is shown in Figure 6 for $\sigma = -1$, $N \in \{50, 200\}$, $\Delta t = 1/N$, and several SBP-SAT finite-difference approximations. Note that for sixth order discretizations the free parameter x leads to spectra with different features.

If $x = x_1 = 342523/518400$, the eigenvalues are more distant from the imaginary axis than for the other x values. On the other hand, this parameter choice also results in two outliers which significantly increase the stiffness of the time discretization operator for large values of N . Two outliers, close to the origin of the complex plane, can be found for $x = x_2 = 89387/129600$ as well. These eigenvalues have a strictly positive real part which increases as N increases. The last parameter choice, $x = x_3 = 0.70127127127\dots$, yields the spectrum closest to the imaginary axis, but it does not have outliers.

As predicted by our analysis, the time discretization operator has eigenvalues with strictly positive real parts. This property allows for provably unique and invertible fully discrete approximations of initial boundary value problems. Another direct consequence of our findings is that the second, fourth, and sixth order accurate first derivative SBP operators D are null-space consistent; i.e., their null-spaces consist only of the vector $\mathbf{1}$. This allows us to conclude that the dual-consistent SBP-SAT time integration methods based on these operators are stiffly accurate, strongly S -stable, and dissipatively stable Runge–Kutta schemes. (See [13] for further details.)

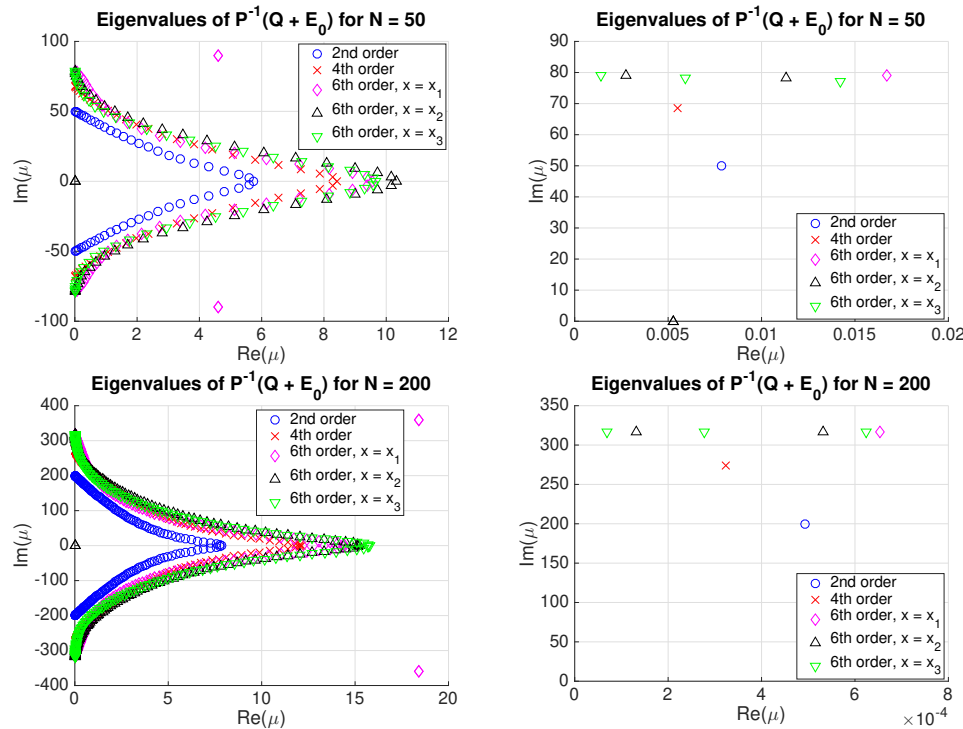


FIG. 6. The spectrum of \mathcal{D} for $\sigma = -1$, $N \in \{50, 200\}$, and $\Delta t = 1/N$ is shown for several SBP-SAT finite difference based approximations. The right figures are magnifications of the left figures.

7. Conclusions. We have identified a necessary and sufficient condition for the existence of eigenvectors to a matrix with repeating stencil. This criterion, which is also a necessary and sufficient condition for the matrix having eigenvalues with strictly positive real parts, has been used to investigate SBP-SAT time discretizations. The condition enabled a detailed eigenvalue analysis for finite difference based second order

approximations.

We have also studied fourth and sixth order approximations of energy-stable initial value problems. Strict positivity of the eigenvalues of these formulations has been shown irrespective of the discretization parameter. In particular, the dual consistent choice leads to Runge–Kutta time integration methods with various stability properties, such as stiff accuracy, strong S -stability, and dissipative stability. Our approach can be used to prove this result for even higher order approximations with repeating stencil.

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