ELSEVIER

Applied Numerical Mathematics 37 (2001) 171–187

APPLIED NUMERICAL MATHEMATICS

www.elsevier.nl/locate/apnum

Fourth- and sixth-order conservative finite difference approximations of the divergence and gradient ☆

J.E. Castillo [a], J.M. Hyman [b], M. Shashkov [b], S. Steinberg [c]

[a] Department of Mathematics, San Diego State University, San Diego, CA 92182-7720, USA

[b] Theoretical Division, Mail Stop B284, Los Alamos National Laboratory, Los Alamos, NM 87545, USA

[c] Department of Mathematics, University of New Mexico, Albuquerque, NM 87131, USA

Received 30 November 1999; accepted 7 August 2000

Abstract

We derive conservative fourth- and sixth-order finite difference approximations for the divergence and gradient operators and a compatible inner product on staggered 1D uniform grids in a bounded domain. The methods combine standard centered difference formulas in the interior with new one-sided finite difference approximations near the boundaries. We derive compatible inner products for these difference methods that are high-order approximations of the continuum inner product. We also investigate defining compatible high-order divergence and gradient finite difference operators that satisfy a discrete integration by parts identity. © 2001 IMACS. Published by Elsevier Science B.V. All rights reserved.

1. Introduction

We are developing a discrete analog of vector and tensor calculus that can be used to accurately approximate continuum models for a wide range of physical processes on logically rectangular, nonorthogonal, nonsmooth grids. These finite difference methods (FDMs) preserve fundamental properties of the original continuum differential operators and allow the discrete approximations of partial differential equations (PDEs) to mimic critical properties, including conservation laws and symmetries, in the solution of the underlying physical problem. The discrete analogs of div, grad, and curl satisfy the identities and theorems of vector and tensor calculus and provide new reliable algorithms for a wide class of PDEs [6–9]. This approach has been used to construct high-quality mimetic finite-difference approximations for the divergence, gradient [16,17], and curl [11]. In [10] this new methodology has been applied to Maxwell's first-order curl equations. We have created higher-order approximations (see [2,3, 5]) in 1D and 2D on smooth curvilinear grids that satisfy a summation by parts identity for the particular case of periodic boundary conditions.

☆ This research was supported by the Department of Energy under contracts W-7405-ENG-36, the Applied Mathematical Sciences Program KC-07-01-01, and the National Science Foundation Grant CCR-9531828.

PII: S0168-9274(00)00033-7

One of the central parts of discrete vector analysis is the discrete analog of integration by parts formula. Compatible discrete divergence ($\nabla\cdot$) and gradient (∇) operators satisfy a discrete analog of the Divergence Theorem:

$$\int_{\Omega} \nabla \cdot \vec{v} f \,\mathrm{d}V + \int_{\Omega} \vec{v} \nabla f \,\mathrm{d}V = \int_{\partial\Omega} f \vec{v} \cdot \vec{n} \,\mathrm{d}S. \tag{1.1}$$

Here Ω is some smooth region in a Euclidean space, $\partial\Omega$ is the boundary of the region, $\vec{n}$ is an outward normal to the boundary, f is a smooth scalar function defined on the closure of the region, and $\vec{v}$ is a smooth vector field defined on the closure of the region (see [15]). The higher-order discrete operators derived in [2,3,5] do not satisfy the discrete analog of this identity for nonperiodic boundary conditions.

Because of its importance, we illustrate how the divergence theorem is used to show stability of solutions of partial differential equations. So assume that $f(x,t)$ is some smooth function for $x \in \Omega$ and satisfies the simple heat equation

$$\frac{\partial f}{\partial t} = \nabla \cdot \nabla f, \tag{1.2}$$

and that f is zero on the boundary $\partial\Omega$. If we introduce the functional

$$E(t) = \frac{1}{2} \int_{\Omega} f^2(x,t) \,\mathrm{d}V, \tag{1.3}$$

then differentiation and the Divergence Theorem give

$$\frac{\partial E}{\partial t}(t) = \int_{\Omega} \frac{\partial f}{\partial t}(x,t) f(x,t) \,\mathrm{d}V = \int_{\Omega} \nabla \cdot \nabla f(x,t) f(x,t) \,\mathrm{d}V = -\int_{\Omega} \big(\nabla f(x,t)\big)^2 \,\mathrm{d}V. \tag{1.4}$$

Consequently, the derivative of E is negative or zero, and thus cannot grow. So in this sense the solutions of the differential equation must be stable.

Similarly one can show that the solutions of the simple wave equation

$$\frac{\partial^2 f}{\partial t^2} = \nabla \cdot \nabla f \tag{1.5}$$

have constant energy

$$E(t) = \frac{1}{2} \int_{\Omega} \left(\frac{\partial f}{\partial t}\right)^2 + \big(\nabla f(x,t)\big)^2 \,\mathrm{d}V, \tag{1.6}$$

by showing that the time derivative of E is zero.

In 1D both divergence and gradient are simple derivatives and the identity (1.1) reduces to integration by parts:

$$\int_0^1 v_x f \,\mathrm{d}x + \int_0^1 v f_x \,\mathrm{d}x = f(1)v(1) - f(0)v(0), \tag{1.7}$$

and when either $f \equiv 1$ or $v \equiv 1$, this becomes a conservation law:

$$\int_0^1 \frac{\mathrm{d}v}{\mathrm{d}x} \,\mathrm{d}x = v(1) - v(0), \qquad \int_0^1 \frac{\mathrm{d}f}{\mathrm{d}x} \,\mathrm{d}x = f(1) - f(0). \tag{1.8}$$

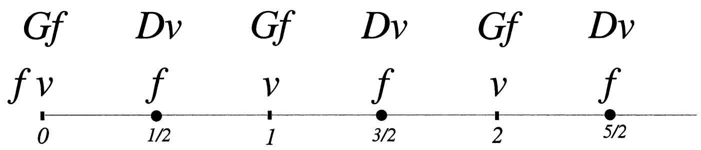

Fig. 1. Staggered grid.

To satisfy a discrete analog of (1.8), we must define a discrete formula for the derivative and a discrete analog of the integral (in general a discrete analog of the inner products in (1.1)). Applications to hyperbolic conservation laws may only contain a divergence, so in this case we need only consider the analog of global conservation (1.8). In this paper we define high-order conservative (that is, satisfying identities (1.8)) finite difference methods (FDMs) for the divergence ($\boldsymbol{D}$) and gradient ($\boldsymbol{G}$) operators on 1D uniform staggered grids in bounded domains. On staggered grids there are two different discrete analogs of this derivative. One, which corresponds to the divergence, has domain consisting of values at the nodes and range consisting of values at the cell centers, and another one, which corresponds to the gradient, has complementary domain and range of values.

The main results of this paper are explicit formulas for fourth- and sixth-order accurate discrete divergence and gradient and corresponding inner products that satisfy a discrete analog of formula (1.8) exactly. Many of the results in this paper require extensive algebraic computations which we have done with a computer algebra system.

In discretization such as ours, it is important to distinguish if a nodal or staggered grid is being used, because this significantly impacts the construction of the difference schemes. Our FDMs for a staggered grid are quite different from those for a nodal grid [1,12,14,18].

For our discretizations we use a uniform staggered grid Fig. 1 with $h = 1/N$ and nodes at $x_i = ih$, $0 \leqslant i \leqslant N$, and cells $[x_i, x_{i+1}]$ with centers $x_{i+1/2} = \frac{1}{2}(x_i + x_{i+1})$. Continuum functions are projected onto the grid using point values:

$$f_{i+1/2} = f(x_{i+1/2}), \quad 0 \leqslant i \leqslant N-1, \qquad v_i = v(x_i), \quad 0 \leqslant i \leqslant N. \tag{1.9}$$

Two auxiliary values for f are introduced at the domain boundaries,

$$f_0 = f(0), \qquad f_N = f(1), \tag{1.10}$$

which is typical for support-operators formulations.

The discrete divergence will act on the v-values, while the discrete gradient will act on the f-values, as illustrated in Fig. 1.

2. Second-order discrete operators

The simplest discrete divergence is defined by

$$(\boldsymbol{D}v)_{i+1/2} = \frac{v_{i+1} - v_i}{h}, \quad 0 \leqslant i \leqslant N-1, \tag{2.1}$$

and the discrete gradient is defined by

$$
\begin{aligned}
(\boldsymbol{G} f)_0 &= \frac{f_{1/2} - f_0}{h/2}, \\
(\boldsymbol{G} f)_i &= \frac{f_{i+1/2} - f_{i-1/2}}{h}, \quad 1 \leqslant i \leqslant N-1, \\
(\boldsymbol{G} f)_N &= \frac{f_N - f_{N-1/2}}{h/2},
\end{aligned} \tag{2.2}
$$

where again the definition of $\boldsymbol{G}$ at the boundary points is standard for the support operators approach. The divergence $\boldsymbol{D}$ is second-order accurate while the gradient $\boldsymbol{G}$ is second-order accurate in the interior and first-order at the boundary. Fig. 1 illustrates the positions of the values of $\boldsymbol{D}v$ and $\boldsymbol{G}f$ in the grid.

Using both the midpoint and trapezoidal rules, we define two *discrete integrals* for cell-centered and nodal quantities by

$$
\boldsymbol{I}_c f = h \sum_{i=0}^{N-1} f_{i+1/2}, \tag{2.3}
$$

$$
\boldsymbol{I}_n v = h \left(\frac{v_0}{2} + \sum_{i=1}^{N-1} v_i + \frac{v_N}{2} \right). \tag{2.4}
$$

An easy computation shows that these are second-order approximations of the continuum integrals and

$$
\begin{aligned}
\boldsymbol{I}_c(\boldsymbol{D}v) &= v_N - v_0, \\
\boldsymbol{I}_n(\boldsymbol{G}f) &= f_N - f_0,
\end{aligned} \tag{2.5}
$$

are analogs of the formulas in (1.8).

2.1. Generalizations

Away from the boundaries, the above considerations generalize to higher-order discretizations. For staggered uniform grids, the half-integer points are obtained from the integer points by translating the points by $1/2$ and vice versa. So the natural higher-order central approximations to the derivative on one grid can be translated by $1/2$ to give an approximation of the derivative on the other grid. Such approximations to the derivative have the form

$$
(\boldsymbol{D}v)_{i+1/2} = \sum_{k=-K+1}^{K} d_k v_{i+k}, \quad 0 \leqslant i \leqslant N-1, \tag{2.6}
$$

$$
(\boldsymbol{G}f)_i = \sum_{k=-K+1}^{K} d_k f_{i+k-1/2}, \quad 1 \leqslant i \leqslant N-1, \tag{2.7}
$$

where K is a positive integer and the d_k are anti-symmetric: $d_k = -d_{1-k}$, $1-K \leqslant k \leqslant K$. (Examples are given below.)

We can set $d_k = 0$ for $k > K$ and $k < 1-K$, while retaining the anti-symmetry of the d_k, and then remove the limits from the sums in (2.6) and (2.7). If we assume that f and v are zero near the boundary, then a natural discretization of the Divergence Theorem (1.1) is

$$\sum_i (\boldsymbol{D}v)_{i+1/2} f_{i+1/2} + \sum_i v_i (\boldsymbol{G}f)_i = 0. \tag{2.8}$$

If we manipulate the sums a bit we get

$$\begin{aligned}\sum_i (\boldsymbol{D}v)_{i+1/2} f_{i+1/2} &= \sum_i \sum_k d_k v_{i+k} f_{i+1/2} = \sum_i \sum_k d_k v_i f_{i-k+1/2} = \sum_i \sum_k d_{1-k} v_i f_{i+k-1/2} \\ &= -\sum_i \sum_k d_k v_i f_{i+k-1/2} = -\sum_i v_i (\boldsymbol{G}f)_i.\end{aligned} \tag{2.9}$$

So away from the boundary, the above simple analog of the Divergence Theorem holds exactly for all antisymmetric approximations of the derivative. One-sided approximations must be used near the boundary, so to have the Divergence Theorem hold exactly, we must modify the definitions of the divergence and gradient and take different approximations to the integrals in (1.1).

Because the d_k are antisymmetric, the higher order divergence $\boldsymbol{D}$ and gradient $\boldsymbol{G}$ both kill constant functions and thus also satisfy the analogs of (1.8) given by (2.5). Our problem is to fix things up so that we get exact discrete analogs of (1.8) up to the boundary.

3. Higher-order discretizations

We define discrete inner products for functions defined on the staggered grid by generalizing the usual inner products using the matrices Q and P:

$$\langle Qf, g\rangle = \sum_{i,j=0}^{N-1} Q_{i+1/2,j+1/2} f_{i+1/2} g_{j+1/2}, \qquad \langle u, Pv\rangle = \sum_{i,j=0}^{N} P_{i,j} u_i v_j. \tag{3.1}$$

For these expressions to be inner products, P and Q have to be symmetric positive-definite operators.

The general divergence and gradient are defined by

$$\begin{aligned}(\boldsymbol{D}v)_{i+1/2} &= \frac{1}{h}\sum_{j=0}^{N} d_{i+1/2,j} v_j, && 0 \leqslant i \leqslant N-1, \\ (\boldsymbol{G}f)_i &= \frac{1}{h}\left(g_{i,0} f_0 + \sum_{j=0}^{N-1} g_{i,j+1/2} f_{j+1/2} + g_{i,N} f_N\right), && 0 \leqslant i \leqslant N,\end{aligned} \tag{3.2}$$

and satisfy a discrete analog of the integration by parts theorem, (1.1) when

$$\langle Q\boldsymbol{D}v, f\rangle + \langle v, P\boldsymbol{G}f\rangle = v_N f_N - v_0 f_0, \tag{3.3}$$

is satisfied. The operators have order of accuracy k when

$$\begin{aligned}(\boldsymbol{D}v)_{i+1/2} - v'\big(\big(i+\tfrac{1}{2}\big)h\big) &= \mathrm{O}\big(h^k\big), && 0 \leqslant i \leqslant N-1, \\ (\boldsymbol{G}f)_i - f'(ih) &= \mathrm{O}\big(h^k\big), && 0 \leqslant i \leqslant N.\end{aligned} \tag{3.4}$$

Our goal is to define Q, P, $\boldsymbol{D}$ and $\boldsymbol{G}$ satisfying (3.3) and (3.4) that are at least fourth order in the interior. Near the boundary $\boldsymbol{D}$ and $\boldsymbol{G}$ should be local operators but they could be lower order. For some PDEs, the reduced accuracy near the boundary has a small effect on the accuracy of the solution.

The leading error term in approximations of the first derivative by finite differences has the form

$$Ch^k \frac{\mathrm{d}^{k+1} f}{\mathrm{d}x^{k+1}}, \tag{3.5}$$

where C is a constant. Therefore, an equivalent formulation of the accuracy requirement is that the derivatives be exact on the polynomials $1, x, \ldots, x^k$:

$$\begin{aligned} &\left(\boldsymbol{D}x^j\right)_{i+1/2} - j\left(\left(i+\tfrac{1}{2}\right)h\right)^{j-1} = 0, \quad && 0 \leqslant i \leqslant N-1, \\ &\left(\boldsymbol{G}x^j\right)_i - j(ih)^{j-1} = 0, && 0 \leqslant i \leqslant N, \end{aligned} \tag{3.6}$$

for $0 \leqslant j \leqslant k$. This condition provides a way of finding constraints on the inner product that are independent of the definitions of $\boldsymbol{D}$ and $\boldsymbol{G}$:

$$m\left\langle Qx^{m-1}, x^n\right\rangle + n\left\langle x^m, Px^{n-1}\right\rangle = 1, \quad 0 \leqslant m \leqslant k,\ 0 \leqslant n \leqslant k,\ m \neq 0 \text{ or } n \neq 0, \tag{3.7}$$

or more explicitly

$$m\sum_{i,j=0}^{N-1} Q_{i+1/2,j+1/2}\left(i+\tfrac{1}{2}\right)^{m-1}\left(j+\tfrac{1}{2}\right)^n + n\sum_{i,j=0}^{N} P_{i,j} i^m j^{n-1} = N^{m+n}. \tag{3.8}$$

That is, the constraints (3.8) on the matrices Q and P and the accuracy constraints on the $\boldsymbol{D}$ and $\boldsymbol{G}$ are independent.

The constraints (3.8) imply that if the approximations $\boldsymbol{D}$ and $\boldsymbol{G}$ are fourth-order accurate then, it is impossible to satisfy (1.7) if Q and P are essentially identity matrices, that is, if Q and P are both diagonal with all but some fixed (with respect to the grid size) number of elements not equal to 1. We proved this fact by assuming Q and P had this form and then using computer algebra to show that not all the conditions could be simultaneously satisfied. This fact is also true for the sixth-order $\boldsymbol{D}$ and $\boldsymbol{G}$ operators.

Because there are no fourth- or sixth-order compatible $\boldsymbol{D}$ and $\boldsymbol{G}$ that are both local operators and satisfy the integration by parts identity (1.7), we first derive local $\boldsymbol{D}$ and $\boldsymbol{G}$ operators satisfying (1.8) and relax the condition that they simultaneously satisfy (1.7). These $\boldsymbol{D}$ and $\boldsymbol{G}$ will satisfy the integration by part formula (1.7) to fourth- and sixth-order of accuracy, respectively. We now look independently at the constraints on the Q and P matrices, the higher-order divergence, and the high-order gradient.

3.1. The divergence

Requiring that the discrete gradient is exact when $f \equiv 1$, that is, $\boldsymbol{G}1 = 0$, reduces the summation by parts formula (3.3) to

$$\langle Q\boldsymbol{D}v, 1\rangle = v_n - v_0. \tag{3.9}$$

This implies that

$$\langle \boldsymbol{D}v, Q^{\mathrm{T}}1\rangle = v_n - v_0. \tag{3.10}$$

If we define the column sums of Q, by

$$\overline{Q}_{i+1/2} = \sum_{j=0}^{N-1} Q_{j+1/2,i+1/2}, \tag{3.11}$$

then

$$\langle \boldsymbol{D}v, \overline{Q}\rangle = v_n - v_0. \tag{3.12}$$

The second-order operator $\boldsymbol{D}$ (2.1) satisfies this condition as does the standard fourth-order approximation

$$(\boldsymbol{D}f)_{i+1/2} = \frac{1}{24h}(f_{i-1} - 27f_i + 27f_{i+1} - f_{i+2}), \tag{3.13}$$

except for the terms near the boundary.

To define a special local boundary formula to be used with this method, by symmetry we only need to consider the upper-left corner of the matrix for the divergence,

$$\boldsymbol{D} = \left(\begin{matrix} a_{11} & a_{12} & a_{13} & a_{14} & a_{15} & a_{16} & a_{17} & a_{18} & \dots \\ a_{21} & a_{22} & a_{23} & a_{24} & a_{25} & a_{26} & a_{27} & a_{28} & \dots \\ a_{31} & a_{32} & a_{33} & a_{34} & a_{35} & a_{36} & a_{37} & a_{38} & \dots \\ a_{41} & a_{42} & a_{43} & a_{44} & a_{45} & a_{46} & a_{47} & a_{48} & \dots \\ a_{51} & a_{52} & a_{53} & a_{54} & a_{55} & a_{56} & a_{57} & a_{58} & \dots \\ 0 & 0 & 0 & 0 & \frac{1}{24} & -\frac{27}{24} & \frac{27}{24} & -\frac{1}{24} & \dots \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{24} & -\frac{27}{24} & \frac{27}{24} & \dots \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{24} & -\frac{27}{24} & \dots \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{24} & \dots \end{matrix}\right. . \tag{3.14}$$

When we display only the upper-left corner of a matrix, we leave off the trailing bracket to make this clear. We settled on modifying the FDM at the first five points after trying a number of examples and finding that with this setup we can find divergences with parameters that can be used to try to satisfy additional conditions.

The following lemma will be helpful in the computations.

Lemma. *Let $d_{i+1/2,j}$, $0 \leqslant i \leqslant N-1$, $0 \leqslant j \leqslant N$, be the matrix defining a divergence and $\overline{Q}_{i+1/2}$, $0 \leqslant i \leqslant N-1$, be the column sums of the weight matrix. Then*

$$\langle \boldsymbol{D}v, 1\rangle = \sum_{j=0}^{N} c_j v_j, \tag{3.15}$$

where

$$c_j = \sum_{i=0}^{N-1} \overline{Q}_{i+1/2} d_{i+1/2,j}, \quad 0 \leqslant j \leqslant N. \tag{3.16}$$

Therefore a fourth-order discrete divergence operator satisfies (3.3) *with* $f \equiv 1$ *provided that* $c_0 = -1$, $c_N = 1$ *and* $c_j = 0$, $1 \leqslant j \leqslant N-1$.

We have shown by direct computation that there are no fourth-order accurate divergences given as above with $\overline{Q} \equiv 1$. On the other hand, there are uniformly fourth-order accurate divergences with non-trivial $\overline{Q}$:

$$\overline{Q}_{1/2} = \tfrac{649}{576}, \qquad \overline{Q}_{3/2} = \tfrac{143}{192}, \qquad \overline{Q}_{5/2} = \tfrac{75}{64}, \qquad \overline{Q}_{7/2} = \tfrac{551}{576}, \qquad \overline{Q}_{9/2} = 1, \qquad \ldots. \tag{3.17}$$

The inner product with these weights is exact for quadratic polynomials and is a fifth-order approximation of the continuous inner product. The formulas are similar to Gregory's boundary corrected trapezoid formulas in [4]. That is, (3.17) is a fifth-order quadrature formula. Using a computer algebra system, we find a three-parameter family of uniformly fourth-order accurate discrete divergence operators,

$$\boldsymbol{D} = \begin{pmatrix} a_{11} & a_{12} & a_{13} & a_{14} & a_{15} & a_{16} & 0 \\ \frac{1}{24}-\alpha & -\frac{27}{24}+5\alpha & \frac{27}{24}-10\alpha & -\frac{1}{24}+10\alpha & -5\alpha & \alpha & 0 \\ -\beta & \frac{1}{24}+5\beta & -\frac{27}{24}-10\beta & \frac{27}{24}+10\beta & -\frac{1}{24}-5\beta & \beta & 0 \\ -\frac{1}{24}-\gamma & \frac{5}{24}+5\gamma & -\frac{3}{8}-10\gamma & -\frac{17}{24}+10\gamma & \frac{11}{12}-5\gamma & \gamma & 0 \\ 0 & 0 & 0 & \frac{1}{24} & -\frac{27}{24} & \frac{27}{24} & -\frac{1}{24} \\ 0 & 0 & 0 & 0 & \frac{1}{24} & -\frac{27}{24} & \frac{27}{24} \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{24} & -\frac{27}{24} \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{24} \end{pmatrix}, \tag{3.18}$$

where

$$\begin{aligned} a_{11} &= -\tfrac{6851}{7788} + \tfrac{39}{59}\alpha + \tfrac{675}{649}\beta + \tfrac{551}{649}\gamma, \\ a_{12} &= \tfrac{8153}{15576} - \tfrac{195}{59}\alpha - \tfrac{3375}{649}\beta - \tfrac{2755}{649}\gamma, \\ a_{13} &= \tfrac{3867}{5192} + \tfrac{390}{59}\alpha + \tfrac{6750}{649}\beta + \tfrac{5510}{649}\gamma, \\ a_{14} &= -\tfrac{9005}{15576} - \tfrac{390}{59}\alpha - \tfrac{6750}{649}\beta - \tfrac{5510}{649}\gamma, \\ a_{15} &= \tfrac{3529}{15576} + \tfrac{195}{59}\alpha + \tfrac{3375}{649}\beta + \tfrac{2755}{649}\gamma, \\ a_{16} &= -\tfrac{24}{649} - \tfrac{39}{59}\alpha - \tfrac{675}{649}\beta - \tfrac{551}{649}\gamma. \end{aligned} \tag{3.19}$$

The special case where the FDM only changes at the boundary is given by $\alpha = 0$, $\beta = \frac{1}{24}$, $\gamma = -\frac{1}{24}$:

$$\boldsymbol{D} = \begin{pmatrix} -\frac{4751}{5192} & \frac{909}{1298} & \frac{6091}{15576} & -\frac{1165}{5192} & \frac{129}{2596} & -\frac{25}{15576} & 0 & 0 \\ \frac{1}{24} & -\frac{27}{24} & \frac{27}{24} & -\frac{1}{24} & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{24} & -\frac{27}{24} & \frac{27}{24} & -\frac{1}{24} & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{24} & -\frac{27}{24} & \frac{27}{24} & -\frac{1}{24} & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{24} & -\frac{27}{24} & \frac{27}{24} & -\frac{1}{24} & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{24} & -\frac{27}{24} & \frac{27}{24} & -\frac{1}{24} \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{24} & -\frac{27}{24} & \frac{27}{24} \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{24} & -\frac{27}{24} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{24} \end{pmatrix}. \tag{3.20}$$

In Appendix A we put this divergence into two more symmetric forms.

3.2. Sixth-order divergence

In Appendix B we give a 10 parameter family of sixth-order divergences. Here we only show the first two rows of the matrix of a divergence where the formula for this divergence is the usual sixth-order approximation of the derivative except for the boundary and first interior point:

$$\begin{matrix} -\frac{1077397}{1273920} & \frac{15668474643803}{32472850116480} & \frac{49955527}{39491520} & -\frac{25369793}{19745760} & \frac{12220145}{15796608} & -\frac{21334421}{78983040} & \frac{460217}{9872880} & -\frac{101017}{39491520} & \frac{3369}{26327680} \\ \frac{31}{960} & -\frac{687}{640} & \frac{129}{128} & \frac{19}{192} & -\frac{3}{32} & \frac{21}{640} & -\frac{3}{640} & 0 & 0 \end{matrix} \tag{3.21}$$

The corresponding Q weights are

$$\frac{41137}{34560}, \quad \frac{15667}{34560}, \quad \frac{2933}{1728}, \quad \frac{2131}{4320}, \quad \frac{41411}{34560}, \quad \frac{33437}{34560}, \quad 1, \quad \ldots. \tag{3.22}$$

3.3. The gradient

Using the exactness when $v \equiv 1$ of the discrete divergence, $\boldsymbol{D}1 = 0$, the summation by parts formula (3.3) reduces to

$$\langle 1, \boldsymbol{P}\boldsymbol{G} f \rangle = f_n - f_0, \tag{3.23}$$

or equivalently,

$$\left\langle \boldsymbol{P}^{\mathrm{T}} 1, \boldsymbol{G} f \right\rangle = f_n - f_0. \tag{3.24}$$

If we define the column sums of $\boldsymbol{P}$ as

$$\overline{P}_i = \sum_{j=0}^{N-1} P_{j,i}, \tag{3.25}$$

then

$$\left\langle \boldsymbol{G} f, \overline{\boldsymbol{P}} \right\rangle = f_n - f_0. \tag{3.26}$$

The operator $\boldsymbol{G}$ given in (2.2) satisfies this condition and is a second-order gradient in the interior with first-order truncation error at the boundary. As for the divergence, we first try for gradients that are a standard fourth-order approximation away from the boundary and local special formulas near the boundaries. The standard fourth-order approximation is

$$(\boldsymbol{G}f)_i = \frac{1}{h}\left(\frac{1}{24}f_{i-3/2} - \frac{27}{24}f_{i-1/2} + \frac{27}{24}f_{i+1/2} - \frac{1}{24}f_{i+3/2}\right). \tag{3.27}$$

As for the divergence, the following will be helpful in doing the computations.

Lemma. *Let $g_{i,0}$, $g_{i,j+1/2}$, $g_{i,N}$, $0 \leqslant i \leqslant N$, $0 \leqslant j \leqslant N-1$, be the matrix defining a gradient and $\overline{P}_i$, $0 \leqslant i \leqslant N$, be the column sums of the weight matrix. Then*

$$\langle P\boldsymbol{G}f, 1\rangle = c_0 f_0 + \sum_{j=0}^{N-1} c_{j+1/2} f_{j+1/2} + c_N f_N, \tag{3.28}$$

where

$$c_j = \sum_{i=0}^{N-1} \overline{P}_i g_{i,j+1/2}, \quad 0 \leqslant j \leqslant N-1. \tag{3.29}$$

The weights are again independent of the particulars of the gradient:

$$\overline{P}_0 = \tfrac{407}{1152}, \qquad \overline{P}_1 = \tfrac{473}{384}, \qquad \overline{P}_2 = \tfrac{343}{384}, \qquad \overline{P}_3 = \tfrac{1177}{1152}, \qquad \overline{P}_3 = 1, \qquad \ldots \tag{3.30}$$

and the resulting discrete inner product is a fifth-order approximation of the continuous inner product. A three-parameter family of uniformly fourth-order accurate gradients is:

$$\boldsymbol{G} = \begin{pmatrix} a_{11} & a_{12} & a_{13} & a_{14} & a_{15} & 0 & 0 \\ \frac{16}{105} - \alpha\frac{128}{35} & -\frac{31}{24} + \alpha 9 & \frac{29}{24} - \alpha 12 & -\frac{3}{40} + \alpha\frac{54}{5} & \frac{1}{168} - \alpha\frac{36}{7} & \alpha & 0 \\ -\beta\frac{128}{35} & \frac{1}{24} + \beta 9 & -\frac{27}{24} - \beta 12 & \frac{27}{24} + \beta\frac{54}{5} & -\frac{1}{24} - \beta\frac{36}{7} & \beta & 0 \\ -\frac{16}{105} - \gamma\frac{128}{35} & \frac{3}{8} + \gamma 9 & -\frac{11}{24} - \gamma 12 & -\frac{27}{40} + \gamma\frac{54}{5} & \frac{51}{56} - \gamma\frac{36}{7} & \gamma & 0 \\ 0 & 0 & 0 & \frac{1}{24} & -\frac{27}{24} & \frac{27}{24} & -\frac{1}{24} \end{pmatrix}, \tag{3.31}$$

where

$$\begin{aligned} a_{11} &= -\tfrac{124832}{42735} + \alpha\tfrac{16512}{1295} + \beta\tfrac{18816}{2035} + \gamma\tfrac{13696}{1295}, \\ a_{12} &= \tfrac{10789}{3256} - \alpha\tfrac{1161}{37} - \beta\tfrac{9261}{407} - \gamma\tfrac{963}{37}, \\ a_{13} &= -\tfrac{421}{9768} + \alpha\tfrac{1548}{37} + \beta\tfrac{12348}{407} + \gamma\tfrac{1284}{37}, \\ a_{14} &= -\tfrac{12189}{16280} - \alpha\tfrac{6966}{185} - \beta\tfrac{55566}{2035} - \gamma\tfrac{5778}{185}, \\ a_{15} &= \tfrac{11789}{22792} + \alpha\tfrac{4644}{259} + \beta\tfrac{5292}{407} + \gamma\tfrac{3852}{259}, \\ a_{16} &= -\tfrac{48}{407} - \alpha\tfrac{129}{37} - \beta\tfrac{1029}{407} - \gamma\tfrac{107}{37}. \end{aligned}$$

The choice $\alpha = \frac{1}{24}$, $\beta = 0$, $\gamma = -\frac{1}{24}$ gives

$$G = \begin{pmatrix} -\frac{1152}{407} & \frac{10063}{3256} & \frac{2483}{9768} & -\frac{3309}{3256} & \frac{2099}{3256} & -\frac{697}{4884} \\ 0 & -\frac{11}{12} & \frac{17}{24} & \frac{3}{8} & -\frac{5}{24} & \frac{1}{24} \\ 0 & \frac{1}{24} & -\frac{27}{24} & \frac{27}{24} & -\frac{1}{24} & 0 \end{pmatrix}, \tag{3.32}$$

and results in a gradient that is only modified at the first interior point.

3.4. *Sixth-order gradient*

In Appendix C we give a 10 parameter family of sixth-order gradients. Here we only show the first three rows of the matrix of a gradient where the formula for this gradient is the usual sixth-order approximation of the derivative except for the boundary and first two interior points:

$$\begin{matrix} -\frac{568557184}{150834915} & \frac{455704609}{83579520} & -\frac{128942179}{41789760} & \frac{15911389}{6964960} & -\frac{142924471}{117011328} & \frac{20331719}{50147712} & -\frac{2688571}{38307280} & \frac{187529}{41789760} & -\frac{6207}{27859840} \\ \frac{496}{3465} & -\frac{811}{640} & \frac{449}{384} & -\frac{29}{960} & -\frac{11}{448} & \frac{13}{1152} & -\frac{37}{21120} & 0 & 0 \\ -\frac{8}{385} & \frac{179}{1920} & -\frac{153}{128} & \frac{381}{320} & -\frac{101}{1344} & \frac{1}{128} & -\frac{3}{7040} & 0 & 0 \end{matrix} \tag{3.33}$$

Again, we only present the rows that are not the same as the usual sixth-order approximation of the derivative. The corresponding P weights are

$$\frac{43531}{138240}, \quad \frac{192937}{138240}, \quad \frac{42647}{69120}, \quad \frac{86473}{69120}, \quad \frac{125303}{138240}, \quad \frac{140309}{138240}, \quad 1, \quad \ldots. \tag{3.34}$$

4. Conclusions and discussion

We derive conservative fourth- and sixth-order finite difference approximations for the divergence and gradient operators and a compatible inner product on staggered 1D uniform grids in a bounded domain. The methods use standard centered difference formulas in the interior with a new one-sided finite difference approximation at the boundary. We derive a compatible inner product for these difference methods, that is, a fifth- and seventh-order approximations, respectively, of the continuum inner product. Our discrete operators satisfy the integration by parts identity (3.3) up to fourth- and sixth-order, respectively.

Our ultimate goal is to define compatible high-order divergence and gradient finite difference operators that satisfy a discrete integration by parts identity (3.3) exactly. Let us note that we have made some substantial but unsuccessful attempts to solve this problem using the general divergence (3.18) and general gradient (3.31). The amount of algebra in this general setting simply overwhelms computer algebra systems. We now list some of the fourth-order cases that we tried that assume special forms for the matrices Q and P in (3.1).

Case 1. No solution. The matrices Q and P have general six-by-six blocks in the upper left (and lower right) corners and are otherwise the identity. Also in the divergence

$$\alpha = 0, \qquad \beta = \frac{1}{24}, \qquad \gamma = -\frac{1}{24}, \tag{4.1}$$

and in the gradient

$$\alpha = \tfrac{1}{24}, \qquad \beta = 0, \qquad \gamma = -\tfrac{1}{24}. \tag{4.2}$$

This choice sets all but the first entries of the first column of the divergence and gradient to zero.

Case 2. No solution. The matrices Q and P are diagonal with diagonal given by the weights (3.22) and (3.34) discussed above, while the divergence is given by the ten-parameter family given in (B.1) and gradient is given by by the ten-parameter family given in (C.1).

Let us note that discrete operators for nodal discretizations in 1D that satisfy summation by part formula have been constructed in [1,12,14,18]. It gives us hope that this also can be done on staggered grids.

Appendix A. Special forms for the divergence

For the fourth-order accurate divergence, it is easy to see that the matrix for the operator $Q\boldsymbol{D}v + v_0$ has a matrix with column sums zero and then that this implies that

$$Q\boldsymbol{D} + v_0 = \frac{1}{h}\delta A v, \tag{A.1}$$

where δ is the simple difference operator, A is an $N+1$ by $N+1$ matrix with upper left corner given by:

$$\begin{aligned}
&A_{1,1} = \tfrac{61}{6912} + \tfrac{143}{192}\alpha + \tfrac{75}{64}\beta + \tfrac{551}{576}\gamma, \qquad A_{1,2} = \tfrac{8153}{13824} - \tfrac{715}{192}\alpha - \tfrac{375}{64}\beta - \tfrac{2755}{576}\gamma,\\
&A_{1,3} = \tfrac{1289}{1536} + \tfrac{715}{96}\alpha + \tfrac{375}{32}\beta + \tfrac{2755}{288}\gamma, \qquad A_{1,4} = -\tfrac{9005}{13824} - \tfrac{715}{96}\alpha - \tfrac{375}{32}\beta - \tfrac{2755}{288}\gamma,\\
&A_{1,5} = \tfrac{3529}{13824} + \tfrac{715}{192}\alpha + \tfrac{375}{64}\beta + \tfrac{2755}{576}\gamma, \qquad A_{1,6} = -\tfrac{1}{24} - \tfrac{143}{192}\alpha - \tfrac{75}{64}\beta - \tfrac{551}{576}\gamma, \qquad A_{1,7} = 0,\\
&A_{2,1} = \tfrac{551}{13824} + \tfrac{75}{64}\beta + \tfrac{551}{576}\gamma, \qquad A_{2,2} = -\tfrac{1715}{6912} - \tfrac{375}{64}\beta - \tfrac{2755}{576}\gamma,\\
&A_{2,3} = \tfrac{161}{96} + \tfrac{375}{32}\beta + \tfrac{2755}{288}\gamma, \qquad A_{2,4} = -\tfrac{4717}{6912} + \tfrac{375}{32}\beta + \tfrac{2755}{288}\gamma,\\
&A_{2,5} = \tfrac{3529}{13824} + \tfrac{375}{64}\beta + \tfrac{2755}{576}\gamma, \qquad A_{2,6} = -\tfrac{1}{24} - \tfrac{75}{64}\beta - \tfrac{551}{576}\gamma, \qquad A_{2,7} = 0,\\
&A_{3,1} = \tfrac{551}{13824} + \tfrac{551}{576}\gamma, \qquad A_{3,2} = -\tfrac{2755}{13824} - \tfrac{2755}{576}\gamma, \qquad A_{3,3} = \tfrac{551}{1536} + \tfrac{2755}{288}\gamma,\\
&A_{3,4} = \tfrac{8791}{13824} - \tfrac{2755}{288}\gamma, \qquad A_{3,5} = \tfrac{1427}{6912} + \tfrac{2755}{576}\gamma, \qquad A_{3,6} = -\tfrac{1}{24} - \tfrac{551}{576}\gamma, \qquad A_{3,7} = 0,\\
&A_{4,1} = A_{4,2} = A_{4,3} = 0, \qquad A_{4,4} = -\tfrac{1}{24}, \qquad A_{4,5} = \tfrac{13}{12}, \qquad A_{4,6} = -\tfrac{1}{24}, \qquad A_{4,7} = 0,\\
&A_{5,1} = A_{5,2} = A_{5,3} = A_{5,4} = 0, \qquad A_{5,5} = -\tfrac{1}{24}, \qquad A_{5,6} = \tfrac{13}{12}, \qquad A_{5,7} = -\tfrac{1}{24}.
\end{aligned} \tag{A.2}$$

Also, because the row sums of $\boldsymbol{D}$ are zero it is possible to write

$$\boldsymbol{D} = \frac{1}{h}B\delta, \tag{A.3}$$

where again δ is the simple difference and

$$B = \begin{pmatrix} a_{11} & a_{12} & a_{13} & a_{14} & a_{15} & 0 \\ -\frac{1}{24}+\alpha & \frac{13}{12}-4\alpha & -\frac{1}{24}+6\alpha & -4\alpha & \alpha & 0 \\ \beta & -\frac{1}{24}-4\beta & \frac{13}{12}+6\beta & -\frac{1}{24}-4\beta & \beta & 0 \\ \frac{1}{24}+\gamma & -\frac{1}{6}-4\gamma & \frac{5}{24}+6\gamma & \frac{11}{12}-4\gamma & \gamma & 0 \\ 0 & 0 & 0 & -\frac{1}{24} & \frac{13}{12} & -\frac{1}{24} \end{pmatrix}, \tag{A.4}$$

where

$$\begin{aligned} a_{11} &= \tfrac{6851}{7788} - \tfrac{39}{59}\alpha - \tfrac{675}{649}\beta - \tfrac{551}{649}\gamma, \\ a_{12} &= \tfrac{5549}{15576} + \tfrac{156}{59}\alpha + \tfrac{2700}{649}\beta + \tfrac{2204}{649}\gamma, \\ a_{13} &= -\tfrac{1513}{3894} - \tfrac{234}{59}\alpha - \tfrac{4050}{649}\beta - \tfrac{3306}{649}\gamma, \\ a_{14} &= \tfrac{2953}{15576} + \tfrac{156}{59}\alpha + \tfrac{2700}{649}\beta + \tfrac{2204}{649}\gamma, \\ a_{15} &= -\tfrac{24}{649} - \tfrac{39}{59}\alpha - \tfrac{675}{649}\beta - \tfrac{551}{649}\gamma. \end{aligned} \tag{A.5}$$

Appendix B. Sixth-order divergence

We have found a ten-parameter family of sixth-order divergences with the following structure:

$$\boldsymbol{D} = \begin{pmatrix} d_{11} & d_{12} & d_{13} & d_{14} & d_{15} & d_{16} & d_{17} & d_{18} & d_{19} & 0 & 0 \\ d_{21} & d_{22} & d_{23} & d_{24} & d_{25} & d_{26} & d_{27} & d_{28} & d_{29} & 0 & 0 \\ d_{31} & d_{32} & d_{33} & d_{34} & d_{35} & d_{36} & d_{37} & d_{38} & d_{39} & 0 & 0 \\ d_{41} & d_{42} & d_{43} & d_{44} & d_{45} & d_{46} & d_{47} & d_{48} & d_{49} & 0 & 0 \\ d_{51} & d_{52} & d_{53} & d_{54} & d_{55} & d_{56} & d_{57} & d_{58} & d_{59} & 0 & 0 \\ d_{61} & d_{62} & d_{63} & d_{64} & d_{65} & d_{66} & d_{67} & d_{68} & d_{69} & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{9}{1920} & \frac{125}{1920} & -\frac{2250}{1920} & \frac{2250}{1920} & -\frac{125}{1920} & \frac{9}{1920} & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{9}{1920} & \frac{125}{1920} & -\frac{2250}{1920} & \frac{2250}{1920} & -\frac{125}{1920} & \frac{9}{1920} \end{pmatrix}, \tag{B.1}$$

where

$$\begin{aligned} d_{11} &= -\tfrac{65098219}{78983040} + \tfrac{34560}{41137}s_1 + \tfrac{241920}{41137}s_2 + \tfrac{34560}{41137}s_3 + \tfrac{241920}{41137}s_4 + \tfrac{241920}{41137}s_6 + \tfrac{34560}{41137}s_5 + \tfrac{34560}{41137}s_7 \\ &\quad + \tfrac{241920}{41137}s_8 + \tfrac{34560}{41137}s_9 + \tfrac{241920}{41137}s_{10}, \\ d_{12} &= \tfrac{4302307}{26327680} - \tfrac{241920}{41137}s_1 - \tfrac{1658880}{41137}s_2 - \tfrac{241920}{41137}s_3 - \tfrac{1658880}{41137}s_4 - \tfrac{1658880}{41137}s_6 - \tfrac{241920}{41137}s_5 - \tfrac{241920}{41137}s_7 \\ &\quad - \tfrac{1658880}{41137}s_8 - \tfrac{241920}{41137}s_9 - \tfrac{1658880}{41137}s_{10}, \\ d_{13} &= \tfrac{3443147}{1974576} + \tfrac{725760}{41137}s_1 + \tfrac{4838400}{41137}s_2 + \tfrac{725760}{41137}s_3 + \tfrac{4838400}{41137}s_4 + \tfrac{4838400}{41137}s_6 + \tfrac{725760}{41137}s_5 + \tfrac{725760}{41137}s_7 \\ &\quad + \tfrac{4838400}{41137}s_8 + \tfrac{725760}{41137}s_9 + \tfrac{4838400}{41137}s_{10}, \\ d_{14} &= -\tfrac{16731259}{7898304} - \tfrac{1209600}{41137}s_1 - \tfrac{7741440}{41137}s_2 - \tfrac{1209600}{41137}s_3 - \tfrac{7741440}{41137}s_4 - \tfrac{7741440}{41137}s_6 - \tfrac{1209600}{41137}s_5 - \tfrac{1209600}{41137}s_7 \\ &\quad - \tfrac{7741440}{41137}s_8 - \tfrac{1209600}{41137}s_9 - \tfrac{7741440}{41137}s_{10}, \end{aligned}$$

$$\begin{aligned}
d_{15} &= \tfrac{282037}{169856} + \tfrac{1209600}{41137}s_1 + \tfrac{7257600}{41137}s_2 + \tfrac{1209600}{41137}s_3 + \tfrac{7257600}{41137}s_4 + \tfrac{7257600}{41137}s_6 + \tfrac{1209600}{41137}s_5 + \tfrac{1209600}{41137}s_7 \\
&\quad + \tfrac{7257600}{41137}s_8 + \tfrac{1209600}{41137}s_9 + \tfrac{7257600}{41137}s_{10}, \\
d_{16} &= -\tfrac{67575371}{78983040} - \tfrac{725760}{41137}s_1 - \tfrac{3870720}{41137}s_2 - \tfrac{725760}{41137}s_3 - \tfrac{3870720}{41137}s_4 - \tfrac{3870720}{41137}s_6 - \tfrac{725760}{41137}s_5 - \tfrac{725760}{41137}s_7 \\
&\quad - \tfrac{3870720}{41137}s_8 - \tfrac{725760}{41137}s_9 - \tfrac{3870720}{41137}s_{10}, \\
d_{17} &= \tfrac{10952047}{39491520} + \tfrac{241920}{41137}s_1 + \tfrac{967680}{41137}s_2 + \tfrac{241920}{41137}s_3 + \tfrac{967680}{41137}s_4 + \tfrac{241920}{41137}s_5 + \tfrac{967680}{41137}s_6 + \tfrac{241920}{41137}s_7 \\
&\quad + \tfrac{967680}{41137}s_8 + \tfrac{241920}{41137}s_9 + \tfrac{967680}{41137}s_{10}, \\
d_{18} &= -\tfrac{34560}{41137}s_1 - \tfrac{34560}{41137}s_3 - \tfrac{34560}{41137}s_5 - \tfrac{34560}{41137}s_7 - \tfrac{34560}{41137}s_9 - \tfrac{2088}{41137}, \\
d_{19} &= -\tfrac{34560}{41137}s_2 - \tfrac{34560}{41137}s_4 - \tfrac{34560}{41137}s_6 - \tfrac{34560}{41137}s_8 - \tfrac{34560}{41137}s_{10} + \tfrac{162}{41137},
\end{aligned}$$

$$\begin{aligned}
d_{21} &= -\tfrac{34560}{15667}s_1 - \tfrac{241920}{15667}s_2 + \tfrac{31}{960}, \qquad d_{22} = \tfrac{241920}{15667}s_1 + \tfrac{1658880}{15667}s_2 - \tfrac{687}{640}, \\
d_{23} &= -\tfrac{725760}{15667}s_1 - \tfrac{4838400}{15667}s_2 + \tfrac{129}{128}, \qquad d_{24} = \tfrac{1209600}{15667}s_1 + \tfrac{7741440}{15667}s_2 + \tfrac{19}{192}, \\
d_{25} &= -\tfrac{1209600}{15667}s_1 - \tfrac{7257600}{15667}s_2 - \tfrac{3}{32}, \qquad d_{26} = \tfrac{725760}{15667}s_1 + \tfrac{3870720}{15667}s_2 + \tfrac{21}{640}, \\
d_{27} &= -\tfrac{241920}{15667}s_1 - \tfrac{967680}{15667}s_2 - \tfrac{3}{640}, \qquad d_{28} = \tfrac{34560}{15667}s_1, \qquad d_{29} = \tfrac{34560}{15667}s_2,
\end{aligned}$$

$$\begin{aligned}
d_{31} &= -\tfrac{1728}{2933}s_3 - \tfrac{1728}{419}s_4 - \tfrac{3}{640}, \qquad d_{32} = \tfrac{1728}{419}s_3 + \tfrac{82944}{2933}s_4 + \tfrac{25}{384}, \\
d_{33} &= -\tfrac{5184}{419}s_3 - \tfrac{34560}{419}s_4 - \tfrac{75}{64}, \qquad d_{34} = \tfrac{8640}{419}s_3 + \tfrac{55296}{419}s_4 + \tfrac{75}{64}, \\
d_{35} &= -\tfrac{8640}{419}s_3 - \tfrac{51840}{419}s_4 - \tfrac{25}{384}, \qquad d_{36} = \tfrac{5184}{419}s_3 + \tfrac{27648}{419}s_4 + \tfrac{3}{640}, \\
d_{37} &= -\tfrac{1728}{419}s_3 - \tfrac{6912}{419}s_4, \qquad d_{38} = \tfrac{1728}{2933}s_3, \qquad d_{39} = \tfrac{1728}{2933}s_4,
\end{aligned}$$

$$\begin{aligned}
d_{41} &= -\tfrac{4320}{2131}s_5 - \tfrac{30240}{2131}s_6, \qquad d_{42} = \tfrac{30240}{2131}s_5 + \tfrac{207360}{2131}s_6 - \tfrac{3}{640}, \\
d_{43} &= -\tfrac{90720}{2131}s_5 - \tfrac{604800}{2131}s_6 + \tfrac{25}{384}, \qquad d_{44} = -\tfrac{75}{64} + \tfrac{151200}{2131}s_5 + \tfrac{967680}{2131}s_6, \\
d_{45} &= -\tfrac{151200}{2131}s_5 - \tfrac{907200}{2131}s_6 + \tfrac{75}{64}, \qquad d_{46} = \tfrac{90720}{2131}s_5 + \tfrac{483840}{2131}s_6 - \tfrac{25}{384}, \\
d_{47} &= -\tfrac{30240}{2131}s_5 - \tfrac{120960}{2131}s_6 + \tfrac{3}{640}, \qquad d_{48} = \tfrac{4320}{2131}s_5, \qquad d_{49} = \tfrac{4320}{2131}s_6,
\end{aligned}$$

$$\begin{aligned}
d_{51} &= \tfrac{3}{640} - \tfrac{34560}{41411}s_7 - \tfrac{241920}{41411}s_8, \qquad d_{52} = -\tfrac{21}{640} + \tfrac{241920}{41411}s_7 + \tfrac{1658880}{41411}s_8, \\
d_{53} &= \tfrac{3}{32} - \tfrac{725760}{41411}s_7 - \tfrac{4838400}{41411}s_8, \qquad d_{54} = -\tfrac{19}{192} + \tfrac{1209600}{41411}s_7 + \tfrac{7741440}{41411}s_8, \\
d_{55} &= -\tfrac{7257600}{41411}s_8 - \tfrac{1209600}{41411}s_7 - \tfrac{129}{128}, \qquad d_{56} = \tfrac{3870720}{41411}s_8 + \tfrac{725760}{41411}s_7 + \tfrac{687}{640}, \\
d_{57} &= -\tfrac{241920}{41411}s_7 - \tfrac{967680}{41411}s_8 - \tfrac{31}{960}, \qquad d_{58} = \tfrac{34560}{41411}s_7, \qquad d_{59} = \tfrac{34560}{41411}s_8,
\end{aligned}$$

$$\begin{aligned}
d_{61} &= -\tfrac{31}{960} - \tfrac{34560}{33437}s_9 - \tfrac{241920}{33437}s_{10}, \qquad d_{62} = \tfrac{443}{1920} + \tfrac{241920}{33437}s_9 + \tfrac{1658880}{33437}s_{10}, \\
d_{63} &= -\tfrac{91}{128} - \tfrac{725760}{33437}s_9 - \tfrac{4838400}{33437}s_{10}, \qquad d_{64} = \tfrac{235}{192} + \tfrac{1209600}{33437}s_9 + \tfrac{7741440}{33437}s_{10}, \\
d_{65} &= -\tfrac{59}{48} - \tfrac{1209600}{33437}s_9 - \tfrac{7257600}{33437}s_{10}, \qquad d_{66} = -\tfrac{211}{640} + \tfrac{725760}{33437}s_9 + \tfrac{3870720}{33437}s_{10}, \\
d_{67} &= \tfrac{1627}{1920} - \tfrac{241920}{33437}s_9 - \tfrac{967680}{33437}s_{10}, \qquad d_{68} = \tfrac{34560}{33437}s_9, \qquad d_{69} = \tfrac{34560}{33437}s_{10}.
\end{aligned}$$

The weights are given in Section 3.2.

Appendix C. Sixth-order gradient

Here is a ten-parameter family of sixth-order gradients:

$$\boldsymbol{G}=\begin{pmatrix} g_{11} & g_{12} & g_{13} & g_{14} & g_{15} & g_{16} & g_{17} & g_{18} & g_{19} & 0 & 0\\ g_{21} & g_{22} & g_{23} & g_{24} & g_{25} & g_{26} & g_{27} & g_{28} & g_{29} & 0 & 0\\ g_{31} & g_{32} & g_{33} & g_{34} & g_{35} & g_{36} & g_{37} & g_{38} & g_{39} & 0 & 0\\ g_{41} & g_{42} & g_{43} & g_{44} & g_{45} & g_{46} & g_{47} & g_{48} & g_{49} & 0 & 0\\ g_{51} & g_{52} & g_{53} & g_{54} & g_{55} & g_{56} & g_{57} & g_{58} & g_{59} & 0 & 0\\ g_{61} & g_{62} & g_{63} & g_{64} & g_{65} & g_{66} & g_{67} & g_{68} & g_{69} & 0 & 0\\ 0 & 0 & 0 & 0 & -\frac{9}{1920} & \frac{125}{1920} & -\frac{2250}{1920} & \frac{2250}{1920} & -\frac{125}{1920} & \frac{9}{1920} & 0\\ 0 & 0 & 0 & 0 & 0 & -\frac{9}{1920} & \frac{125}{1920} & -\frac{2250}{1920} & \frac{2250}{1920} & -\frac{125}{1920} & \frac{9}{1920} \end{pmatrix}, \tag{C.1}$$

where

$$\begin{aligned}
g_{11} &= -\frac{501295888}{178259445}+\frac{47185920}{3351887}s_1+\frac{47185920}{478841}s_2+\frac{47185920}{3351887}s_3+\frac{47185920}{478841}s_4-\frac{2359296}{6224933}s_5+\frac{82575360}{6224933}s_6\\
&\quad+\frac{47185920}{3351887}s_7+\frac{47185920}{478841}s_8+\frac{47185920}{3351887}s_9+\frac{47185920}{478841}s_{10},\\
g_{12} &= \frac{7327275}{2785984}-\frac{1797120}{43531}s_1-\frac{12441600}{43531}s_2-\frac{1797120}{43531}s_3-\frac{12441600}{43531}s_4+\frac{48384}{43531}s_5-\frac{1555200}{43531}s_6\\
&\quad-\frac{1797120}{43531}s_7-\frac{12441600}{43531}s_8-\frac{1797120}{43531}s_9-\frac{12441600}{43531}s_{10},\\
g_{13} &= \frac{14680151}{5571968}+\frac{3594240}{43531}s_1+\frac{24192000}{43531}s_2+\frac{3594240}{43531}s_3+\frac{24192000}{43531}s_4-\frac{96768}{43531}s_5+\frac{2419200}{43531}s_6\\
&\quad+\frac{3594240}{43531}s_7+\frac{24192000}{43531}s_8+\frac{3594240}{43531}s_9+\frac{24192000}{43531}s_{10},\\
g_{14} &= -\frac{179817489}{27859840}-\frac{5391360}{43531}s_1-\frac{34836480}{43531}s_2-\frac{5391360}{43531}s_3-\frac{34836480}{43531}s_4+\frac{145152}{43531}s_5-\frac{2177280}{43531}s_6\\
&\quad-\frac{5391360}{43531}s_7-\frac{34836480}{43531}s_8-\frac{5391360}{43531}s_9-\frac{34836480}{43531}s_{10},\\
g_{15} &= \frac{142907685}{19501888}+\frac{35942400}{304717}s_1+\frac{31104000}{43531}s_2+\frac{35942400}{304717}s_3\\
&\quad+\frac{31104000}{43531}s_4-\frac{138240}{43531}s_5+\frac{35942400}{304717}s_7+\frac{31104000}{43531}s_8\\
&\quad+\frac{35942400}{304717}s_9+\frac{31104000}{43531}s_{10},\\
g_{16} &= -\frac{596065}{124128}-\frac{2995200}{43531}s_1-\frac{16128000}{43531}s_2-\frac{2995200}{43531}s_3-\frac{16128000}{43531}s_4+\frac{80640}{43531}s_5+\frac{2016000}{43531}s_6\\
&\quad-\frac{2995200}{43531}s_7-\frac{16128000}{43531}s_8-\frac{2995200}{43531}s_9-\frac{16128000}{43531}s_{10},\\
g_{17} &= \frac{9908595}{5571968}+\frac{10782720}{478841}s_1+\frac{43545600}{478841}s_2+\frac{10782720}{478841}s_3+\frac{43545600}{478841}s_4-\frac{290304}{478841}s_5-\frac{21772800}{478841}s_6\\
&\quad+\frac{10782720}{478841}s_7+\frac{43545600}{478841}s_8+\frac{10782720}{478841}s_9+\frac{43545600}{478841}s_{10},\\
g_{18} &= -\frac{22977393}{72435584}-\frac{138240}{43531}s_1-\frac{138240}{43531}s_3+\frac{48384}{565903}s_5+\frac{10886400}{565903}s_6-\frac{138240}{43531}s_7-\frac{138240}{43531}s_9,\\
g_{19} &= \frac{648}{43531}-\frac{138240}{43531}s_2-\frac{138240}{43531}s_4-\frac{138240}{43531}s_6-\frac{138240}{43531}s_8-\frac{138240}{43531}s_{10},
\end{aligned}$$

$$\begin{aligned}
g_{21} &= \frac{496}{3465}-\frac{47185920}{14856149}s_1-\frac{47185920}{2122307}s_2, \qquad g_{22}=-\frac{811}{640}+\frac{1797120}{192937}s_1+\frac{12441600}{192937}s_2,\\
g_{23} &= \frac{449}{384}-\frac{3594240}{192937}s_1-\frac{24192000}{192937}s_2, \qquad g_{24}=-\frac{29}{960}+\frac{5391360}{192937}s_1+\frac{34836480}{192937}s_2,\\
g_{25} &= -\frac{11}{448}-\frac{35942400}{1350559}s_1-\frac{31104000}{192937}s_2, \qquad g_{26}=\frac{13}{1152}+\frac{2995200}{192937}s_1+\frac{16128000}{192937}s_2,\\
g_{27} &= -\frac{37}{21120}-\frac{10782720}{2122307}s_1-\frac{43545600}{2122307}s_2, \qquad g_{28}=\frac{138240}{192937}s_1, \qquad g_{29}=\frac{138240}{192937}s_2,
\end{aligned} \tag{C.2}$$

$$g_{31} = -\frac{8}{385} - \frac{23592960}{3283819}s_3 - \frac{23592960}{469117}s_4, \qquad g_{32} = \frac{179}{1920} + \frac{898560}{42647}s_3 + \frac{6220800}{42647}s_4,$$
$$g_{33} = -\frac{153}{128} - \frac{1797120}{42647}s_3 - \frac{12096000}{42647}s_4, \qquad g_{34} = \frac{381}{320} + \frac{2695680}{42647}s_3 + \frac{17418240}{42647}s_4,$$
$$g_{35} = -\frac{101}{1344} - \frac{17971200}{298529}s_3 - \frac{15552000}{42647}s_4, \qquad g_{36} = \frac{1}{128} + \frac{1497600}{42647}s_3 + \frac{8064000}{42647}s_4,$$
$$g_{37} = -\frac{3}{7040} - \frac{5391360}{469117}s_3 - \frac{21772800}{469117}s_4, \qquad g_{38} = \frac{69120}{42647}s_3, \qquad g_{39} = \frac{69120}{42647}s_4,$$

$$g_{41} = -\frac{20}{143} + \frac{1179648}{12365639}s_5 - \frac{41287680}{12365639}s_6, \qquad g_{42} = \frac{519}{1280} - \frac{24192}{86473}s_5 + \frac{777600}{86473}s_6,$$
$$g_{43} = -\frac{145}{192} + \frac{48384}{86473}s_5 - \frac{1209600}{86473}s_6, \qquad g_{44} = \frac{15}{256} - \frac{72576}{86473}s_5 + \frac{1088640}{86473}s_6,$$
$$g_{45} = \frac{69120}{86473}s_5, \qquad g_{46} = \frac{475}{768} - \frac{40320}{86473}s_5 - \frac{1008000}{86473}s_6,$$
$$g_{47} = -\frac{771}{3520} + \frac{145152}{951203}s_5 + \frac{10886400}{951203}s_6, \qquad g_{48} = \frac{105}{3328} - \frac{24192}{1124149}s_5 - \frac{5443200}{1124149}s_6, \qquad g_{49} = \frac{69120}{86473}s_6,$$

$$g_{51} = \frac{8}{385} - \frac{47185920}{9648331}s_7 - \frac{47185920}{1378333}s_8, \qquad g_{52} = -\frac{39}{640} + \frac{1797120}{125303}s_7 + \frac{12441600}{125303}s_8,$$
$$g_{53} = \frac{15}{128} - \frac{3594240}{125303}s_7 - \frac{24192000}{125303}s_8, \qquad g_{54} = -\frac{113}{960} + \frac{5391360}{125303}s_7 + \frac{34836480}{125303}s_8,$$
$$g_{55} = -\frac{447}{448} - \frac{35942400}{877121}s_7 - \frac{31104000}{125303}s_8, \qquad g_{56} = \frac{137}{128} + \frac{2995200}{125303}s_7 + \frac{16128000}{125303}s_8,$$
$$g_{57} = -\frac{673}{21120} - \frac{10782720}{1378333}s_7 - \frac{43545600}{1378333}s_8, \qquad g_{58} = \frac{138240}{125303}s_7, \qquad g_{59} = \frac{138240}{125303}s_8,$$

$$g_{61} = -\frac{496}{3465} - \frac{47185920}{10803793}s_9 - \frac{47185920}{1543399}s_{10}, \qquad g_{62} = \frac{163}{384} + \frac{138240}{10793}s_9 + \frac{12441600}{140309}s_{10},$$
$$g_{63} = -\frac{335}{384} - \frac{276480}{10793}s_9 - \frac{24192000}{140309}s_{10}, \qquad g_{64} = \frac{433}{320} + \frac{414720}{10793}s_9 + \frac{34836480}{140309}s_{10},$$
$$g_{65} = -\frac{1745}{1344} - \frac{2764800}{75551}s_9 - \frac{31104000}{140309}s_{10}, \qquad g_{66} = -\frac{355}{1152} + \frac{230400}{10793}s_9 + \frac{16128000}{140309}s_{10},$$
$$g_{67} = \frac{1189}{1408} - \frac{829440}{118723}s_9 - \frac{43545600}{1543399}s_{10}, \qquad g_{68} = \frac{138240}{140309}s_9, \qquad g_{69} = \frac{138240}{140309}s_{10}.$$

The weights are given in Section 3.4.

References

[1] M.H. Carpenter, D. Gottlieb, S. Abarbanel, Time-stable boundary conditions for finite difference solving hyperbolic systems: Methodology and applications to high-order compact schemes, J. Comput. Phys. 111 (1994) 220–236.

[2] J.E. Castillo, J.M. Hyman, M.J. Shashkov, S. Steinberg, The sensitivity and accuracy of fourth order finite-difference schemes on non-uniform grids in one dimension, Comput. Math. Appl. 30 (8) (1995) 41–55.

[3] J.E. Castillo, J.M. Hyman, M.J. Shashkov, S. Steinberg, High-order mimetic finite-difference schemes on non-uniform grids, ICOSAHOM '95; Houston J. Math. (1996).

[4] R.W. Hamming, Numerical Methods for Scientists and Engineers, 2nd Edition, McGraw-Hill, New York, 1973.

[5] J.M. Hyman, R.J. Knapp, J.C. Scovel, High order finite volume approximations of differential operators on nonuniform grids, Phys. D 60 (1992) 112–138.

[6] J.M. Hyman, M. Shashkov, Natural discretizations for the divergence, gradient, and curl on logically rectangular grids, Internat. J. Comput. Math. Appl. 33 (1997) 81–104.

[7] J.M. Hyman, M. Shashkov, The adjoint operators for the natural discretizations for the divergence, gradient, and curl on logically rectangular grids, IMACS J. Appl. Numer. Math. 25 (1997) 413–442.

[8] J.M. Hyman, M. Shashkov, The approximation of boundary conditions for mimetic finite difference methods, Internat. J. Comput. Math. Appl. 36 (1998) 79–99.

[9] J.M. Hyman, M. Shashkov, The orthogonal decomposition theorems for mimetic finite difference methods, SIAM J. Numer. Anal. 36 (1999) 788–818.
[10] J.M. Hyman, M. Shashkov, Mimetic discretizations for Maxwell's equations, J. Comput. Phys., in press.
[11] J.M. Hyman, M. Shashkov, S. Steinberg, The numerical solution of diffusion problems in strongly heterogeneous non-isotropic materials, J. Comput. Phys. 132 (1997) 130–148.
[12] H.-O. Kreiss, G. Scherer, Finite element and finite difference methods for hyperbolic partial differential equations, in: C. De Boor (Ed.), Mathematical Aspects of Finite Elements in Partial Differential Equations, 1974, pp. 195–212.
[13] S.K. Lele, Compact finite-difference schemes with spectral-like resolution, J. Comput. Phys. 103 (1) (1992) 16–42.
[14] P. Olsson, Summation by parts, projections, and stability I, Math. Comp. 64 (211) (1995) 1035–1065.
[15] M. Shashkov, Conservative Finite-Difference Methods on General Grids, CRC Press, Boca Raton, FL, 1995.
[16] M. Shashkov, S. Steinberg, Support-operator finite-difference algorithms for general elliptic problems, J. Comput. Phys. 118 (1995) 131–151.
[17] M. Shashkov, S. Steinberg, Solving diffusion equations with rough coefficients in rough grids, J. Comput. Phys. 129 (1996) 383–405.
[18] B. Strand, Summation by parts for finite difference approximations for $\mathrm{d}/\mathrm{d}x$, J. Comput. Phys. 110 (1994) 47–67.