Summation by parts methods for the spherical harmonic decomposition of the wave equation in arbitrary dimensions

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Splitting a solution of the wave equation in $n + 1$ space dimensions into spherical harmonic components on $n$-spheres and reducing to first order results in the pair of first-order partial differential equations in radius and time $\pi = \psi' + \psi' \psi/\sigma$ and $\psi = \pi'$ for each spherical harmonic, where $p = 2l + n$, and $l$ is a spherical harmonic index. The $\psi/r$ term gives rise to numerical stability problems near the origin, and also poses the key numerical difficulty in related systems of equations. We propose a class of summation by parts finite differencing methods that converge pointwise, including at $r = 0$, and are stable because they admit a discrete energy. We explicitly construct such schemes that are 2nd and 4th order accurate at interior points, and first and 2nd order accurate at the spherical outer boundary $r = R$. We use the projection method to impose a class of boundary conditions for which the discrete energy is non-increasing.

Keywords: Finite differencing, summation by parts, wave equation, spherical harmonics.

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I. INTRODUCTION

We consider the wave equation
\[ \ddot{\Phi} = \Delta \Phi \] (1)
in \( n + 1 \) space dimensions and time. In spherical coordinates, the Laplace operator \( \Delta \) in \( n + 1 \) space dimensions can be split into radial and angular derivatives as
\[ \Delta = \frac{1}{r^n} \frac{\partial}{\partial r} \left( r^n \frac{\partial}{\partial r} \right) + \frac{1}{r^2} \Delta S^a. \] (2)
The Laplacian on \( S^a \) has eigenfunctions \( Y_l \ldots \) that obey
\[ \Delta S^a Y_l \ldots = -l(l + n - 1)Y_l \ldots \] (3)
We can therefore make the separation of variables ansatz
\[ \Phi(r, t, \theta) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \phi_{l,m}(r, t)e^{\pm il\theta} \] (4)
in 2 space dimensions,
\[ \Phi(r, t, \theta, \varphi) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \phi_{l,m}(r, t)Y_{l,m}(\theta, \varphi) \] (5)
in 3 space dimensions, and
\[ \Phi(r, t, \text{angles}) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \phi_{l,m}(r, t)Y_{l,m}(\text{angles}) \] (6)
in higher space dimensions, where the \( Y_{l,m} \ldots \) are the familiar scalar spherical harmonics, and \( Y_l \ldots \) their generalisation to higher dimension. The nonstandard notation for the Fourier series in the \( n = 1 \) case was chosen to give \( l \) the range \( l \geq 0 \) for all \( n \geq 1, n = 1 \) is then a regular case in what follows. Each \( \phi_{l,m} \ldots \) now obeys
\[ \ddot{\phi} = \phi'' + \frac{n}{r} \phi' - \frac{(l + n - 1)}{r^2} \phi. \] (7)
Here a dot denotes a t-derivative, and a prime an \( r \)-derivative. We no longer write the suffix \( \pm l, \ldots \) or \( l \ldots \) that labels the spherical harmonic. Regularity of \( \Phi \) at \( r = 0 \), in the sense that it admits an expansion in positive integer powers of the Cartesian coordinates \( x, y, z \), requires that \( \phi(r, t) = r^l \phi(r, t) \), where \( \phi \) is even and regular, in the sense that it admits an expansion in positive even powers of \( r \). \( \phi \sim r^l \) is difficult to enforce numerically. This may lead to a loss of convergence or to instability, and it is preferable to evolve \( \phi \) with
\[ \ddot{\phi} = \phi'' + \frac{p}{r} \phi', \] (8)
where
\[ p = 2l + n. \] (9)
Therefore \( p \) is an even integer in an odd number (in particular, three) of space dimensions, and an odd integer in an even number of space dimensions. With the first-order auxiliary variables
\[ \pi \equiv \dot{\phi}, \quad \psi \equiv \phi', \] (10)
this is equivalent to
\[ \dot{\psi} = \pi', \quad \ddot{\pi} = \psi' + \frac{\psi}{r}. \] (11)
Regularity implies
\[ \pi(-r, t) = \pi(r, t), \quad \psi(-r, t) = -\psi(r, t), \] (12)
if we formally extend the functions to negative values of \( r \).

In this paper, we use the summation by part ideas (SBP) of Strand [1] to construct finite differencing schemes of a given accuracy for (11), for positive integer \( p \), with the regularity conditions (12) at \( r = 0 \), which admit a discrete energy whose time derivative is a boundary term at a spherical outer boundary \( r = R \). We then use the projection method of Olsson [2] to impose boundary conditions of one of the three forms
\[ \rho \pi + \sigma \psi = 0, \quad r = R, \quad \rho \sigma \geq 0, \] (13)
(maximally dissipative boundary conditions),
\[ \rho \pi + \mu \pi' = 0, \quad r = R, \quad \rho \mu \geq 0, \] (14)
or
\[ \sigma \psi + \nu \left( \psi' + \frac{\nu}{r} \psi \right) = 0, \quad r = R, \quad \sigma \nu \geq 0. \] (15)
Any of these guarantee that a discrete energy exists that is positive definite and non-increasing. Hence the numerical scheme is stable. (A continuum energy exists and implies well-posedness also for the more general class of boundary conditions \( \rho \pi + \sigma \psi + \mu \pi' + \nu(\psi' + p\psi/r) = 0 \), but we have not been able to find an equivalent discrete energy.)

We are aware of two other SBP schemes for (11) in the literature.

The scheme proposed in [3] and used in [4] is SBP including at the outer boundary \( r = R \), and is second-order accurate at fixed \( r \). However, it has error terms that behave as \( h^2/r^2 \). Therefore, at a fixed grid point \( i \) near the origin the error scales as \( 1/i^2 \), and is independent of \( h \). Therefore, the error does not converge in the maximum norm, although for \( p \neq 2, 3 \) it converges with \( h^2 \) in the energy norm [24] defined below [3]. By contrast, the schemes we present here have an error of \( O(h^2) \) or \( O(h^3) \) at all grid points including the origin.

A second-order accurate (including at the origin) finite differencing scheme for (11) was described by Evans [6] and is widely used, see for example [7] for \( p = 2 \) and [8] for \( p \geq 2 \). Although this method was not explicitly
designed as an SBP scheme, it actually is SBP at interior points and at the origin. This may explain its empirical robustness. Here, we complete it as an SBP scheme on the finite range \(0 \leq r \leq R\) by a suitable modification at the outer boundary.

Our paper is structured as follows. Sec. II discusses general considerations. In Sec. II A we introduce our notation for the discretisation in \(r\). In Sec. II B we identify the summation by parts (SBP) property that our difference operators must obey for a discrete energy to exist. In Sec. II C we discuss the accuracy of these operators and in Secs. II D and II E we discuss the symmetry boundary conditions stated above.

In Sec. II F we derive another 2nd-order accurate SBP method, and in Sec. II G we generalise this to 4th-order accuracy. It should be possible to construct implementations with arbitrary order of accuracy at interior points by extending our two examples. Sec. III D summarises our results and comments on their generalisation to the three subclasses of boundary conditions in numerical experiments.

Sec. IV summarises our results and comments on their implementation with arbitrary order of accuracy at interior points by extending our two examples. Sec. III D summarises our results and comments on their generalisation to the three subclasses of boundary conditions in numerical experiments.

The continuum equations admit the energy
\[
E = \frac{1}{2} \int_0^R (\pi^2 + \psi^2) r^p \, dr
\]
with time derivative
\[
\frac{dE}{dt} = \left[ \pi^p \psi \right]_0^R, \tag{19}
\]
where the second equation is obtained after using the evolution equations and integrating by parts. In order to control the growth of \(E\), the boundary term at \(r = R\) must be controlled by a suitable boundary condition. The boundary condition
\[
\rho \pi + \sigma \psi = 0, \quad r = R \tag{20}
\]
clearly guarantees \(dE/dt \leq 0\) for \(\rho, \sigma \geq 0\). Such boundary conditions are called maximally dissipative. We show in Appendix C that the more general boundary condition (C1) also guarantees \(dE_b/dt \leq 0\) for a generalised energy \(E_b\).

By contrast, the boundary at \(r = 0\) is not a physical boundary, but rather a point in the interior of the ball \(r \leq R\). Indeed regularity alone implies that \(\psi(0,t) = 0\), and so the boundary term at \(r = 0\) vanishes.

As is well-known, the continuum equations are well-posed in the norm provided by \(E\) because \(E\) is conserved. A summation by parts (SBP) finite differencing scheme exactly conserves a discrete equivalent \(\hat{E}\) of the continuum energy \(E\). This guarantees that it is stable (the discrete equivalent of well-posed).

We consider the discrete energy
\[
\hat{E} = \frac{1}{2} h^{p+1} \left( \Pi^t \Pi + \Psi^t \hat{W} \Psi \right) \tag{21}
\]
where
\[ W^t = W', \quad W^t = W, \quad W > 0, \quad W > 0, \] (22)
and write the finite differencing scheme as
\[ \Psi = h^{-1} D\Pi, \quad \Pi = h^{-1} \hat{D} \Psi. \] (23)
The powers of \( h \) have been introduced so that \( W, W, D, \hat{D} \) are all dimensionless and independent of \( h \). The quantity \( r_i/h = i \) also has this property. The SBP property that guarantees that \( \hat{E} \) is constant up to boundary terms is
\[ W \hat{D} + (W D)^t = B, \] (24)
where the boundary operator \( B \) is defined by
\[ \Pi^t B \Psi = \chi M^t \Pi_M \Psi_M, \] (25)
and the constant \( \chi \) obeys \( \chi \to 1 \) in the continuum limit \( M \to \infty \) as \( h \to 0 \) at fixed \( r = R \). As \( W \) is positive definite, it is invertible, and we can consider \( \hat{D} \) as determined by \( D, W, \hat{W} \) and \( B \):
\[ \hat{D} = -W^{-1} D^t \hat{W} + W^{-1} B. \] (26)

C. Accuracy

A useful reparameterisation of the difference operator coefficients \( \hat{D}_{ij} \) is obtained by expressing \( \psi(r) \) through the Taylor expansion of \( \psi(r) \) about the fixed grid point \( r_i \). We can then write
\[ h^{-1}(\hat{D} \psi)_i = c_0 h^{-1} \psi(r_i) + c_1 h \psi'(r_i) + c_2 h^2 \psi''(r_i) + \ldots + c_{2K} h^{2K} \psi^{(2K)}(r_i) + O(h^{2K}) \] (27)
with a straightforward linear relation between the \( c_{ai} \) and the \( \hat{D}_{ij} \) at each point \( i \). In the following we adopt a simplified notation where the \( c_{ai} \) (with \( \alpha = 0, \ldots, 2K \)) are written as \( c_{ai} \), \( \psi(r_i) \) simply as \( \psi \), etc., and \( r_i \) simply as \( r \). That is, we do not write the dependence on \( i \), and all continuum quantities are evaluated at \( r = r_i \).

Our difference operators are defined to be accurate to order \( 2N \) if they obey (using our abbreviated notation)
\[ h^{-1}(D\Pi)_i = \psi' + O(h^{2N}), \] (28)
\[ h^{-1}(\hat{D} \psi)_i = \frac{p}{r} \psi + \psi' + O(h^{2N}). \] (29)

A key observation for our problem is that the \( O(h^{2N}) \) error needs to be obtained formally in the limit \( h \to 0 \), both at (approximately) constant \( r \), and at constant \( i \). The possible problem with the latter limit are error terms of the form \( h^{m}/r^{p} \), which are \( O(h^{m}) \) at constant \( r \), but only \( O(h^{m-n}) \) at constant \( i \). As an example, the identity
\[ \psi' + \frac{p}{r} \psi = \frac{(r^p \psi')'}{r^p} \] (30)
suggests the finite differencing operator
\[ (\hat{D} \psi)_i = \frac{(i + 1)^p \Psi_{i+1} - (i - 1)^p \Psi_{i-1}}{2ip}. \] (31)
However, for \( \psi = r \) and \( p = 2 \), the local error of the finite differencing operator \( h^{-1} \hat{D} \) is exactly \( h^2/r^2 = 1/i^2 \). (For higher \( p > 0 \), terms up to \( (h/r)^p \) also appear.) This does not go to zero with \( h \) at fixed \( i \).

We assume in the following that the operator \( h^{-1} \hat{D} \) is a standard representation of \( d/dr \) with known accuracy, and concentrate on the difference operator \( \hat{D} \), where the \( p/r \) term may cause accuracy problems at the origin.

The point \( r = 0 \), which arises (only) on a centered grid, must be treated specially. Taking the limit \( r \to 0 \) of \( (29) \) at finite \( h \) we see that at \( r = 0 \) the accuracy conditions are
\[ c_1 = 1 + p, \quad c_3 = c_5 = \ldots = c_{2N-1} = 0, \] (32)
with the even \( c_{ai} \) undetermined because \( \psi = \psi'' = \ldots = 0 \) for an odd function at the origin. For the methods with a centred grid that we have considered, these conditions will be discussed below for each specific method.

Turning now to generic points with \( r > 0 \), naively one would expect the accuracy requirement for \( \hat{D} \) to be equivalent to the following constraints on the coefficients of the difference operator (as defined above):
\[ c_0 = \frac{ph}{r}, \quad c_1 = 1, \quad c_2 = \ldots = c_{2N} = 0. \] (33)

Clearly, we need a stencil of width \( 2N + 1 \) or larger to control all these \( c_{ai} \).

However, we shall now see that we can replace some of the equalities \( (33) \) with inequalities, which gives us additional freedom to impose the SBP conditions. Rather than devising a general notation, we present the cases \( N = 1 \) and \( N = 2 \).

For \( N = 1 \), we make the following ansatz:
\[ c_0 = \frac{ph}{r} + \delta_0 \left( \frac{h}{r} \right)^3, \] (34)
\[ c_1 = 1 - \delta_0 \left( \frac{h}{r} \right)^2, \] (35)
\[ c_2 = \delta_1 \left( \frac{h}{r} \right), \] (36)
where the \( \delta_\alpha \) may depend on \( i \). The special case \( \delta_0 = \delta_1 = 0 \) gives \( (33) \). Substituting this ansatz into \( (27) \) gives
\[ h^{-1}(\hat{D} \psi)_i = \frac{p}{r} \psi + \psi' + \delta_0 h^2 \left[ r^{-2} \left( \frac{\psi'}{r} - \psi \right) \right] + \delta_1 h^2 \left[ r^{-1} \psi'' \right] + R_2. \] (37)
Here
\[ R_2 = c_3 h^2 \psi''' + c_4 h^3 \psi'''' + \ldots, \] (38)
where for a 3-point stencil $c_3$, $c_4$, ... are known linear functions of $c_0$, $c_1$ and $c_2$. Now, because of (12) and regularity, both square brackets in (37) are actually $O(1)$ as $r \to 0$. Therefore, as long as $\delta_0$ and $\delta_1$ are bounded uniformly in $i$, the coefficients of $h^4$ in (37) are bounded. Similarly, as $c_3$, $c_4$, ... are regular functions of $\delta_0$ and $\delta_1$, $h^2$ and all higher powers of $h$ in (38) are also explicitly regular at $r = 0$ and so we have the desired second-order accuracy.

For $N = 2$ we make the ansatz

$$c_0 = \frac{ph}{r} + \delta_0 \left( \frac{h}{r} \right)^5,$$  
$$c_1 = 1 - \delta_0 \left( \frac{h}{r} \right)^4,$$  
$$c_2 = \left( \frac{\delta_0}{3} + \delta_1 \right) \left( \frac{h}{r} \right)^3,$$  
$$c_3 = -\delta_1 \left( \frac{h}{r} \right)^2,$$  
$$c_4 = \delta_2 \left( \frac{h}{r} \right),$$  

which gives

$$h^{-1}(\tilde{D}\psi)_i = \frac{h}{r} \psi + \psi' + \delta_0 h \left[ r^{-3} \left( \frac{\psi'}{r^2} - \frac{\psi''}{h^2} \right) \right] + \delta_1 h \left[ r^{-2} \left( \frac{\psi''}{r^2} - \frac{\psi'''}{3} \right) \right] + \delta_2 h \left[ r^{-1} \psi''' \right] + R_4,$$  

where $R_4 = O(h^4)$ in the sense discussed above. Again, all the square brackets are regular at $r = 0$, and so we have fourth order accuracy if and only if the $\delta_{ik}$ are bounded uniformly in $i$.

The values of $\delta_1$ in the methods we construct below are plotted against $i$ and $p$ in Figs. 1 and 2.

It is clear that this method extends to arbitrary $N$, giving $N$ equations to be solved and $N + 1$ inequalities (uniform in $i$ bounds on the $\delta_{ik}$) to be then verified.

Informally, our method can be described as “trading $r$ for $h$”. It works because the terms in square brackets above are all $O(1)$ as $r \to 0$, which in turn requires $\psi(r, t)$ to be a regular odd function of $r$.

Note that for $r \gg h$, our $c_0$ given by (45) and (46) approach the values (33). Similarly, $R_2$ and $R_4$ approach the values they take for the standard stencils $D$ given below in (39) and (40), which are precisely the minimum width stencils for a given accuracy that obey (33).

D. The symmetry boundary $r = 0$

In numerical simulations using polar coordinates one is faced with the fact that $r = 0$ is a boundary of the numerical grid, but is not in fact a boundary of the physical domain. As a result, there are (typically) no physical boundary conditions one can or must impose in the continuum limit, but the numerical simulation does require boundary conditions. These are derived from the assumption that the desired solution is not less differentiable at $r = 0$ than for $r > 0$ (usually implicitly assumed smooth). The standard general approach to such “symmetry boundary conditions” or “regularity conditions” is to identify variables which under the assumption of regularity are either even functions of $r$ (for example $\pi$) or odd functions of $r$ (for example $\psi$), and then to extend standard centered finite difference methods to the boundary by extending the numerical grid into a small number of “ghost points” representing negative $r$ and which are populated by the assumed even or odd parity of the grid functions.

From a strict SBP point of view, there are no ghost points, and finite difference operators are necessarily skewed near the boundary. The fact that $r = 0$ is not a physical boundary is represented by the fact that $\tilde{B}$ is zero at the boundary $r = 0$.

However, we find that the use of ghost points allows a clearer derivation of our results, in that we do not need to discuss $r = 0$ explicitly as a boundary. Rather than introduce a few ghost points, for our derivation we extend all grid objects from 1/2 or 0, ... , $M$ to $-M$, ... , $M$, corresponding to $-R \leq r \leq R$.

We extend the grid functions to negative $i$ as

$$\Pi_{-i} = \Pi_i, \quad \Psi_{-i} = -\Psi_i. \quad (45)$$

Because of how $W$ and $\tilde{W}$ define $\dot{E}$, we can assume without loss of generality that

$$W_{i,j} = W_{ij}, \quad W_{-i,j} = W_{i,-j} = 0, \quad i,j > 0, \quad (46)$$

and similarly for $\tilde{W}$, $\tilde{B}$ is extended by $B_{-M,-M} = -B_{MM}$. In Appendix A we prove from these assumptions that (45) holds at all times if and only if

$$D_{-i,j} = -D_{ij}. \quad (47)$$

When coding our method, we implement $D$ and $\tilde{D}$ with a few ghost points. Equivalently, the ghost points can be explicitly eliminated. A rigorous treatment is relegated to Appendix A as it introduces additional notation not required for our main argument.

E. The outer boundary $r = R$

We begin by reviewing the one-dimensional wave equation

$$\tilde{x} = \psi', \quad \psi = \pi', \quad a \leq x \leq b \quad (48)$$

with energy

$$E = \int_a^b (\pi^2 + \psi^2) \, dx, \quad \frac{dE}{dt} = [\pi\psi]_a. \quad (49)$$
with energy
\[ E = \frac{h}{2} \left( \Pi^T W_0 \Pi + \Psi^T W_0 \Psi \right). \]
and SBP condition
\[ W_0 D_0 + (W_0 D_0)^\ast = B_0. \]

Notice that this problem is translation-invariant, and so \( D_0 \) and \( W_0 \) will naturally be translation-invariant in the interior, except for finite-sized end points. \( D_0 \) and \( W_0 \) with various orders of accuracy in the interior and at the boundaries have been constructed by Strand \( [1] \).

In \( [1] \) with \( p > 0 \) additional problems result because the equations are not translation-invariant but depend explicitly on \( r \). In the previous two sections we have addressed these problems at interior points and at the pseudo-boundary \( r = 0 \). Intuitively, the problem of imposing SBP at the outer boundary \( r = R \) should be similar to those solved by Strand because with increasing resolution \( r \) varies less over a finite number of near-boundary grid points, and we should be able to make use of Strand’s results. We now formalise this idea.

Strand provides, among others, norms \( W_0 \) that are the unit matrix except near the boundaries. We shall later construct norms \( W' \) and \( \bar{W}' \) for the problem without an outer boundary (on the range \( 0 \leq r < \infty \)) which are diagonal everywhere except near \( r = 0 \). In this subsection we denote their restrictions to \( 0 \leq r \leq R \) by the same names. We now set
\[ W = W_0 W', \]
\[ \bar{W} = W_0 \bar{W}', \]
\[ B = B_0 \bar{W}', \]
\[ D = D_0, \]
where \( W_0, D_0 \) and \( B_0 \) are the Strand operators with diagonal \( W_0 \) on \( -R \leq r \leq R \). Then from \( [20] \) and \( [22] \) we obtain
\[ \bar{D} = W'^{-1} D_0 \bar{W}'. \]
Let us assume we have already shown that this is accurate to some given order at the interior points where \( D_0 \) takes a simple translation-invariant form. Let us also assume that \( D_0 \) is accurate to some order \( \tau \) at the boundary points, and let us assume that
\[ W' = \text{diag} \left[ p^r (1 + O(i^{-\tau})) \right], \]

near the boundary and similarly for \( \bar{W}' \). Then near the boundary, at \( r \lesssim R \), for fixed \( R \),
\[ \bar{D} = D_0 + \frac{p}{2} \left[ 1 + O(i^{-\tau}) \right] = D_0 + \frac{p}{2} \left[ 1 + O(h^{-\tau}) \right], \]
which is accurate to order \( \tau \).

III. SPECIFIC EXAMPLES

A. The “Evans method”

1. Interior points

We concentrate at first on interior grid points by considering the range \( 0 \leq r < \infty \). Furthermore, points near the boundary \( r = 0 \) can be treated like interior points if we use ghost points, as discussed in Sec. \( [1] \). We use the notation \( D' \) etc. for operators on \( -\infty < r < \infty \), and \( D \) etc. for operators on \( 0 \leq r \leq R \).

The identity
\[ \left( \frac{d}{dr} + \frac{p}{r} \right) \psi = (p + 1) \frac{d(r^p \psi)}{dr^{p+1}} \]

motivates the difference operator
\[ h^{-1}(D' ) = (p + 1) \frac{r^p \Psi_{i+1} - r_{i-1}^p \Psi_{i-1}}{r_{i+1} - r_{i-1}}, \]

which is the generalisation to arbitrary even \( p \) of a difference operator introduced in \( [6] \). It is second-order accurate including at \( r = 0 \). We combine it with the usual second-order accurate 3-point symmetric difference operator
\[ (D' ) = (i+1)^{-1} - \frac{2i}{w_i}, \]
\( \Psi_i \) and \( \Pi_i \) for negative \( i \) are defined by \( [35] \). Consider now
\[ W' = \text{diag}(w_i), \quad \bar{W}' = \text{diag}(v_i). \]
The SBP formula \( [20] \) then gives
\[ (D' ) = \frac{v_{i+1}^p \Psi_{i+1} - v_{i-1}^p \Psi_{i-1}}{2w_i}. \]
Comparing \( [64] \) with \( [61] \) we see that the Evans method is of this form with \( (\text{using our convention } r_i = ih) \)
\[ v_i = i^p, \]
\[ w_i = \frac{(i+1)^{p+1} - (i-1)^{p+1}}{2(p+1)}. \]

We note that these are well defined for all \( i \) including \( i = 0 \). Indeed, the accuracy conditions at the origin \( [32] \) for a method with diagonal energy \( [33] \) reduce to
\[ v_1 = (1 + p)w_0, \]
for the ansatz \( [65][66] \) for even \( p \). Note that the Evans method does not work for odd \( p \) (the wave equation in even space dimensions) on a staggered grid, as then \( w_0 = 0 \).
2. The outer boundary

We now address the outer boundary. Following the general prescription of Sec. [11E] we set

$$D = \begin{pmatrix} -\frac{1}{2} & 0 & \frac{1}{2} \\ -\frac{1}{2} & 0 & \frac{1}{2} \\ -1 & 1 \end{pmatrix}, \quad (67)$$

$$B = \begin{pmatrix} 0 \\ 0 \\ v_M \end{pmatrix}, \quad (68)$$

$$W = \text{diag}(\ldots, w_{M-2}, w_{M-1}, \frac{w_M}{2}), \quad (69)$$

$$\hat{W} = \text{diag}(\ldots, v_{M-2}, v_{M-1}, \frac{v_M}{2}). \quad (70)$$

Note that this gives $\chi = 1$. From [24] we read off

$$\hat{D} = \begin{pmatrix} -\frac{w_{M-1}}{2w_{M-2}} & 0 & \frac{w_{M} - w_{M-1}}{w_M} \\ -\frac{w_{M-1}}{2w_{M-2}} & 0 & \frac{w_{M} - w_{M-1}}{w_M} \\ \frac{v_{M}}{w_M} & \frac{v_{M}}{w_M} & \frac{v_{M}}{w_M} \end{pmatrix}. \quad (71)$$

We read off

$$(\hat{D}\Psi)_M = \frac{v_{M-1}}{w_M} h\psi' + \frac{v_{M} - v_{M-1}}{w_M} \psi + O(h^2)$$

$$= [1 + O(M^{-1})] h\psi'$$

$$+ \left[1 + O(M^{-1})\right] \frac{p}{M} \psi + O(h^2)$$

$$= h \left[\psi' + \frac{p}{R} \psi + O(h)\right], \quad (72)$$

where the last equality holds because $M = R/h$, and hence this method is first-order accurate at the boundary point $i = M$.

3. Generalization to higher accuracy

The identity [30] suggests a generalization of the Evans method to accuracy order $2N$, discretizing $d/dr + p/r$ as

$$(p + 1) \frac{D(r^p \psi)}{D(r^{p+1})}. \quad (73)$$

where $D$ is some discretization of $d/dr$ of accuracy order $2N$. If we take the norms

$$v_i = v_i^p, \quad w_i = \frac{1}{p + 1} D(p + 1), \quad (74)$$

then [73] also obeys the SBP property. However, for the minimal-width centered stencils $D$ of order larger than 2 this does not work. To see this we differentiate $\psi(r) = ar + br^3$ using the operators $D$ of accuracy $N = 1$ and $N = 2$. The discretization errors are, respectively,

$$b(p + 3)(2p + 1) h^2 + O(h^3), \quad (75)$$

$$-\frac{2b(p + 3)(p - 1)}{15} \frac{h^4}{r^2} + O(h^5). \quad (76)$$

In the latter case we see an error of the form $h^4/r^2$, which becomes $h^2$ near the centre.

We have not been able to generalize Evan’s method to avoid this type of singular error term. Now we present a new, general approach to this problem, which allows high-order SBP methods that are regular at the centre.

B. Another 2nd-order accurate implementation (SBP2)

1. General considerations

There are many ways of solving both the SBP conditions and the accuracy conditions for any required order of accuracy. We choose as our priority to make $D$ and $\hat{D}$ as narrow as possible. For given $D$, wider $W$ and $\hat{W}$ make $\hat{D}$ [given by (26)] wider, so we try to make them as narrow as possible. Finally, we choose $\hat{W}$ to be diagonal in order to make it easy to invert. We note that an overall constant factor in $W$ (and its inverse in $\hat{W}$) cancels out from $\hat{D}$.

Given that $h^{-1}D$ represents $d/dr$, it is natural to make the extended finite difference operator $D'$ the “standard” minimal width operator for a given order of accuracy $2N$ at interior points.

2. Interior points

We concentrate at first on interior grid points. We assume again that $D'$ is given by [72], and we look for $W'$ and $\hat{W}'$ of the form

$$W' = \hat{W}' = \text{diag}(w_i), \quad (77)$$

where $w_{-1} = w_i$. The SBP formula (26) gives

$$(\hat{D}'\Psi)_i = \frac{w_{i+1} \Psi_{i+1} - w_{i-1} \Psi_{i-1}}{2w_i}, \quad (78)$$

where $\Psi_j$ for negative $j$ is defined by [15].

We can now read off $c_0, c_1$ and $c_2$ in terms of $w_i$. The one equality contained in [33-39], namely

$$\left(\frac{r}{h}\right) c_0 + c_1 = 1 + p, \quad (79)$$

gives the linear recurrence relation of degree 2 for $w_i$

$$(i + 1)w_i - (i - 1)w_{i-1} = 2(p + 1)w_i. \quad (80)$$

The other two accuracy conditions are taken to define $\delta_1$ and $\delta_2$ in terms of $w_i$. On a staggered grid, we have
We initially fix an arbitrary value for \( w_{1/2} \), and can then solve the recursion for \( w_i \) for all \( i \geq 3/2 \).

(\footnote{\( D' \) is unchanged if \( W' \) is multiplied by a constant factor.})

On a centered grid, evaluating the accuracy conditions \( (32) \) with \( w_{-1} = w_1 \) gives \( w_1 = (1 + p) w_0 \). We initially fix an arbitrary value of \( w_0 \) and can then solve the recursion for \( w_i \) for all \( i \geq 2 \). We note in passing that the method \( [3] \) is given at interior points by

\[
\tilde{w}_i > \frac{1}{2}(w_i + w_{i+1}) - \frac{1}{12}(w_i - w_{i+2}) + \frac{1}{12}(w_i - w_{i-2}) \tag{87}
\]

(hence \( \bar{w}_i \) tends to a constant \( \bar{w}_i \), as we show in Fig. \( \ref{fig:1} \)).

Finally, we adjust the arbitrary overall factor such that \( \lim_{i \to \infty} \tilde{w}_i = 1 \). On the centered grid we need

\[
\tilde{w}_0 = \frac{p_1}{2p} \tag{90}
\]

for any value of \( p \). \( \tilde{w}_i \) for \( i > 0 \) is then actually given by the asymptotically constant polynomial \( (84) \). (For even \( p \), this is true for all \( i \), but not for \( i = 0 \) with odd \( p \), where the special form of the accuracy condition at the centre needs to be used.)

On the staggered grid we need for even \( p \)

\[
\bar{w}_{1/2} = \frac{[(p + 1)!!]^2}{p + 1} \tag{91}
\]

which also leads to the polynomials \( (83) \). However for odd \( p \) the symmetry condition at the centre is incompatible with having only the asymptotically constant mode, and we need a contribution from the oscillating mode \( (83) \). For \( \lim_{i \to \infty} \tilde{w}_i = 1 \) we now need

\[
\bar{w}_{1/2} = \frac{2}{\pi} \frac{[(p + 1)!!]^2}{p + 1} \tag{92}
\]

3. The outer boundary

This works exactly as in Sec. \( \ref{sec:3.1} \) except that \( v_i = w_i \) and \( \chi = \tilde{v}_M = \tilde{w}_M \to 1 \) only in the continuum limit.

C. A 4th-order accurate implementation (SBP4)

1. Interior points

For \( N = 2 \), we have found a scheme where \( D' \) is the unique 4-th order accurate 5-point difference operator,

\[
(D' \Pi)_i = \frac{8(\Pi_{i+1} - \Pi_{i-1}) - (\Pi_{i+2} - \Pi_{i-2})}{12} \tag{93}
\]

and where \( W' \) is diagonal and \( \tilde{W}' \) is band-diagonal with three bands. We parameterize them as

\[
W_{i,i} = \bar{w}_i, \quad w_{i,i} = w_i, \quad \bar{W}_{i,i} = v_i, \quad u_{i,i} = v_i, \quad \bar{W}_{i,i+1} = u_{i+1/2}, \quad u_{i+1/2} = u_i, \quad \bar{W}_{i,i-1} = u_{i-1/2}, \quad u_{i-1/2} = u_i, \tag{94-97}
\]

and all other components zero, where on the staggered grid the index on \( v \) and \( w \) takes half-integer values and
the index on \( u \) takes integer values, and the other way around on the centred grid. \( u_0 = 0 \) on the staggered grid and \( u_{1/2} = u_{-1/2} = 0 \) on the centred grid because we assumed in (40) that the off-diagonal blocks of \( W' \) vanish.

If we take temporarily \( u_i \) as given, we can solve the accuracy conditions for the \( \delta_{0i} \) and \( \delta_{1i} \), plus a linear recurrence relation of order 4 for \( v_i \). On the staggered grid, we can fix \( v_{1/2} = v_{-1/2} \) and \( v_{3/2} = v_{-3/2} \) arbitrarily, and solve the recurrence relation for \( v_i \) for \( i \geq 5/2 \) starting from those four points and our choice of \( u_j \). On the centred grid, the accuracy conditions (42) at the origin reduce to \( (1 + p)u_0 = v_1 - (1/8)u_{3/2} + (5/8)u_{5/2} \) and \( v_2 = v_1 + (63/8)u_{3/2} - (27/8)u_{5/2} \). We can fix \( v_1 \) and choose the the \( u_j \) arbitrarily and then compute \( v_i \) for \( i \geq 3 \) from the recurrence relation. (Note that \( v_0 \) and \( u_{1/2} \) multiply \( \Psi_0 \), which vanishes, and hence do not participate in the recurrence.)

As we shall see, it is sufficient to set all \( u_i = 0 \) except for \( u_1 \) on the staggered grid and \( u_{3/2} \) and \( u_{5/2} \) on the centered grid. In compact form, we can write

\[
(\hat{D}'\Psi)_i = \frac{8(\hat{\Psi}_{i+1} - \hat{\Psi}_{i-1}) - (\hat{\Psi}_{i+2} - \hat{\Psi}_{i-2})}{12u_i},
\]

where we have introduced the shorthand

\[
\hat{\Psi}_{1/2} \equiv v_{1/2} \Psi_{1/2} + u_{1/2} \Psi_{3/2},
\]

\[
\hat{\Psi}_{3/2} \equiv v_{3/2} \Psi_{3/2} + u_{3/2} \Psi_{1/2},
\]

\[
\hat{\Psi}_i \equiv v_i \Psi_i, \quad i \geq 5/2.
\]

for the staggered grid and

\[
\hat{\Psi}_0 \equiv 0,
\]

\[
\hat{\Psi}_1 \equiv v_1 \Psi_1 + u_3/2 \Psi_2,
\]

\[
\hat{\Psi}_2 \equiv v_2 \Psi_2 + u_{3/2} \Psi_1 + u_{5/2} \Psi_3,
\]

\[
\hat{\Psi}_3 \equiv v_3 \Psi_3 + u_{5/2} \Psi_2,
\]

\[
\hat{\Psi}_i \equiv v_i \Psi_i, \quad i \geq 4.
\]

for the centred grid.

FIG. 1. Values of \( \delta_0 \) and \( \delta_1 \) for our second-order accurate \((N = 1)\) methods, for \( p = 1, \ldots, 10 \). SBP2 is in the left column and Evans in the right column. The staggered grids (half-integer \( i \)) and centred grids (integer \( i \)) are shown on the same plot. In all cases increasing values of \( p \) correspond to increasing \( |\delta_i| \), with even values of \( p \) shown in blue (dark) and odd values in orange (light). Note that the Evans method does not exist for odd \( p \) on the centred grid, and the corresponding dots are absent. We see a rapid convergence towards the respective asymptotic values (86) and (87) for SBP2, and \( \delta_0 \to (p + 2)p(1 - p)/3(p + 1) \) and \( \delta_1 \to p/2 \) for the Evans method. Note that the \( i \) axis is logarithmic.
With the equivalent of (S1) and (S3) for \( v_i \), the fourth-order linear recurrence for \( \bar{v}_i \) has four independent asymptotic solutions with

\[
\rho = 1, \quad -1, \quad 4 + \sqrt{15}, \quad 4 - \sqrt{15}, \tag{107}
\]

all with \( k = 0 \). The linearity of the recurrence implies that the general solution \( \bar{v}_i \) is a linear combination of the four corresponding modes \( \bar{v}_i^{(p)} \). It is possible to show that if the linear combination contains any contribution of the growing or oscillating modes then the \( \delta_0 \) are not bounded. Hence we must find a solution which only contains the asymptotically constant and the decaying modes. The freedom in \( u_1, v_{1/2} \) and \( v_{3/2} \) on the staggered grid, and in \( u_{3/2}, u_{5/2} \) and \( v_1 \) on the centred grid allows us precisely to cancel simultaneously the growing mode and the oscillating non-decaying mode and fix an overall constant factor. To do that we proceed as follows.

We first compute three arbitrary solutions of the recurrence up to some high value of \( i \), say 1000. For example, on the staggered grid we can set each of \( u_1, v_{1/2} \) and \( v_{3/2} \) to 1 and the other two to 0. The three solutions are dominated by the growing mode, and reach very high values, of order \( (4 + \sqrt{15})^{1000} \times 10^{-996} \). We have detected extreme sensitivity of the solution in the initial conditions, roughly losing one decimal digit of precision per iteration, and hence the recurrence is solved with exact rational arithmetics, using Mathematica.

Then we compute the asymptotic form of the modes, up to order \( O(i^{-8}) \). For instance for the asymptotically constant mode we have

\[
\bar{v}_i^{(1)} = 1 + \frac{(2p - 1)(p - 1)p(p + 1)(p + 3)}{60i^4} + \frac{(2p - 3)(p - 3)(p - 2)(p - 1)p(p + 1)(p + 3)}{504i^6} + O(i^{-8}). \tag{108}
\]

(for \( p = 2 \) this is simply \( 1 + 3/(2i^4) + O(i^{-8}) \).) However, in contrast to the \( N = 1 \) case, these are only finite polynomials for odd \( p \), but not for even \( p \). For \( i \sim 1000 \) this expression will give results correct up to relative errors smaller than \( 10^{-18} \) for \( p \leq 10 \). We take three such values of \( i \) and construct a linear system to find which linear combination of our three solutions gives that mode \( \bar{v}_i^{(1)} \).

For such high values of \( i \) we can neglect the contribution of the decaying mode. In this way we determine the values of \( \bar{v}_i \) up to \( i = 1000 \). For larger \( i \), and \( p \leq 10 \), the asymptotic series are accurate to 16 digits. In our experiments below we shall use up to \( p = 22 \), for which values up to \( i = 2000 \) must be computed to use the given asymptotic expansions with relative errors below double precision. Note that we do not know if these series are convergent.

From \( v_i \) we can compute \( w_i \). This gives the following asymptotic behaviour for \( \bar{w}_i \),

\[
\bar{w}_i = 1 + \frac{(2p + 1)(p + 1)p(p - 1)(p - 3)}{60i^4} + \frac{(p - 1)(p - 5)(p - 3)(p - 2)(p - 1)p(p + 1)}{504i^6} + O(i^{-8}). \tag{109}
\]

For \( i \geq 9/2 \) on the staggered grid and \( i \geq 6 \) on the centred grid the \( \delta \) can be computed from \( v_i \) and \( w_i \) as follows,

\[
\delta_{0i} = i^5 \frac{v_{i-2} - 8v_{i-1} + 8v_{i+1} - v_{i+2}}{12w_i}, \tag{110}
\]

\[
\delta_{1i} = i^2 \frac{v_{i-2} - v_{i-1} - v_{i+1} + v_{i+2}}{9w_i}, \tag{111}
\]

\[
\delta_{2i} = i \frac{2v_{i-2} - v_{i-1} + v_{i+1} - 2v_{i+2}}{36w_i}. \tag{112}
\]

The previous expansions imply that the \( \delta \) are bounded and have finite limits:

\[
\delta_{0i} = -p(p - 1)^2 + O(i^{-2}), \tag{113}
\]

\[
\delta_{1i} = \frac{p(p - 1)}{3} + O(i^{-2}), \tag{114}
\]

\[
\delta_{2i} = -\frac{p}{6} + O(i^{-2}). \tag{115}
\]

The limit value of \( \delta_0 \) is cubic in \( p \). That means that \( \delta_0 \) is very large for large values of \( p \). Comparing with \( N = 1 \) it is plausible that \( \delta_0 \) has an asymptotic limit which grows like \( p^{N+1} \).

We provide in our webpage [9] data files with double-precision results for \( \bar{v}, \bar{w} \) and the \( \delta \) for \( 1 \leq s \leq 22 \) and \( i \leq 2000 \). Formulas (108) and (109) can be used to compute \( \bar{v} \) and \( \bar{w} \) for these \( p \) and \( i \geq 2000 \) to 16 digits.

We find that for \( p = 1 \) and \( p = 2 \) (the wave equation in cylindrical and spherical symmetry), on the staggered grid, \( v_{1/2} < 0 \), so that \( \bar{W} \) is then not positive definite. This problem is absent for \( p \geq 3 \), or on the centred grid. It is possible that allowing for \( u_i \) other than \( u_1 \) to be nonzero, this could be fixed, but we have not tried this.

2. The outer boundary

Strand provides boundary operators with interior accuracy order \( 2N \) (2s in the notation of Strand) and different boundary accuracy orders \( \tau \), depending on the number \( r \) of boundary points used and the form of the \( W_0 \) (\( W \) in the notation of Strand) operator. He finds that \( \tau \leq N \) with \( r \) ranging from \( r = \tau + 1 \) for a general \( W_0 \) to \( r = 2\tau \) for diagonal \( W_0 \). In our case \( 2N = 4 \) and we want to have diagonal \( W_0 \), so there are two possibilities: \( (\tau = 1, r = 2) \) and \( (\tau = 2, r = 4) \).

For \( \tau = 1 \), following the general prescription of Sec. II.E we set

\[
D = \left( \begin{array}{cccc}
\frac{1}{12} & \frac{2}{3} & 0 & -\frac{1}{12} \\
\frac{1}{3} & \frac{2}{3} & -\frac{8}{9} & 0 \\
\frac{2}{3} & -\frac{8}{9} & \frac{2}{3} & -\frac{1}{12} \\
-\frac{1}{12} & 0 & -\frac{1}{12} & \frac{1}{3}
\end{array} \right), \tag{116}
\]
FIG. 2. Values of $\delta_0$, $\delta_1$ and $\delta_2$ for SBP4 on the centred grid (left column) and on the staggered grid (right column), with $p = 1, \ldots, 10$. In all cases increasing values of $p$ correspond to lines further from the axis $\delta_i = 0$, with even values of $p$ shown in blue (dark) and odd values in orange (light). Again, we see a rapid convergence towards their respective asymptotic values (113–115). The fact that $u_1$ (for the staggered grid) and $u_{5/2}$ or $u_{5/2}$ (for the centred grid) appear explicitly in the recurrence for a few low $i$ points, but not beyond, produces some irregular behaviour at those points.

\[
B = \begin{pmatrix}
0 \\
0 \\
v_M
\end{pmatrix}, \quad (117)
\]

\[
W = \text{diag} \left( \ldots, w_{M-2}, \frac{13w_{M-1}}{12}, \frac{5w_M}{12} \right), \quad (118)
\]

\[
\tilde{W} = \text{diag} \left( \ldots, v_{M-2}, \frac{13v_{M-1}}{12}, \frac{5v_M}{12} \right). \quad (119)
\]
From (24) we read off
\[ \tilde{D} = \begin{pmatrix}
\frac{v_{M-4}}{12w_{M-2}} & \frac{2v_{M-3}}{3w_{M-2}} & 0 & \frac{2v_{M-1}}{w_{M-2}} & \frac{v_M}{5w_M} \\
\frac{v_{M-4}}{12w_{M-2}} & \frac{2v_{M-3}}{3w_{M-2}} & 0 & \frac{2v_{M-1}}{w_{M-2}} & \frac{v_M}{5w_M} \\
0 & \frac{8v_{M-2}}{5w_{M-1}} & \frac{7v_{M-1}}{5w_M} & \frac{6v_M}{5w_M} & \frac{12v_{M-2}}{5w_{M-1}} \\
\frac{4v_{M-4}}{43w_{M-2}} & \frac{4v_{M-3}}{43w_{M-2}} & \frac{4v_{M-1}}{43w_{M-2}} & \frac{4v_{M-1}}{43w_{M-2}} & \frac{4v_{M-1}}{43w_{M-2}} \\
0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0
\end{pmatrix} \]  
(120)

This \( \tilde{D} \) is fourth-order accurate in the interior, and first-order accurate at \( i = M - 1, M \).

For \( \tau = 2 \), following the general prescription we set
\[ \tilde{W} = \text{diag}(\ldots, \frac{49v_{M-3}}{48}, \frac{43v_{M-2}}{48}, \frac{59v_{M-1}}{48}, \frac{17v_M}{48}), \]
(121)
\[ \tilde{D} = \begin{pmatrix}
\frac{v_{M-6}}{12w_{M-2}} & \frac{2v_{M-5}}{3w_{M-2}} & 0 & \frac{2v_{M-3}}{w_{M-2}} & \frac{v_M}{5w_M} \\
0 & \frac{4v_{M-4}}{43w_{M-2}} & \frac{4v_{M-3}}{43w_{M-2}} & \frac{4v_{M-1}}{43w_{M-2}} & \frac{4v_{M-1}}{43w_{M-2}} \\
0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0
\end{pmatrix} \]  
(122)

The expressions for \( D \) and \( W \) are obtained by setting \( u_i \) and \( w_i \) to 1.

D. Numerical tests

We have tested our 2nd and 4th order accurate implementations as described above, combined with 4th-order Runge-Kutta discretisation in time, with a Courant factor \( \Delta t/h = 1/4 \). In SBP4 we use the numerical coefficients \( \tilde{D}_{ij} \), or equivalently \( u_i, \bar{u}_i \) and \( \bar{w}_i \), calculated by the relaxation method described above up to \( i \sim 2000 \), and using the asymptotic results [103], [109] for larger \( i \).

Initial data are set with \( \pi \) a smooth function of compact support bounded away from \( r = 0 \) and \( R \), and \( \bar{\psi} = 0 \), so that at early times we can verify accuracy without the complication of boundary conditions.

To determine the accuracy of the method we have investigated self-convergence. This means that we check that \( e_t \) as defined by
\[ \Pi_t(t) = \pi(r_i, t) + \pi^4 e_t(r_i, t) + o(h^4) \]  
(123)
(the Richardson expansion, here assuming 4th-order accuracy) is approximately independent of \( h \). Starting from a reference resolution, we refine twice (by a factor of 2 on the centred grid, and a factor of 3 on the staggered grid). We can then obtain two independent estimates of \( e_t(r, t) \) (or \( e_3 \) or \( e_2 \) if we are testing for third or second-order accuracy) and we compare these. Using refinement by a factor of 3 allows us to combine a staggered grid with fixed \( r_M = R \), and still have appropriate grid points of all refined grids align with the coarsest grid. Keeping \( R \) exactly resolution-independent is necessary to compare different resolutions, while aligned grids avoid the need for high-order interpolation to the same values \( r \) in comparing different resolutions. Both \( \pi \) and \( \bar{\psi} \) and their associated errors scale as \( r^{-p/2} \) to leading order, and we therefore plot \( r^{-p/2} \pi \) and \( r^{-p/2} \bar{\psi} \). This is sensible also because technically speaking we expect convergence to the continuum in the energy norm \( E \), rather than the usual \( L^2 \) norm, or in other words we expect convergence of \( r^{-p/2} \pi \) and \( r^{-p/2} \bar{\psi} \) in the standard \( L^2 \) norm.

We have tested Evans, SBP2, SBP41 and SBP42, for \( 0 \leq p \leq 22 \), on the staggered and centred grids, with representative outer boundary conditions (see below). We note two exceptions. 1. The Evans method does not exist on the centred grid for odd \( p \), because \( v_0 \) is then not defined. 2. The energy of SBP4 is not positive definite on the staggered grid for \( p = 1, 2 \), and so we would not expect it to be stable. However, we do not see signs of instability in our numerical experiments.

In all other cases, our numerics confirm theoretical expectations, as follows. At short times, before the solution has interacted with the boundary \( r = R \), we see convergence at precisely the expected order, that is second order for Evans and SBP2, and fourth order for SBP41 and SBP42. As expected, the error \( e_1 \) is identical for SBP41 and SBP42, because they are the same method except at the boundary. Surprisingly, the error \( e_2 \) is almost identical also between Evans and SBP2. This may be because they agree more and more with each other, and the naive method, with increasing \( i \).

Once the solution has interacted with the boundary, we
still see precise second-order convergence for Evans and SBP2. For SBP41 we see second-order convergence and for SBP42 we see third-order convergence. Note that in each case this global accuracy is one order higher than the accuracy at the boundary. We do not know if this was to be expected, see Sec. 12.7 of [10]. For SBP41 and SBP42 after the wave has interacted with the boundary, the error is dominated by grid noise, and hence the strict Richardson expansion is lost, but the envelope of $e_3$ or $e_2$ respectively is still approximately resolution-independent.

We have also evaluated the discrete energy at every time step. With the boundary conditions $\sigma \dot{r} + \mu \dot{\psi} = 0$ and $\sigma \dot{\psi} + \nu (\dot{\psi}^2 + \dot{\psi}/r) = 0$ discussed in Appendix A we have $d\hat{E}/dt = 0$. With the maximally dissipative boundary condition $\sigma \dot{r} + \mu \dot{\psi} = 0$ we have $d\hat{E}/dt = \chi M M \dot{\psi} M \leq 0$, and we have evolved the expected value of $\hat{E}$ by discretising this in $t$ using 4th-order Runge-Kutta. In all these cases the discrepancy between the evaluated and predicted numerical energy is of relative size $10^{-8}$, essentially independent of the method (Evans, SBP2, SBP41 or SBP42) and of $h$, and increases linearly with $t$. As expected, it is due only to accumulated roundoff error (machine precision).

IV. CONCLUSIONS

The wave equations (7), (8) or (11) appear in many areas of mathematical physics. In a larger class of applications, these evolution equations are modified by $r$-dependent coefficients (for example in the wave equation on a curved spacetime), lower-order nonlinear terms (for example a scalar field potential), or couplings through lower-order terms to other equations in a larger system (for example stellar perturbation theory).

Our experience suggests that the key stability problems in such systems of equations arise already in the simple linear system considered here. Prior to the results presented here, we are not aware of any completely stable finite differencing scheme for these equations. Methods which appear to be stable at first fail to converge at sufficiently high resolution or large $p$, with problems either at the origin $r = 0$ or the outer boundary $r = R$.

It is surprising that the lower order term $p \dot{\psi}/r$ in (11) alone can make standard schemes unstable, and that an elaborate SBP scheme is necessary. Note however that a standard centered finite difference implementation of the one-dimensional wave equation is already SBP except possibly at the boundaries, while the equivalent naive finite differencing of (11) for $p > 0$ is not SBP even at interior points. It seems highly unlikely to us that any boundary conditions can be devised to make such a scheme stable.

Finally, the reader may be used to adding numerical dissipation to keep numerical methods stable. However, strictly linear equations such as the ones we consider here should not require explicit dissipation, which should be reserved for dealing with nonlinearities. Moreover, in a naive finite differencing of our equations, the amount of dissipation required increases rapidly with $p$, so that this is not a feasible approach if large $p$ are required.

The answer is then two-fold: first, to make the numerical scheme SBP at interior points and second, to make it SBP also at the boundary and to use the Olsson projection method to impose suitable boundary conditions. In hindsight, the Evans method is already SBP at interior points, which explains why it works much better than a naive scheme. However, SBP at the outer boundary is also necessary to make it into a demonstrably stable scheme. This is not difficult to achieve, but without an explicit reference to discrete energy methods would not be at all obvious, especially as SBP methods appear to require a reduction in the order accuracy at boundary points [11]. Furthermore, the Evans method does not have an obvious generalisation to higher order accuracy, and does not work for odd $p$ on a centred grid.

As the main result of this paper, we have therefore constructed 2nd and 4th-order accurate SBP methods by using discrete energies that are non-diagonal near the origin. These can be made 1st and 2nd-order accurate, respectively, at the boundary $r = R$, leading to global 2nd and 3rd-order accuracy after the solution has interacted with the boundary. (Our SBP4 is not positive definite for $p = 1, 2$ on a staggered grid.) It is clear that our ansatz can be generalized to order $2N$ in the interior and order $N$ at the boundary, giving rise to global accuracy of order $N + 1$.

In the Appendix, we have used the SBP property to construct discretisations of the boundary conditions [15] that give rise to a strictly non-increasing discrete energy, and hence guarantee numerical stability.

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Appendix A: Rigorous treatment of ghost points

Consider $\hat{\psi}_i$ for physical grid points $i > 0$. We can write the use of ghost points explicitly as

$$\hat{\psi}_i = h^{-1} \sum_{j > 0} (D_{ij} \Pi_j + D_{i-\quad j} \Pi_{-j}) = h^{-1} \sum_{j > 0} D_{ij}^+ \Pi_j,$$

where

$$D_{ij}^+ \equiv D_{ij} + D_{i-\quad j}, \quad i, j > 0. \quad (A1)$$

Consider $\hat{\Psi}_i$ for physical grid points $i > 0$. We can write the use of ghost points explicitly as

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where

$$D_{ij}^+ \equiv D_{ij} + D_{i-\quad j}, \quad i, j > 0. \quad (A2)$$
We think of this as “folding over the ghost points”. A similar observation holds for $D$, except that as $\Psi_i$ is odd, the equivalent of (A2) is
\[
\tilde{D}_{ij}^+ \equiv \tilde{D}_{ij} - \tilde{D}_{i,-j}, \quad i, j > 0.
\] (A3)
Note that $D_{ij}^+ \neq D_{ij}$ even for $i, j > 0$, thus requiring a separate symbol. (The symbol $D^+$ is a reminder of the range $i, j > 0$.) The split of $D_{ij}^+$ into $D_{ij}$ and $D_{i,-j}$ for $i, j > 0$ is in general not unique. We do, however, have a natural prescription for this split if we assume that $D_{ij}$ is translation-invariant, i.e., depends only on $i - j$ even at the boundary.

In order to extend $D_{ij}$ and $\tilde{D}_{ij}$ to negative $i$, we use the requirement that (A5) hold at all times, or
\[
\tilde{1}_{i-1} = \tilde{1}_i, \quad \tilde{\Psi}_{-1} = -\tilde{\Psi}_i.
\] (A4)
The first equation of (A5) and the second equation of (A4) immediately give, for $i, j > 0$, that
\[
D_{ij} + D_{i,-j} + D_{-ij} + D_{-i,-j} = 0.
\] (A5)
The second equation of (A5) and the first equation of (A4), after substituting (26) and using (46), give, for $i, j > 0$, that
\[
(W^{-1})_{ik} (D_{kl} - D_{k,-l} - D_{-kl} + D_{-k,-l}) W_{ij} = 0,
\] (A6)
and hence
\[
D_{ij} - D_{i,-j} - D_{-ij} + D_{-i,-j} = 0.
\] (A7)
Taking the sum and difference of (A5) and (A7), we obtain (A8).

Finally, we have, for $i, j > 0$, that
\[
\tilde{D}_{ij}^+ = \sum_{k,l>0} - (W^{-1})_{ik} (D_{lk} - D_{-lk}) \tilde{W}_{ij}
\]
\[
= \sum_{k,l>0} - (W^{-1})_{ik} (D_{lk} + D_{l,-k}) \tilde{W}_{ij}
\]
\[
= \sum_{k,l>0} - (W^{-1})_{ik} (D_{lk}^+ + D_{lk}^-) \tilde{W}_{ij},
\] (A8)
and so (24) holds for the operators $D^+$ and $\tilde{D}^+$ with ghost points folded in if and only if it holds for the extended operators $D$ and $\tilde{D}$. This confirms that the introduction of ghost points is just a matter of notation.

Appendix B: The projection method for imposing boundary conditions

For completeness, this Appendix summarises relevant methods from [2]. Suppose a first-order in space and time system of PDEs in one spatial dimension has been discretised in space as
\[
\dot{u} = Du
\] (B1)
Note that the vector $u$ in general ranges over multiple variables (for example $\pi$ and $\psi$) as well as grid points (for example $i$), and we use calligraphic letters such as $D$ for operators on this vector space.

Suppose this system has a discrete energy
\[
\dot{E} \equiv \frac{1}{2} u^tWu
\] (B2)
and obeys the SBP property that
\[
\mathcal{B} \equiv \frac{1}{2} (WD + D^tW)
\] (B3)
is a boundary operator. Then
\[
\frac{dE}{dt} = u^tBu
\] (B4)
is a boundary term.

We want to impose one or several homogenous linear boundary conditions that we write as
\[
Lu = 0.
\] (B5)
In matrix notation where $u$ is a column vector, $L$ is a matrix that has one row for each boundary condition.

To focus on the essential idea, we define the inner product
\[
(u, v) \equiv u^t\Psi v.
\] (B6)
In this notation we can write
\[
\dot{E} = \frac{1}{2}(u, u), \quad \frac{dE}{dt} = (u, Du).
\] (B7)
The adjoint with respect to this inner product is defined by
\[
(Au, v) \equiv (u, A^tv),
\] (B8)
and is therefore given by
\[
A^t = \Psi^{-1}A^t\Psi.
\] (B9)
The operator
\[
\mathcal{P} \equiv 1 - W^{-1}L^t(\mathcal{L}W^{-1}L)^{-1}\mathcal{L}
\] (B10)
clearly obeys
\[
\mathcal{P}^2 = \mathcal{P}, \quad \mathcal{L}\mathcal{P} = 0, \quad \mathcal{P}^t = \mathcal{P},
\] (B11)
and so is a self-adjoint projection operator into the space of grid functions that obey the boundary conditions. If we now use the semi-discrete evolution equation
\[
\dot{u} = \mathcal{P}Du
\] (B12)
instead of (B11), we have $\mathcal{L}\dot{u} = 0$ exactly, and hence $\mathcal{L}u = 0$ and therefore $\mathcal{P}u = u$ at all times if it holds initially. Then we have
\[
\frac{dE}{dt} = (u, \mathcal{P}Du) = (\mathcal{P}u, Du) = (u, Du)
\] (B13)
as before and so both the discrete energy bound and the desired boundary conditions hold.
Appendix C: Continuum boundary conditions involving derivatives

Consider the class of boundary conditions of the form
\[ \rho \pi + \sigma \psi + \mu \pi' + \nu \left( \psi' + \frac{\rho}{r} \psi \right) = 0, \quad r = R \]
(C1)

or equivalently
\[ \rho \pi + \sigma \psi + \mu \dot{\psi} + \nu \ddot{\pi} = 0, \quad r = R \]
(C2)

for \( \rho, \sigma, \mu, \nu \) not all vanishing at once. To fix an overall sign, we also assume that at least one of them is positive. We now use an energy argument to show that these boundary conditions give rise to a stable initial-boundary value problem if \( \rho, \sigma, \mu, \nu \geq 0 \) with \( \rho \mu + \sigma \nu > 0 \). The maximally dissipative special case \( \mu = \nu = 0 \) with \( \rho \sigma \geq 0 \) is also stable based on the energy \( E \) defined in (18).

We consider the energy
\[ E_b = E + \frac{\rho}{2s}(\mu \psi + \nu \pi)^2 \]
(C3)

where \( E \) is given by (18), \( E_b \) stands for \( E \) modified by a boundary term, and \( s \) is
\[ s \equiv \rho \mu + \sigma \nu. \]
(C4)

Its time derivative is
\[ \frac{dE_b}{dt} = R^p \left[ \pi \psi + \frac{1}{s}(\mu \psi + \nu \pi) \left( \mu \dot{\psi} + \nu \ddot{\pi} \right) \right]_{r=R} \]
\[ = R^p \left[ \pi \psi - \frac{1}{s}(\mu \psi + \nu \pi) (\rho \pi + \sigma \psi) \right]_{r=R} \]
\[ = \frac{-R^p}{s}(\mu \sigma \psi^2 + \nu \rho \pi^2)_{r=R}, \]
(C5)

The necessary and sufficient conditions for \( E_b \) to be positive definite and its time derivative to be non-positive are
\[ \rho \geq 0, \quad \sigma \geq 0, \quad \mu \geq 0, \quad \nu \geq 0. \]
(C6)

We have \( dE_b/dt = 0 \) if \( \rho \sigma = \rho \pi = 0 \), and \( dE_b/dt < 0 \) otherwise. However, the limiting case \( \mu \sigma = \sigma \nu = 0 \) is not allowed because it would give \( s = 0 \), except for the maximally dissipative sub-case \( \mu = \nu = 0 \), where \( E \) and \( dE/dt \) are given by (18) and (19) instead of (18) and (19).

Appendix D: Numerical boundary conditions involving derivatives

We define the modified numerical energy
\[ \hat{E}_b = \hat{E} + \frac{\chi h^p M^p}{2s} (\mu \Psi_M + \nu \Pi_M)^2, \]
(D1)

where \( \chi \) parameterises finite differencing error in the boundary term, as defined by [25]. We find
\[ \frac{d\hat{E}_b}{dt} = \chi h^p M^p \left[ \Pi_M \dot{\Psi}_M + \frac{1}{s}(\mu \dot{\Psi}_M + \nu \dot{\Pi}_M) \left( \mu \Psi_M + \nu \Pi_M \right) \right], \]
(D2)

so if the numerical boundary could be chosen to be
\[ \rho \pi_M + \sigma \psi_M + \mu \dot{\psi}_M + \nu \ddot{\pi}_M = 0, \]
(D3)

the argument could be completed as in the continuum case. However, \( \hat{u} = P \hat{D} u \) and not \( \hat{D} u \). We have not been able to find an ansatz for \( \hat{L} \) and \( \hat{E}_b \) such that \( \hat{dE}_b/dt \leq 0 \).

Consider however the two subclasses of boundary conditions where \( \hat{dE}_b/dt \) is in the continuum. Consider first the case \( \sigma = \nu = 0 \) with \( \rho \mu > 0 \). Then [22] reduces to
\[ \frac{d\hat{E}_b}{dt} = \chi h^p M^p \left( \Pi_M \dot{\Psi}_M + \frac{1}{\rho} \Psi_M \dot{\Psi}_M \right) \]
\[ = \chi h^p M^p \left( \Pi_M \Psi_M + \frac{1}{\rho} \Psi_M \Pi_M h^{-1}(D\Pi)_M \right) \]
\[ = 0, \]
(D4)

where the second equality holds because in this special case the boundary condition is independent of \( \Psi \) so that \( P \) only acts on \( \Pi \), and the last equality holds if we implement \( \hat{L} u = 0 \) as
\[ \rho \Pi_M + \mu h^{-1}(D\Pi)_M = 0. \]
(D5)

The case \( \rho = \mu = 0 \) with \( \nu \sigma > 0 \) works the same way, with the roles of \( \Pi \) and \( \Psi \) interchanged.

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