

A MULTIGRID FORMULATION FOR FINITE DIFFERENCE METHODS ON SUMMATION-BY-PARTS FORM: AN INITIAL INVESTIGATION

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Abstract. *Several multigrid iteration schemes for high order finite difference methods are studied by comparing the effect of different interpolation operators. The usual choice of prolongation and restriction operators based on linear interpolation in combination with the Galerkin condition leads to coarse grid operators which are less accurate than their fine grid counterparts.*

Moreover, these operators do not mimic the integration-by-parts property possessed by the original fine grid summation-by-part schemes and hence are intuitively less stable. In this paper, an alternative class of interpolation operators is considered to overcome these issues and improve the stability of the overall multigrid iteration scheme. As a pleasant side effect we find that also the efficiency of the iteration scheme is improved.

1 INTRODUCTION

The multigrid method is a convergence acceleration technique based on a hierarchy of grids [1, 2]. The solution of a discrete problem on a fine grid is computed by solving a system of equations on the coarsest grid level. This technique is applied to problems in various branches of applied mathematics and engineering, such as the Helmholtz equation [3], magnetohydrodynamics [4] and computational fluid dynamics [5].

One of the main issues associated with this method is the construction of restriction and prolongation operators which transfer the information between grids. In this work we make use of a general relation between prolongation and restriction operators which was originally proposed in a different context [6]. These interpolation operators are consistent at the boundaries and guarantee that the accuracy of the original scheme is retained at the interior nodes on each grid level.

By using this result, we combine the multigrid method with an energy stable discretization for high order finite difference methods, based on the Summation–by–Parts (SBP) and Simultaneous–Approximation–Term (SAT) approach described in [7]. The improved stability of the new multigrid method is shown through numerical simulations of a hyperbolic problem in one dimension.

The rest of this paper is organized as follows: in Section 2 the main features of the two-level multigrid algorithm are presented. Section 3 introduces the SBP operators and the SAT penalty terms for high order finite difference discretizations. Section 4 deals with the construction of multigrid algorithms for SBP–SAT discretizations using the new class of interpolation operators. In Section 5 the new algorithm is compared to a multigrid scheme with conventional prolongation and restriction operators. Conclusions are drawn in Section 6.

2 THE MULTIGRID ALGORITHM

In this Section the multigrid approach is outlined by means of a two–level algorithm[1, 2, 8]. Let us consider the following steady–state problem

$$\begin{aligned} Lu &= f, \quad \text{in } \Omega, \\ Hu &= g, \quad \text{on } \partial\Omega, \end{aligned} \tag{1}$$

where L is a differential operator, H is a boundary operator, f and g are given functions, and Ω is a domain. We assume that the boundary conditions are assigned in a way such that (1) is well–posed. The multigrid algorithm for solving (1) can be written in four steps:

1. Discretization;
2. Error smoothing;
3. Coarse–grid correction;
4. Fine–grid update.

2.1 Discretization

Construct a discretization for (1) on a grid $\Omega_1 \subset \Omega \cup \partial\Omega$ called *fine grid*. The resulting problem has the form

$$L_1 \mathbf{u} = \mathbf{f}, \tag{2}$$

where L_1 is a discretization of the operator L in (1) which also includes the boundary conditions defined by H . The vector \mathbf{f} is a grid function which approximates f on the nodes of Ω_1 , possibly augmented with boundary data, and \mathbf{u} is an approximate solution to (1). Typically Ω_1 has many nodes, and therefore it may be expensive to solve (2) directly.

The discrete operator L_1 is assumed to be invertible, since its continuous counterpart L in (1), with the boundary conditions defined by H , leads to a well-posed problem. Even though we do not want to compute the inverse of L_1 , the solution to (2) will be indicated by $L_1^{-1}\mathbf{f}$ in the rest of the paper.

2.2 Error smoothing

Define an error smoothing procedure. As an example, we may consider to march toward the solution to (2) from an initial guess $\mathbf{u}^{(0)}$ by solving

$$\begin{aligned} \left(\frac{d}{dt} + L_1\right)\mathbf{w}(t) &= \mathbf{f}, & t > 0, \\ \mathbf{w}(0) &= \mathbf{u}^{(0)}, \end{aligned} \quad (3)$$

for a given finite time $\Delta t > 0$ called *smoothing step*. The solution to (3) is

$$\mathbf{w}(\Delta t) = e^{-L_1\Delta t}\mathbf{u}^{(0)} + (I - e^{-L_1\Delta t})L_1^{-1}\mathbf{f}, \quad (4)$$

where I indicates the identity matrix on Ω_1 . Note that this technique yields a smoothing effect on the grid function $\mathbf{u}^{(0)}$ if all the eigenvalues of L_1 have positive real part. In particular, $\mathbf{w}(\Delta t) \rightarrow \mathbf{u} = L_1^{-1}\mathbf{f}$ as $\Delta t \rightarrow +\infty$.

By similarity, we may define a general smoothing technique for (2) as

$$\begin{aligned} \mathbf{v}^k &= S\mathbf{v}^{k-1} + (I - S)L_1^{-1}\mathbf{f}, & k = 1, \dots, \nu, \\ \mathbf{v}^0 &= \mathbf{u}^{(0)}, \end{aligned} \quad (5)$$

where the exponential smoother $S_{exp} = e^{-L_1\Delta t}$ yields a procedure based on time-marching as in (4). After ν steps, the iterative method (5) provides the grid function

$$\mathbf{v} = S^\nu\mathbf{u}^{(0)} + (I - S^\nu)L_1^{-1}\mathbf{f}. \quad (6)$$

This step of the algorithm is necessary since the high frequency modes on Ω_1 may be unresolved on coarser grids (see Figure 1).

2.3 Coarse-grid correction

Consider $\Omega_2 \subsetneq \Omega_1$, called the *coarse grid*, and solve a correction problem on Ω_2 :

$$L_2\mathbf{d} = I_r(\mathbf{f} - L_1\mathbf{v}) \quad (7)$$

which is obtained from (2) and (4) by making use of

- a restriction operator $I_r : \Omega_1 \rightarrow \Omega_2$,
- a coarse-grid operator $L_2 : \Omega_2 \rightarrow \Omega_2$.

The coarse-grid operator can be built by using the Galerkin Condition [2]

$$L_2 = I_r L_1 I_p, \quad (8)$$

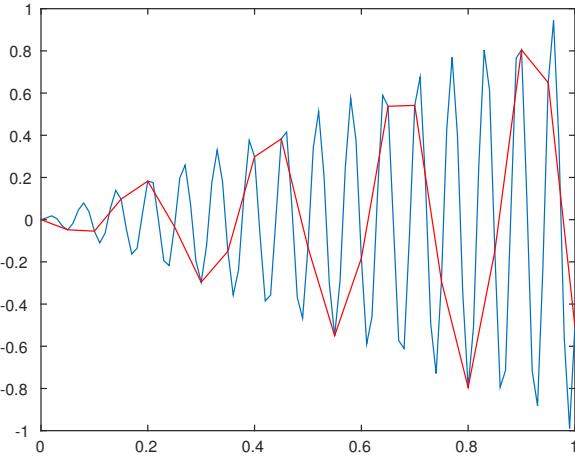


Figure 1: The function $x \sin(100x)$, $x \in [0, 1]$, is represented on a fine (blue line) and on a coarse grid (red line). The fine grid is given by 101 equidistant points, while the coarse grid has got 21 nodes. The restricted grid function has a lower frequency than the original one.

where $I_p : \Omega_2 \rightarrow \Omega_1$ is a prolongation operator.

A common choice for I_p in the one dimensional case is based on linear interpolation. Assuming for example that $\Omega_1 = \{x_j : x_j = jh, \quad j = 0, \dots, N\}$ with $h = 1/N$, and that Ω_2 consists of the odd nodes of Ω_1 , we may write

$$(I_p \mathbf{v})_m = \begin{cases} v_j, & m = 2j, \\ \frac{1}{2}(v_j + v_{j+1}), & m = 2j + 1, \end{cases} \quad j = 0, \dots, N/2, \quad (9)$$

while the restriction operator is usually given in terms of the prolongation operator

$$I_r = \frac{1}{2} I_p^T. \quad (10)$$

2.4 Fine-grid update and multigrid iteration scheme

Update the fine grid solution \mathbf{v} with an estimate of the correction \mathbf{d} in (7), obtained through prolongation with I_p

$$\mathbf{u}^{(1)} = \mathbf{v} + I_p \mathbf{d}. \quad (11)$$

This relation, together with (6) and (7), provides an iterative method for solving (1):

$$\mathbf{u}^{(n+1)} = M \mathbf{u}^{(n)} + N \mathbf{f}, \quad (12)$$

where

$$M = CS^\nu, \quad C = I - I_p L_2^{-1} I_r L_1 \quad \text{and} \quad N = (I - M) L_1^{-1}. \quad (13)$$

We will refer to M as the multigrid iteration matrix and to C as the coarse-grid correction operator.

The role of M in the convergence of the iterative method (12) is central: by considering the errors $\mathbf{e}^{(n)} = \mathbf{u}^{(n)} - L^{-1} \mathbf{f}$, we get

$$\mathbf{e}^{(n+1)} = M \mathbf{e}^{(n)}, \quad (14)$$

which leads to convergence if the spectral radius of M is less than 1.

2.5 The coarse-grid correction operator

In Section 2.3 we claimed that the Galerkin condition (8) may be used to build a coarse-grid operator L_2 . This choice leads to some interesting theoretical properties about the coarse-grid correction operator C in (12), (13). To start with, we prove

Lemma 2.1. *If the Galerkin condition (8) holds, then the coarse-grid correction operator C in (12), (13) is idempotent, i.e. $C^k = C$ for every $k \in \mathbb{N}$.*

Proof. By multiplying C by itself we get

$$C^2 = (I - I_p L_2^{-1} I_r L_1) (I - I_p L_2^{-1} I_r L_1) = I - 2I_p L_2^{-1} I_r L_1 + I_p L_2^{-1} I_r L_1 I_p L_2^{-1} I_r L_1 = C,$$

since the Galerkin condition $L_2 = I_r L_1 I_p$ is fulfilled. \square

The idempotency of C implies that its eigenvalues are given by zeros and ones [9]. Moreover, it is possible to show

Corollary 2.2. *If the Galerkin condition (8) holds, the image of the prolongation operator I_p is contained in the nullspace of C .*

Proof. Consider a vector $\mathbf{y} \in \text{Im}(I_p)$, i.e. $\mathbf{y} = I_p \mathbf{z}$. When the coarse-grid correction operator acts on this vector, we find

$$C\mathbf{y} = (I - I_p L_2^{-1} I_r L_1) I_p \mathbf{z} = I_p \mathbf{z} - I_p L_2^{-1} I_r L_1 I_p \mathbf{z} = \mathbf{0},$$

since the Galerkin condition holds. \square

The main consequence of Corollary 2.2 is that C cancels all the grid functions which can be represented through the prolongation operator I_p . This implies that C deals with smooth errors while the smoother S damps the remaining high frequency modes.

3 THE SBP–SAT DISCRETIZATION

In this Section we introduce the Summation-by-Parts operators (SBP) and the Simultaneous-Approximation-Term (SAT) technique. The first ones mimic integration by parts, whereas the second one introduces penalty-like terms enforcing the boundary conditions weakly [7].

Definition 3.1. *We say that $D = P^{-1}Q$ is a (p, q) -accurate first derivative SBP operator, if $Q + Q^T = B = \text{diag}(-1, 0, \dots, 0, 1)$, P is a symmetric positive definite matrix, and the associated truncation errors are $\mathcal{O}(h^p)$ in the interior and $\mathcal{O}(h^q)$ at the boundaries.*

SBP operators based on diagonal norms P are available for even orders $p = 2q$ in the interior, while the boundary closure is q th order accurate. Even though this is not the only possible choice, we will only consider these $(2q, q)$ -accurate operators with diagonal P . For further details on the construction of SBP operators for the first derivative with $q \leq 4$, see [10].

The SBP finite difference operators together with a strong treatment of the boundary conditions only admits stability proofs for very simple problems. This was shown in [11], where SAT technique was proposed to complement the SBP schemes. By discretizing a well-posed Initial-Boundary-Value-Problem (IBVP) with both SBP operators and SAT penalty terms (the SBP–SAT approach), it is possible to prove that the corresponding semi-discrete problem is stable. As an example, we consider the advection equation in one dimension.

3.1 The advection problem

Consider

$$\begin{aligned} u_t + u_x &= 0, \quad 0 < x < 1, \quad t > 0, \\ u(x, 0) &= f(x), \quad 0 < x < 1, \\ u(0, t) &= g(t), \quad t > 0, \end{aligned} \tag{15}$$

where both f and g are known data. The problem (15) is well-posed, since the analytical solution is a traveling wave, and the boundary condition is imposed at the inflow.

Let us consider an $(N + 1)$ -point uniform grid on $[0, 1]$, given by $x_j = jh$ for $j = 0, \dots, N$, where $h = 1/N$. We introduce the grid function $f_j = f(x_j)$ and to each grid point we also associate the approximate solution u_j . By applying the SBP-SAT discretization in space to (15), we get

$$\begin{aligned} \mathbf{u}_t + P^{-1}Q\mathbf{u} &= P^{-1}\sigma(u_0 - g)\mathbf{e}_0, \quad t > 0, \\ \mathbf{u}(0) &= \mathbf{f}, \end{aligned} \tag{16}$$

where $\mathbf{u} = (u_0, \dots, u_N)$, $\mathbf{f} = (f_0, \dots, f_N)$, $\sigma \in \mathbb{R}$ is a penalty parameter which can be tuned for stability, and $\mathbf{e}_0 = [1, 0, \dots, 0]^T \in \mathbb{R}^{N+1}$. By defining the matrix $\tilde{Q}_\sigma = Q - \sigma\mathbf{e}_0\mathbf{e}_0^T$ and the vector $\mathbf{F} = -P^{-1}\sigma g\mathbf{e}_0$ we can rewrite (15) in a more compact form

$$\begin{aligned} \mathbf{u}_t + P^{-1}\tilde{Q}_\sigma\mathbf{u} &= \mathbf{F}, \quad t > 0, \\ \mathbf{u}(0) &= \mathbf{f}, \end{aligned} \tag{17}$$

where $\tilde{Q}_\sigma + \tilde{Q}_\sigma^T = \text{diag}(-(1 + 2\sigma), 0, \dots, 0, 1)$.

We want to find σ such that the problem (17) is strongly stable, i.e. such that

$$\|\mathbf{u}(\cdot, t)\|^2 \leq K(t) \left(\|\mathbf{f}\|^2 + \max_{\tau \in [0, t]} \|g(\tau)\|^2 \right) \tag{18}$$

in a suitable norm, with $K(t)$ bounded for any finite t and independent of the data (for further details, see [7]). By multiplying the equation (17) by $\mathbf{u}^T P$ and adding the transpose we find

$$\frac{d}{dt} \|\mathbf{u}\|_P^2 = -u_N^2 + (1 + 2\sigma)u_0^2 - 2\sigma gu_0$$

where $\|\mathbf{u}\|_P = \sqrt{\mathbf{u}^T P \mathbf{u}}$. For $g = 0$ the method is stable for $\sigma \leq -\frac{1}{2}$. If $g \neq 0$ and assuming that $\sigma \neq -\frac{1}{2}$, we get

$$\frac{d}{dt} \|\mathbf{u}\|_P^2 = -\frac{\sigma^2}{1 + 2\sigma}g^2 - u_N^2 + \frac{[(1 + 2\sigma)u_0 - \sigma g]^2}{1 + 2\sigma},$$

which lead to an estimate of the form (18). Therefore, the semi-discrete problem (16) is strongly stable if $\sigma < -\frac{1}{2}$.

4 THE SBP-SAT-MG SCHEME

In the previous Section we have shown that operators which mimic integration by parts leads to stable semi-discrete problems. We conjecture that preserving this property on both fine and coarse levels should lead to an improved multigrid method.

Let us consider the following steady model problem

$$\begin{aligned} u_x &= f, \quad 0 < x < 1, \\ u(0) &= g. \end{aligned} \tag{19}$$

By applying the SBP–SAT method (see Section 3.1) we get

$$P^{-1}\tilde{Q}_\sigma \mathbf{u} = \mathbf{F}, \quad (20)$$

where $\mathbf{F} = \mathbf{f} - P^{-1}\sigma g \mathbf{e}_0$ and \tilde{Q}_σ is defined above. Since our problem is written on the same form as (2), we can apply the multigrid scheme in Section 2 directly. The time–marching smoothing procedure (3) yields the semi–discrete problem (17), whose solution is stable. Following the remaining steps of the algorithm, we define a coarse grid correction problem using the Galerkin Condition (8). Unfortunately, the resulting coarse–grid operator does not satisfy the SBP property if standard restriction and prolongation operators like (9) and (10) are used.

By looking closely at the multigrid algorithm, we realize that the restriction operator chosen in (10) is consistent only in the interior. Hence, instead of using this relation, we use

$$I_r = P_2^{-1} I_p^T P \quad (21)$$

proposed in [6], where P_2 is a symmetric positive definite matrix of the same type as P on the coarse grid. By satisfying (21) it is possible to build pairs of consistent and p th–order accurate prolongation and restriction operators according to the following definition of SBP–preserving interpolation operators given in [6].

Definition 4.1. *Let the row–vectors \mathbf{x}_1^k and \mathbf{x}_2^k be the projections of the monomials x^k onto equidistant 1–D grids corresponding to a fine and coarse grid, respectively. We say that I_r and I_p are $2q$ th–order accurate SBP–preserving interpolation operators if $I_r \mathbf{x}_1^k - \mathbf{x}_2^k$ and $I_p \mathbf{x}_2^k - \mathbf{x}_1^k$ vanish for $k = 0, \dots, 2q - 1$ in the interior and for $k = 0, \dots, q - 1$ at the boundaries.*

The SBP–preserving interpolation operators with minimal bandwidth for $q = 1$ are given by

$$I_p = \begin{bmatrix} 1 & & & & \\ \frac{1}{2} & \frac{1}{2} & & & \\ & 1 & & & \\ & \frac{1}{2} & \frac{1}{2} & & \\ & & \ddots & \ddots & \\ & & & 1 & \\ & & & \frac{1}{2} & \frac{1}{2} \\ & & & & 1 \end{bmatrix}, \quad I_r = \frac{1}{2} \begin{bmatrix} 1 & 1 & & & \\ \frac{1}{2} & 1 & \frac{1}{2} & & \\ & \frac{1}{2} & 1 & \frac{1}{2} & \\ & & \ddots & \ddots & \ddots \\ & & & \frac{1}{2} & 1 & \frac{1}{2} \\ & & & & 1 & 1 \end{bmatrix}. \quad (22)$$

Note that in this case I_p coincides with the prolongation operator (9).

The SBP–preserving interpolators, together with the Galerkin Condition (8), lead to the following coarse grid operator

$$P_2^{-1}\tilde{Q}_{2,\sigma} = I_r (P^{-1}\tilde{Q}_\sigma) I_p = P_2^{-1} I_p^T P (P^{-1}\tilde{Q}_\sigma) I_p = P_2^{-1} (I_p^T \tilde{Q}_\sigma I_p),$$

where obviously $\tilde{Q}_{2,\sigma} = I_p^T \tilde{Q}_\sigma I_p$.

We claim

Proposition 4.2. *The interpolation operators satisfying (21) lead to a coarse grid operator $\tilde{Q}_{2,\sigma}$ which satisfies the Summation–By–Parts property.*

The proof will be given in the full paper. Hence, through the Galerkin Condition (8) it is possible to build new SBP operators on the coarse grid. Moreover, these operators are consistent with (19) and can retain the accuracy of the original scheme at the interior nodes. We can show

Proposition 4.3. Consider the $2q$ th-order accurate SBP-preserving interpolation operators I_p and I_r , with $q \geq 1$. If D is a $(2q, q)$ -first derivative SBP-operator in the fine grid, then $D_2 = I_r D I_p$ is a first derivative SBP-operator in the coarse grid. Moreover, it is $2q$ th-order accurate in the interior nodes, while the accuracy on the boundary nodes is at least $q - 1$.

The proof will be given in the full paper.

Remark 4.4. For $q = 1$ the coarse grid operator D_2 has the same structure as D and is first-order accurate at the boundaries.

The operators for higher orders will be provided in the full paper.

5 NUMERICAL EXPERIMENTS

In this Section we perform numerical computations to test the properties of the new multigrid iteration scheme. Consider (19) as model problem with a manufactured solution given by

$$v(x) = e^{-x} (\cos(10\pi x) + \cos(2\pi x)), \quad 0 < x < 1.$$

To discretize (19) we use the formulation (20) on an $(N+1)$ -point uniform grid on $[0, 1]$. The tests are carried out using a single-step smoother based on a modified Runge–Kutta scheme which was proposed in [12] for first order systems:

$$S = I - \Delta t L_1 + 0.6\Delta t^2 L_1^2 - 0.36\Delta t^3 L_1^3. \quad (23)$$

In the following tests, we consider that the multigrid iteration has reached convergence if $\|\mathbf{u}^{n+1} - \mathbf{u}^n\| < \varepsilon$, where $\varepsilon = \text{tolerance}$.

5.1 IMPROVED CONVERGENCE

Consider a $(2, 1)$ -order accurate discretization on a grid with $N = 500$ and a smoothing step $\Delta t = 5 \cdot 10^{-4}$. Figure 2 shows the spectral radius and the distribution of the eigenvalues of the multigrid iteration matrix M in (13) by varying the interpolation operators. In particular, the SBP-preserving interpolation operators of 2nd order are tested against the classical choices (9) and (10). Note that even if in this case the prolongation operator is the same (see (22)), a minor change in the restriction operator affects the distribution of the eigenvalues of M .

To test the convergence properties, we have used both the tolerance 10^{-10} and 10^{-3} . The results, shown in Table 1, suggest that the new class of operator is clearly superior.

	SBP-preserving	Conventional
Number of iterations (10^{-10})	2372	$> 10^6$
Number of iterations (10^{-3})	1470	1541

Table 1: The number of iterations to convergence for the multigrid scheme with tolerance 10^{-10} and 10^{-3} .

Another test with tolerance $\varepsilon = 10^{-10}$ and an increased smoothing step $\Delta t = 6.3 \cdot 10^{-4}$ makes the spectral radius for the SBP-preserving choice decrease, while the classical linear prolongation and restriction lead to instability. As a side effect, the number of iterations to convergence for the new interpolation operators drops to 1873. In Figure 3 the distributions of the eigenvalues are shown for this case. Note that the current smoothing step is close to the

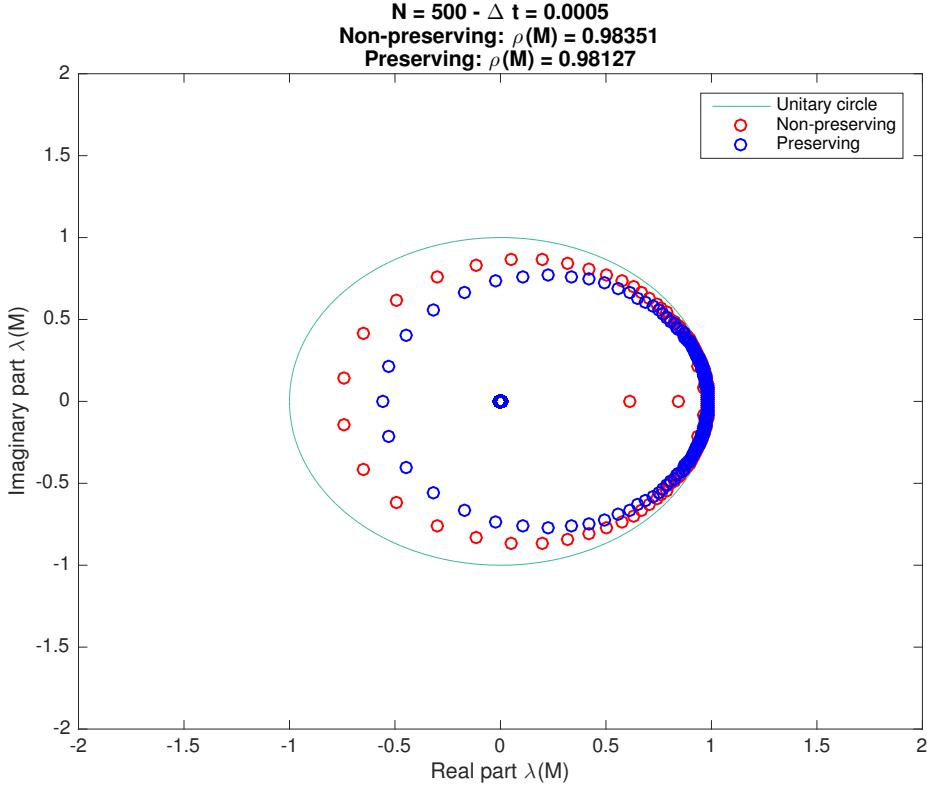


Figure 2: Eigenvalues of the multigrid iteration matrix for different choices of interpolation operators. The spectral radius of M with SBP-preserving interpolators is less than the one with the conventional prolongation and restriction.

stability limit. This phenomenon can be evaluated by looking at the eigenvalues on the left side of the picture: increasing the time-step Δt , the magnitude of these eigenvalues becomes bigger.

These numerical experiments suggest that the SBP-preserving interpolation operators yield multigrid iteration schemes with significantly improved convergence properties.

5.2 HIGHER ORDER METHODS

The following tests are carried out by raising the order of accuracy of the fine grid first-derivative operator. The tolerance $\varepsilon = 10^{-10}$ was used.

	Minimum iterations	Δt	$\rho(M)$	Δt^*
(4, 2), SBP-preserving	1435	$5.8 \cdot 10^{-4}$	0.96882	$5.9 \cdot 10^{-4}$
(4, 2), Conventional	6358	$1.3 \cdot 10^{-4}$	0.99404	$3.4 \cdot 10^{-4}$
(6, 3), SBP-preserving	1278	$5.1 \cdot 10^{-4}$	0.96955	$6.8 \cdot 10^{-4}$
(6, 3), Conventional	7030	$9.8 \cdot 10^{-5}$	0.99485	$2.6 \cdot 10^{-4}$
(8, 4), SBP-preserving	1856	$6.8 \cdot 10^{-4}$	0.98502	$7.2 \cdot 10^{-4}$
(8, 4), Conventional	10817	$7.9 \cdot 10^{-5}$	0.99667	$2.3 \cdot 10^{-4}$

Table 2: The minimum number of iterations and the corresponding smoothing step are presented for each order of accuracy. For the SBP-preserving choice the minimum amount of iterations is almost the same for any order. The spectral radius $\rho(M)$ and the time-step limit Δt^* are also given for each scheme.

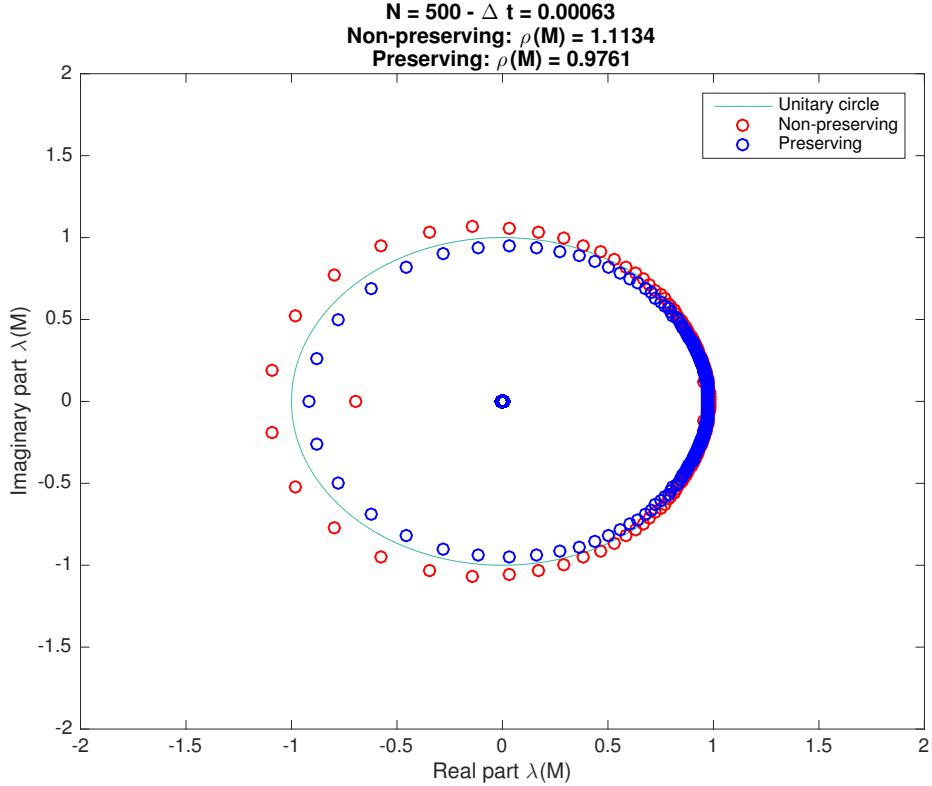


Figure 3: Increasing the smoothing step to $\Delta t = 6.3 \cdot 10^{-4}$ leads to an unstable multigrid iteration scheme, if the non-preserving choice is made.

In Table 2 the effects of the interpolation operators on the multigrid iteration scheme are shown. For each order of accuracy, the SBP-preserving interpolators lead to faster convergence. Moreover, the minimum amount of iterations does not change considerably for higher orders. Conversely, when the order of accuracy of the fine-grid operator is increased and the classical linear interpolation (9) and (10) is used, the number of iterations grows and the time-step limit Δt^* decreases.

6 CONCLUSIONS

A new multigrid scheme for SBP-SAT discretizations has been proposed. So called SBP-preserving interpolation operators have been used to convey information between grids. When the Galerkin condition is considered, these prolongation and restriction operators lead to coarse-grid operators which satisfy the summation-by-part property.

Numerical experiments show that when compared to a multigrid scheme with the conventional choice of prolongation and restriction based on linear interpolation, the new scheme allows the use of larger smoothing steps and reaches convergence in fewer iterations. Hence, for every order of accuracy the SBP-preserving interpolation operators lead to multigrid iteration schemes which are more stable and have better convergence properties.

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