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Development of arbitrary-order multioperators-based schemes for parallel calculations. Part 2: Families of compact approximations with two-diagonal inversions and related multioperators

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Abstract

One-parameter families of compact approximations to grid functionals with inverses of two-point operators and their properties are described. As particular examples, interpolation/extrapolations operators, quadratures formulas and approximations to derivatives are presented. Using operators from the families with fixed parameters values as basis operators, their linear combinations providing formally arbitrary-order approximations (multioperators) are constructed. Numerical illustrations are presented. Special emphasis is placed on first derivatives discretizations in the context of conservation laws. As an example, a highly accurate tenth-order scheme is outlined and tested against the Burgers' equation. It is shown how extrapolation multioperators can be used to create boundary closures.

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1. Introduction

The multioperators idea proposed previously by the author [1] is aimed at construction formally arbitrary-order approximation to any grid functional (midpoint values, integrals, derivatives at nodes etc.). It cardinally differs from the standard way of enlarging stencils to get higher orders formulas. Operators of conventional approximations may be viewed as summation over stencils with some coefficients . In contrast, multioperators may be viewed as sums of basis operators with some coefficients, the basis operators being formed by setting

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distinct values to parameters in one-parameter operators families. Increase of multioperators orders can be achieved by simply increasing numbers of basis operators, that is, by increasing numbers of the parameter values. Supposing that the number of the parameters and hence the number of the basis operators is M, the orders are linear functions in M. Since M is an arbitrary number, multioperators actions on grid functions may be viewed as arbitrary-order approximations.

To calculate multioperators actions, it is sufficient to calculate the actions of each basis operator, multiply the results by known coefficients and perform summation of the multiplied values. Since the basis operators differ only in the parameters values, the calculations can be carried out in a parallel and synchronous manner when using parallel machines with at least M processors. In the case of negligible times of data exchange processes, the CPU times for multioperators are equal to those for the corresponding basis operators. Assuming that speedup is the ratio of the CPU times needed to calculate multioperators actions in the case of single processor and multiprocessors machines, the "idealized" speedup is equal to M. It should be emphasized that this type of speedup concerns only multioperators actions rather than parallelism of calculations in the framework of final algorithms. Thus multioperators parallelism can be combined with other ways of parallelization of multioperators-based methods (for example, parallel calculations for spatial coordinates, using domain decomposition principle etc.).

Clearly, the multioperators concept is quite general. It can be applied to various problem in various forms. However since approximation order is not unique property of efficient algorithms, additional studies concerning other properties of the multioperators in particular cases are needed. For example, stability of the resulting schemes and accurate representation of small scales may be viewed as important properties in the context of CFD calculations.

In the previous papers [3–6], the methodology was applied to fluid dynamics equations, one-parameter family of Compact Upwind Differencing (CUD) operators from [2] being used as basis operators. The companion paper [8] reflects the recent results in this area presenting remarkably accurate high resolution conservative ninth-order multioperators approximations to convection-type terms based on the fifth-order CUD. However, other types of multioperators (for example, central ones with artificially introduced free parameters) were also considered [7]. The brief outlines of the multioperators activity can be found in [8].

In the above cited papers, compact approximations are understood as those with narrow stencils containing no more than three nodes thus justifying the label "compact". Such types of operators allow one to use three-diagonal inversions and to calculate actions of the involved explicit operators at the internal grid points of bounded domains without using values outside the domains or changing their forms near boundaries. At present, it is clear that any approximation with one-parameter inverse operators (that is, a compact approximation in a broad sense) has potential for generating basis operators, the parameter being either "natural" (as in the CUD case) or artificially introduced.

In the present paper, the further results in the multioperators area are presented. They concern with novel one-parameter families of compact approximation to grid functionals as a source of basis operators. The families were briefly outlined in short paper [9]. The approximations can be viewed as rational functions of two-point and three-point operators and are in line with the previous strategy of using narrow stencils only.

Inversions of two-point operators with *fixed numerical constants* is the well known procedure which can be used as a part of calculations related to compact approximations to derivatives. In particular, the implicit part of the earliest third-order CUD operators [2] reduces to two-point operators for particular values of the involved parameter. Compact approximations with two-point inverse operators were considered also in [10]. In contrast, the below described families *depend on a free parameter* thus allowing one to construct multioperators. Moreover they concern with various types of grid functionals, the derivatives at grid points being a particular example.

In some instances, the operators families can be used to increase orders of standard formulas. However, their more important property seems to be their ability to provide basis operators for novel types of multioperators characterized by very small operation counts per node and by possibly negligible influence of boundary conditions for two-diagonal operators inversions. Their obvious extensions we are not presently interested in are rational functions of two-point and more-than-three-point operators.

The rest of the paper consist of the description of the families and their properties (Section 2) and the resulting multioperators (Section 3). Due to the corresponding numerous possibilities and options, the paper is aimed at outlining main ideas rather then at presenting sufficiently documented algorithms. Thus numerical illustrations of Section 3 may be viewed only as simple examples showing possible performance of the multi-operators technique.

2. One-parametric families of compact approximations with two-diagonal inversions

2.1. Definitions and properties

2.1.1. Using inverses of two-point operators

Supposing that a uniform mesh $\omega_h = (x_j = jh, j = 0, \pm 1, \pm 2, \dots)$ with a constant mesh size h is introduced, we denote by Δ_0 and Δ_2 the central three-point operators given by

$$\Delta_0 = T_1 - T_{-1}, \quad \Delta_2 = T_1 - 2I + T_{-1}, \quad T_{\pm 1} v_j = v_{j\pm 1}.$$

where I is the identity operator. Consider now the "left" and "right" grid operators defined respectively by

$$N_l(c) = (I + c(I - T_{-1}))^{-1} \quad N_r(c) = (I + c(I - T_1))^{-1},$$

where c is supposed to be a non-zero free parameter.

The actions $w_j = N_k u_j, k = l, r$ of N_l and N_r on known grid functions u_j, $j = 1, 2, \dots, n-1$ in the case of bounded domains $x_0 \leqslant x \leqslant x_n$ can be calculated using the following procedures.

$$\begin{aligned} & w_j = \alpha w_{j-1} + u_j/(1+c), \ w_0 \quad \text{is given}, \ j = 1, 2, \dots n-1 \\ & w_j = \alpha w_{j+1} + u_j/(1+c), \ w_n \quad \text{is given}, \quad j = n-1, \ n-2, \dots, 1 \\ & \alpha = c/(1+c), \quad c \neq 0. \end{aligned} \tag{1}$$

The sweeps are stable if $-0.5 < c$. However it is advantageous to use the parameter satisfying $| c | \ll 1$. In that case, the impact of the initial values u_0 and u_n on the values u_k and u_{n-k} decays very rapidly (as $O(c^k)$)) with increasing the distances kh from the boundaries.

Let $U_h(\omega_h)$ be the Hilbert space of grid functions $u_h = (u_j, j = 0, \pm 1, \pm 2, \dots)$ with summable squares. Introducing the inner product as $(u_h, v_h) = h\sum_{j=-\infty}^{\infty} u_j v_j$, $u_h, v_h \in U_h$, it is easy to see that Δ_2 and Δ_0 are self-adjoint and skew-symmetric operators $U_h \to U_h$ respectively. It means that $(\Delta_2 u_h, v_h) = (u_h, \Delta_2 v_h)$ or $\Delta_2 = \Delta_2^*$ and $(\Delta_0 u_h, v_h) = -(u_h, \Delta_0 v_h)$ or $\Delta_0 = -\Delta_0^*$, $u_h, v_h \in U_h$. Operators inequalities for linear operators like $A_h \geqslant B_h$ will be used below meaning that $(A_h u_h, u_h) \geqslant (B_h u_h, u_h)$, $u_h \in U_h$. In particular, one has $\Delta_2 < 0$ and $-\Delta_2 \leqslant 4I$. Skipping the outlines of the underlying theory, the commuting property of all grid operators introduced in the rest of the paper was used to perform algebraic manipulations considering them as variables.

In the terms of Δ_0 and Δ_2 operators, the inverses of N_l and N_r can be cast in the form

$$N_l^{-1} = I + c(\Delta_0 - \Delta_2)/2, \quad N_r^{-1} = I - c(\Delta_0 + \Delta_2)/2. \tag{2}$$

Denoting by upper indexes "(0)" and "(1)" self-adjoint and skew-symmetric components of operators, one can see that

$$(N_l^{-1})^{(0)} = (N_r^{-1})^{(0)} = I - c/2\Delta_2 > 0 \quad \text{for } c > -.5 \quad \text{and} \quad (N_l^{-1})^{(1)} = -(N_r^{-1})^{(1)} = c/2\Delta_0,$$

the positivity of the self-adjoint components being due to the operators inequality $-\Delta_2 \leqslant 4I$.

Thus $N_r^{-1} = (N_l^{-1})^*$. The same properties of the N_l and N_r operators can be presented in the form of the following:

Theorem 1. *Let $c > -0.5$. Then*

$$N_l^{(0)} = N_r^{(0)} > 0, \ N_l^{(1)} = -N_r^{(1)}$$

and therefore $N_r = N_l^*$.

Proof. We note first that

$$G = N_l N_l^* = N_r N_r^* = ((I - c\Delta_2/2)^2 - c^2 \Delta_0^2/4)^{-1}, \quad G^* = G > 0.$$

Using the equality $(N_l^{-1})^* = (N_l^*)^{-1}$ and the same equality for the N_r operator, one can write

$$N_l = (N_l N_l^*)(N_l^{-1})^*, \quad N_r = (N_r N_r^*)(N_r^{-1})^*.$$

Taking into account Eq. (2), one obtains $N_l = G((N_l^{-1})^{(0)} - (N_l^{-1})^{(1)})$ and $N_r = G((N_l^{-1})^{(0)} + (N_l^{-1})^{(1)})$ which proves the formulation of the theorem. □

2.1.2. Approximations to grid functionals

Consider $[Lu]_j$, the action of a linear operator L associated with a node j on a function $u(x) \in U$ of the continuous argument x (the notation [.] is used to define the projection operator $U \to U_h$). For example, $[Lu]_j$ can be viewed as integrals with respect to x between the limits in a vicinity of x_j, as values for shifted arguments $u(x_j + kh)$ with a fixed parameter k, as derivatives at x_j etc.. In the following it will be always supposed that U is a space of functions which are as smooth as needed for the relevant reasoning.

Following the strategy of using three-point stencils only, suppose that the functional is approximated by three-point formula which general form can be written as $[Lu]_j \approx L_h u_j = (aI + d\Delta_0 + e\Delta_2)u_j$ with constants a, d, e.

In [8], one-parameter families of the Compact Upwind Differencing (CUD) operators from [2] were considered as multiplicative and additive corrections to three-point differencing operator $\Delta(s) = (\Delta_0 - s\Delta_2)/2$. Following the similar representation, it is possible to construct compact approximations which can be viewed as additive and multiplicative corrections to L_h. They can be written as "left" and "right" operators $L_l(c)$ and $L_r(c)$ of the forms

$$L_l(c) = L_{h,l} + N_l(c)(a_l\Delta_0 + b_l\Delta_2), \quad L_r(c) = L_{h,r} + N_r(c)(a_r\Delta_0 + b_r\Delta_2), \tag{3}$$

or

$$\widetilde{L}_l(c) = N_l(c)(L_{h,l} + \tilde{a}_l\Delta_0 + \tilde{b}_l\Delta_2), \quad \widetilde{L}_r(c) = N_r(c)(L_{h,r} + \tilde{a}_r\Delta_0 + \tilde{b}_r\Delta_2), \tag{4}$$

where $a_l, b_l, a_r, b_r, \tilde{a}_l, \tilde{b}_l, \tilde{a}_r, \tilde{b}_r$ are parameters generally depending on c. It is assumed here that different three-point formulas $L_{h,l}$ and $L_{h,r}$ can serve as L_h used to approximate $[Lu]_j$. The parameters in (3) and (4)are supposed to be obtained by maximizing the approximation orders of the left and right operators. It can be accomplished by setting zero as many terms in the Taylor expansion series for the operators actions on sufficiently smooth functions as possible. The multiplicative corrections (4) can be written simply as $N_l L_{h,l}$ and $N_r L_{h,r}$. However, the form (4) is introduced to emphasize the possibility of using standard numerical analysis formulas for $L_{h,l}$ and $L_{h,r}$ with added second-order terms to maximize the resulting orders.

The operators from one-parameter families defined by (3), (4) should not be confused with widely used compact approximations with fixed numerical coefficients requiring two-diagonal inversions. For example, the third-order approximation to first derivatives (CUD-3) investigated in depth in [2] looks as

$$\left(I + \frac{1}{6}\Delta_0 - \frac{s}{4}\Delta_2\right)^{-1}\Delta(s)/h,$$

its early version with $|s| = 1$ being dated back to seventies [2]. The three-diagonal inverse operator can be reduced to two-diagonal one simply by setting $|s| = 2/3$ thus removing the free parameter. Two-diagonal inversions were used also in [10] as well as in other publications. That type of compact approximations corresponds to the particular case of derivatives discretizations using multiplicative corrections Eq. (4) with the particular value $c = 1/3$.

The merits of the above approximations follow from the inversion procedures equations (1). They are very small operation count per node and one-sided boundary conditions with negligible impact on calculated nodal values outside near-boundary regions in the case of $|c| \ll 1$. Moreover in some instances there is a possibility of further increasing the orders of (3), (4). It can be achieved by using the products $N_l(c)N_l(\bar{c})$ and $N_r(c)N_r(\bar{c})$ instead of $N_l(c)$ and $N_r(c)$ where $\bar{c}$ is another parameter. The orders can be increased if there exists a real function $\bar{c} = \phi(c)$ annihilating the next term in the expansion series for (3), (4). The resulting operators may be referred to as "double left" and "double right" ones. Examples of that option will be presented below. However, only left and right operators will be considered in the present paper in the context of the resulting multioperators.

Before presenting particular examples of left and right operators, it is worth examining their general properties. First of all supposing that the parameters with the "l" indexes are found, their counterparts with the "r" indexes can be determined using the following considerations based on the conjugate properties of the involved operators.

Let $L_{h,r} = L^*_{h,l}$. Then $L^*_l = L_{h,r} + N_r(-a_l\Delta_0 + b_l\Delta_2)$ and it is natural to set $a_r = -a_l$ and $b_r = b_l$ thus obtaining $L_r = L^*_l$. If $L_{h,r} = -L^*_{h,l}$ then $L_r = -L^*_l$ with $a_r = a_l$ and $b_r = -b_l$. First derivatives approximations fit neatly in the latter case while those for interpolation/extrapolation operators, for integrals etc. correspond to the former one.

More information can be obtained by considering the Tailor expansion series for the actions of the operators on $[u]_j, u \in U$ where $u(x)$ is a sufficiently smooth function. In the following it will be always assumed that U is a space of functions which are as smooth as needed for the relevant considerations.

Starting with the multiplicative corrections, Eqs. (4) can be rewritten as products of N_l, N_r and three-point operators. Thus

$$\widetilde{L}_l = N_l(q_0 I + q_1\Delta_0 + q_2\Delta_2)$$

where coefficients q_0, q_1, q_2 are supposed to be determined from the condition of annihilation of the low order truncation error terms.

For the sake of convenience, we introduce the following symbolic representation of functions with shifted arguments:

$$u(x+kh) = \sum_{l=0}^{\infty} \frac{(kh)^l}{l!} u_x^{(l)}(x) = \mathrm{e}^{kZ}u(x)$$

where $u^{(0)}(x) = u(x)$ and the operator Z is defined by $Z = h(\mathrm{d}/\mathrm{d}x)$. In the above expansion, $u(x)$ is considered as an analytic function otherwise it is supposed that the expansion is truncated with adding the corresponding remainder.

Considering formally Z as a variable and setting $x = x_j$, one can write

$$\widetilde{L}_l(c) = \frac{q_0\,\mathrm{e}^{-Z} + q_1 + q_2\,\mathrm{e}^{Z}}{1 + c(1-\mathrm{e}^{-Z})} = F(Z).$$

Expanding $F(Z)$ near $Z = 0$, one obtains

$$F(Z) = \sum_{l=0}^{\infty} \tilde{p}_l(c)Z^l \tag{5}$$

where $\tilde{p}_l(c), l = 0, 1, 2, \ldots$, as can be shown, are l-degree polynomials in c. Suppose now that the expansion for the target functional looks as

$$[Lu]_j = (g_0 + g_1 Z + g_2 Z^2 + g_3 Z^3 + g_4 Z^4 + \ldots)[u]_j.$$

For example, the only non-zero coefficient is $g_1 = 1/h$ in the case of $[Lu]_j = (\mathrm{d}u/\mathrm{d}x)_{x=x_j} = Z/h$. The coefficients q_0, q_1, q_2 can be found now from a linear system obtained by equating to zero low-order terms in the expansion for the truncation error $[Lu]_j - \widetilde{L}_l(c)[u]_j$. It gives

$$\widetilde{L}_l(c)[u]_j = [Lu]_j + \left(\frac{1}{6}(g_1 + 3c(g1 - g2))Z^3 + \sum_{l=2}^{\infty} \bar{p}_l(c)Z^{l+2}\right)[u]_j$$

where $\bar{p}_l(c)$ are l-degree polynomials in c.

In the case of additive corrections operators L_l , similar considerations lead to a linear system for the coefficients providing $\mathrm{O}(Z^4)$ truncation errors. However, the coefficients satisfying the maximum orders conditions are not linearly independent. In fact it can be shown the systems are solvable if the coefficients q_1 and q_2 are related through

$$q_2 = q_1 + \frac{1+3c}{6c}g_1 - g_2 - \frac{1}{3}g_3$$

Thus a lot of correction terms can be introduced satisfying the maximum order conditions. They provide a unique expression for the L_l operator. It looks as

$$L_l(c)[u]_j = [Lu]_j + \left(\frac{1}{12}(12g_4 + 6(1+2c)g_3 - g_2 - (1+2c)g_1)Z^4 + \sum_{l=2}^{\infty} p_l(c)Z^{l+3}\right)[u]_j.$$

Concerning the right operators $\widetilde{L}_r(c)$ and $L_r(c)$, the above described conjugate properties suggest that the expansions for their actions differ from those for the left operators only in signs of either odd or even powers of Z. The latter case corresponds to first derivatives approximations. In fact, the expansions can be obtained by substituting $-Z$ instead of Z in Eq. (5) or in the similar representation of the L_l operator. Then, for example, one has either $\widetilde{L}_r = F(-Z)$ or $\widetilde{L}_r = -F(-Z)$. The relation between the expansions is illustrated below by presenting two terms in the truncation errors for particular examples. Due to the relation, it is advantageous in some instances to use either sums or differences of left and right operators. When doing so, one can increase approximation orders in specific cases. Moreover, the resulting expansion series contain either odd or even powers of Z which can be beneficial when constructing multioperators.

Considering various types of grid functionals, it is well to bear in mind that $\mathrm{O}(Z^3)$ and $\mathrm{O}(Z^4)$ truncation errors are not necessarily $\mathrm{O}(h^3)$ and $\mathrm{O}(h^4)$ ones since the coefficients of initial formulas may contain powers of h. For example, the coefficient g_1 is proportional to h^{-1} in the case of first derivatives.

2.2. Application to typical grid functionals

Using the general representations (3), (4), it is possible to construct one-parameter compact approximations to various grid functionals. Below we restrict ourselves to presenting several examples. They do not cover all possible options and serve merely as illustrations of the approach. The main attention will be paid to the approximations which can be used for constructing schemes for PDE's. Though they can be viewed as a novel class of numerical formulas, we consider them primarily as an important source of basis operators for creating high-order multioperators.

2.2.1. Midpoint interpolation

In some instances, one needs to calculate grid functions defined on the grid $\bar{\omega}_h = \{x_{j+1/2} = (j+1/2)h,\ h = \mathrm{const}, j = 0, \mp 1, \mp 2, \ldots\}$ using those defined on ω_h. We consider as an example additive corrections to the "left" and "right" approximations

$$u(x_{j+1/2}) \approx (3u(x_j) - u(x_{j-1}))/2, \quad u(x_{j-1/2}) \approx (3u(x_j) - u(x_{j+1}))/2.$$

Adding the correction terms with N_l and N_r operators with the coefficients a_l, b_l, a_r, b_r chosen to get the highest approximation orders, one can arrive at the following left and right midpoint operators denoted here by M_l and M_r respectively.

$$\begin{aligned} M_l &= (3I/2 - T_{-1}/2) + (3/8 - 1/16c)\Delta_2 + N_l\Delta_2/16c, \\ M_r &= (3I/2 - T_1/2) + (3/8 - 1/16c)\Delta_2 + N_r\Delta_2/16c. \end{aligned} \tag{6}$$

It can be shown that they are forth-order accurate, the first three terms of the Taylor expansion series being

$$\begin{aligned} M_l[u]_j &= u(x_{j+1/2}) + \frac{5+8c}{128}h^4u_j^{(4)} - \frac{3+16c+16c^2}{256}h^5u_j^{(5)} + \mathrm{O}(h^6), \\ M_r[u]_j &= u(x_{j-1/2}) + \frac{5+8c}{128}h^4u_j^{(4)} + \frac{3+16c+16c^2}{256}h^5u_j^{(5)} + \mathrm{O}(h^6), \quad u_j^{(k)} = [u_x^{(k)}]_j. \end{aligned} \tag{7}$$

It is worth noting that the expansions (7) hold even if $c = 0$ though the value is not allowed due to the inequality $c \neq 0$ in Eq. (1).

Taking into account the equalities $N_r = N_l^*$ and $T_1 = T_{-1}^*$, one can deduce from (6) that $M_r = M_l^*$. It explains why the terms with the fifth-order derivatives in Eqs. (7) have opposite signs.

2.2.2. Approximations to shift operators

Extrapolation operators are often needed to create boundary closures for difference schemes. Consider simple extrapolation formulas

$$u(x_{j+2}) \approx 2u(x_{j+1}) - u(x_j), \quad u(x_{j-2}) \approx 2u(x_{j-1}) - u(x_j).$$

Performing additive corrections, one can get the following forth-order compact approximations denoted by E_l and E_r.

$$E_l = 2T_1 - I + (1 + 1/c)\Delta_2 - N_l\Delta_2/c \quad E_r = 2T_{-1} - I + (1 + 1/c)\Delta_2 - N_r\Delta_2/c.$$

The operators are related through $E_r = E_l^*$ and the corresponding Taylor expansion series read

$$\begin{aligned} E_l[u]_j &= u(x_{j+2}) - (1 + c)h^4u_j^{(4)} + (c + c^2)h^5u_j^{(5)} + \mathrm{O}(h^6), \\ E_r[u]_j &= u(x_{j-2}) - (1 + c)h^4u_j^{(4)} - (c + c^2)h^5u_j^{(5)} + \mathrm{O}(h^6). \end{aligned} \tag{8}$$

The fifth-order extrapolation formulas can be obtained by using the double left and the double right operators. The modified extrapolation operators are given by

$$\begin{aligned} \overline{E}_l &= 2T_1 - I + (1 + 1/(c + \bar{c}))\Delta_2 - N_l(c)N_l(\bar{c})\Delta_2/(c + \bar{c}), \\ \overline{E}_r &= 2T_{-1} - I + (1 + 1/(c + \bar{c}))\Delta_2 - N_r(c)N_r(\bar{c})\Delta_2/(c + \bar{c}). \end{aligned}$$

The $\overline{E}_l$ and $\overline{E}_r$ operators reduce to E_l and E_r for $\bar{c} = 0$. Setting $\bar{c} = \sqrt{(}1 - 2c - 3c^2) - 1 - c$, one obtains the following leading term of the truncation errors for both operators

$$\frac{2c^2(1 + c)}{1 - c - \sqrt{1 - 2c - 3c^2}}h^5u_j^{(5)}$$

where it is assumed that $c \leqslant 1/3$.

Small values of $|\, c \,|$ allow one to obtain the fourth- or fifth-order accurate boundary values of extrapolated grid functions which are practically independent of starting values at the corresponding opposite boundaries.

2.2.3. Compact quadrature formulas

Considering integrals over x between limits in the vicinity of x_j (for example, $\int_{x_j}^{x_{j+1}} u(\xi)\,\mathrm{d}\xi$, $\int_{x_{j-1/2}}^{x_{j+1/2}u(\xi)\mathrm{d}\xi}$, $\int_{x_{j-1}}^{x_j} u(\xi)\mathrm{d}\xi$), the corresponding compact approximations can be constructed in the form of corrections to the standard two- or three-point operators. Though the resulting order can be higher than that of standard formulas, there is no point to viewing them as alternatives to powerful high-order numerical integration tools like the Simpson and Gauss rules. However, they can serve as basis operators in the case of extremely high-order multioperators approximations.

Correcting, for example, the trapezoid rule for $[x_{j-1}, x_j]$, one can obtain the left operator

$$Q_l = \frac{1}{2}(I + T_{-1}) - \frac{1}{12}N_l\Delta_2$$

for which

$$Q_l(c)[u]_j = \frac{1}{h}\int_{x_{j-1}}^{x_j} u(\xi)\mathrm{d}\xi - \frac{1}{24}(1 + 2c)h^3u_j^{(3)} + \frac{1}{360}(2 + 15c - 30c^2)h^4u_j^{(4)} + \mathrm{O}(h^5).$$

Similarly, the expansion series for the right operator

$$Q_l = \frac{1}{2}(I + T_1) - \frac{1}{12}N_r\Delta_2$$

looks as

$$Q_r(c)[u]_j = \frac{1}{h}\int_{x_j}^{x_{j+1}} u(\xi)\mathrm{d}\xi + \frac{1}{24}(1 + 2c)h^3u_j^{(3)} + \frac{1}{360}(2 + 15c - 30c^2)h^4u_j^{(4)} + \mathrm{O}(h^5).$$

In the above example, the additive correction increases approximation order of the trapezoid rule. In the context of multioperators, it makes sense to consider also compact approximations which order is less than that of an initial formula. As another example, consider the following multiplicative correction to the modified Simpson rule.

$$Q_{1,l} = N_l\left(\frac{1}{3}(4I + T_1 + T_{-1}) - c(\Delta_0 - \Delta_2)\right),\ Q_{1,r} = N_r\left(\frac{1}{3}(4I + T_1 + T_{-1}) - c(\Delta_0 + \Delta_2)\right).$$

It gives in the case of the left operator

$$Q_{1,l}(c)[u]_j = \frac{1}{h}\int_{x_{j-1}}^{x_{j+1}} u(\xi)\mathrm{d}\xi - \frac{1}{3}ch^3u_j^{(3)} + \frac{1}{90}(1 + 15c + 30c^2)h^4u_j^{(4)} + \mathrm{O}(h^5). \tag{9}$$

Thus the approximation order of the Simpson rule is not increased. It can be increased however when using additive corrections with the double left and double right operators.

$$\overline{Q}_{1,l} = \frac{1}{3}(4I + T_1 + T_{-1}) + \Delta_2 - N_l(c)N_l(\bar{c})\Delta_2$$
$$Q_{1,r} = N_r\left(\frac{1}{3}(4I + T_1 + T_{-1}) + \Delta_2\right) - N_r(c)N_r(\bar{c})\Delta_2.$$

Setting $\overline{Q} = (\overline{Q}_{1,l} + \overline{Q}_{1,r})/2$ and

$$\bar{c} = \frac{1}{60}\left(\sqrt{5}\sqrt{53 - 180c - 540c^2} - 30c - 15\right),$$

with $c < c_* \approx .188$ one obtains

$$\overline{Q}(c)[u]_j = \frac{1}{h}\int_{x_{j-1}}^{x_{j+1}} u(\xi)\mathrm{d}\xi + h^6\varphi_6(c)u_j^{(6)} + h^8\varphi_8(c)u_j^{(8)} + \mathrm{O}(h^{10})$$

where the lengthy expressions for $\varphi_6(c)$ and $\varphi_8(c)$ are not presented here. One can see that the $\overline{Q}$ operator is the sixth-order accurate one. Besides, its expansion series contain only even order powers of h.

2.3. Approximations to convection-type terms

2.3.1. Approximation to first derivatives

As in the case of CUD operators from [2], we consider three-point operator $\Delta(s) = (\Delta_0 - s\Delta_2)/2$ with a free parameter s as a generic operator L_h. It is advantageous to use the additive correction approach (3) to obtain third-order differencing formulas. Adding the correction terms with $N_l(c)$ and $N_r(c)$ operators and following the above described procedure, one arrives at the expressions for the left and right differencing operators D_l and D_r given by

$$D_l = \frac{1}{2}\left(\Delta_0 - \frac{1}{3c}\Delta_2\right) + \frac{1}{6c}N_l\Delta_2, \quad D_r = \frac{1}{2}\left(\Delta_0 + \frac{1}{3c}\Delta_2\right) - \frac{1}{6c}N_r\Delta_2.$$

The corresponding Taylor expansion series read

$$\begin{aligned} D_l[u]_j/h &= [u_x]_j + \left(\frac{1}{12} + \frac{c}{6}\right)h^3u_j^{(4)} - \left(\frac{1}{30} + \frac{c}{6} + \frac{c^2}{6}\right)h^4u_j^{(5)} + \mathrm{O}(h^5) \\ D_r[u]_j/h &= [u_x]_j - \left(\frac{1}{12} + \frac{c}{6}\right)h^3u_j^{(4)} - \left(\frac{1}{30} + \frac{c}{6} + \frac{c^2}{6}\right)h^4u_j^{(5)} + \mathrm{O}(h^5) \end{aligned} \tag{10}$$

One can verify that the coefficients for $\mathrm{O}(h^k)$ terms not included in (10) are $(k-2)$-th order degree polynomials in c. One can verify also that the expansions for D_l and D_r differ only in signs of the coefficients for the odd powers of h.

The N_l and N_r operators can be used also to get "mixed" fourth-order approximations to $\partial u/\partial x$ based on midpoint operators. Integrating the equality $g = \partial f/\partial x$, one obtains the identically accurate formula

$$\int_{x_{j-1/2}}^{x_{j+1/2}} g\,\mathrm{d}x = f_{j+1/2} - f_{j-1/2} \tag{11}$$

Using, for example, the operator M_l from Eq. (6) to approximate the right hand side of (11) and the operator $h(I+\Delta_2/24)g_j$ as a quadrature formula for the integral in its left hand side, one obtains the following left approximation $\overline{D}_l$ to the derivative.

$$\overline{D}_l[u]_j/h = [u_x]_j + \frac{26+45c}{720}h^4 f_j^{(5)} + O(h^5),$$
$$\overline{D}_l = (I+\Delta_2/24)^{-1}(E-T_{-1})M_l$$

Using M_r in (11), one obtains the similar expression for the right operator $\overline{D}_r = (I+\Delta_2/24)^{-1}(T_1 - I)M_r$. The corresponding expansion differs from that for $\overline{D}_l$ only in signs of the coefficients for odd powers of h.

The calculations with the fourth-order operators $\overline{D}_l, \overline{D}_r$ require two-diagonal and three-diagonal inversions. Thus they are more computationally expensive than the third-order D_l and D_r operators.

The pairs $D_l(c), D_r(c)$ and $\overline{D}_l(c), \overline{D}_r(c))$ are similar to the CUD pairs $L(s)$ and $L(-s)$ from [2] in that they can be used for constructing upwind biased approximations. However, changing their "orientation" is due to changing the index l by r or vice versa with the same values of the parameter c. Mathematically, this property can be expressed in the form of the following

Theorem 2. *Let $\mathcal{D}_l$ and $\mathcal{D}_r : U_h \to U_h$ be left and right operators $D_l, \overline{D}_l$ and D_r, $\overline{D}_r$, respectively defined for $c > -0.5$. Then*

$$\mathcal{D}_l^* = -\mathcal{D}_r, \quad \mathcal{D}_l > 0$$

Proof. Consider, for example, the pair D_l and D_r. Introducing the conjugate operators, the left operators can be cast in the form

$$D_l = \frac{1}{2}\Delta_0 - \frac{1}{6c}\Delta_2 + \frac{1}{6c}N_l N_l^*(N_l^*)^{-1}\Delta_2,$$

Similarly, the right operators look as

$$D_r = \frac{1}{2}\Delta_0 + \frac{1}{6c}\Delta_2 - \frac{1}{6c}N_r N_r^*(N_r^*)^{-1}\Delta_2.$$

Using the previous notation

$$G = N_l N_l^* = N_r N_r^*, \quad G = G^* > 0$$

and the expressions (2)for N_l^{-1} and N_r^{-1}, one obtains the skew-symmetric and the self-adjoint components of D_l

$$D_l^{(1)} = D_r^{(1)} = \frac{1}{2}\Delta_0 - \frac{1}{12}G\Delta_0\Delta_2, \quad D_l^{(0)} = -D_r^{(0)} = -\frac{1}{6c}\Delta_2\Big(I - G\Big(I - \frac{c}{2}\Delta_2\Big)\Big).$$

Thus one has $D_l = -D_r^*$.

To prove the corresponding operators inequality, it is sufficient to estimate operator $D_l^{(0)}$. It can be written as

$$-\frac{\Delta_2 G}{6c}\Big(G^{-1} - \Big(I - \frac{c}{2}\Delta_2\Big)\Big).$$

Using the expression for G^{-1} and the equality $\Delta_0^2 = 4\Delta_2 + \Delta_2^2$, one obtains upon simple manipulations $D_l^{(0)} = \frac{G}{12}(1+2c)\Delta_2^2 > 0$.

The proof for the $\overline{D}_l$ and $\overline{D}_r$ can be accomplished in the similar manner.

Positivity of the operators allows one to construct upwind-biased schemes. □

2.3.2. Application to conservation laws

Consider the model equation

$$u_t + f(u)_x = 0. \tag{12}$$

The standard approach to construct an upwind semi-discretized scheme is to use for the x-derivative $\mathcal{D}_l$ and $\mathcal{D}_r$ operators if $f'(u) > 0$ and $f'(u) < 0$ respectively. It will be conservative approximation since the actions of the $\mathcal{D}_l, \mathcal{D}_r$ operators on a grid function f can be presented as the difference of numerical fluxes across midpoint cell boundaries. Considering, for example, D_l, one can write

$$D_l f_j = (q_{l,j+1/2} - q_{l,j-1/2}),$$
$$q_{l,j+1/2} = \frac{1}{2}\left(f_{j+1} + f_j - \frac{1}{3c}(f_{j+1} - f_j)\right) - \frac{1}{6c} N_l(f_{j+1} - f_j).$$

In the case of $\overline{D}_l$ operator, one has the left midpoint numerical fluxes given by $q_{l,j+1/2} = (I + \Delta_2/24)^{-1} M_l f_j$.

The above described scheme requires switching from left to right operators or vice versa. Besides it is not in general an entropy-consistent one. Thus it is advantageous, as in [8], to use the flux splitting

$$f(u) = F^+ + F^-, \quad F^+ = \frac{1}{2}(f(u) + Cu), \quad F^- = \frac{1}{2}(f(u) - Cu), \quad C = \text{const} > 0.$$

Introducing

$$D^+ = (\mathcal{D}_l + \mathcal{D}_r)/2, \quad D^- = (\mathcal{D}_l - \mathcal{D}_r)/2,$$

the conservative entropy-consistent scheme can be written in the index-free form as

$$\frac{\partial u}{\partial t} + \frac{1}{h}(D^+F^+ + D^-F^-) = 0. \tag{13}$$

Scheme (13) does not require the operators switching. It is a scheme with a positive operator (in the frozen coefficients sense) and hence is stable in the discrete L_2 norm. It can be presented in the equivalent form

$$\frac{\partial u}{\partial t} + \frac{1}{2h}((\mathcal{D}_l + \mathcal{D}_r)f(u)) + C(\mathcal{D}_l - \mathcal{D}_r)u = 0. \tag{14}$$

In Eq. (14) the sum and the difference of the operators can be readily recognized as skew-symmetric and positive self-adjoint operators respectively if it is supposed that $f(u) = au$, $a = \text{const}$.

The extensions of the scheme to systems of conservation laws and multidimensional problems are outlined in [8]. In all cases, the Runge–Kutta time stepping or iterative procedures can be applied to form fully discretized schemes.

3. Multioperators

3.1. General forms

We return to the one-parameter operators families defined by Eqs. (3) or (4) in the previous section. Their general properties discussed therein show that the coefficients in the Taylor expansion series for the operators actions are polynomial in the parameter c of successively increased degrees. In particular, the above examples present the first two coefficients as the first and second degree polynomials in c. It suggests using operators from the families as basis operators composing uniquely defined multioperators.

At this point, it is worth reminding the general multioperators approach [1]. It is based on the assumption that there exists an one-parameter operators family $L_h(s)$ with the expansion

$$[Lf]_j = L_h(s)[f]_j + \sum_{k=m}^{m+M-2} a_{kj} c_k(s) h^k + \mathrm{O}(h^{m+M-1}) \tag{15}$$

(the high-order derivatives are included in the coefficients a_{kj}), satisfying the following. For fixed distinct values of s ($s = s_i$, $i = 1, 2, \ldots, M$), the matrix A defined by

$A = \{b_{ij}\}$, $b_{1j} = 1$, $b_{ij} = c_{m+i-2}(s_j)$ $\quad i = 2, 3, \ldots, M$, $j = 1, 2, \ldots, M$ does not degenerate.

If the above one-parameter family of grid operators $L_h(s)$ do exist, the procedure of constructing multioperators starts from solving the linear system

$$A\mathbf{g} = \mathbf{r}, \quad \mathbf{g} = (\gamma_1, \gamma_2, \ldots, \gamma_M)^{\mathrm{T}}, \tag{16}$$

where M-component vector $\mathbf{r}$ is given by $\mathbf{r} = (1, 0, 0, \ldots 0)$. Once $\gamma_1, \gamma_2, \ldots, \gamma_M$ coefficients are obtained, the final step is forming the linear combination $L_M = \sum_{i=1}^{M} \gamma_i L_h(s_i)$ referred to as multioperator in which $L_h(s_i)$ may be viewed as basis operators.

Since the γ coefficients are a partition of unity, the summation over i of the equations obtained from Eq. (15) by setting $s = s_i$ and multiplying by γ_i preserves the resulting left hand side. At the same time, the sum of the second terms in the right hand sides of the equations vanishes. Thus one has $L_M[u]_j = [Lu]_j + \mathrm{O}(h^{m+M-1})$.

Since M is supposed to be arbitrary, the multioperator's action is the arbitrary-order approximation to the target grid functional. Clearly the above procedure can be applied to the case of the expansions for $L_h(s)[u]_j$ containing either odd or even powers of h thus increasing the resulting multioperators orders for fixed M.

In the present case, we set $s = c$ and consider the operators of the previous section as the required one-parameter families. Following the general procedure and denoting by L_l either of the two mth-order left operators, we fix M different values $c_1, c_2, \ldots, c_M$ and construct the left linear combination

$$L_{M,l} = \sum_{i=1}^{M} \gamma_i^{(l)} L_l(c_i),$$

where coefficients $\gamma_i^{(l)}, i = 1, 2, \ldots, M$ is a partition of unity. To annihilate $M - 1$ expansion terms, the coefficients are required to satisfy the linear system

$$\sum_{i=1}^{M} \gamma_i^{(l)} = 1, \quad \sum_{i=1}^{M} p_1(c_i)\gamma_i^{(l)} = 0, \quad \sum_{i=1}^{M} p_2(c_i)\gamma_i^{(l)} = 0, \quad \ldots, \sum_{i=1}^{M} p_{M-1}(c_i)\gamma_i^{(l)} = 0, \tag{17}$$

where $p_k, \; k = 1, 2, \ldots, M$ are kth-degree polynomials served as coefficients in the Taylor expansion series for $L_l(c_i)[u]_j$. Successively extracting from Eqs. (17) equalities for the sums $\sum_{i=1}^{M} c_i \gamma_i^{(l)}$, $\sum_{i=1}^{M} c_i^2 \gamma_i^{(l)}, \ldots,$ $\sum_{i=1}^{M} c_i^{M-1} \gamma_i^{(l)}$, one arrives at a system with the Vandermonde matrix

$$\sum_{i=1}^{M} \gamma_i^{(l)} = 1, \quad \sum_{i=1}^{M} c_i \gamma_i^{(l)} = r_1, \quad \sum_{i=1}^{M} c_i^2 \gamma_i^{(l)} = r_2, \ldots, \sum_{i=1}^{M} c_i^{M-1} \gamma_i^{(l)} = r_m, \tag{18}$$

where $r_1, r_2, \ldots, r_{M-1}$ are numerical constants defined by the coefficients of $p_k(c)$.

The similar system arises when constructing the right operator $L_{M,r}$ based on linear combinations $L_{M,r} = \sum_{i=1}^{M} \gamma_i^{(r)} L_r(c_i)$ where L_r is either of the two right operators from Eqs. (3) and (4). Having in mind the invertibility of the Vandermonde matrices, the following statement is true.

Theorem 3. *Let $c_i < -.5, i = 1, 2, \ldots, M$ be distinct real numbers while $\gamma_i^{(l)}, \gamma_i^{(r)}, i = 1, 2, \ldots, M$ satisfy (18) with the right hand sides $r_i = r_i^{(l)}$ and $r_i = r_i^{(r)}$ respectively. Then there exist uniquely defined linear combinations $L_{M,l} = \sum_{i=1}^{M} \gamma_i^{(l)} L_l(c_i), L_{M,r} = \sum_{i=1}^{M} \gamma_i^{(r)} L_r(c_i)$ for which*

$$L_{M,l}[u]_j = [Lu]_j + \mathrm{O}(h^{m+M-1}), \quad L_{M,r}[u]_j = [Lu]_j + \mathrm{O}(h^{m+M-1}).$$

The combinations form left and right multioperators. As evident from the expressions for the basis operators considered in the previous section, the left and the right basis operators differ only in signs of their either skew-symmetric or self-adjoint components. It means that (as illustrated by Eqs. (7)–(10)) the polynomial $p_k(c)$ in the corresponding Taylor expansion series are the same while the series differ only in signs of their terms. Hence it follows that the initial linear system (17) holds for both left and right basis operators. In turn, it leads to equalities which can be summarized in the form of the following

Theorem 4. *Let (L_l, L_r) be the pairs of the left and right basis operators. Then*

$$\gamma_i^{(l)} = \gamma_i^{(r)}, i = 1, 2, \ldots, M,$$

and

$$L_{M,l} = -L_{M,r}^* \text{ if } L_l = -L_r^*, \quad L_{M,l} = L_{M,r}^* \text{ if } L_l = L_r^*$$

As in the case of other types of multioperators, the actions of $L_{M,l}$ $L_{M,r}$ on known grid functions can be calculated simultaneously and independently when using M parallel processors. In all cases, the coefficients γ_i can be obtained in analytical forms without solving (18) numerically.

3.1.1. Choice of the parameters

Though existence of arbitrary-order multioperators for any set of distinct values of c exceeding $-.5$ is guaranteed, some limitations on their choice can be important.

First of all, conditions numbers of the Vandermonde matrices dramatically increase with increasing M, the number of the parameters values. Though it does not influence analytical solutions for the γ coefficients, their absolute values can be quite large thus adversely affecting round-off errors. Practically, it means that 64-bits arithmetics may be insufficient to get solutions errors like 10^{-15} for $M = 5$. To reduce the absolute values increasing with M, it is worth choosing c_i as the zeroes of the Mth-order Chebyshev polynomials for chosen intervals $(c_{\min}, c_{\max})$. The lesser are values of $| c_i |$ the greater is the effect of decaying influence of boundary conditions in (1). However, the excessively small values may considerably increase condition numbers of (18) even in the case of the Chebyshev distribution.

Once the resulting multioperators $L_{M,l}(c_{\min}, c_{\max})$, $L_{M,r}(c_{\min}, c_{\max})$ are defined, $c_{\min}, c_{\max}$ can be used as parameters controlling some desirable properties in particular cases. For example, behavior of the Fourier transforms of the multioperators in ranges of the highest wave numbers admitted by meshes may be of importance in the case of spatial discretizations of hyperbolic conservation laws. Another example is using the parameters to minimize truncation error leading term (terms) of the multioperators.

3.1.2. Central multioperators

Operators $L_{M,l}$ and $L_{M,r}$ are essentially non-central ones. This property can be useful in the case of extrapolation procedures, when constructing upwind schemes etc.. However, in certain instances it is more appropriate to use central approximations. Examples are discretization of second derivatives and quadratures. There are two ways to obtain central multioperators.

The first one is to use their combinations $(L_{M,l} + L_{M,r})/2$ or $(L_{M,l} - L_{M,r})/2$, the latter case being appropriate for creating dissipative mechanisms in the case of first derivatives.

Another way is to use the combinations of the central operators $L_0 = (L_l(c) + L_r(c))/2$ or $L_1 = (L_l(c) - L_r(c))/2$ as generators of basis operators. Fixing M values of c, one obtains the basis operators $L_0(c_i)$, $L_1(c_i)$, $i = 1, 2, \ldots, M$ allowing to annihilate more powers of h in the corresponding truncation errors than in the case of $L_l(c)$ and $L_r(c)$. The expansions are given by Eq. (5) with missed either odd or even powers of Z. Some penalty for this advantage is the necessity to investigate domains in free parameters spaces for which the multioperators do exist. Luckily, the solvability of the linear systems for the γ coefficients can be checked numerically for any set of parameters.

3.2. Examples of multioperators

Using the above described general procedure, one can create multioperators for various grid functionals. In particular, one-parameter quadrature, interpolation and extrapolation formulas of Section 2 can be converted into prescribed-order ones using expansions Eqs. (9), (7) and (8) with added (if needed) the next terms. As an illustration, we consider simple cases of the sixth-order extrapolation and numerical integration multioperators ($M = 3$) for which the information given in Eqs. (8) and (9) is sufficient to get the required $\gamma_1, \gamma_2, \gamma_3$ coefficients.

3.2.1. Extrapolation operators

Inspecting the two terms in the truncation error in Eq. (8), one can see that the first one generates equation $\sum_{i=1}^{3} c_i\gamma_i = -1$. Taking it into account, one obtains using the second term another equation $\sum_{i=1}^{3} c_i^2\gamma_i = 1$. With the partition of unity condition, it gives the system whose analytical solution is

$$\gamma_1 = \frac{1 + c_3 + c_2 + c_3c_2}{(c_1 - c_2)(c_1 - c_3)}, \quad \gamma_2 = -\frac{1 + c_1 + c_3 + c_1c_3}{(c_2 - c_1)(c_2 - c_3)}, \quad \gamma_3 = \frac{1 + c_1 + c_2 + c_1c_2}{(c_3 - c_1)(c_3 - c_2)}.$$

Considering the further term in the expansion (8) for $c = c_1, c = c_2, c = c_3$, one can obtain the coefficient for the leading $O(h^6)$ term in the multioperators truncation error. Thus one has, for example, in the case of the left multioperator

$$E_{M,l}[u]_j = \sum_{i=1}^{3} \gamma_i E_l(c_i)[u]_j = u(x_{j+2}) + (1+c_1)(1+c_2)(1+c_3)h^6 u_j^{(6)} + O(h^7).$$

Left extrapolation multioperators can be used for formulating boundary conditions at right boundaries.

3.2.2. Multioperators quadratures

We choose the corrections to the Simpson rule, that is $(Q_{1,l}, Q_{1,r})$ as the basis operators. From the Taylor expansion series (9) one can easily obtain the right hand sides of (18) in the case $M = 3$. They are (1, 0, −1/30). Retaining more terms in (9), one can construct desired order approximations to $\int_{x_{j-1}}^{x_{j+1}} u(\xi)\mathrm{d}\xi$. Consider an integration interval $[a, b]$. Taking advantage of the decaying influence of boundary conditions, one can use left multioperators for $[(b-a)/2, b]$ and right multioperators for $[a, (b-a)/2]$ with the basis operators actions as starting values in the procedures Eq. (1). As an illustration, the integration errors for the Simpson formula, the 5th- and 7th-order multioperators quadratures (denoted by I_{simp}, I_5 and I_7 respectively) are presented in Table 1 with the corresponding orders estimates k for several mesh sizes $h = 1/N$. In the calculations, more or less arbitrary chosen the uniform and the Chebyshev distributions with $c_{\min} = .08, c_{\max} = .12$ and $c_{\min} = .01, c_{\max} = .1$ were used for the fifth-order and the seventh-orders multioperators respectively.

As seen, the fifth-order multioperator outperforms the sevenths-order one if $N = 8$ but the latter shows striking increase of accuracy when N increases. Its loss of accuracy for $M = 8$ seems to be due to the large numerical coefficients for the truncation errors which are considerably greater for $M = 5$ than those for $M = 3$ as a result of increasing condition numbers of system (18).

3.3. Multioperators for derivatives discretizations

Using the above described differencing operators $D_l, D_r, \overline{D}_l, \overline{D}_r$ as basis ones, the procedure for constructing the corresponding multioperators is quite straightforward. Following the standard approach, the $(M+2)$-order left and right multioperators based, for example, on the former pair with a set $c_1, c_2, \ldots, c_M$ read

$$D_{M,l} = \sum_{i=1}^{M} \gamma_i D_l(c_i), \quad D_{M,r} = \sum_{i=1}^{M} \gamma_i D_r(c_i).$$

However the positivity of the basis operators does not necessary mean that the resulting multioperators are also positive. To guarantee their positivity, a search for "admissible" intervals $(c_{\min}, c_{\max})$ is needed. Supposing that the intervals are found, the multioperators can be used to approximate the flux function in Eq. (12) in the flux-splitted form. As a result, the semi-discretized scheme for Eq. (12) can be written using the index-free notations as

$$u_t + \frac{1}{2h}(D_{M,l} + D_{M,r})f(u) + \frac{C}{2h}(D_{M,l} - D_{M,r})u = 0, \tag{19}$$

where $C > 0$ is a constant. The sum and the difference of the multioperators are skew-symmetric and self-adjoint operators respectively, the latter being positive if $D_{M,l}$ is positive.

Table 1
Accuracy of multioperators-based quadrature formulas

N	8	16	32	64
I_{simp}	5.81e−6	3.28e−7	2.05e−8	1.28e−9
I_5	2.38e−7	1.35e−8	4.77e−10	1.57e−11
k		4.13	4.82	4.92
I_7	2.18e−4	1.83e−8	7.99e−13	7.19e−15
k		13.5	14.5	6.79

Comparing with the differencing multioperators described in [8], more parameters c_i are needed to obtain a given approximation order resulting in larger values of the γ coefficients. We do not follow the above strategy in the present paper. Instead, we use below the basis operators generated by the central skew-symmetric and the self-adjoint operators $D_1(c) = (D_l + D_r)/2h$ and $D_2(c) = (D_l - D_r)/2h$ defined by left and right differencing operators of Section 2 with possibly different sets of parameters. As mentioned, the advantage of the approach follows from the structure of the corresponding Taylor expansion series containing either odd or even powers of h. Thus larger approximation orders can be obtained for fixed numbers of parameters. Besides, one thus has a good opportunity to control efficiently the dispersion and dissipation properties of the resulting schemes.

As an illustration, we consider the pair D_l, D_r with the expansion series (10). The symbolic representation of the skew-symmetric operator then reads

$$D_1(c) = D_x + \sum_{k=1}^{\infty} p_{2k}(c) h^{2k+2} D_x^{2k+3}, D_x = \partial/\partial x.$$

Fixing M values $c_1, c_2, \ldots, c_M$, one obtains the linear system

$$\sum_{i=1}^{M} \gamma_i = 1, \sum_{i=1}^{M} p_2(c_i)\gamma_i = 0, \quad \sum_{i=1}^{M} p_4(c_i)\gamma_i = 0, \ldots, \sum_{i=1}^{M} p_{2M-2}(c_i)\gamma_i = 0, \tag{20}$$

where $p_2(c)$ is given by the coefficient for h^4 in series (10). Its solution (if exists) defines the skew-symmetric multioperator

$$D_{1,M} = \sum_{i=1}^{M} \gamma_i D_1(c_i), \quad D_{1,M}[f(x)]_j = [f_x]_j + \mathrm{O}(h^{2M+2}).$$

Similarly, the expansion for the self-adjoint basis operator looks as

$$D_2(c) = \sum_{k=1}^{\infty} p_{2k-1}(c) h^{2k+1} D_x^{2k+2}.$$

Fixing possibly other set $\bar{c}_1, \bar{c}_2, \ldots, \bar{c}_M$, the linear system for the coefficients $\bar{\gamma}_i$ of the self-adjoint multioperator

$$D_{2,M} \sim h^{2M+1} D_x^{2M+2}$$

is

$$\sum_{i=1}^{M} \bar{\gamma}_i = 1, \sum_{i=1}^{M} p_1(\bar{c}_i)\bar{\gamma}_i = 0, \sum_{i=1}^{M} p_3(\bar{c}_i)\bar{\gamma}_i = 0, \ldots, \sum_{i=1}^{M} p_{2M-3}(\bar{c}_i)\bar{\gamma}_i = 0, \tag{21}$$

where $\bar{p}_1(c)$ is given by the coefficient for h^3 in series (10).

Systems (20) and (21) do not reduce to those of the Vandermonde type so their solvability should be either investigated or simply checked for particular sets of the parameters. Assuming some distributions $c_i = c_i(c_{\min}, c_{\max})$ and $\bar{c}_i = \bar{c}_i(\bar{c}_{\min}, \bar{c}_{\max})$, one can use $c_{\min}, c_{\max}$ and $\bar{c}_{\min}, \bar{c}_{\max}$ to control the multioperators spectral properties. In particular, the last pair should be chosen to guarantee positivity of $D_{2,M}$.

Using both multioperators, the x-derivative in Eq. (12) can be approximated now as

$$[f(u)_x]_j = D_{1,M}[f]_j + CD_{2,M}[u]_j + \mathrm{O}(h^{2M+2}), \quad C = \text{const} > 0,$$

with the $D_{2,M}$ operator playing the role of the built-in filter of high frequency numerical noise. Thus the sum and difference of the multioperators in Eq. (19) are changed by the multioperators based on the sum and the difference of the basis operators.

Setting $D^+ = D_{1,M}$ and $D^- = D_{2,M}$ in Eq. (13) and using extensions outlined in Subsection 2.3, one can construct flux-splitting forms of multioperators schemes for equations with convection terms, for systems of conservation laws, for the fluid dynamics equations etc. It is easy to show that their semi-discretized versions are conservative, entropy-consistent and stable in the discrete L_2 norms (in the frozen coefficients sense).

Considering Eq. (12) with $f(u) = au$, $a = \text{const}$ and performing the Fourier transforms for $D_{1,M}$ and $D_{2,M}$, one can estimate the spectral contents of the normalized numerical phase velocity r defined as the ratio of the numerical phase velocity to the exact one a and the amplitude errors introduced by $D_{2,M}$.

As an example, we consider the twelfth-order skew-symmetric multioperator $D_{12} = D_{1,M}(c_1, c_2, c_3, c_4, c_5)$ depending on chosen parameters c_i. To construct it, it is sufficient to solve for $\gamma_1, \gamma_2, \gamma_3, \gamma_4, \gamma_5$ the system obtained from Eqs. (20) by setting $M = 5$. In this way, the $O(h^4), O(h^6), O(h^8), O(h^{10})$ terms are annihilated. The system is not of the Vandermonde type so we fix the uniform parameters distribution considering $c_1 = c_{\min}$ and $c_5 = c_{\max}$ as controlling parameters.

Fig. 1 shows the relative numerical phase velocity in the case of the above advection equation semi-discretized with $D_{12}(c_{\min}, c_{\max})$. The function $r(\alpha)$ in the Figure is defined by $r(\alpha) = \mathrm{Im}\hat{D}_{1,M}(\alpha)/\alpha$ where $\hat{D}_{1,M}(\alpha)$ and $\alpha = kh$ are the Fourier transform of $D_{1,M}$ and the dimensionless wave number respectively. The deviations of $r(\alpha)$ from unity, $er = \mid 1 - r \mid$, characterize the phase errors. The function $er \times 10^5$ is shown by the dashed line in Fig. 1. The uniform distribution with $c_{\min} = c_1 = -.404$ and $c_{\max} = c_5 = .41$ was chosen more or less arbitrary by observing the $r(\alpha)$ function. As seen, the phase errors satisfy $er < 10^{-5}$ for $\alpha_* < 1.7$ and $er < 7 \times 10^{-5}$ for $\alpha_* < 2.1$.

Using two multioperators for constructing numerical fluxes allows one to use optimization procedures independently for amplitude and phase errors. For instance, one can formulate the following problem. Given an interval $[0, \alpha_*]$, find $(c_{\min}, c_{\max})$ for which $\max_{[0,\alpha_*]} er = \min$. Solving the optimization problems as well as detailed investigation into the relevant schemes are beyond the scope of the present paper.

Instead, we restrict ourselves to presenting the results of calculations with the D_{12} operators in the case standard periodic problem for the Burgers' equation (see, for example, [11]) considered in the companion paper [8]. It reads

$$\frac{\partial u}{\partial t} + \frac{\partial}{\partial x}\frac{u^2}{2} = 0, \quad -1 \leqslant x \leqslant 1$$
$$u(0, x) = 1 + 0.5\sin(\pi x)$$

The exact solution up to certain time moment $t = t_*$ is smooth. It can be obtained using an iterative procedure described in [11] with the machine precision.

The calculations were carried out with the D_{12} operator for x-derivatives, the dissipation multioperator being excluded by setting $C = 0$. The fourth-order Runge–Kutta time stepping was found to be sufficient to guarantee stability of the scheme for the present particular example and relatively small time interval $t \leqslant .3$.

In Table 2, the maximum norm of the solution errors at $t = .3 < t_*$ and the corresponding estimates of the mesh convergence orders k are presented for numbers of nodes $N = 16, 32, \ldots, 256$. For comparison, the similar results obtained with the ninth-order multioperators scheme from [8] are also included in the Table as reference ones. The scheme is based on a version of the fifth-order CUD operator and denoted here by L_{59}.

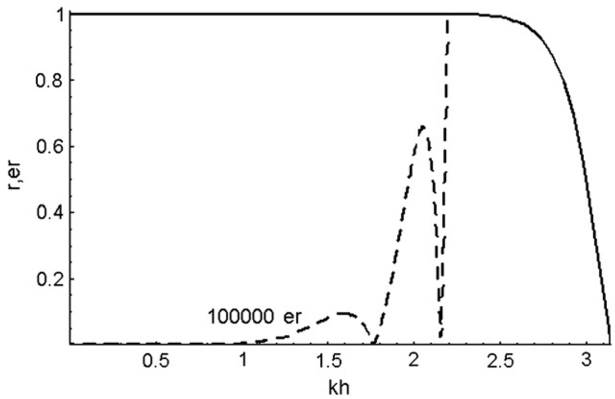

Fig. 1. Twelfth-order multioperator for advection equation: normalized numerical phase velocity and phase error vs. dimensionless wave number.

Table 2
Maximum norms of solution errors for the Burgers' equation

N	16	32	64	128	256
L_4	1.80e−2	2.486e−3	2.052e−4	1.40e−5	9.30e−7
k_c		2.6	3.6	3.9	3.9
L_{59}	1.86e−3	2.16e−5	5.02e−8	4.7e−11	9.96e−14
k_c		6.4	8.7	10.0	9.2
L_{10}	1.55e−3	7.56e−6	1.37e−8	6.16e−12	1.35e−14
k		7.7	9.1	11.1	8.8

As seen, both schemes show remarkably high accuracy, the twelfth-order one being several times more accurate than the ninth-order one in the case of the finest mesh. It is partly due to the ninth-order dissipation mechanism of the latter with the dissipation constant $C = 1$ used to deal with the discontinuous solution at $t > t^*$. However, calculations with L_{59} and $C = 0$ showed that the dissipation can decrease solution errors only by a factor O(1) for the considered relatively small time interval.

In the Table, solution errors in the case of the fourth-order basis operators denoted here by L_4 illustrate the striking difference between relatively low- and high-order multioperators approximations.

The considered case does not bear relation to very high values of the dimensionless wave numbers $\alpha = kh$ supported by the meshes. To illustrate the ability of the multioperator-based approximation to resolve very small scales ($\alpha > \pi/2$), the calculations for the benchmark problem proposed in [12] were carried out (the problem was considered also in our previous publication [8]). The initial value problem was formulated as follows. The advection equation

$$\frac{\partial u}{\partial t} + \frac{\partial u}{\partial x} = 0$$

with the initial condition

$$u(0,x) = [2 + \cos(\beta x)][\exp(-2\ln(2)(x/10)^2)]$$

should be discretized using the uniform mesh with $h = 1$ and numerically solved to provide the comparison with the exact solution at $t = 400$ and $t = 800$. In view of the above prescribed mesh size, the parameter β is equal to our parameter α. The value was used in the calculations. Moreover the greater value $\alpha = 1.9$ was used as well. Though a ninth-order multioperators-based dissipation operator was created to deal with the problem, it was found that (surprisingly) the above D_{12} skew-symmetric operator can do the job alone. The comparisons with the exact solutions at $t = 800$ are presented in Figs. 2 and 3 for $\alpha = 1.7$ and $\alpha = 1.9$ respectively. As seen, there is no visual difference between the exact and numerical solutions in both cases.

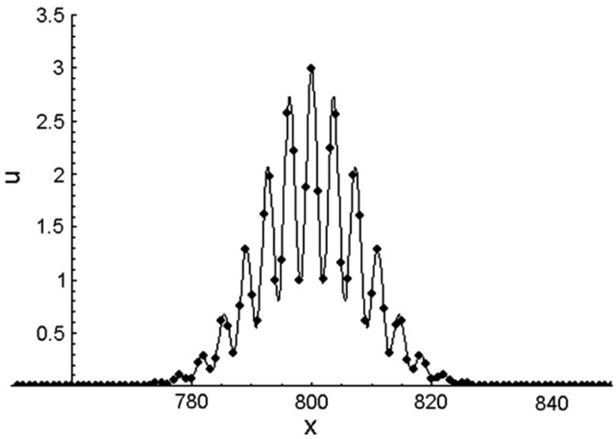

Fig. 2. Linear advection equation: comparison of the exact (solid line) and numerical (dots) solutions at $t = 800$ for $\alpha = 1.7$.

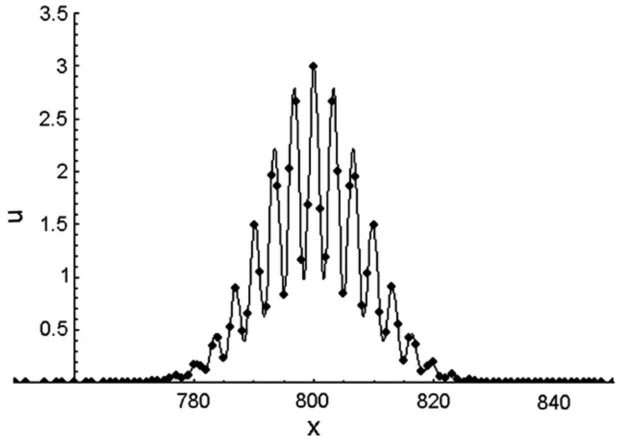

Fig. 3. Linear advection equation: comparison of the exact (solid line) and numerical (dots) solutions at $t = 800$ for $\alpha = 1.9$.

It should be emphasized that no in-depth optimization was used. In fact, the $c_{\max} = .41$ was chosen arbitrary while $c_{\min}$ was tuned by observing the dispersion errors curves.

3.4. Using extrapolation multioperators for constructing high-order boundary conditions

As follows from the definition of multioperators, calculations of their actions on known grid functions reduce to calculations of underlying basis operators actions on the functions. As far as basis compact approximations are concerned, the required boundary conditions can be readily constructed without decrease of approximation orders. They are needed to perform operators inversions and should not be confused with boundary conditions coming from mathematical formulations.

Now the problem arises how to formulate them in such a way that the summation over i with γ_i coefficients provides the claimed multioperators orders at boundary (and hence, near boundary) nodes. To explain the problem, it is worth emphasizing that the estimates of multioperators approximation orders are based on the implicit assumption that the Taylor expansion series Eq. (15) can be constructed for each node of computational domains. Unfortunately, it is not the case of boundary grid points if bounded domains are considered without imposing periodicity conditions. In general, the introduced boundary operators produce expansions with other high-order terms which are not annihilated as a result of the summation with the γ_i coefficients. Since the coefficients are a partition of unity, standard boundary closers result in the multioperators orders near boundaries which are equal to those of the basis operators.

A possible way to handle the problem is to use high order extrapolation operators. The idea behind this can be explained in the following way. Suppose one can extrapolate the results of inversions of operators to the boundary node $j = 0$ with as high order as needed. It means that the corresponding Taylor expansion series are extrapolated as well thus allowing to annihilate the low order terms.

To be specific, consider numerical differentiation procedure for a known grid function $u_j, j = 0, 1, 2, \dots, N$ performed with the left $(M + 2)$-order multioperator $D_{l,M}$ for which the starting values $w_0(c_i)$ are required to calculate the grid function $w_j(c_i) = N_l(c_i)\Delta_2 u_j, i = 1, 2, \dots, M$. Clearly, $w_j(c_i)$ are linear functions in $w_0(c_i)$ obtained as the output of the left sweep (1) for each c_i. Choosing another set $\bar{c}_1, \bar{c}_2, \dots, \bar{c}_M$ (in particular, the (c_i) set can be chosen), one can construct the right shift multioperator $E_{r,M}$ defining for sufficiently smooth $v(x)$ the extrapolation procedure $v(x_j) = E_{r,M}v(x_{j+1}) + O(h^{M+3})$. Performing the right sweeps (1) for $i = 1, 2, \dots, M$ to calculate the extrapolated values $w^e_j(c_i) = E_{r,M}w_{j+1}(c_i)$ with the right starting values, say, with $w_{N-1}(c_i)$, one obtains $w^e_0(c_i)$ which are practically independent of the starting conditions. Due to the linearity of $E_{r,M}$, they are also linear functions in $w_0(c_i)$. Thus $w^e_0(c_i) = a(c_i)w_0(c_i) + b(c_i)$ where the coefficients a and b can be obtained by giving two distinct values to $w_0(c_i)$ (for example, 0 and 1). Setting $w_0(c_i) = w^e_0(c_i)$, one obtains the target values $w_0(c_i) = b/(1 - a)$.

Table 3
Local near-boundary errors for numerical differentiation for $cos(\pi x), x \in [0, 1]$ with 5th-order multioperator

Node number	1	2	3	4	5	6	7
$N = 16$, A, $e_1 = 2.8\text{e}{-5}$	−6.1e−5	−5.4e−5	−4.8e−5	−4.2e−5	−3.6e−5	−3.0e−5	−2.2e−5
$N = 16$, B, $e_1 = 1.0\text{e}{-4}$	0	5.2e−4	−6.0e−4	−2.0e−4	−6.7e−5	−3.5e−5	−2.3e−5
$N = 32$, A, $e_1 = 8.7\text{e}{-7}$	−1.6e−6	−1.5e−6	−1.5e−6	−1.4e−6	− 1.4e−6	−1.3e−6	−1.3e−6
$N = 32$, B, $e_1 = 5.9\text{e}{-6}$	0	6.9e−5	−7.1e−5	−2.2e−5	−5.2e−6	−1.9e−6	−1.34e−6
$N = 64$, A, $e_1 = 2.8\text{e}{-8}$	−4.6e−8	−4.6e−8	−4.6e−8	−4.5e−8	−4.5e−8	−4.4e−8	−4.4e−8
$N = 64$, B, $e_1 = 3.5\text{e}{-7}$	0	8.8e−6	−8.8e−6	−2.6e−6	−5.3e−7	−1.2e−7	−5.5e−8

Rows B and A correspond to boundary conditions for the inverting procedures with exact values at node $j = 1$ and multioperators-extrapolated values at node $j = 0$, e_1 stands for l_1 norm of the errors.

The calculations were carried out for $u(x) = \cos(\pi x)$, $x \in [0, 1]$ using the fifth-order $D_{M,l}$ operator and the sixth-order right extrapolation operator $E_{M,r}$ ($M = 3$). The set $(c_1, c_2, c_3) = (.05, .1, .15)$ was chosen in both cases.

In Table 3, the columns contain the absolute values of errors at the nodes $x_j = jh$, $j = 0, 1, 2, \ldots, 7$, $h = 1/N$ where N is the total number of grid points. There are two rows for each value of N. The first row corresponds to the results of the above described technique while the second one contains the data obtained by using the exact derivative value at $x = h$ and therefore the value of $N_l \Delta_2[u]$ at $x = x_1$ as a starting one. The l_1 norms of the numerical differentiation errors denoted by e_1 are also presented in the table.

As seen, the fifth-order is excellently preserved everywhere in the vicinity of $x = 0$ if the multioperators extrapolation procedure is used. In contrast, the exact boundary value gives zero error at $x = h$ but only the third-order local errors at near-boundary nodes thus increasing the l_1 norms.

Upon inspecting the table, another observation concerns with the decaying influence of the "wrong" boundary condition at $x = h$. One can see that the differentiation errors in both cases are very close to each other at some distance from the boundary.

4. Conclusions and discussion

A novel one-parameter families of compact approximations with two-points inverse operators for various grid functionals are described. They may be viewed as left and right operators depending on the orientation of the corresponding stencils in respect to center nodes. Their merits are due to very small operation counts per node and the possibility of rapidly decaying influence of boundary conditions needed for inversion procedures. Though they can be used as a tool for increasing orders of standard three-point formulas, their main property in the context of the present paper is the potential for generating basis operators for formally arbitrary-order multioperators.

General properties of the basis operators and of the resulting multioperators are described. As particular cases, interpolation/extrapolations operators, quadratures and approximation to first derivatives are considered. The presented numerical examples illustrate high accuracy and claimed mesh convergence orders of the multioperators approximations. As shown, extrapolation one-sided multioperators can be efficiently used for generating numerical boundary conditions.

Concerning multioperators for hyperbolic conservation laws, it may be advantageous to construct multioperators based on halve sums and halve differences of left and right one-parameter operators instead of constructing left and right multioperators. It allows one to perform independently optimization of phase and amplitude errors introduced by multioperators schemes. Calculations in the case of the standard problem for the Burgers' equation show remarkably high performance of the scheme with the tenth-order multioperator.

In general, it follows from the multioperators principle that formally arbitrary-order approximations can be constructed with great ease without enlarging stencils and adding complexity to the basis operators by simply increasing numbers M of the involved parameters. However it makes sense to obtain *reasonably high orders*, the notion "reasonably high" being problem dependent. For example, Table 3 shows that near PC machine precision accuracy is obtained in the case of the Burgers equation with the mesh size $h = 1/256$. If such size is minimal for accurate representation of the smallest solution scales in other cases while the accuracy is preserved, there is no need in using higher-than-tenth orders schemes. Instead, it is worth concentrating at proper optimization procedures allowing to deal with highest wave numbers supported by meshes. There is a good opportunity to do so due to large numbers of multioperators controlling parameters. The numbers can be further increased by increasing M without increasing the number of the γ coefficients.

Many other options of the multioperators strategy are possible. They are not covered by the present paper and can be a subject matter of further publications.

Acknowledgments

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