Available online at www.sciencedirect.com
ScienceDirect

Journal of Computational Physics 225 (2007) 2333–2353

JOURNAL OF COMPUTATIONAL PHYSICS

www.elsevier.com/locate/jcp

Development of arbitrary-order multioperators-based schemes for parallel calculations. 1: Higher-than-fifth-order approximations to convection terms

Andrei I. Tolstykh

Computing Center of Russian Academy of Sciences, 119991 Moscow GSP-1, Vavilova Strasse 40, Russian Federation

Received 13 November 2006; received in revised form 19 March 2007; accepted 22 March 2007
Available online 6 April 2007

Abstract

Further results concerning arbitrary-order approximations to grid functionals via linear combinations of basis operators obtained by fixing sets of free parameters (multioperators) are presented. A parallel algorithm for their calculations is described. As basis operators, a version of one-parametric families of the fifth-order compact upwind differencing operators (CUD) as well as the fourth-order non-centered approximations to first derivatives are considered. The resulting conservative schemes for fluid dynamics type of equations (or other equations with convection terms) are outlined. The existence and uniqueness of the corresponding multioperators are discussed. It is shown that for properly chosen parameters, multioperators preserve the upwind (downwind) properties of the basis operators, that is their positivity (negativity) in appropriate Hilbert spaces of grid functions. As examples, the seventh- and ninth-order multioperators-based schemes with very good dispersion and dissipation properties are described, their possible optimization being discussed. Numerical examples illustrating their extremely high accuracy are presented.

PACS: 65M06; 76M20

Keywords: Compact approximations; Basis compact operators; Multioperators; Parallel algorithm; High-order and arbitrary-order schemes; Convection terms; Fluid dynamics equations

1. Introduction

The concept of multioperators was introduced by the author in [1]. It was aimed at constructing prescribed-order approximations (formally, arbitrary-order ones) to various grid functionals by exploiting linear combinations of basis operators having relatively simple structures and depending on at least one free parameter. It is an alternative to the commonly used ways of increasing of approximation orders by adding complexities to approximating expressions (in particular, by increasing numbers of grid points in operators supports

E-mail address: tol@ccas.ru

0021-9991/$ - see front matter
doi:10.1016/j.jcp.2007.03.021

(stencils)). In the case of parallel machines, execution times for multioperators-based methods of very high accuracy can be approximately the same as those for relatively low-order basis operators so the multioperators principle seems to be quite attractive when high-order schemes are needed.

For completeness, we reproduce here the formulation of the main idea. Suppose that there is a family of operators $L_h(s)$ depending on, at least, one parameter s and approximating a linear operator L on a uniform grid $\omega_h = (x_j = jh, j = 0, \pm 1, \pm 2, \ldots)$ with a mesh size h. Suppose further that for sufficiently smooth functions f from some space U one has the following Taylor expansion series at grid points $x = x_j = jh, j = 0, \pm 1, \pm 2, \ldots$

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

where high-order derivatives are included in the coefficients a_{kj} and $[\cdot] : U \to U_h(\omega_h)$ is a projection operator into a space U_h of grid functions defined on ω_h. Assume also that for M fixed distinct values of s $(s = s_i, i = 1, 2, \ldots, M)$, one has

$$\det A \neq 0, \tag{2}$$

where $A = \{b_{ij}\}, b_{1j} = 1, b_{ij} = c_{m+i-2}(s_j)\ i = 2, 3, \ldots, M,\ j = 1, 2, \ldots, M$. Then it is possible to find a partition of unity γ_i, $i = 1, 2, \ldots, M$ such that Eq. (1) upon the multiplication by γ_i followed by the summation over i reduces to

$$[Lf]_j = \sum_{i=1}^{M} \gamma_i L_h(s_i)[f]_j + \mathrm{O}(h^{m+M-1}).$$

The required γ_i coefficients are the solution of the linear system with matrix A and the right-hand side vector having only the first non-zero component equal to unity. The above equality means that $L_M = \sum_{i=1}^{M} \gamma_i L_h(s_i)$ labelled as multioperator is a $(m + M - 1)$th-order approximation to L for arbitrary M. The mth-order operators $L_h(s_i)$ are viewed here as basis operators. The potential for being basis operators satisfying (2) is an inherent feature of compact approximations having free parameters in their inverse operators. It is the case of the one-parametric families of compact upwind differencing (CUD) operators from [2] (their examples can be found also in [7]), the upwinding parameter s being viewed as the free parameter in (1). The third-order CUD operator was considered in the initial paper [1].

In the subsequent works [3–6], the emphasis was placed on approximations to the first derivatives in convection, convection–diffusion and fluid dynamics types of equations. As basis operators, third- and fifth-order CUD operators from [2] were used. It was found that matrix A in (2) can be cast in the form of the product of a non-degenerate triangular matrix and the transpose of the Vandermonde matrix whose rows are powers (or inverse powers) of $s_1, s_2, \ldots, s_M$. It guaranties existence and uniqueness of the considered multioperators. Moreover, the γ_i coefficients of the multioperators can be obtained in analytical forms thus avoiding numerical solution procedures. Though arbitrary-order multioperators can be constructed with arbitrary sets of distinct free parameters values, a limitation on their choice comes from the stability criteria for the resulting schemes. The sets were viewed as admissible if they allowed one to construct upwind biased multioperators schemes. The above cited papers contain an analysis of the admissible values of the parameters in the case of the third-order CUD basis operators and the corresponding fifth-order multioperators conservative schemes ($M = 3$). In [6], the analysis was extended to the case of the fifth-order CUD basis operators described in [7] and seventh-order schemes for conservation laws. Numerical examples concerning the Burgers, Euler and Navier–Stokes equations showed their superior performance when solving both unsteady and steady-state problems. The CUD operators with the upwinding parameter present natural one-parametric families for constructing multioperators approximating the first derivatives in fluid dynamics equations. Using upwind multioperators-based schemes allows one in many cases to obtain good quality spurious oscillations-free solutions without introducing artificial dissipation. However, there exists a variety of problems which do not require upwinding. Small Reynolds number flows may serve as an example. Moreover, the upwinding concept is senseless in the case of discretization procedures for self-adjoint operators, say, for the second derivatives in the Poisson equation appearing in the vorticity-stream function formulation for incompressible flows, in the wave equation for acoustic problems, etc. Thus, it is natural to look for multioperators which are linear combinations of centered basis operators. It was shown in [8] that it is possible to create multioperators for centered differencing formulas as well. In this case, it is sufficient to change in the well known Collatz [9] or Numerov formulas for the first or second derivatives the numerical constants in the inverse operators by the free parameter (thus reducing their order to 2) and then to fix its M values. Using the resulting M operators as the basis ones and proceeding in the above described manner, one can obtain extremely accurate $2M$th-order formulas. Moreover, it was shown in [8], that the left-hand side term of Eq. (1) need not be viewed as a derivative at a grid point. Indeed, it can be other functionals, for example, such as midpoint values of a functions, and integral over cells. The constructed approximations are applied in [8] to a finite-volume type of schemes for convection-diffusion equations and the Poisson equation. In the recent paper [10], the ninth-order multioperators with the CUD fifth-order basis operators from [7] were constructed. They were used for the direct numerical simulation of generation and decay of 2D turbulence in the case of a shear layer instability described by the incompressible Navier–Stokes equations. It was shown that the smallest scales up to the Reynolds number $Re = 400{,}000$ were properly resolved due to good dispersion and dissipation properties of the scheme.

In the present paper, further results concerning arbitrary-order approximations to convection terms are presented. The basis operators this time are obtained by fixing parameters in the fifth-order CUD operator from ([2]) which previously did not receive the attention it needs. Additionally, to illustrate the flexibility of the multioperators principle, a fourth-order one-parametric family of compact approximations is created by following the finite volume strategy. Both families are then used to construct a novel type of multioperators for convection, convection–diffusion and fluid dynamics equations. In all cases, interior approximations are considered only. The results of the recent paper [11] can be used to formulate multioperators boundary closures. It will be a part of the subject of the ongoing publication.

The rest of the paper consists of three sections with the description and analysis of the basis operators, the corresponding multioperators and conclusions. As a particular realization of the theory, the seventh- and ninth-order schemes with illustrating numerical examples are presented in Section 3. Additional details of the previous results in the multioperators area can be found in Appendix A.

2. Basis operators

We consider first the version of the CUD operators families described in [2] and a family of fourth-order compact approximations to first derivatives obtained using quadratures and non-centered compact interpolation formulas. In both cases, the resulting parameter-depending operators can serve as basis operators for novel types of multioperators.

2.1. One-parameter family of fifth-order differencing operators

The third- and fifth-order compact upwind differencing (CUD) operators from [2] approximating first derivatives may be viewed as rational functions of three-point operators depending at least on one free parameter. They do not require grid functions values outside computational domains when applied to derivatives at internal nodes. Following the notations of [2,7], they can be expressed in terms of the unity operator I and three-point central differences Δ_0, Δ_2 defined by

$$\Delta_0 = T_1 - T_{-1}, \quad \Delta_2 = T_1 - 2I + T_{-1}, \quad T_{\pm 1}v_j = v(jh \pm h).$$

In the condensed forms, the rth-order CUD families ($r = 3, 5$) look as

$$\begin{aligned} &\left[\frac{\partial u}{\partial x}\right]_j = L(s)u_j + \mathrm{O}(h^r), \quad r = 3, 5, \\ &L(s) = \left(\Delta(s) + \frac{s}{2}R_1^{-1}(s)Q_1(s)\Delta_2\right)/h \quad \text{or} \\ &L(s) = R_2^{-1}(\Delta(s) + Q_2\Delta_2)/h, \end{aligned} \tag{3}$$

where $\Delta(s) = 0.5(\Delta_0 - s\Delta_2)$, s is the upwinding parameter, h is a constant mesh size, $Q_1 = I, Q_2 = 0$ for $r = 3$, $Q_i = \widetilde{Q}_i(I + \Delta_2/12)^{-1}, i = 1, 2$ for $r = 5$ while three-diagonal operators R_i, $\widetilde{Q}_i$ can be expressed in terms of Δ_0 and Δ_2.

Eq. (3) present two types of compact differencing formulas depending at least on one free parameter. They may be considered as additive and multiplicative corrections, respectively, to the first-order upwind (downwind) differencing operator $\Delta(s)/h$. In the previous publications [2,7] they were referred to as CUD-II-m and CUD-m where $m = 3, 5$ denotes their orders.

A version of the fifth-order operators from [2] was described in [7] where the expressions for R_1 and $\widetilde{Q}_1$ can be found. Now we consider another version from [2] denoting it by $L_5(s)$. In this case, R_1 and $\widetilde{Q}_1$ are defined by

$$R_1(s) = I + \frac{1}{6s}\Delta_0 + \frac{1}{5}\Delta_2, \quad \widetilde{Q}_1(s) = I + \left(\frac{17}{60} - \frac{1}{9s^2}\right)\Delta_2.$$

To calculate the action of $L_5(s) = (\Delta(s) + \frac{s}{2}R_1^{-1}(s)Q_1\Delta_2)/h$ on a grid function, say on $u_j, j = 0, 1, \dots, N$, it is sufficient to calculate first $v_j = (I + \Delta_2/12)^{-1}\Delta_2 u_j$ by inverting the tridiagonal matrix $(I + \Delta_2/12)$, then to calculate $w_j = R_1^{-1}(\widetilde{Q}_1 v_j)$ by inverting again tridiagonal matrix and finally to calculate $\Delta(s)u_j + \frac{s}{2}w_j$. As seen, three-point operators only are involved in the calculations thus using only internal grid values and requiring $O(N)$ operations. It is supposed that boundary conditions are formulated to perform the inversions.

In some instances it is convenient to cast $L(s)u_j$ in the conservative form

$$L_5(s)u_j = (q_{j+1/2} - q_{j-1/2})/h, \tag{4}$$

where $q_{j+1/2}, j = 0, 1, \dots, N-1$ can be calculated in the above described manner with changing $\Delta_0 u_j$ and $\Delta_2 u_j$ by $(u_{j+1} + u_j) - (u_j + u_{j-1})$ and $(u_{j+1} - u_j) - (u_j - u_{j-1})$, respectively. Thus,

$$q_{j+1/2} = G(s)u_j = \frac{u_{j+1} + u_j}{2} - s\frac{u_{j+1} - u_j}{2} + sR_1^{-1}(s)Q_1(s)\frac{u_{j+1} - u_j}{2}. \tag{5}$$

Thus, two different fluxes $q^+_{j+1/2}$ and $q^-_{j+1/2}$ can be calculated for $s > 0$ and $s < 0$, respectively. Obviously, Eq. (4) solves the following reconstruction problem: given grid function u_j, find numerical fluxes $q_{j+1/2}$ in such a way that the divided difference $(q_{j+1/2} - q_{j-1/2})/h$ is the fifth-order approximation to $[\partial u/\partial x]_j$. One can easily verify by using the Taylor expansion series that the above algorithm for calculating $G(s)u_j$ with known u_j can be used for the finite volume reconstruction, that is, given the cell averages

$$\bar{u}_j = \frac{1}{h}\int_{x_{j-1/2}}^{x_{j+1/2}} u(\xi)\mathrm{d}\xi,$$

find $u_{j+1/2} = G(s)\bar{u}_j = [u]_{j+1/2} + O(h^5)$. Form Eq. (4) is typical for all members of the CUD families. It is appropriate for constructing conservative schemes in the case of discontinuous solutions allowing to use flux limiters in shock capturing calculations. Examples of the calculations are presented in [2]. As to the schemes with the above fifth-order approximation with flux limiters, they were tested against the Riemann problem and the supersonic flows described by the Euler equations in [12].

Another important property of the $L_5(s)$ operator concerns with its ability to provide upwind biased approximations. Mathematically, it can be formulated in two ways depending on the assumed spaces U_h of grid functions.

Let U_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 $(u_h, v_h) = h\sum_{j=-\infty}^{\infty} u_j v_j$ and the norm $\|u_h\|_{U_h} = (u_h, u_h)^{1/2}$, it is easy to show that upon presenting $L_5(s)$ as sums of the skew-symmetric $L_5^{(1)}$ and self-adjoint $L_5^{(0)}$ parts $\left(L_5 = L_5^{(1)} + L_5^{(0)}\right)$, one can write

$$L_5^{(1)}(s) = L_5^{(1)}(-s), \quad L_5^{(0)}(s) = -L_5^{(0)}(-s). \tag{6}$$

It was shown in [2] that L_5 is a positive operator, that is $(L_5 u_h, u_h) > 0$ (which means that $\left(L_5^{(0)} u_h, u_h\right) > 0), u_h \in U_h$ if $s > \sqrt{5/3}$. In the similar way, it can be proved that $(L_5 u_h, u_h) < 0$ if $0 < s < 3/2\sqrt{2}$. In terms of the conjugate operation, Eq. (6) can be written as $L(s)^* = -L(-s)$.

Considering the corresponding Fourier space, the real part of the Fourier transform $\widehat{L}_5(s)$ of $L_5(s)$ can be shown to be a non-negative and non-positive function of the Fourier variable for $s > \sqrt{5/3}$ and

$0 < s < 3/2\sqrt{2}$, respectively. It satisfies $\mathrm{Re}\widehat{L}_5(s) = -\mathrm{Re}\widehat{L}_5(-s)$, the imaginary part being invariant under the transformation $s \to -s$.

Suppose now that $\overline{U}_h$ is the space of bounded grid functions $u_j, j = 0, \pm 1, \pm 2, \ldots$ supplied with the norm $\|u_j\| = \max_j |u_j|$. Then it is easy to verify that $L_5 : \overline{U}_h \to \overline{U}_h$ has the eigenfunctions $w_n = \exp(\mathrm{i}\alpha n)$, $0 \leqslant \alpha \leqslant 2\pi, w_n \in \overline{U}_h$. The expressions for the real parts of its eigenvalues are those for the real parts of $\widehat{L}_5$ if one considers $k = \alpha/h$ as the Fourier variable.

By adjusting the sign of s to the slopes of characteristics of convection equations (or directions of a blowing wind), one can obtain semi-discretized schemes which are linearly stable if $\|\cdot\|_{U_h}$ norm is used. The schemes also satisfy the spectral stability criteria if one prefers to use the discrete C-norms and the spectral theory. Thus, there exists the potential for constructing stable fully-discretized schemes when proper time stepping procedures are introduced.

2.2. Fourth-order upwind and downwind operators

Following the integro-interpolation (finite volume type) principle [13], consider the simplest equality:

$$g = \frac{\partial f}{\partial x} \tag{7}$$

and corresponding exact integral relation

$$\int_{jh-h/2}^{jh+h/2} g\,\mathrm{d}x = f_{j+1/2} - f_{j-1/2}. \tag{8}$$

To discretize the RHS of (8), we construct a midpoint interpolation formulas using compact approximations. Considering three-point operators, the required one-parametric family can presented as the interpolation from the left

$$\begin{aligned} &f(x_{j+1/2}) = S_l f_j + \mathrm{O}(h^4), \\ &S_l = \left(I + \left(16s - \frac{1}{8}\right)\Delta_0 + \left(\frac{3}{16} - 8s\right)\Delta_2\right)^{-1}\left(I + \left(16s - \frac{1}{8}\right)\Delta_0 + \left(\frac{3}{16} - 8s\right)\Delta_2\right) \end{aligned} \tag{9}$$

and from the right

$$\begin{aligned} &f(x_{j-1/2}) = S_r f_j + \mathrm{O}(h^4), \\ &S_r = \left(I - \left(16s - \frac{1}{8}\right)\Delta_0 + \left(\frac{3}{16} - 8s\right)\Delta_2\right)^{-1}\left(I - \left(16s + \frac{1}{8}\right)\Delta_0 + \left(\frac{3}{16} + 8s\right)\Delta_2\right). \end{aligned} \tag{10}$$

The RHS of (8) can be approximated as either $(I - T_{-1})S_l f_j$ or $(T_1 - I)S_r f_j$. Using the quadrature formula

$$\int_{jh-h/2}^{jh+h/2} g\,\mathrm{d}x = h\left(I + \frac{1}{24}\Delta_2\right)g_j + \mathrm{O}(h^5)$$

and Eqs. (9) and (10), one arrives at the fourth-order approximations to $\partial f/\partial x$ shown by the following Taylor expansion series:

$$\begin{aligned} &L_{4,l} = \left(I + \frac{1}{24}\Delta_2\right)^{-1}(I - T_{-1})S_l/h, \\ &L_{4,l}[f]_j = \left[\frac{\partial f}{\partial x}\right]_j - \left(\frac{17}{5760} + s\right)h^4 f^{(5)} + \left(32s^2 - \frac{1}{512}\right)h^5 f^{(6)} + \mathrm{O}(h^6), \end{aligned} \tag{11}$$

$$\begin{aligned} &L_{4,r} = \left(I + \frac{1}{24}\Delta_2\right)^{-1}(T_1 - I)S_r/h, \\ &L_{4,r}[f]_j = \left[\frac{\partial f}{\partial x}\right]_j + \left(\frac{17}{5760} + s\right)h^4 f^{(5)} - \left(32s^2 - \frac{1}{512}\right)h^5 f^{(6)} + \mathrm{O}(h^6). \end{aligned} \tag{12}$$

To estimate the positivity (negativity) properties of the "left" and "right" operators $E_{4,l}$ and $E_{4,r}$ respectively, it is worth noting first that their skew-symmetric and self-adjoint components $E_{4,l}^{(1)}, E_{4,r}^{(1)}$ and $E_{4,l}^{(0)}, E_{4,r}^{(0)}$, respectively, satisfy the equalities

$$E_{4,l}^{(1)} = E_{4,r}^{(1)}, \quad E_{4,l}^{(0)} = -E_{4,r}^{(0)}. \tag{13}$$

To prove them, it is sufficient to take into account the commuting property of the involved operators and to cast the operators in the form $A^{-1}B$ or, equivalently, in the form $(A*A)^{-1}(A*B)$. The inverse operator is a self-adjoint positive one while the product $A*B$ can be readily calculated using algebraic manipulations with the linear functions in Δ_0 and Δ_2 and taking into account the easily provable relation $\Delta_0^2 = 4\Delta_2 + \Delta_2^2$. Upon doing so, one can obtain the resulting skew-symmetric and self-adjoint components and verify that the above equalities are true. Thus, if $E_{4,l}$ is positive then $E_{4,r}$ is negative and vice versa. It means that the operators can be used as upwind or downwind approximations to convection terms. However, in contrast to the CUD operators, the switching from the upwind to downwind options occurs when changing the operators indexes rather then when changing the sign of the parameter s. More information can be obtained by considering their Fourier transforms $\widehat{E}_{4,l}(\alpha)$ and $\widehat{E}_{4,r}(\alpha)$ or, equivalently, their eigenvalues. Considering, for example, the real part $\mathrm{Re}\widehat{E}_{4,l}(\alpha)$, one can find that

$$h\mathrm{Re}\widehat{E}_{4,l}(\pi) = \frac{12 - 1536s}{5 + 640s}.$$

Thus, the real part is positive (negative) if $|s| < 1/128$ ($|s| > 1/128$). It agrees with the negativity (positivity) of the third term in the RHS of Eq. (11).

As in the CUD case, the actions of $L_{4,l}$ and $L_{4,r}$ operators can be expressed in terms of numerical fluxes. They look as

$$L_{4,l}f_j = (q^l_{j+1/2} - q^l_{j-1/2})/h, \quad q^l_{j+1/2} = \left(I + \frac{1}{24}\Delta_2\right)^{-1} S_l f_j,$$

$$L_{4,r}f_j = (q^r_{j+1/2} - q^r_{j-1/2})/h, \quad q^r_{j+1/2} = \left(I + \frac{1}{24}\Delta_2\right)^{-1} S_r f_{j+1}.$$

2.3. Related compact schemes

Using the pairs $\{L_5(s), L_5(-s)\}, \{L_{4,l}, L_{4,r}\}$ operators for convection, convection–diffusion equations, hyperbolic and fluid dynamics systems allows one to construct robust stable schemes with positive operators (in the frozen coefficients sense). Optionally, either finite difference or finite-volume type approximations can be constructed in non-linear cases. Below the former strategy will be always followed. One of the possible options [2,7] looks as follows. Consider systems of conservation laws:

$$\frac{\partial \mathbf{u}}{\partial t} + \frac{\partial \mathbf{f}(\mathbf{u})}{\partial x} = 0, \tag{14}$$

where $\boldsymbol{u}$ and $\boldsymbol{f}$ are p-components vectors.

Let L^+ and L^- be the operators from any pair $\{L_5(s), L_5(-s)\}, \{L_{4,l}, L_{4,r}\}$ satisfying $L^+ > 0$ and $L^- < 0$, respectively. Then the semi-discretized scheme for Eq. (14) in the index-free form can be written as

$$\frac{\partial \mathbf{u}}{\partial t} + \mathscr{L}u = 0, \quad \mathscr{L}u = \frac{1}{2}(L^+(\mathbf{f}(\mathbf{u}) + C\mathbf{u}) + L^-(\mathbf{f}(\mathbf{u}) - C\mathbf{u})) = 0, \tag{15}$$

where C is a diagonal matrix with positive entries $(c_1, c_2, \ldots, c_p)$, $c_i > 0, i = 1, 2, \ldots, p$. Now the spatial discretization of Eq. (14) can be presented as

$$\mathscr{L}u = (1/2)(L^+ + L^-)\mathbf{f}(\mathbf{u}) + (1/2)C(L^+ - L^-)\mathbf{u}.$$

The sum and the difference of the operators can be readily recognized as the skew-symmetric and the self adjoint parts of our basis operators, respectively. Depending on the chosen pair, the former can be shown to provide $O(h^6)$ or $O(h^4)$ approximation to $\partial f/\partial x$ while the latter is the positive self-adjoint operator which action on $[f]_j$

can be estimated as $O(h^5)$. Due to positivity of c_i, the second term of the above sum is the positive operator as well (in the frozen coefficients case). It represents a dissipative mechanism which may be viewed as a built-in filter of non-physical oscillations of numerical solutions. The flux splitting in Eq. (15) is similar to the Lax–Friedrichs one, the difference being due to the absence of the direct relation to the Jacobian matrix $\partial \mathbf{f}/\partial \mathbf{u}$.

Assuming $\mathbf{f}(\mathbf{u}) = A\mathbf{u}$ where A is a constant symmetric matrix, it is easy to see that (15) is conditionally stable in the L_2-norm generated by the introduced inner product. It is worth noting that the theoretical stability for the frozen coefficients is guaranteed by the positivity of C and any relation between its entries and the eigenvalues of the corresponding Jacobian matrix is not required. However, practically, it is desirable to use c_i which are of the same orders of magnitude as the eigenvalues are. Otherwise, excessively small or large dissipation may lead to either spurious oscillations of numerical solutions or some loss of accuracy due to large coefficients in the $O(h^5)$ terms.

Specifying time stepping procedures, one can construct various conditionally or unconditionally stable fully discretized schemes. In particular, the Runge–Kutta technique is appropriate for unsteady problems while the following two-level scheme can be used to get steady-state solutions:

$$(I + \tau L_1)\frac{u^{m+1} - u^m}{\tau} + \mathscr{L}u^m = 0, \quad t_m = m\tau, \;\; m = 0, 1, 2, \ldots \tag{16}$$

where L_1 is a preconditioner admitting relatively simple inversion of the time stepping operator and preserving stability of the scheme. One of the possible options is to choose L_1 as a first-order approximation to the x-derivative.

Considering (14) as the scalar equation ($p = 1$) with $f(u) = au, a = \text{const}$, one can estimate in the standard way dispersion and dissipation properties of the semi-discretized scheme with $\mathscr{L}$ operator. To perform the analysis, we use, for example, the space $\overline{U}_h$ of bounded grid functions. Now operator $\mathscr{L} : \overline{U}_h \to \overline{U}_h$ has the eigenfunctions $w_n = \exp(\mathrm{i}\alpha n), 0 \leqslant \alpha \leqslant 2\pi, n = 0, \pm 1, \pm 2, \ldots, w_n \in \overline{U}_h$. Assuming w_n to be the initial value for Eq. (14), the solution of (15) can be readily obtained to give

$$u_n(t) = \mathrm{e}^{-c_1 ad(\alpha)t/h}\mathrm{e}^{\mathrm{i}(\alpha n - a\varphi(\alpha)t/h)} = \mathrm{e}^{-c_1 ad(\alpha)t/h}\mathrm{e}^{\mathrm{i}k(x_n - a\varphi(\alpha)t/\alpha)}, \tag{17}$$

where c_1 is the flux splitting constant, $d(\alpha; s)/h$ and $\varphi(\alpha; s)/h$ are the real and imaginary parts of the eigenvalues while $k = \alpha/h$ is the wave number and $x_n = nh$. The term $a\varphi(\alpha; s)/\alpha = ar(\alpha; s)$ may be viewed as the numerical phase velocity and the deviation of $r(\alpha)$ from unity defines the phase errors introduced by the scheme. Since the parameter s is supposed to be chosen in such away that $ad(\alpha; s) > 0$, the positive function $c_1|d|$ characterizes the attenuation of the initial harmonics during time interval $t = h/|a|$ and may be considered as a measure of the amplitude errors. The phase and amplitude errors can be shown to be $O(\alpha^6)$ for L_5 operators. In the case of the fourth-order operators, they are $O(\alpha^4)$ and $O(\alpha^6)$, respectively.

One can easily extend schemes (15) and (16) to the case of the Euler equations written as conservation laws in curvilinear coordinates. In that case, it is sufficient to construct $\mathscr{L}$ operators corresponding to each spatial coordinate. As to the Navier–Stokes equations, the terms with viscosity coefficients can be approximated quite independently with desired order. In particular, centered compact approximations can be used.

3. Multioperators

The above defined operators families depending on the parameter s can be used for constructing higher-order approximations to first derivatives or convection terms. They differs from those previously investigated in [1,3–5,8].

3.1. Multioperators based on $L_5(s)$ family

The potential for constructing prescribed-order multioperators using basis operators $L_5(s_1), L_5(s_2), \ldots, L_5(s_M)$ where $s_1, s_2, \ldots, s_M$ is a set of distinct values of s is due to the specific form of the Taylor expansion series like (1) for $L_5(s)$. Performing manipulations with the series for Δ_0 and Δ_2, one can arrive at the following expression for the action of $L(s_i)$ on a sufficiently smooth function u

$$
\begin{aligned}
&L_5(s_i)[u]_j = [\partial u/\partial x]_j + \sum_{k=5}^{l} p_{k-4}(s_i)\left[\partial^{k+1}u/\partial x^{k+1}\right]_j h^k + \mathrm{O}(h^{l+1}),\\
&p_{k-4}(s_i) = a_k s_i + \sum_{l=1}^{k-4} b_{kl} s_i^{-l}, \quad i = 1,2,\ldots,M
\end{aligned}
\tag{18}
$$

where a_k and b_{kl} are numerical constants. To prove the second equality in (18), one can use the series manipulation rules and the induction procedure. As an illustration, functions p_1, p_2 and p_3 look as

$$
p_1(s) = \frac{1}{135s} - \frac{s}{120}, \quad p_2(s) = \frac{41}{12600} - \frac{1}{405s^2}, \quad p_3(s) = \frac{160s^{-3} - 291s^{-1} + 54s}{194400}.
$$

Fixing M values $s_1, s_2, \ldots, s_m$ and introducing a partition of unity $\sum_{i=1}^{M}\gamma_i = 1$, the system annihilating $\mathrm{O}(h^k)$ terms, $k = 5, 6, \ldots M + 4$, in (18) reads

$$
\sum_{i=1}^{M}\gamma_i = 1, \quad \sum_{i=1}^{M}\gamma_i p_1(s_i) = 0, \quad \sum_{i=1}^{M}\gamma_i p_2(s_i) = 0, \ldots \sum_{i=1}^{M}\gamma_i p_{M-1}(s_i) = 0. \tag{19}
$$

In the above cited publications, the matrices of the systems like (19) were reduced to transposes of the Vandermonde matrix whose entries are powers of s_i or s_i^{-1}. Thus, the existence and uniqueness of the solutions were guaranteed. However, it is not the case of Eq. (19). It can be shown that there exist hyperplanes in the $(s_1, s_2, \ldots, s_M)$ spaces containing "wrong" values of the parameters.

For example, in the case of $M = 3$, relatively simple algebraic manipulations show that "good" parameters s_1, s_2, s_3 may not satisfy the relation

$$
s_1 s_2 + s_1 s_3 + s_2 s_3 + 8/9 = 0. \tag{20}
$$

Practically, the solvability of (19) can be readily checked by solving it numerically for fixed values of the parameters. Moreover, the search for the solvability domains in the parameters spaces is greatly simplified if one specifies a distribution of the parameter s inside some chosen interval $[s_{\min}, s_{\max}]$. In that case, the determinant of system (19) is a function of two variables and can be readily investigated while $s_{\min}, s_{\max}$ can be used as parameters controlling the multioperators properties.

Suppose now that the existence and uniqueness of the solution of (19) is verified for a particular value of M and a particular parameter distribution for a chosen admissible pair $[s_{\min}, s_{\max}]$. Then one has

$$
L_M[u]_j = \sum_{i=1}^{M}\gamma_i L_5(s_i)[u]_j = \left[\frac{\partial u}{\partial x}\right]_j + \mathrm{O}(h^{M+4}). \tag{21}
$$

Formally, one can assign any integer value to M to obtain arbitrary-order approximation to first derivatives. Moreover, changing M does not influence execution times for calculating $L_M u_j, j = 0, 1, 2, \ldots J$ if parallel machines are used and the corresponding broadcasting and gathering expenses are not taken into account. It can be explained in the following manner.

Suppose that one can use M processors. Choosing any set of M distinct values of s, the task for the ith processor is to calculate the action $L_5(s_i)u_j$ with assumed boundary conditions for L_5 calculations. Performing in the parallel manner, the processors provide outputs which are summed with γ coefficients to give $L_M u_j, j = 0, 1, 2, \ldots J$. Note that increasing M adds no complexity to the execution procedure for each processor. The parallel algorithm is schematically presented in Fig. 1 where the set $u_j, j = 0, 1, 2, \ldots J$ is denoted by u (see Fig. 2).

It can be shown that the multioperator L_M defined by (21) satisfies the equality which is similar to (6)

$$
\begin{aligned}
L_M^{(1)}(s_1, s_2, \ldots, s_M) &= L_M^{(1)}(-s_1, -s_2, \ldots, -s_M),\\
L_M^{(0)}(s_1, s_2, \ldots, s_M) &= -L_M^{(0)}(-s_1, -s_2, \ldots, -s_M).
\end{aligned}
\tag{22}
$$

The proof is based on the fact that the polynomials in (19) are either odd or even functions of s in accordance with the dependencies on s of the skew-symmetric and self-adjoint components of the $L_5(s)$. Due to the zero right-hand sides of all equations in (19) except of the first one corresponding to the partition of unity, the sys-

u

Calculate $L_5(s_1)u$ | Calculate $L_5(s_2)u$ | ... Calculate $L_5(s_M)u$

Calculate $\quad L_M u = \sum_{k=1}^{M} L_5(s_k)u$

Fig. 1. Parallel algorithm.

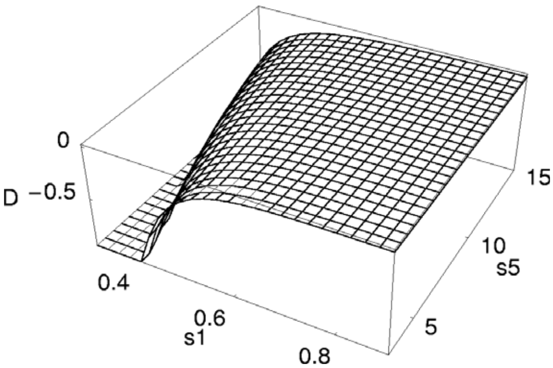

Fig. 2. Determinant of the system for the multioperator coefficients, $M = 5$ (ninth-order multioperator).

tem and therefore its solution is invariant under the change $s \to -s$. Taking into account Eq. (6), the above operators equalities can be easily established.

Now we are interested in pairs $s_{\min}$, $s_{\max}$ defining multioperators with positive (negative) self-adjoint components $L_M^{(0)}(s_1, s_2, \ldots, s_M)$. The bounds of positivity in the plane ($s_{\min}$, $s_{\max}$) can be obtained numerically by solving the following problem.

Find $s_{\min}$, $s_{\max}$ so that $L_M^{(0)}(s_{\min}, s_{\max}) > 0$ or $L_M^{(0)}(s_{\min}, s_{\max}) < 0$.

The problem can be solved by calculating the real part of the Fourier transform $\widehat{L}_M(\alpha), \alpha = kh$, of L_M at each grid point of a grid in the ($s_{\min}$, $s_{\max}$) plane and checking if they are positive or negative for $\alpha \in [0, \pi]$. Supposing that the solution exists, any resulting "good" pair $s_{\min}$, $s_{\max}$ can serve as the multioperators parameters providing positive or negative approximations. In the latter case it is sufficient to use $-s_{\min}, -s_{\max}$ to guarantee multioperators positivity.

As in the case of the basis operators, multioperators actions on grid functions can be presented as a difference of numerical fluxes at the neighbor midpoints. It can be accomplished by multiplying both sides of the Eq. (4) written for $s = s_i$ by γ_i and performing the summation over i. As a result, one arrives at

$$\begin{aligned} &L_M(s)f_j = ((q_M)_{j+1/2} - (q_M)_{j-1/2})/h, \quad (q_M)_{j+1/2} = G_M u_j, \\ &G_M = \sum_{i=1}^{M} \gamma_i G(s_i), \end{aligned} \tag{23}$$

where $G(s)$ is defined in (5). Again, one has the reconstruction procedure which can be applied to the finite volume formulation as well. In that case, one has the equality written for midpoint values in terms of the cell averaged values $\bar{u}_j$:

$$f_{j+1/2} = G_M \bar{u}_j = f(x_{j+1/2}) + \mathrm{O}(h^{M+4}).$$

3.2. Multioperators with $L_{4,l}, L_{4,r}$ basis operators

The Taylor expansion series for $L_{4,l}, L_{4,r}$ operators, Eqs. (11) and (12), show that the coefficients for h^k, $k = 4, 5$, are $(k-3)$th-order polynomials in s. Using the induction procedure, it is possible to show that it is true also for $k > 5$. It means that upon fixing M distinct values of s and introducing a partition of unity $\sum_{i=1}^{m}\gamma_i = 1$, the sums $\sum_{i=1}^{m} s_i\gamma_i, \sum_{i=1}^{m} s_i^2\gamma_i, \ldots, \sum_{i=1}^{m} s_i^{M-1}\gamma_i$ can be obtained successively by equating to zero the coefficients. As a result, one arrives at the following system

$$Sg = \mathbf{r}, \tag{24}$$

where

$$S = \begin{vmatrix} 1 & 1 & \ldots & 1 \\ s_1 & s_2 & \ldots & s_M \\ s_1^2 & s_2^2 & \ldots & s_M^2 \\ \vdots & \vdots & \ddots & \vdots \\ s_1^{M-1} & s_2^{M-1} & \ldots & s_M^{M-1} \end{vmatrix}$$

$\mathbf{g} = (\gamma_1, \gamma_2, \ldots \gamma_M)^T$, $\mathbf{r} = (1, r_2, \ldots r_M)^T$, $r_k, k = 2, 3, \ldots M$ being numerical constants. The system holds for both operators $L_{4,l}, L_{4,r}$ with the same RHS since the corresponding Taylor expansion series differ only in signs of the odd powers to h. The system is known to be always solvable, the solution being readily obtainable in an analytic form. This proves the existence and uniqueness of the left and right multioperators defined by

$$L_{M,l} = \sum_{i=1}^{M}\gamma_i L_{4,l}(s_i), \quad L_{M,r} = \sum_{i=1}^{M}\gamma_i L_{4,r}(s_i), \tag{25}$$

where γ_i are the solution of (24). They approximate first derivatives with $O(h^{M+3})$ truncation errors.

Unfortunately, the condition numbers of systems like (24) dramatically increase with growing M. It adversely effects the accompanied round-off errors. To considerably improve the situation, the distributions of the parameters s_i should be defined as zeroes of the Chebyshev polynomials for chosen intervals $(s_{\min}, s_{\max})$. The zeroes read as

$$s_i = \frac{s_{\min} + s_{\max}}{2} + \frac{s_{\max} - s_{\min}}{2}\cos\frac{(2i-1)\pi}{2M}, \quad i = 1, 2, \ldots, M$$

Practically, using the above parameters distribution allows to construct near 10th-order approximations with quite acceptable round-off errors supported by 64 bits arithmetics. The approximation order can be considerably increased by increasing machine accuracies.

The conjugate properties of $L_{M,l}$ and $L_{M,r}$ defined by Eq. (25) follow immediately from those of the basis operators, Eq. (13):

$$L_{M,l}^{(1)}(s_{\min}, s_{\max}) = L_{M,r}^{(1)}(s_{\min}, s_{\max}), \quad L_{M,l}^{(0)}(s_{\min}, s_{\max}) = -L_{M,r}^{(0)}(s_{\min}, s_{\max}).$$

Thus, the "switching" of the self-adjoint components results from changing of the operator indexes rather than from changing the parameters signs. As in the case of the L_M operators, we consider as "good" values $(s_{\min}, s_{\max})$ those which provide positivity of either of two operators $L_{M,l}, L_{M,r}$. Now the task is to find $(s_{\min}, s_{\max})$ so that the real part of the operators Fourier transforms are either positive or negative. It can be readily accomplished in the same manner as in the case of L_M operator.

3.3. Multioperators-based schemes

Though the multioperators approach can result in formally arbitrary-order approximation to various grid functionals and, in particular, to derivatives at nodal points, their use as a discretization tool for convection terms requires special investigations. It concerns first of all with the search for positivity regions in the $(s_{\min}, s_{\max})$-plane for chosen parameters distributions. Of course, the positivity requirement can be relaxed in the case of stabilized time stepping devices (for example, implicit ones), but its fulfilment important if one follows the strategy of constructing robust schemes. Once the required parameters domains are specified, the next step is a fine tuning of the parameters aimed at some desirable optimization.

To be definite, suppose that $L_M(s_{\min}, s_{\max}) > 0$ or $L_{M,l}(s_{\min}, s_{\max}) > 0$. Denoting the operators by L^+, we define then L^- as $L_M(-s_{\min}, -s_{\max})$ or $L_{M,r}(s_{\min}, s_{\max})$. With the notations, the semi-discretized scheme (15) and its extensions to the described in Section 2.3 fully-discretized forms may serve as examples of conservative linearly stable multioperators-based schemes. They can be rewritten in terms of numerical fluxes needed if flux limiters are used in shock capturing calculations. Optionally, one can set the flux splitting matrix C equal to zero to obtain dissipation-free non-robust schemes.

In the case of diffusion terms, the centered desired-order multioperators approximations described in [8] or other high-order approximations can be used.

3.3.1. Dispersion and dissipation

Returning to the solution (17) of the advection equation with a constant coefficient $a > 0$ for the x-derivative, the numerical phase velocity resulting from the multioperators approximations is $a^* = a\varphi(\alpha)/\alpha, \varphi(\alpha) = h\mathrm{Im}\hat{L}^+(\alpha), \alpha = kh$. The deviation of the relative phase velocity from the unity $e_p = |a^*/a - 1|$ may be considered as a measure of the phase errors. Similarly, $e_a = d(\alpha) = h\mathrm{Re}\widehat{L}^+$ may be viewed as a dissipation parameter characterizing the amplitude errors.

In the long wave limit, the phase velocity and amplitude errors can be estimated as $\mathrm{O}(\alpha^{K+1})$ where the approximation order K is supposed to be odd. Thus, very accurate harmonics representation can be expected for some interval $0 \leqslant \alpha \leqslant \alpha_*$. As in the case of the basis operators, the growth of the phase errors beyond this interval is accompanied by increasing dissipation which plays role of a built-in filter of spurious oscillations. As to the actual values of α_*, high approximation orders of multioperators do not necessary mean that α_* is considerably greater than those in the case of the corresponding basis operators. To increase the values in the case of traditional high-order finite difference schemes, some optimization procedures were suggested (see, for example, [14,15,17]). Optimization can be used in the present case as well by considering $s_{\min}$ and $s_{\max}$ as controlling parameters. Several strategies depending on problems to be solved can be thought of. For example, target functionals for selected wave numbers intervals can be constructed to minimize phase errors e_{p}, to minimize amplitude errors e_{a} or to minimize simultaneously both phase and amplitude errors e_{p} and e_{a}. The number of controlling parameters can be increased when using the following options.

(i) If one uses the flux splitting in Eq. (4), the dissipation can be controlled by the diagonal entries of the matrix C (or by the constant c_1 in the scalar case). In particular, one can obtain dissipation-free schemes by setting the constants to zeroes.
(ii) Calculations of multioperators actions can be organized in the following way. Instead of calculating the L^+ and L^- actions on positive and negative fluxes respectively, one can calculate the action of $L^+ + L^-$ on f_j and the action of $L^+ - L^-$ on u_j using different pairs ($s_{\min}$, $s_{\max}$). In the former case one can use the pair which is the best choice in the dispersion preserving sense while in the latter case another pair can be chosen to provide near zero dissipation errors for the obtained interval of near zero dispersion errors.
(iii) Additional free parameters can be introduced by increasing the number of the parameters s_i without increasing approximation orders.

Various optimization procedures are beyond the scope of the present paper. In the following subsection, we shall restrict ourselves to examples of the dispersion and dissipation functions obtained by calculating the Fourier transforms of the operators for several values of parameters pairs and choosing visually the "best looking" functions in α.

3.3.2. Comments on boundary conditions

Boundary conditions for calculations of the multioperators actions are essentially those needed in the case of the corresponding basis operators. Thus, in contrast to conventional approximations, no extra numerical boundary conditions are required when increasing approximation orders. However, there is the following latent difficulty emerging if one tries to get approximation orders at boundaries conforming with those of multioperators.

When killing the low-order terms in the expansion (1) for $L_h(s)$, it was implicitly assumed that the latter holds everywhere in a computational domain. Generally, boundary operators in non-periodic cases of bounded domains has expansions different from (1) thus producing mismatch near the boundaries. Consequently, multiplying by γ_i with summing over i does not annihilate higher-order terms near boundaries. The exception is periodic problems when no special boundary operators are needed. One way out is to construct boundary operators for each s_i which preserve the main expansion at internal points at least with certain degree of accuracy. It can be accomplished by using other multioperators which extrapolate with a prescribed order actions of basis operators at near-boundary grid points. Such multioperators are planned to be presented in Part II of the present paper. The technique can be used for conventional compact schemes as well.

The possibility of non-conforming boundary and interior schemes is also worth discussing. It should be noted that matrices to be inverted may, on occasion, posses noticeable diagonal dominance. It means that the influence of boundary values decays rapidly with increasing distances from boundaries. Therefore, local higher-order and higher accuracy can be obtained almost everywhere in computational domains, the exception being only boundary and near boundary nodes where orders and accuracy are expected to be those of the basis operators. Having in mind that the basis operators can be quite accurate, the idea of using their "native" boundary conditions may be viewed as quite acceptable from the practical viewpoint at least in some instances.

3.4. Schemes with seventh- and ninth-order multioperators

As a particular realizations of the above presented theory, consider the schemes based on the seventh- and ninth-order L_M operators ($M = 3, 5$).

In the simplest case of $M = 3$ one has $L_5(s_1), L_5(s_2), L_5(s_3)$ basis operators. Assuming an uniform distribution $(s_1, (s_1 + s_3)/2, s_3)$, it is easy to see that the LHS of (20) reduces to $((s_1 + s_3)^2 + 2s_1s_3)/2 + 8/9$ which is positive if $s_1s_3 > 0$. Under this condition, equality (20) is never satisfied and seventh-order multioperators do exist. Fixing, for example, positive values of s_1 and s_3, $s_1 < s_3$, one can solve the linear system of three equations to obtain coefficients $\gamma_1, \gamma_2, \gamma_3$ giving the seventh-order multioperator depending on two parameters. We denote it by L_{57},

$$L_{57}(s_1, s_3) = \sum_{k=1}^{3} \gamma_k L_5(s_k),$$

thus specifying the orders of basis operators and the resulting multioperator. To estimate the domains in the (s_1, s_3)-plane where $L_{57}(s_1, s_3) > 0$, the Fourier transform

$$\widehat{L}_{57}(\alpha; s_1, s_3) = \sum_{k=1}^{3} \gamma_k \widehat{L}_5(\alpha; s_k)$$

was calculated. It was found that its real part $d_7(\alpha; s_1, s_3) = h\mathrm{Re}\widehat{L}_{57}(\alpha; s_1, s_3)$ is a negative function in $\alpha, 0 \leqslant \alpha \leqslant \pi$, at least if $(s_1, s_5) \in \Omega_7$ where Ω_7 is defined by

$$\Omega_7 = \{.8 \leqslant s_{\min} < s_{\max}, 2 \leqslant s_{\max} \leqslant 20\} \tag{26}$$

with $s_{\min} = s_1$ and $s_{\max} = s_3$. Hence, the operator can be viewed as a positive one for the pairs $(-s_1, -s_3)$ satisfying $(s_1, s_3) \in \Omega_7$.

Consider now the case $M = 5$, that is, ninth-order multioperator. Fixing, for example, an uniformly distributed five parameters $s_1 < s_2 < \cdots < s_5$, one obtains the linear system which solution (if exists) gives five values of the coefficients depending on two parameters, say, s_1 and s_5. The resulting multioperator is defined by

$$L_{59}(s_1, s_5) = \sum_{k=1}^{5} \gamma_k L_5(s_k).$$

Unfortunately, analytical estimates of the parameters domains guaranteeing multioperators existence become too complicated in this case. However, the existence can be readily checked (at least locally) by calculating the determinant of the system $D(s_1, s_5)$ as a function of two variables. The calculations for $1 \leqslant s_1, s_5 \leqslant 15$ give the surface $D(s_1, s_5)$ shown in Fig. 1. As seen, it has no common points with the plane $D(s_1, s_5) = 0$.

The search for a positivity domain in (s_1, s_5)-plane can be carried out in the above described manner. In the case of the uniform parameters distribution, the calculations show that $d_9(\alpha; s_1, s_5)$, the real part of the Fourier transform $h\widehat{L}_{59}(s_1, s_5)$, is negative if $(s_1, s_5) \in \Omega_9$ where Ω_9 can be defined approximately by (26) with $s_{\max} = s_5$.

Once the positivity domains are found, the $s_{\min}$ and $s_{\max}$ values can be used to control the dispersion and dissipation properties in the case of advection equations with constant coefficients. Avoiding introducing functionals to be minimized, we use this opportunity by varying the parameters and observing the phase velocity and dissipation functions $r(\alpha)$ and $d(\alpha)$. The procedure was aimed at producing an example rather than obtaining the best possible results.

In the present case, the dispersion relation preserving property may be characterized by the relative numerical phase velocity given by $r_k(\alpha) = h\mathrm{Im}\widehat{L}_{5k}(\alpha)/\alpha, k = 7, 9$. Unexpectedly, it was found that "good" values of s_1 for fixed $s_{\max} = s_3, s_5$ from the interval $5 \leqslant s_{\max} \leqslant 15$ in the seventh- or ninth-order case, respectively, are close to 0.8 for both multioperators. The functions $r(\alpha) = r_m(\alpha), m = 7, 9, \alpha = kh$ are shown in Fig. 3 for $s_1 = .82, s(3) = 10$ and $s_1 = .835, s(5) = 15$ in the case of the seventh-order and ninth-order multioperators, respectively. Though the curves for $M = 3$ and $M = 5$ look almost identical, the numerical values of the phase errors were found to be considerably smaller in the latter case for the long and medium waves, the estimates being $O(\alpha^8)$ and $O(\alpha^{10})$ for $M = 3$ and $M = 5$, respectively. Accordingly, the calculations give, for example, $|1 - r_7(\pi/4)| = 2.1 \times 10^{-6}, |1 - r_9(\pi/4)| = 1.2 \times 10^{-7}$.

The dispersion errors $|1 - r(\alpha)|$ are shown in Fig. 4 for $M = 3$ and $M = 5$. As seen, the phase errors introduced by the ninth-order multioperator are very small in the interval $0 \leqslant kh \leqslant \pi/2$, their maximum value being 1.66×10^{-5} at $kh = \pi/2$. The upper limit of kh for which the errors are less than 5×10^{-5} is about 1.9.

It is worth comparing the above errors with those for existing optimized schemes, for example, for the schemes from [17]. Following the definition of resolving efficiency first introduced in [16] and using notations from [17], we rewrite the dispersion errors as $E_k = |k^*\Delta x - k\Delta x|/\pi, \Delta x = h$ where k^* is the effective wave number. In our notations, $E_k = |1 - r| * kh/\pi$. The criteria introduced in [17] are $E_k < 5 \times 10^{-4}$ and $E_k < 5 \times 10^{-5}$.

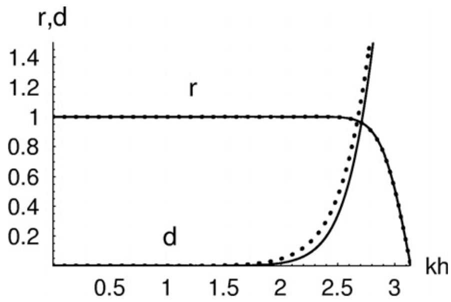

Fig. 3. Relative phase velocity and dissipation parameter vs. dimensionless wave number. Solid and dashed lines correspond to ninth- and seventh-order multioperators.

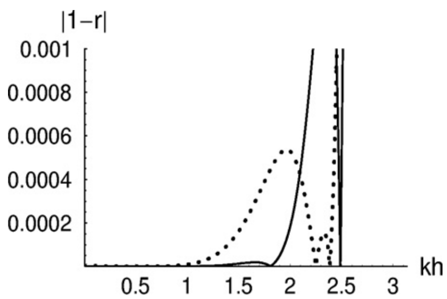

Fig. 4. Dispersion errors vs. dimensionless wave number. Solid and dashed lines correspond to ninth- and seventh-order multioperators.

They were viewed as indications of maximum wave numbers properly and accurately resolved by schemes and were expressed in terms of numbers of points per wave length, $\lambda_p/\Delta x$ and $\lambda_a/\Delta x$ respectively. In the ninth-order case, the values are 2.9 and 3.25 as compared with 3.36 and 4.66, the data corresponding to the best results from [17].

The dissipation functions $d(\alpha) = d_m(\alpha), m = 7, 9$ shown in Fig. 3 are also found to be practically independent of the maximal parameters values $s_{\max}$. Though they are visually closely aligned, the small dissipation wave number upper limit is slightly larger in the $M = 5$ case (see Fig. 3). Moreover, the values of $d_9(\alpha)$ are considerably smaller than those of $d_7(\alpha)$ for $kh < \pi/2$. For example, $|d_7(\pi/4)| = 1.7 \times 10^{-5}$, $|d_9(\pi/4)| = 4.1 \times 10^{-7}$, respectively.

Comparing the low dispersion and low dissipation wave number domains, it should be noted that (as seen in Fig. 3) the latter is slightly narrower than the former for the present parameters choices. However, as was mentioned previously, it is possible to optimize both errors individually by choosing different parameters pairs.

Outlining briefly the seventh- or ninth-order multioperators Eq. (25) based on the operators $L_{4,l}$ and $L_{4,r}$, Eqs. (11) and (12), the following specific issues should be emphasized.

(i) The multioperators existence is guaranteed for distinct values of the parameters. Their best choice is the Chebyshev distributions for chosen pairs ($s_{\min}$, $s_{\max}$).
(ii) Since the operators are the fourth-order ones, one should set $M = 4$ and $M = 6$ to get the multioperators with $O(h^7)$ and $O(h^9)$ dissipative leading terms in their Taylor expansion series.
(iii) Once the positivity domains are found for each multioperator, their negative counterparts can be obtained using the "opposite" basis operators (that is, the operators with the index r instead of l or vice versa) rather than changing the signs of the parameters, the γ coefficients being unchanged. Considering, for example, the ninth-order left multioperator:

$$L_{49,l}(s_{\min}, s_{\max}) = \sum_{k=1}^{6} \gamma_k L_{4,l}(s_k),$$

it was found to be positive at least if the $(s_{\min}, s_{\max})$ pair belongs to the region marked by "+" in Fig. 5.

It was found also that the optimization procedures turn out to be more efficient if different pairs from the domain are used for the dispersion and dissipation tunings. As an illustration of the individual approximate tuning, Fig. 6 displays the phase and amplitude curves obtained for the pairs (−0.1793, −0.3) and (−0.189, −0.3), respectively. As seen, this time the small dissipation region is wider than the dispersion preserving one.

The scheme with the multioperators pair $(L_{49,l}, L_{49,r})$ used in the calculations presented below is referred to as the scheme with the L_{49} multioperator.

3.5. Numerical examples

3.5.1. Inviscid Burgers' equation

Consider first the periodic IVP problem for the Burgers equation which is often used as a testing one (see, for example [18,15])

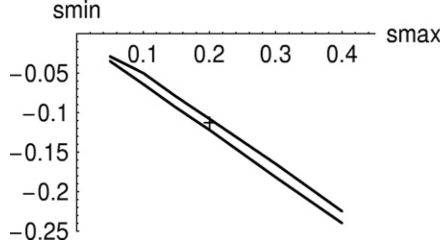

Fig. 5. Domain of positivity for the $L_{M,l}$ ninth-order multioperator (marked by "+").

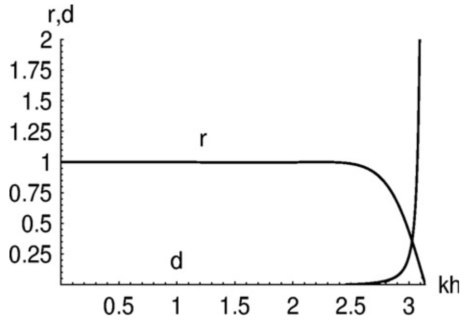

Fig. 6. Relative phase velocity and dissipation parameter vs. dimensionless wave number in the case of $L_{M,l}$ ninth-order multioperator.

$$\begin{aligned}&\frac{\partial u}{\partial t}+\frac{\partial}{\partial x}\frac{u^2}{2}=0, \quad -1\leqslant x\leqslant 1,\\ &u(0,x)=1+0.5\sin(\pi x), \quad -1\leqslant x\leqslant 1.\end{aligned} \tag{27}$$

The exact solution up to $t = 2/\pi$ is smooth. It can be obtained using an iterative procedure described in [15] with the machine precision. Its values at grid points will be denoted by u_j^{ref}.

The calculations with the splitting constant $c_1 = 1$ were carried out using the fourth-order Runge–Kutta method. To exclude the influence of the relatively low order of the time stepping technique, sufficiently small values of the CFL number were used. The accuracy was estimated using the discrete C-norm giving numerical solution errors and approximate mesh convergence orders as

$$E_{\mathrm{c}}(n)=\max_j|u_j-u_j^{\mathrm{ref}}|, \quad k_{\mathrm{c}}=\log_2\frac{E_{\mathrm{c}}(n)}{E_{\mathrm{c}}(2n)}.$$

In Table 1, the results for L_{57}, L_{49} and L_{59} multioperators corresponding to time $t = 0.3$ are presented for several meshes with the number of nodes n. For comparison, the data from [10] obtained with the previous versions of ninth-order multioperators (denoted here by $L_{59\mathrm{a}}$ and L_{39}) are included in the table. The multioperators are based on another fifth-order operator from [2,7] (denoted here by $L_{5\mathrm{a}}$) and one of the third-order CUD basis operators from [2]. The table contains also the results of calculations with the fifth-order WENO scheme presented in [10]. As seen, the schemes with L_{57} and L_{59} outperform all other schemes demonstrating remarkably high accuracy (especially, in the latter case). Note that the claimed convergence orders of the

Table 1
1D Burgers' equation: the discrete C-norms of the solution errors and the convergence orders obtained by different methods

n		8	16	32	64	128	256
WENO-5	E_c	6.47e − 2	1.25e − 2	1.20e − 3	9.50e − 5	3.31e − 6	8.66e − 8
	k_c		2.4	3.4	3.7	4.8	5.3
L_{5a}	E_c	3.99e − 2	6.10e − 3	4.35e − 4	1.63e − 5	5.11e − 7	1.56e − 8
	k_c		2.71	3.81	4.74	5.00	5.03
L_{39}	E_c	4.96e − 2	7.86e − 3	3.85e − 4	9.01e − 6	7.76e − 8	3.58e − 10
	k_c		2.66	4.35	5.42	6.86	7.76
L_{49}	E_c	1.95e − 2	2.11e − 3	1.22e − 4	1.07e − 6	5.85e − 9	3.79e − 11
	k_c		3.24	4.07	6.83	7.51	7.27
L_{59a}	E_c	3.30e − 2	2.89e − 3	1.30e − 4	2.17e − 6	1.30e − 8	3.46e − 11
	k_c		3.51	4.47	5.91	7.38	8.55
L_{57}	E_c	1.82e − 2	2.14e − 3	3.61e − 5	2.21e − 7	8.03e − 10	3.38e − 12
	k_c		3.1	5.9	7.3	8.1	7.9
L_{59}	E_c	1.74e − 2	1.86e − 3	2.16e − 5	5.02e − 8	4.7e − 11	9.96e − 14
	k_c		3.2	6.4	8.7	10	9.2

schemes settle earlier when doubling the number of nodes as compared with those for other ninth-order multioperators. The last were found to provide the ninth-order mesh-convergence only in the case of more refined meshes than those presented in the table.

Comparing the schemes with L_{49} and L_{59a}, the present calculations show their approximately similar performances. However, slight preference may be given to the former due to its relative simplicity. The L_{39} operator is seen to be less accurate than other ninth-order operators. It can be explained by the fact than the condition number of the corresponding Vandermonde matrix for $M = 7$ can be greater than that for $M = 5$ resulting in larger absolute values of the γ_i coefficients. In turn, it leads to relatively large numerical constants in the truncation errors. At the same time, the operation counts when calculating the operators actions in the case of the fifth-order CUD basis operators are nearly twice as large as those for the third-order CUD ones.

Though Table 1 gives a general idea of the multioperators performances, it is worth noting that the presented results concern particular choices of the involved parameters which are not necessarily optimal for each scheme. Thus, the possibility exists of further decreasing the corresponding solution errors. In turn, it may influence the estimates of the relative efficiency of the schemes.

3.5.2. *Discontinuous solutions*

Exploiting exact solutions smoothness, the present paper does not concern with shock capturing calculations. It should be emphasized however that once multioperators numerical fluxes are calculated, it is possible to correct them to suppress spurious oscillations well localized near discontinuities. To do so, one can look for a flux limiter best suited to the present case. To illustrate the capability of the multioperators schemes to deal with discontinuous solutions, the calculations for Eq. (27) were carried out up to $t = 1.1$. For that time moment, the exact solution of Eq. (27) is no longer smooth. As an example of possible limiters, one of the earliest devices [20] was used. In Fig. 7, the corrected numerical solution $u(x_j, t), x_j = -1 + jh, j = 0, 1, \dots n, n = 320, t = 1.1$ (shown by markers) is compared with the exact one (shown by the solid line). Although some loss of accuracy can be detected near the discontinuity, the numerical and the exact solutions are visually undiscernible. It should be noted that the numerical solutions obtained without correcting numerical fluxes (not presented here) show only marginal non-monotone behavior.

3.5.3. *3D inviscid Burgers' equation*

We consider now the example presented in [19]. The IVP periodic problem reads

$$
\begin{aligned}
&\frac{\partial u}{\partial t} + \frac{\partial}{\partial x}\frac{u^2}{2} + \frac{\partial}{\partial y}\frac{u^2}{2} + \frac{\partial}{\partial z}\frac{u^2}{2} = 0, \\
&u(0, x) = 0.25 + \sin(\pi x)\sin(\pi y)\sin(\pi z), \quad -1 \leqslant x \leqslant 1, -1 \leqslant y \leqslant 1, -1 \leqslant z \leqslant 1.
\end{aligned} \tag{28}
$$

Its exact solution can be readily obtained using an iteration procedure for solving algebraic equations [19]. The calculations were carried out with the fourth-order Runge–Kutta time stepping and the ninth-order multioperators based on $L_5(s)$ operators corresponding to the x, y, z coordinates, the parameters distribution being the

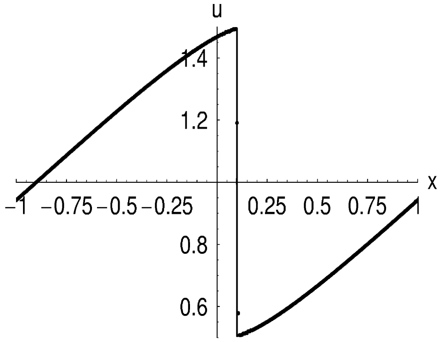

Fig. 7. Comparison of numerical and exact solutions of the Burgers' equation at $t = 1.1$ (shown by markers and solid line, respectively).

Table 2
3D Burgers' equation: the l_1-norms of the solution errors and the convergence orders obtained by the present ninth-order scheme

n		5	10	20	40	80
L_{59}	l_1	5.89e − 3	1.94e − 4	1.57e − 7	1.48e − 10	9.10e − 14
	k_c		4.92	10.27	10.51	10.66

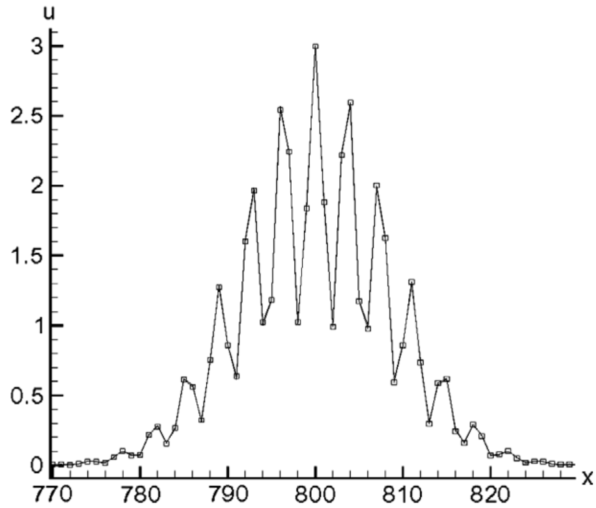

Fig. 8. Exact and numerical solutions of the linear advection equation at grid points shown by solid line and markers, respectively ($t = 800$).

same. The l_1 norm of the numerical solutions errors and mesh convergence orders are shown in Table 2. Again, extremely high accuracy of the technique can be deduced from the Table. For example, the error for $n = 80$ is about five orders of magnitude less than that in the case of the fifth-order ADER5 scheme from [19].

3.5.4. Acoustic benchmark problem

To illustrate resolution properties of schemes with L_{59} operators, consider the following initial value problem

$$\frac{\partial u}{\partial t} + \frac{\partial u}{\partial x} = 0, \quad u(0,x) = [2 + \cos(\beta x)][\exp(-2\ln(2)(x/10)^2)], \quad \beta = 1.7$$

to be discretized using the uniform mesh with $h = 1$. The comparison of the exact solutions and the obtained numerical solution at times $t = 400$ and $t = 800$ is needed. The problem was proposed by C. Tam in [21].

In our notations, the dimensionless wave number $\alpha = \beta = 1.7 > \pi/2$ approximately corresponds to the domain of small phase and amplitude errors of the scheme for very short wave lengths.

Fig. 8 shows the comparison of the calculations at $t = 800$ with the solid line and markers presenting the exact and numerical solutions respectively. Visually, no difference between the solutions is seen in the figure.

4. Conclusions

Further results in the framework of the multioperators arbitrary-order approximation are presented. Two types of upwind (downwind) parameter-dependent operators of the fifth and the fourth-order are described. They can serve as a basis operators by setting different values to the parameters. Linear combinations of the basis operators (referred to as multioperators) allow to construct prescribed order approximations to convection terms. It is shown that the approximations can be cast in the form of numerical fluxes differences. It provides the potential for creating conservative schemes with possible flux corrections in the case of discontinuous solutions.

The solvability of the linear systems for the combination coefficients is either guaranteed or can be verified numerically. Since basis operators differ only in their parameters values, calculations of the multioperators actions on known grid functions can be organized in a parallel manner. In that case, an increase of approximation orders can be achieved simply by adding more parameters and more processors involved in the calculations.

Following the strategy of constructing upwind schemes, the sets of the basis operators parameters should be chosen to ensure the positivity (negativity) of the resulting multioperators in the standard Hilbert spaces of grid functions. This can be accomplished by calculating the real parts of their Fourier transforms.

The paper concerns with spatial discretizations only. To construct fully discretized schemes, one can use any reasonable time stepping procedure. It can be, for example, the Runge–Kutta technique for unsteady calculations or a two-level preconditioned implicit scheme for getting steady-state solutions. In both case, a flux splitting of the Lax-Friedrichs type with positive splitting constants instead of maximum absolute values of flux function derivatives is suggested.

In the case of the advection equation with a constant coefficient, semi-discretized multioperators schemes show very small amplitude and phase errors for physically relevant wave numbers supported by meshes. In the highest wave numbers regions, the multioperators dissipative mechanism plays role of a built-in filter of spurious oscillations. Using several options of choosing schemes parameters, it is possible to considerable enlarge the dispersion relation preserving domains of the wave numbers.

As particular examples of the realization of the multioperators principle, semi-discretized schemes with the seventh- and ninth-order multioperators are presented. Their dispersion and dissipation properties are outlined. It was shown that the upper limits of the dimensionless wave numbers for which the phase and amplitude errors are very small (about 10^{-5}) can be noticeably greater than $\pi/2$ for particular choices of the parameters distributions. However, the same property for fully discretized schemes is critically dependent on chosen time stepping techniques.

Generally, multioperators schemes are multipurpose ones. They can be used for solving various CFD problems allowing to construct sufficiently smooth meshes. However, their main areas of applications seem to be DNS, LES, aeroacoustics and other problems requiring calculations for large time intervals. Possibly, higher-than-fourth-order low dissipative and low dispersive Runge–Kutta methods are needed in many cases.

Acknowledgements

This work has been supported by Russian Fund of Basic Researches (Grant 05-01-0584) and by Basic-Research Program No. 3 of the Department of Mathematical Sciences, Russian Academy of Sciences (Project No. 3.15).

Appendix A. Brief outlines of the previous multioperators results

The idea of increasing approximation orders of numerical formulas by using appropriate linear combinations of operators from one- parameter operators families was first presented by the author at the Manchester parallel CFD conference (1997) [1]. It resulted from close examination of the Taylor expansion series for the earliest form of the compact upwind differencing (CUD) operators [2]. The series at grid point x_j look as

$$\frac{1}{h}\left(I+\frac{1}{6}\Delta_2-\frac{s}{4}\Delta_0\right)^{-1}\Delta(s)[f]_j=\left[\frac{\partial f}{\partial x}\right]+\frac{s}{24}h^3f_j^4+\left(\frac{s^2}{48}-\frac{1}{180}\right)h^4f_j^5+\cdots \tag{A.1}$$

where Δ_0 and Δ_2 operators are those used in Eq. (3). It was observed that the $O(h^3)$ and $O(h^4)$ terms can be killed by substituting in Eq. (A.1) distinct values of the parameter $s=s_1,s_2,s_3$ and summing the resulting equations pre-multiplied by a partition of unity $\gamma_1,\gamma_2,\gamma_3,\sum_{i=1}^{3}\gamma_i=1$. Equating the coefficients for h^3 and h^4 to zero and taking into account the partition of unity condition, the linear system for γ_i then reeds

$$\sum_{i=1}^{3}\gamma_i = 1, \quad \sum_{i=1}^{3}s_i\gamma_i = 0, \quad \sum_{i=1}^{3}s_i^2\gamma_i = \frac{1}{180}. \tag{A.2}$$

The system is always solvable for distinct values s_i since its matrix is of the Vandermonde type. Retaining more terms in the above expansion series, one can verify that the successive powers of s, that is $s^3, s^4, \ldots$, appear in the expressions for the expansion coefficients. It is a particular manifestation of the general property of the expansion series in the case of inverse operators depending on a parameter. More terms in the sums of the pre-multiplied expansions (A.1) can be cancelled by fixing more values of s. Denoting the left-hand sides of Eq. (A.1) by $L_3(s_i)[f]_j, i = 1, 2, \ldots, M$, the linear combination $L_M = \sum_{i=1}^{M}\gamma_i L_3(s_i)$ was referred to as the "multioperator" generated by the basis operators $L_3(s_i)$. It defines $O(h^{M+2})$ approximation to the first derivatives of $f(x)$ at grid points.

In the subsequent studies, other CUD operators from [2] depending on the upwinding parameter s were used as basis ones. The sole exception was the fifth-order operator of the present paper (it was erroneously supposed that investigation into the corresponding multioperator will not provide additional useful information).

For brevity, we denote below any CUD-based multioperator by L_M. In all cases, it was found that matrices of the systems for the coefficients γ_i are the Vandermonde matrices whose entries are powers either of s_i or of s_i^{-1}. It guarantees existence and uniqueness of the related multioperators for *all sets of the parameter values*. Moreover, solutions of the systems can be obtained in analytical forms.

In the theoretical studies, the emphasis was on the properties of the skew-symmetric and self adjoint components of L_M's viewed as operators in the standard Hilbert spaces of grid functions. The studies were considerably simplified by writing them in terms of the Δ_0 and Δ_2 operators used in Eq. (A.1). Of interest were, in particular, their response to the transformation $s_i \to -s_i, i = 1, 2, \ldots, M$. It was found that L_M's change signs of their self-adjoint components when changing signs of the underlying basis operators while the skew-symmetric components are invariant under the transformation. Denoting by $\widehat{L}_M(kh; s_1, s_2, \ldots, s_M)$ the multioperators Fourier transforms, it means that

$$\begin{aligned}
\mathrm{Re}\widehat{L}_M(kh; s_1, s_2, \ldots, s_M) &= -\mathrm{Re}\widehat{L}_M(kh; -s_1, -s_2, -\ldots, s_M),\\
\mathrm{Im}\widehat{L}_M(kh; s_1, s_2, \ldots, s_M) &= \mathrm{Im}\widehat{L}_M(kh; -s_1, -s_2, -\ldots, s_M).
\end{aligned}$$

The algebraically equivalent expressions can be written for the real and imaginary parts of the eigenvalues of L_M if the space of bounded grid functions with the discrete C-norm is assumed. Thus, the multioperators preserve the similar property of the underlying basis operators. Having in mind multioperators-based schemes for CFD applications, it was assumed that L_M must satisfy other two conditions characterizing their basis operators. The conditions are as follows:

(i) There exists a domain in the parameters space for which multioperators are positive. In the terms of the Fourier transforms, it means the existence of a set $s_1, s_2, \ldots, s_M$ such that $\mathrm{Re}\widehat{L}_M(kh; s_1, s_2, \ldots, s_M) > 0$.
(ii) The dissipation may not vanish for the shortest waves theoretically supported by meshes, that is $\mathrm{Re}\widehat{L}_M(kh; s_1, s_2, \ldots, s_M) \neq 0$ in the vicinity of $kh = \pi$.

The first condition means the possibility of constructing upwind schemes while the second one suggests the existence of a built-in filter of spurious oscillations of numerical solutions.

It was found that the second condition rules out multioperators based on CUD operators with multiplicative corrections in Eq. (3) and, in particular, multioperators resulting from the expansion series Eq. (A.1). In fact, the values $\mathrm{Re}\widehat{L}_M(\pi; s_1, s_2, \ldots, s_M)$ were found in that case to be proportional to $\sum_{i=1}^{3}s_i\gamma_i$. The sum is equal to zero since it is the left-hand side of the second equation in both (A.2) and the similar system in the case of the fifth-order multiplicative correction operator in Eq. (3). Thus, only the remaining additive correction CUD operators were used as basis ones. Their description can be found in [7].

To improve the conditioning of the linear systems for the γ coefficients, the values of the parameter s were always chosen as zeroes of the Chebyshev polynomials for some intervals $[s_{\min}, s_{\max}]$. Thus, the search for parameters sets satisfying (i) was reduced to finding domains in the $s_{\min}$, $s_{\max}$ plane providing positive values of $\mathrm{Re}\widehat{L}_M(kh; s_{\min}, s_{\max}), 0 \leqslant kh \leqslant \pi$. In some instances the simplest case $M = 3$, the estimates of the positivity domains were obtained analytically.

The flux-splitting schemes outlined in Section 2.3 with the CUD-based multioperators were used for both Euler and Navier–Stokes calculations. It was found that multioperators schemes can be advantageous over the fifth-order CUD ones even though a single processor machine is used. It is due to the superior resolution properties of the higher-order methods allowing to use coarser meshes for good representation of fine solution details.

Calculations of thin shear layers instability reported in [10] were carried out using partly a cluster parallel system. They were characterized by a noticeable speed-up factor. However it was less than the''ideal'' one (which is equal to the number of involved processors) due to data exchange operations.

More details concerning the CUD-based multioperators can be found in the papers mentioned in Section 1.

A.1. Multioperators with central compact differencing operators

Families of high-order compact approximations to various grid functionals (and, in particular, to derivatives at grid points) were proposed by Lele in his well-known paper [16]. In the simplest case of the first or second derivatives and three-point stencils, the differencing formulas in our notations look as

$$\frac{1}{2h}\left(I + \frac{1}{6}\Delta_2\right)^{-1}\Delta_0[f]_j = \left[\frac{\partial f}{\partial x}\right]_j + \mathrm{O}(h^4),$$
$$\frac{1}{h^2}\left(I + \frac{1}{12}\Delta_2\right)^{-1}\Delta_2[f]_j = \left[\frac{\partial^2 f}{\partial x^2}\right]_j + \mathrm{O}(h^4).$$

They are known as Collatz and Numerov formulas, respectively (note that the Collatz operator can be obtained by setting $s = 0$ in the operator in the left-hand side of Eq. (A.1)). Due to the lack of free parameters, it is not possible to use them as basis operators. However, it is possible to obtain the necessary basis operators by inserting a parameter in the inverse operators. The corrected formulas then define one-parameter families of the second-order compact approximations. Denoting the parameter by c, the corresponding $D_1(c)$ and $D_2(c)$ operators and the expansions for their actions read

$$\begin{aligned} D_1(c)[f]_j &= \frac{1}{2h}(I + c\Delta_2)^{-1}\Delta_0[f]_j = \left[\frac{\partial f}{\partial x}\right]_j + \left(\frac{1}{6} - c\right)h^2 f_j^{(3)} + \left(\frac{1}{120} - \frac{c}{4} + c^2\right)h^4 f_j^{(5)} + \mathrm{O}(h^6), \\ D_2(c)[f]_j &= \frac{1}{h^2}(I + c\Delta_2)^{-1}\Delta_2[f]_j = \left[\frac{\partial^2 f}{\partial x^2}\right]_j + \left(\frac{1}{12} - c\right)h^2 f_j^{(4)} + \left(\frac{1}{360} - \frac{c}{6} + c^2\right)h^4 f_j^{(6)} + \mathrm{O}(h^6), \end{aligned} \tag{A.3}$$

the coefficients for further terms being polynomials of successively increasing degrees.

Upon setting $c = c_1, c_2, c_3$, the systems for the $\gamma_1, \gamma_2, \gamma_3$ coefficients annihilating $\mathrm{O}(h^2)$ and $\mathrm{O}(h^4)$ terms in the sums of the pre-multiplied series (A.3) are similar to system (A.2), the difference being only due to the notations for the parameters and other right-hand sides. The last are now $(1, 1/6, 1/30)$ and $(1, 1/12, 1/90)$, respectively, in the particular case of $M = 3$. The solutions written in either analytical or numerical form gives the sixth-order approximations to the first and second derivatives.

Fixing M parameters $c_1, c_2, \ldots, c_M$ and retaining more terms in the expansions, $2M$th-order multioperators $\sum_{i=1}^{M}\gamma_i D_1(c_i)$ can be constructed as compared with $(M + m - 1)$th-order ones in the case of mth-order CUD basis operators ($m = 3, 5$). Thus, the central multioperators for the same M are superior over non-central ones from the viewpoint of their orders and accuracy.

In the CFD context, schemes with central multioperators for the first derivatives can be efficient when supplied with some artificial high-order dissipative mechanisms. Multioperators with $D_2(c)$ basis operators can be used for approximations to the second and cross derivatives in the viscous terms as well as for approximations to the Poisson operator in the case of the vorticity-stream function formulation for incompressible flows. More details and numerical examples showing highest accuracy of schemes withy central multioperators can be found in [8].

A.2. Other types of multioperators

Though main emphasis in the multioperators investigations was placed on derivatives approximations, other grid functionals can be of interest when constructing high-order methods for PDE's or other applications. Examples are midpoint interpolations, integrals over cells, etc. To create multioperators for target functionals, it is sufficient to modify the corresponding standard formulas by introducing inverse operators depending on a parameter. The idea was used in [8] and in Section 2.2 of the present paper.

Recently, novel families of one-parameter compact approximations to various functionals were suggested [11], the crucial point being the use of two-point inverse operators. They can generate basis operators for multioperators with some attractive properties. Relevant topics will be the subject matter of forthcoming papers.

References

[1] A.I. Tolstykh, Multioperator high-order compact upwind methods for CFD parallel calculations, in: D.R. Emerson et al. (Eds.), Parallel Computational Fluid Dynamics, Elsevier, Amsterdam, 1998, pp. 383–390.
[2] A.I. Tolstykh, High Accuracy Non-centered Compact Difference Schemes for Fluid Dynamics Applications, World Scientific, Singapore, 1994.
[3] A.I. Tolstykh, Multioperator arbitrary-order schemes based on non-centered compact approximations, Dokl. Akad. Nauk 336 (3) (1999) 319–322 (Engl. transl. in Doklady Mathematics 59 (3) (1999) 409–412).
[4] A.I. Tolstykh, On constructing prescribed order schemes via linear combinations of compact differencing operators, J. Comput. Math., Math. Phys. 140 (8) (2000) 1159–1172 (transl. from Russian).
[5] A.I. Tolstykh, On multioperators principle for constructing arbitrary-order difference schemes, Appl. Numer. Math. 46 (2003) 411–423.
[6] M.V. Lipavskii, A.I. Tolstykh, Fifth- and seventh-order accurate multioperator compact schemes, J. Comput. Math., Math. Phys. 43 (7) (2003) 975–990 (transl. from Russian).
[7] A.I. Tolstykh, M.V. Lipavskii, On performance of methods with third- and fifth-order compact upwind differencing, J. Comput. Phys. 140 (1998) 205–232.
[8] A.I. Tolstykh, Centered prescribed-order approximations with structured grids and resulting finite-volume schemes, Appl. Numer. Math. 49 (2004) 431–440.
[9] L. Collatz, The Numerical Treatment of Differential Equations, Springer, Berlin, 1960.
[10] M.V. Lipavskii, A.I. Tolstykh, E.N. Chigirev, A parallel computational scheme with ninth-order multioperator approximations and its application to direct numerical simulation, Comput. Math., Math. Phys. 46 (8) (2006) 1433–1452 (transl. from Russian).
[11] A.I. Tolstykh, A family of compact approximations and related multioperators of a given order, Dokl. Akad. Nauk 403 (1) (2005) 172–177, Engl. transl. in Doklady Mathematics 72 (2) (2005) 519–524.
[12] A.I. Tolstykh, D.A. Shirobokov, Fifth-order compact upwind method and its applications to three-dimensional compressible Navier–Stokes equations, Comput. Fluid Dyn. J. 5 (1997) 425–428.
[13] A.A. Samarskii, The Theory of Difference Schemes, Nauka, Moscow, 1977 (in Russian).
[14] C.K.W. Tam, J.C. Webb, Dispersion-relation preserving finite difference schemes for computational acoustics, J. Comput. Phys. 107 (1993) 262.
[15] N.A. Adams, K. Shariff, A high resolution Compact-ENO schemes for shock-turbulence interaction problems, J. Comput. Phys. 127 (1996) 27–51.
[16] S.K. Lele, Compact finite-difference schemes with spectral-like resolution, J. Comput. Phys. 103 (1992) 16–42.
[17] C. Bogey, C. Baily, A family of low dispersive and low dissipative explicit schemes for flow and noise computations, J. Comput. Phys. 194 (2004) 194–214.
[18] X-D. Liu, S. Osher, Non-oscillatory high-order accurate self-similar maximum principle satisfying shock capturing schemes, SIAM J. Numer. Anal. 33 (1996) 760–779.
[19] E.F. Toro, V.A. Titarev, ADER schemes for scalar non-linear hyperbolic conservation laws with source terms in three-space dimensions, J. Comput. Phys. 202 (2004) 196–215.
[20] S.T. Zalesak, Fully multidimensional flux-corrected transport algorithms for fluids, J. Comput. Phys. 31 (1979) 335.
[21] C.K.W. Tam, Problem 1-aliasing, In: Fourth Computational Aeroacoustics (CAA) in: Proceedings of the Workshop on Benchmark Problems, NASA/CP-2004-2159, 2004.