Summation-by-Parts Operators with Minimal Dispersion Error for Coarse Grid Flow Calculations

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Abstract

We present a procedure for constructing Summation-by-Parts operators with minimal dispersion error both near and far from numerical interfaces. Examples of such operators are constructed and compared with purely periodic stencils as well as non-optimised Summation-by-Parts operators of higher order. Experiments show that the optimised operators are superior for wave propagation and turbulent flows involving large wavenumbers, long solution times and large ranges of resolution scales.

Keywords: Summation-by-Parts; Dispersion relation; Finite differences; Wave propagation

1. Introduction and motivation

It is well known that maximising the formal order of accuracy with respect to the bandwidth of a finite difference stencil may lead to a suboptimal numerical scheme for problems involving high frequency waves over large time spans. In order to properly resolve such waves, a very small spatial increment is typically required. However, severe restrictions on the spatial increment naturally has a negative impact on the efficiency of the solver. Problems of this type are common in fields such as fluid dynamics, acoustics, meteorology, electromagnetism and seismology, and have been addressed accordingly, see e.g. [1, 2, 3, 4, 5]. For these problems, the errors in the numerical solutions are dominated by inaccurate approximations of the dispersion relations related to the governing partial differential equations. Wave properties encoded within
the dispersion relation include phase velocity, group velocity, anisotropy and dissipation. It is therefore of interest to develop finite difference schemes that preserve the analytic dispersion relation of the governing equations for a wide range of spatial increments. In [6], a discussion and comparison is made of many stencils that attempt to do so. For more recent approaches, see e.g. [7, 8, 9].

Discussions of numerical dispersion has in the literature largely been concerned with central finite difference stencils suitable for purely periodic problems. However, in realistic simulations numerical interfaces will generally be present, at which departure from centrality may be required, and questions of numerical stability must be addressed. In this paper we will present a procedure for designing new finite difference operators on Summation-by-Parts (SBP) form [10, 11, 12, 13, 14] that approximate first derivatives both near and far from numerical interfaces. SBP operators combined with weakly imposed interface conditions lead to provably stable schemes, and may be constructed at high orders. The new operators have suboptimal order of accuracy relative to the bandwidth, leaving a set of free stencil parameters that are used to minimise the dispersion error.

SBP operators based on dispersion relation preserving schemes [15] have previously been constructed in [16], however no particular procedure was applied in order to minimise the dispersion near interfaces. In this paper we will construct SBP operators based on the local stencils presented in [9], where the dispersion error of central difference stencils were minimised in the $L^\infty$-sense. We extend this work by analogously minimising the dispersion error of the non-central stencils arising near the interface. This minimisation problem is shown to be quasiconvex and may thus be solved fast and reliably using standard optimisation packages.

This paper is structured as follows: We introduce relevant notation and mathematical concepts in Section 2. In Section 3 we discuss the definition, properties and structure Summation-by-Parts operators. We discuss the procedure of obtaining optimal SBP operators and show a few examples in Section 4. In Section 5 we illustrate the performance of the new SBP operators by solving relevant test problems. Finally, concluding remarks are made in Section 6.
2. Preliminaries

Before we proceed we introduce the notation and theoretical concepts that will be required.

2.1. Notation

Throughout this paper we will separate analytic quantities and approximated quantities, the latter of which we mark with an overbar. Thus, for example \( \bar{\xi} \) would represent a numerical approximation of the analytic quantity \( \xi \).

Matrices will in general be denoted by capitalised letters. Functions will be denoted by lower case letters, e.g. \( u(x, t) \), unless otherwise specified. If a function is evaluated on a discrete grid we write it as a vector, e.g. \( u = (u_0, \ldots, u_N)^T \). Here \( u_j \) is the \( j \)th element of the \( (N + 1) \)-dimensional vector \( u(t) \), given by the function value of \( u(x, t) \) at the point \( x = x_j, 0 \leq j \leq N \). In this paper we assume that all grids are equidistant and let \( \Delta x = x_{j+1} - x_j \) be the spatial increment.

2.2. Dispersion of local finite difference stencils

Consider a local finite difference approximation at the point \( x_j \) defined as a weighted sum of function evaluations at \( L \) points to the left and \( R \) points to the right of \( x_j \);

\[
\left( \frac{\partial f}{\partial x} \right)_j \approx \frac{1}{\Delta x} \sum_{m=-L}^{R} c_m f_{j+m}.
\]  

(1)

Here, \( f_j \) is the \( j \)th element of the vector \( f \), which is obtained by projecting the function \( f(x) \) onto the grid, and \( c_m \) denote the corresponding weights. Following the derivation in [15], we note that the above equation is a special case of

\[
\frac{\partial f(x)}{\partial x} \approx \frac{1}{\Delta x} \sum_{m=-L}^{R} c_m f(x + m\Delta x).
\]  

(2)

when \( x = j\Delta x \). By the inverse Fourier transform we may write

\[
f(x) = \int_{-\infty}^{\infty} \hat{f}(\kappa) \exp(i\kappa x) d\kappa,
\]
where $\hat{f}(\kappa)$ is the Fourier transform of $f$ and $\kappa$ is a wavenumber. Inserting this into (2), multiplying by $-i\Delta x$ and cancelling common terms gives

$$\Delta x \kappa \approx -i \sum_{m=-L}^{R} c_m \exp (im\Delta x \kappa).$$

(3)

Thus, the finite difference stencil provides an approximation of the analytic wavenumber in terms of a truncated Fourier-type series.

We introduce the notation $\xi = \kappa \Delta x$ as the normalised wavenumber. As the smallest resolvable wavelength is $\lambda_{\min} = 2\Delta x$, the largest resolvable wavenumber is $\kappa_{\max} = 2\pi/\lambda_{\min} = \pi/\Delta x$, implying that $|\xi| \leq \pi$. Typically we will consider some smaller range of wavenumbers, $\xi \in [0, \kappa_{\max}]$.

We define the dispersion error as

$$E(\xi, c) = \xi - \bar{\xi}(\xi, c) = \xi - \left(-i \sum_{m=-L}^{R} c_m \exp (im\xi)\right),$$

(4)

where $\bar{\xi}(\xi, c)$ is the numerical approximation of the normalised wavenumber, henceforth referred to as the numerical wavenumber. The vector $c$ contains the coefficients $c_m$.

We make a special note of the case when $L = R = n$, i.e. when the stencil is central. To distinguish this case from the non-central stencils we will refer to the vector of coefficients by the letter $a$. In this case we have the relations $a_m = -a_{-m}$, $a_0 = 0$. Thus, by (4) the dispersion error for the central difference stencil is given by

$$E(\xi, a) = \xi - 2 \sum_{m=1}^{n} a_m \sin (m\xi).$$

(5)

In this case the numerical wavenumber is purely real. Hence, the stencil causes no growth or decay of the solution.

3. Summation-by-Parts operators

Summation-by-Parts (SBP) operators were first derived in [10, 11] and further developed in [12]. Augmented with Simultaneous Approximation Terms (SAT) [17] that weakly enforce boundary conditions, the SBP-SAT technique allows for stable and high order discretisations of partial differential equations if well posed boundary conditions are available. For reviews of the SBP-SAT technique and its development, see [13, 18] and the references therein.
3.1. Definition

A Summation-by-Parts operator \( D = P^{-1}Q \) may be defined by the properties

1. \( \partial u / \partial x \big|_{x=x_j} \approx e_j^T D u, \quad j = 0, \ldots, N, \)
2. \( P = P^T > 0, \)
3. \( Q + Q^T = \text{diag}(-1, 0, \ldots, 0, 1), \)

where \( P \) and \( Q \) are matrices of dimension \((N + 1) \times (N + 1)\), and \( u \) is the projection of the function \( u(x, t) \) onto the grid. Here, \( e_j \) is the \( j \)th unit vector.

Remark 1. There are more general formulations than 1,2,3 above that extend the definition of Summation-by-Parts operators to non-cartesian grids, see [19, 20, 21].

3.2. Stability

To illustrate the use of the SBP-SAT technique we consider the periodic model problem

\[
\begin{align*}
  u_t + a u_x &= 0, & x &\in [0, 1], & t &\geq 0 \\
  u(x, 0) &= f, & x &\in [0, 1] \\
  u(0, t) &= u(1, t), & t &\geq 0,
\end{align*}
\]

(6)

where we let \( a > 0 \). Multiplying by \( u \) and integrating in space gives the energy rate

\[
\frac{d}{dt} \| u \|^2 = 0,
\]

(7)

which leads to a bounded solution, thus implying that the model problem is well posed.

Consider now discretising in space. Rather than using a periodic operator we will introduce a numerical interface connecting the grid points at \( x = 0 \) and \( x = 1 \) by imposing periodic boundary conditions. A discretisation of (6) using an SBP operator yields

\[
u_t + aP^{-1}Q u = \sigma_0 P^{-1}(u_0 - u_N)e_0 + \sigma_N P^{-1}(u_N - u_0)e_N,
\]

(8)

where the right-hand side consists of SAT terms that weakly impose the periodic interface condition at the first and last grid points in the domain.
Here, \(e_0\) and \(e_N\) are the first and last columns of the identity matrix with dimension \(N + 1\). Multiplying by \(u^T P\) and adding the transpose of the resulting equality yields

\[
\frac{d}{dt} \|u\|_P^2 = u_0^2(2\sigma_0 + a) + u_N^2(2\sigma_N - a) - 2u_0u_N(\sigma_0 + \sigma_N),
\]

where we have used point 2 in the definition of the SBP operator to define the norm \(\|u\|_P^2\) as \(u^T Pu\). Additionally, we have used point 3 in the definition in order to extract the boundary terms from \(Q\). In order to bound the right hand side we let the penalty parameters take the form \([22]\)

\[
\sigma_0 = -\frac{a + \theta}{2}, \quad \sigma_N = \frac{a - \theta}{2},
\]

for some constant \(\theta\). Inserting this into (9) and simplifying gives the final discrete energy rate

\[
\frac{d}{dt} \|u\|_P^2 = -\theta(u_0 - u_N)^2,
\]

which is bounded if \(\theta \geq 0\). Thus the discretisation (8) is a stable approximation of the model problem (6). Note that the discrete energy rate (10) mimics the continuous one (7) exactly if \(\theta = 0\), and adds a small dissipative term otherwise.

### 3.3. Structure and accuracy

As an example of the typical structure of \(Q\) we consider

\[
Q = \begin{pmatrix}
-1/2 & q_{12} & q_{13} & q_{14} \\
-q_{12} & 0 & q_{23} & q_{24} \\
-q_{13} & -q_{23} & 0 & q_{34} & a_2 \\
-q_{14} & -q_{24} & -q_{34} & 0 & a_1 & a_2 \\
 & -a_2 & -a_1 & 0 & a_1 & a_2 \\
\end{pmatrix},
\]

where \(a = (a_1, a_2)\) is the vector of coefficients of a (given) central difference stencil, and \(q_{ij}\) are stencil coefficients to be determined. Thus, \(Q\) consists of an interior set of central difference stencils augmented with blocks of size \(r \times r\) to account for the discretisation near domain interfaces.
For stability reasons [23, 24] we will in this paper limit our analysis to the case when $P$ is a diagonal matrix of the form

$$P = \Delta x \text{ diag}(p_1, \ldots, p_r, 1, \ldots, 1, p_r, \ldots, p_1),$$

where $p_j$, $j = 1, \ldots, r$ are positive real numbers.

In order for the matrices $P$ and $Q$ to be compatible they must satisfy certain linear accuracy conditions, first described in [10]. Let us impose that $D = P^{-1}Q$ should exactly differentiate polynomials up to degree $p$. Then, for the monomial $x^j$ (where the exponent is to be taken elementwise and $x^{-1} = 0$, where 0 is the all zeros vector), we have

$$Qx^j = jPx^{j-1}, \quad j = 0, \ldots, p. \quad (11)$$

Multiplying (11) from the left by $(x^i)^T$ and adding the resulting equality with swapped indices gives the identity

$$(x^i)^TQx^j + (x^j)^TQx^i = j(x^i)^TPx^{j-1} + i(x^j)^TPx^{i-1} = (i + j)1^TPx^{i+j-1},$$

where $1$ is the all ones vector and we have used the diagonal structure of $P$ in the final equality. Let $s = i + j$. Simplifying using property 3 in the definition of the SBP operator gives

$$s1^TPx^{s-1} = x_N^s - x_0^s, \quad s = 1, \ldots, 2p. \quad (12)$$

Note that (12) defines a set of $2p$ linear conditions on $P$ (the case $s = 0$ is trivially satisfied). In applications we will typically rearrange these conditions such that they take the simpler form

$$A_0\mathbf{p} = \mathbf{b}_0, \quad (13)$$

where the vector $\mathbf{p}$ contains the diagonal elements in $P$.

Consider now $Q$. Assuming that $P$ has been determined by solving (13), the equality (11) defines a set of linear accuracy conditions on the elements in $Q$. With a suitable rearrangement this may be written in the form,

$$A_1\mathbf{q} = \mathbf{b}_1, \quad (14)$$

where the vector $\mathbf{q}$ contains the elements of $Q$.  

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Remark 2. If the interior stencil $\mathbf{a}$ is predefined, the conditions (13) and (14) can generally be written down only for the $r$ rows near the interface. For details of how to obtain such restricted conditions, see [10].

If the interior stencil $\mathbf{a}$ of $D = P^{-1}Q$ has formal order of accuracy $O(\Delta x^{2p})$, then each of the $r$ rows near the interface can only reach accuracy of order $O(\Delta x^{p})$ [10]. It can be shown that this leads to solutions with global order $O(\Delta x^{p+1})$ if the approximation is pointwise stable and the problem is first order hyperbolic [25].

In summary, given a desired order of accuracy $p$, an interior stencil $\mathbf{a}$, and a given dimension of the boundary closure $r$, a Summation-by-Parts operator $D$ may be constructed by satisfying the accuracy conditions on $P$ and $Q$ simultaneously while ensuring that $P$ is positive definite. Certainly for many (in fact most) feasible parameter choices there will be some degrees of freedom left after all conditions are satisfied. In the next section we will utilise this freedom in order to minimise the dispersion errors of each row at the interface block of $D$.

4. SBP operators with minimal dispersion errors

We now turn to the problem of obtaining SBP operators with minimal dispersion errors. It should be noted that defining the objective function for the minimisation can be done in many different ways. Here, we attempt to define this function in a way analogous to the optimisation that was performed in [9] for central difference stencils.

4.1. Optimisation procedure

In [9] the problem of uniformly minimising the dispersion error for a central difference stencil of arbitrary width and order of accuracy was formulated as

$$\text{Find } \arg \min_{\mathbf{a}} \| E(\xi, \mathbf{a}) \|_{\infty} \quad \text{subject to } A_{\text{int}} \mathbf{a} = \mathbf{b}_{\text{int}} \quad (15)$$

where $E(\xi, \mathbf{a})$, given by (5), is the dispersion error of a central difference stencil and $A_{\text{int}}$ and $\mathbf{b}_{\text{int}}$ correspond to the conditions on the interior stencil $\mathbf{a}$ ensuring accuracy of order $O(\Delta x^{2p})$. Our goal in this paper is to analogously minimise the dispersion error at each row close to the boundary of the SBP operator $D = P^{-1}Q$. 

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Let, as before, \( r \) be the number of rows in the interface block of the SBP operator, and let and \( q \) and \( p \) be vectors containing the boundary coefficients of \( Q \) and \( P \) respectively. Each of the \( r \) rows near the interface defines a finite difference stencil of the form (1) and therefore has an associated dispersion error of the form (4).

**Remark 3.** In what follows we will restrict our attention to the real part of the dispersion errors as this determines the speed of the propagating solution. The imaginary part locally affects the amplitude of the solution. However, as seen from the discrete energy rate (10), the change in energy of the solution is unaffected by the specific stencil parameters. Thus, even if some small redistribution of energy among modes can occur, we will henceforth ignore the imaginary part of the dispersion errors.

With a slight abuse of notation, we let the real part of the dispersion error at the \( j \)th row of the boundary block of \( D \) be given by

\[
E_j(\xi, q, p) = \xi - \bar{\xi}_j(\xi, q, p),
\]

where \( \bar{\xi}_j(\xi, q, p) \) is the real part of the numerical wavenumber of the stencil at row \( j \).

We define the index set \( J_r = \{1, 2, \ldots, r\} \). We may now formulate our problem as follows:

Find \( \arg \min_{q, p} \max_{j \in J_r} \| E_j(\xi, q, p) \|_{\infty} \)

subject to \( A_0 p = b_0 \)

and \( A_1 q = b_1 \) \quad (16)

where \( A_0, A_1, b_0 \) and \( b_1 \) correspond to the conditions (13) and (14) ensuring accuracy \( O(\Delta x^{p+1}) \) of the resulting scheme. In words, we track all \( r \) dispersion errors near the boundary simultaneously and look for the choice of \( q \) and \( p \) that makes the largest among them as small as possible.

In order to solve (16) with reasonable efficacy we let \( x^T = (q^T, p^T) \) and define the objective function

\[
\phi(x) = \max_{j \in J_r} \| E_j(\xi, x) \|_{\infty} = \max_{j \in J_r} \sup_{\xi \in [0, \xi_{\text{max}}]} | E_j(\xi, x) |,
\]

where \( \xi_{\text{max}} \leq \pi \) is the upper limit of the wavenumber domain of interest. Problem (16) can now be written

Find \( \arg \min_x \phi(x) \)

subject to \( Ax = b \) \quad (17)
where $A$ and $b$ are suitable concatenations of $A_0, A_1, b_0$ and $b_1$.

Recall from (4) that $E_j$ takes the form

$$E_j = \xi - \left( -i \sum_{m=-L}^{R} c_m \exp(im\xi) \right).$$

Here, $c_m$ are the stencil coefficients of $D = P^{-1}Q$ at row $j$. Thus, $c_m = q_{jm}/p_j$ and hence, $E_j$ is a linear function of the elements in $Q$ and an inversely linear function of the strictly positive elements in $P$. Such a function is quasiconvex (see [26] for a definition and details). Quasiconvexity is preserved both under the supremum and the maximum operations, and thus $\phi(x)$ is a quasiconvex function of $x$.

There are many algorithms for solving the quasiconvex problem (17). For a review, see e.g. [27]. Here we have used an approach based on the repeated solution of associated convex programs, outlined in [26], which merely requires a convex program solver. To this end we have used the CVX package [28, 29], which allows us to obtain optimised SBP operators, typically in a matter of seconds.

4.2. Examples of SBP operators

We have seen that SBP operators may be defined through the triplet $(p, r, a)$ where, as before, $p$ is the order of accuracy of the resulting operator, $r$ is the dimension of the matrix block near the interface, and $a$ contains the coefficients of the repeated interior stencil, which is of order $2p$. The cost of using a given SBP operator depends on its sparsity, which in turn depends on $r$ and the number of elements in $a$.

To exemplify our procedure we will henceforth primarily consider two types of SBP operators, each with $r = 8$ and four elements in $a$. The complete sets of coefficients are found in Appendix A. The first of these operators is a "classical" (in the sense of non-optimised) SBP operator based on an eighth order central difference scheme. We will refer to this operator as SBP(4,0,8) as it corresponds to $p = 4$, has zero optimised parameters in the interior stencil and has a boundary block of dimension $8 \times 8$. It should be noted that there are three free parameters in the interface block of SBP(4,0,8). These are chosen in such a way that the truncation error is minimised [30].

The second type of operator is based on a fourth order central difference scheme optimised as in [9]. Note that this scheme has the same bandwidth as the SBP(4,0,8) operator despite the reduced order of accuracy. Again, we
Figure 1: Dispersion errors of SBP operators.
use an $8 \times 8$ boundary block where all free parameters resulting from the reduced accuracy are used to minimise the dispersion error as described in the previous section. We will refer to this operator as SBP(2,2,8) or, when it is not clear from context, SBP(2,2,8,$\xi_{\text{max}}$), where $[0,\xi_{\text{max}}]$ is the wavenumber domain over which the operator is optimised. All such operators correspond to $p = 2$, has two optimised parameters in the interior stencil and has a boundary block of dimension $8 \times 8$.

Example of operators are shown in Fig. 1, where the dispersion errors of the first eight rows of SBP(4,0,8) and and SBP(2,2,8) operator, optimised for $\xi \in [0,\pi/3]$, are plotted. Note that the largest error of SBP(2,2,8) is reduced by a factor of 25 compared to SBP(4,0,8). In Fig. 2 the dispersion errors of the interior stencils are shown. For consistency with [9] we denote

![Figure 2: Dispersion errors of interior stencils.](image-url)
the interior stencil of SBP(4,0,8) as Classical(8,9) and that of SBP(2,2,8) as Remez(4,9). The first number is the formal order of accuracy of the stencil and the second number is the stencil width. The max norm dispersion error of Classical(8,9) is about $1.8 \times 10^{-3}$ whereas that of Remez(4,9) is $3.7 \times 10^{-5}$; an improvement by a factor close to 50.

5. Numerical examples

We proceed by illustrating the performance of the optimised SBP operators compared to the classical ones through three numerical examples. The first is a narrow Gaussian pulse solution to the one-dimensional advection equation. This simple illustration exemplifies the use of optimised operators for solutions with high frequency spectral content. The second example is the propagation of an Euler vortex using the Euler equations, which is a common example of a non-linear problem exhibiting unphysical dispersive phenomena if not properly resolved [31, 9]. The third example is a calculation of the Taylor-Green vortex (TGV) using the Navier-Stokes equations, which illustrates how optimised operators regain much of the resolving capacity of higher order central differences for periodic problems.

5.1. Gaussian pulse

Consider the periodic advection equation

$$u_t + u_x = 0, \quad -3.5 \leq x \leq 3.5, \quad t \geq 0$$

with exact solution

$$u(x, t) = 2 \exp \left( -3200(x - t + 3)^2 \right).$$

This pulse is narrow and thus its Fourier transform is wide resulting in a significant contribution from a broad range of wavenumbers.

We use the SBP(4,0,8) and SBP(2,2,8) operators described in the previous section. Additionally, another classical SBP operator based on a fourth order interior stencil with $r = 4$ is used to compare the performance of SBP(2,2,8) with a scheme of the same order of accuracy. This operator will be denoted SBP(2,0,4). We set $\Delta x = 1/120$ and integrate in time using the classical fourth order Runge-Kutta scheme with time step $\Delta t = 10^{-3}$ so that the contribution to the error from the temporal discretisation is insignificant. A numerical interface is introduced at $x = 0$. The condition $u_L(0, t) = u_R(0, t)$
Figure 3: Numerical solutions to the polychromatic advection problem before and after the pulses pass through the numerical interface. The pulses have been separated vertically for clarity.
is imposed weakly using the SAT technique, where $u_{L,R}$ respectively are the solutions on the left-hand and right-hand sides of the interface. This problem is identical to (6) apart from the location of the interface. The stability analysis is identical and the SAT penalties have been parametrised with $\theta = 0$ to yield a discrete energy rate identical to the continuous one; see (10).

The exact and numerical solutions are shown in Figure 3, where we have separated the pulses vertically for clarity. All numerical solutions quickly disperse into a train of pulses with decaying amplitude trailing behind the main peak. This is due to the fact that the stencils underestimate the wavenumber $\xi$, resulting in a reduction of the wavespeed. This effect is increasingly pronounced as $\xi$ increases. See [9] for details of this phenomenon. Note that the trail behind the SBP(2,2,8) operator is smaller than the others as is expected from the smaller dispersion errors shown in Figure 1.

Numerical reflections of unresolved Fourier modes are seen after the pulses
pass through the interface. Clearly the reflection is smaller when using the SBP(2,2,8) operator compared to the non-optimised SBP stencils. Note also that the spurious reflections propagate out of the domain faster by the optimised stencil than by the classical SBP operators. This results from the fact that the classical stencils underestimate the wave speed of high frequency modes [9], whereas this effect is significantly reduced after minimising the dispersion error.

The $L^2$ error as a function of time is plotted in Figure 4. The disturbance around $t = 3$ is due to interactions with the numerical interface. This interaction is smaller for the SBP(2,0,4) operator, largely because the main peak is significantly reduced. Again it is seen that the optimised SBP(2,2,8) stencil is the better performer both near and far from the interface. Clearly the SBP(2,0,4) operator is significantly worse than SBP(2,2,8) despite the schemes having the same formal order of accuracy. The small error reductions seen for SBP(4,0,8) at time $t \approx 4.75$ and for SBP(2,2,8) at time $t \approx 4.25$ are a consequence of the numerical reflections leaving the computational domain. The reflections arising when using SBP(2,0,4) never propagate out of the domain during the simulation time, hence no reduction is visible for this operator.

5.2. The Euler vortex

The compressible Euler equations in two dimensions, written in conservative form, are given by

$$ U_t + F_x + G_y = 0, \quad (18) $$

where

$$ U = \begin{pmatrix} \rho \\ \rho u \\ \rho v \\ e \end{pmatrix}, \quad F = \begin{pmatrix} \rho u \\ \rho u^2 + p \\ \rho uv \\ u(e + p) \end{pmatrix}, \quad G = \begin{pmatrix} \rho v \\ \rho uv \\ \rho v^2 + p \\ v(e + p) \end{pmatrix}. $$

Here, $\rho$ is the density; $u$ and $v$ are the velocity components in the $x$- and $y$-directions respectively; $e$ is the total energy density; $p$ is the pressure, related to the conserved variables through the equation of state,

$$ p = (\gamma - 1) \left( e - \frac{1}{2} \rho (u^2 + v^2) \right), $$

where $\gamma = 1.4$ is the ratio of specific heats.
In [31] a vortex model that solves (18) was introduced. The model assumes a uniform background flow along the \( x \)-axis of pressure \( P_\infty \), temperature \( T_\infty \) and a Mach number \( M_\infty \). A vortical movement, characterised by the radius \( R \) and the vortex strength \( \beta \), centered around the coordinates \((x_0, y_0)\), is superposed. The local velocity components and the temperature assume the form

\[
\begin{align*}
u &= M_\infty \beta \exp \left(-\frac{r^2}{2}\right), \\
T &= T_\infty - \frac{1}{2} M_\infty^2 \beta^2 \exp \left(-\frac{r^2}{2}\right),
\end{align*}
\]

where \( r^2 = R^2 \left( (x - x_0)^2 + (y - y_0)^2 \right) \).

The Euler vortex is largely dominated by small wavenumbers, though with an increasing contribution from higher ones as the vortex strength, \( \beta \), is increased, as well as when coarse grids are used. In the following experiment we use a moderately strong vortex with \( \beta = 2.5 \) while setting \( M_\infty = R = 0.5 \). We use a square domain with \( x \in [0, 10] \), \( y \in [-5, 5] \) and periodic boundaries.

The problem is discretised on a \( 65 \times 65 \) point grid in space using the non-optimal SBP(4,0,8) operator previously described, and a series of SBP(2,2,8) operators optimised in different wavenumber regimes, \( \xi \in [0, \xi_{\text{max}}] \). Here we let \( \xi_{\text{max}} \in \{\pi/3, \pi/4, \pi/5, \pi/6\} \). The periodic boundary conditions are enforced using the SBP-SAT framework by introducing numerical interfaces in the same fashion as for the advection problem. For the temporal discretisation we use an adaptive fourth order Runge-Kutta method with a sufficiently small error to not have a significant impact on the experiment. A small amount of artificial dissipation is added for stability.

To separate the dispersive from the dissipative sources of error we define the quantity \( E_{\text{disp}} \) defined as

\[
E_{\text{disp}} = \sqrt{\left(x^{(a)}_{\text{min}} - x^{(n)}_{\text{min}}\right)^2 + \left(y^{(a)}_{\text{min}} - y^{(n)}_{\text{min}}\right)^2}, \tag{19}
\]

where \( (x, y)^{(a,n)}_{\text{min}} \) are the coordinates of the locations of minimum pressure of the analytic and numerical solutions of (18), which we may use as the definition of the centers of the vortices. Since (19) only depends on the coordinate of minimum pressure, it is a function of the speed of the vortex, and hence estimates the dispersive qualities of the scheme while ignoring the dissipative ones. A procedure for obtaining \( E_{\text{disp}} \) is described in [9].
In Fig. 5, $E_{\text{disp}}$ is shown for the different SBP operators as it evolves in time. By the end of the simulation, the vortex has passed through the numerical interface ten times. Traces of the interactions with the interface can be seen as small humps in the data at times 10, 30, 50, . . . . It is clear that with a careful tuning of the wavenumber domain over which the optimisation is performed, it is possible to outperform the classical high order SBP(4,0,8) operator also for non-linear problems. SBP(4,0,8) may be seen as the result of the optimisation procedure in the limit $\xi_{\text{max}} \rightarrow 0$. Thus, Fig. 5 suggest that there is some wavenumber domain with $0 < \xi_{\text{max}} < \pi/6$ at which the dispersion error is minimal for this particular problem. Finding that domain for a given problem may be a delicate task. However, as the experiment demonstrates, improvements compared to the non-optimal stencils can be made even with limited knowledge of the solution.

5.3. The Taylor-Green vortex

In this final example we consider the Taylor-Green vortex (TGV). Though the errors in a TGV simulation may not necessarily be dominated by dispersive effects, this example demonstrates that the resolving capacity of the operator SBP(2,2,8), optimised over a wavenumber domain $[0, \pi/3]$, yields at least as good, if not better results than the higher order SBP(4,0,8) operator for an underresolved solution.

The Taylor-Green vortex flow in a three-dimensional periodic box is a model for the non-linear transfer of kinetic energy among eddies with a large range of sizes. Velocity shear generates kinetic energy, which is dissipated by the viscosity at smaller scales. Thus, the TGV provides a model problem for the evolution of a turbulent flow and the energy transfer to successively smaller spatial scales.

The governing equations for the TGV will here be the three-dimensional compressible Navier-Stokes equations with constant physical properties and a low Mach number, $M_{\infty} = 0.1$. We assume that the fluid is a perfect gas at Reynolds number $Re = 1600$ with heat capacity ratio $\gamma = 1.4$ and Prandtl number $Pr = 0.71$. The initial temperature field is assumed to be constant.
Figure 5: Dispersion error development for a non-optimal and several optimised SBP operators.

The initial conditions are given by

\begin{align*}
  u &= +V_0 \sin \left( \frac{x}{L} \right) \cos \left( \frac{y}{L} \right) \cos \left( \frac{z}{L} \right) \\
  v &= -V_0 \cos \left( \frac{x}{L} \right) \sin \left( \frac{y}{L} \right) \cos \left( \frac{z}{L} \right) \\
  w &= 0 \\
  p &= 1 + \frac{V_0^2}{16} \left( \cos \left( \frac{2x}{L} \right) + \cos \left( \frac{2y}{L} \right) \right) \left( \cos \left( \frac{2y}{L} \right) + 2 \right),
\end{align*}

where \( u, v, w \) and \( p \) respectively represent the flow field in the \( x, y \) and \( z \) directions, and the pressure. Here \( V_0 = 0.1 \) and \( L = 2\pi \) is the dimension of the periodic box. The duration of the flow is taken to be \( 20t_c \) where \( t_c = L/V_0 \)
is the characteristic convective time.

As a measure of the quality of the schemes we compute the kinetic energy of the solution and compare it to data from a direct numerical simulation obtained using a dealiased pseudo-spectral code with vanishingly small numerical dissipation and dispersion errors, run on a $512^3$ point grid [32, 33]. Additionally we compute the kinetic energy dissipation rate, which allows us to remark on the dissipative effects of the SBP operators.

We consider two possible scenarios: The first is a purely periodic problem for which the central difference stencils at the interior of the SBP operators are used everywhere. As before, we refer to the interior stencil of the SBP($4,0,8$) operator as Classical($8,9$). In this case, without any interface treatment, Classical($8,9$) constitutes an 8th order accurate scheme with a bandwidth of 9 points. Similarly, consistent with the notation in [9], the interior of the SBP($2,2,8$) operator will be referred to as Remez($4,9$), which is 4th order accurate and also utilises a bandwidth of 9 points. Here we use the SBP($2,2,8$) operator optimised for wavenumbers in the range $[0, \pi/3]$.

In the second scenario we introduce numerical interfaces at the edges of the box, enforcing periodic boundary conditions by using the weak SAT formulation. The SBP operators in this scenario reduces the accuracy of the schemes for SBP($4,0,8$) and SBP($2,2,8$) to $O(\Delta x^5)$ and to $O(\Delta x^3)$ respectively. Additionally, the resolving capacities near the interfaces are reduced.

We consider two grid resolutions; a $64^3$ point grid and a $128^3$ point grid. All simulations use a Courant number of 0.1 and a small amount of artificial dissipation is added for stability. In Figure 6 the time evolution of the kinetic energy is plotted for the two scenarios when the $64^3$ point grid is used. In this case the solution is underresolved and the energy transfer to the smallest spatial scales is not captured accurately, as seen by the overly dissipated energy in the transfer to turbulence at $t/t_c \sim 9$. Nonetheless, in the purely periodic case, the resolving capacities of both Classical($8,9$) and Remez($4,9$) are sufficient to capture the behaviour of the solution near the end of the simulation. Note that when the numerical interfaces are introduced, SBP($4,0,8$) seems to lose this resolving capacity whereas it is retained by the optimised SBP($2,2,8$) operator.

In Figure 7 the kinetic energy dissipation rate is shown for the $64^3$ point grid. It is indeed clear that in both the purely periodic and the interface cases, all solutions are overly dissipative. However, note that the optimised SBP($2,2,8$) operator appears to capture the transition to turbulence somewhat better than the SBP($4,0,8$) operator; in particular the peak energy
Figure 6: Kinetic energy evolution for the purely periodic and the interface problems using $64^3$ grid points.
dissipation at \( t/t_c \sim 9 \).

In Figs 8 and 9 the same experiments are shown for the 128\(^3\) point grid. This time the solutions are well resolved, and in both the periodic and the interface cases the kinetic energy and the energy dissipation rate are captured satisfactorily. It is remarkable to note that the performance of the lower order SBP(2,2,8) operator is comparable to that of the higher order SBP(4,0,8) operator also on this finer grid. This suggests that improved dispersion properties of finite difference operators may be a useful tool in turbulence simulations.

6. Conclusions

An inaccurate representation of the analytic dispersion relation by finite difference stencils may, for problems involving high wavenumbers or large time scales, be the dominant source of error. To remedy this, a variety of central difference schemes have been presented in the literature that preserves the dispersion relation of the governing equations. In this paper we have developed Summation-by-Parts operators that extend this dispersion relation preservation to stencils near interfaces, thus allowing for a much broader range of problems to be solved with high resolution while retaining stability and high order.

We have optimised the SBP operators by finding the stencil coefficients that minimise the largest dispersion error associated with the stencil near numerical interfaces. The problem of constructing such operators is quasi-convex and can therefore be solved using any standard convex optimisation package, typically in a matter of seconds.

Comparisons of an optimised and a non-optimised SBP operator of the same order has revealed that significant error reductions can be obtained for propagating solutions with high frequency content. Further comparisons with a higher order operator has shown that maximising the formal order of accuracy with respect to the bandwidth of the stencil is inferior to minimising the dispersion error, both for problems involving high frequencies and for long time simulations. This is expressed partly in terms of a severe underestimation of the wavespeed of high frequency waves, and partly in terms of reflections at numerical interfaces. Both these effects are significantly reduced when the dispersion error is minimised.

Similar improvements are seen for non-linear systems of equations as has been demonstrated by solving the Euler vortex problem. A careful tuning
Figure 7: Kinetic energy rate for the purely periodic and the interface problems using $64^3$ grid points.
Figure 8: Kinetic energy evolution for the purely periodic and the interface problems using $128^3$ grid points.
Figure 9: Kinetic energy rate for the purely periodic and the interface problems using $128^3$ grid points.
of the wavenumber domain over which the SBP operator is optimised has significant impact on the resulting quality of the scheme. In this paper we have not attempted to find the perfect tuning for a given problem. Rather, it has been demonstrated that even with limited knowledge of the solution to the problem at hand, improvements can be made.

Finally, by solving the Taylor-Green vortex it has been demonstrated that an optimised SBP operator gives improved performance for an underresolved solution as compared to higher order SBP operators. For a better resolved solution the SBP operators show excellent agreement with data obtained on a much finer grid, even in the presence of artificial interfaces. This suggests that optimised SBP operators are promising tools for turbulence simulations governed by initial boundary value problems with a physical geometry. Further research into this approach will be the topic of a future paper.
Appendix A. Stencil coefficients

**SBP(4,0,8)**

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\[ SBP(2,2,8,\pi/6) \]

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References


