29th Congress of the International Council of the Aeronautical Sciences
St. Petersburg, Russia; September 7-12, 2014

EXTREMELY HIGH ORDER AND HIGH RESOLUTION MULTIOPERATORS – BASED SCHEMES FOR CFD APPLICATIONS,

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Keywords: *multioperators, high-order schemes, Navier-Stokes equations, aeroacoustics, hybrid*

Abstract

The main idea of highly accurate multioperators schemes for CFD applications is briefly outlined, their optimization being discussed.. Several examples of numerical simulations related to aeroacoustics are presented. Hybrid schemes with multioperators for shock capturing calculations are considered.

1 Introduction

The idea of constructing arbitrary-order approximation and schemes via linear combinations of basis operators depending on a parameter (multioperators) was proposed by the author at 1997 ParCFD conference [1]. It is an alternative to increasing approximation orders by increasing numbers of degrees of freedom (for example, by enlarging stencils). It allows to calculate actions of multioperators on known grid functions by calculating actions of basis operators in a parallel and synchronous manner. In this way, execution times can be nearly independent of approximation orders provided that broadcasting and gathering expenses are small when compared with each processor's execution time. The detailed description of the multioperators technique and its applications to Computational Fluid Dynamics (CFD) can be found in [2], [3], [4],[5].

Multioperators-based schemes are aimed primarily at CFD problems requiring high accuracy, high resolution and long-time integration (examples are DNS, LES and some aeroacoustics problems). Using free parameters which are essential features of multioperators, it is possible to optimize the schemes for enlarginge domains of small phase and amplitude errors.

Several options of the schemes were used for numerical simulations of instabilities, the emphasize being placed on aeroacoustics. In particular, hot subsonic jets were considered in [6]. Calculations of supersonic underexpanded jets generating screech waves are reported in [7].

Below high-order multioperators and their implementation in CFD schemes are briefly described. Examples of numerical simulations are presented. A way of using hybrid multioperators schemes for capturing strong discontinuities is outlined.

2 Multioperators-based schemes

2.1 Multioperators

For completeness, we reproduce here the formulation of the main idea. Suppose that there is an one-parameter family of operators $L_h(s)$ which are m th-order approximations to a linear operator L on a uniform grid with a mesh size h. Considering sufficiently smooth function $f(x)$, we construct the Taylor expansion series for $L_h f$ at a grid point , the expansion coefficients being functions of s. We fix M distinct values of $s = s_i, i = 1,2,\ldots M$. Upon introducing coefficients $\gamma_i, i = 1,2,\ldots,M$ satisfying

$\sum_{i=1}^{M}\gamma_i = 1$ and summing the expansions at $s = s_i$ multiplied by γ_i, one arrives at the new expansion. Equating to zero each coefficient of that expansion, one obtains $M-1$ linear equations for γ_i with zero right hand side. The system is closed by the $\sum_{i=1}^{M}\gamma_i = 1$ equation. Supposing that the system is solvable, its solution gives

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

The sum $L_M = \sum_{j=1}^{M}\gamma_i L_h(s_i)[f]_j$ was labeled in [1] as multioperator while the m-th order operators $L_h(s_i)$ were viewed as basis operators. The truncation error in Eq. (1) becomes $O(h^{2M+m})$ if the basis operators are central ones.

The crucial point is how to get one-parameter families $L_m(s)$ providing solvable systems for γ_i coefficients. It turns out that any compact approximation having free parameters in its inverse operator (or operators) has the potential for being the required family. In the case of CFD applications, we previously used one-parameter families of Compact Upwind Differencing (CUD) operators from [2] , the upwinding parameter s being viewed as the free parameter in $L_h(s)$. Three-diagonal inversions are needed for calculations of basis operators actions (see [2] for details).

A lot of multioperators approximating convection terms in the Euler or the Navier-Stokes equations can be constructed. Presently, we use versions of multioperators generated by the one-parameter families of compact approximation with two-diagonal inversions described in [5]. The families are formed by the left and right operators $L_r(c)$ and $L_r(c)$ depending on a parameter c. They provide the third-order approximations to the first derivatives and can be viewed as an upwind-downwind pair:

$L_l(c) = (I + c\Delta_-)^{-1}A_l$, $L_r(c) = (I + c\Delta_+)^{-1}A_r$,

where $\Delta_- u_j = u_j - u_{j-1}$, $\Delta_+ u_j = u_{j+1} - u_j$ while A_l and A_r are two- or three-point operators defined in [5]. In the latest versions, we use Δ_- and Δ_+ operators as A_l and A_r ones thus reducing the approximation error but narrowing the stencils. As an option, the half-sum of the left and right centered operators $(L_l + L_r)/2$ can serve as the generator of the fourth-order basis operators. Since the expansion series for the basis operators contain only even-order powers of h in that case, the 10th- and 18th –order multioperators $L_M(c_1, c_2, \ldots c_M)$ were constructed by fixing M =4 and M =8 parameters $c_1, c_2, \ldots c_M$. The resulting centered multioperators are dissipation-free ones. To provide a high-order dissipation mechanism, the 9th -and 17th-order multioperators were created using the half difference of the left and right operators.

2.2 Creating CFD schemes

Desirable approximation orders can be obtained for more or less arbitrary sets of the parameters s or c. However, high orders should be accompanied by other important properties characterized efficient schemes.. Thus the parameter sets must be chosen first of all to provide their stability. To simplify the analysis of multioperators-based schemes, distributions of the parameters values between their minimal and maximal values $s_{\min}, s_{\max}$ or $c_{\min}, c_{\max}$ are introduced. Thus multioperators and their Fourier images become dependent on two parameters. In the case of the CUD-based multioperators, $s_{\min}, s_{\max}$ should be chosen such that

$$L_M(s_{\min}, s_{\max}) \text{ and } L_M(-s_{\min}, -s_{\max})$$

can be used as an upwind-downwind pair [4]. The task can be accomplished by looking for the parameters which provide positive and negative real parts of the Fourier images of the multioperators.

In the case of the left and the right basis operators, the values of $c_{\min}, c_{\max}$ must be chosen to meet the same requirement. Finally, $c_{\min}, c_{\max}$ must be chosen to provide positivity of dissipation multioperators in the case of centered multioperators which are dissipation-free ones.

Assuming that the requirements are met, the general structure of the schemes can be illustrated using 1D equation $u_t + f(u)_x = 0$ where u and f are vectors. If a upwind-downwind pairs with switching the upwinding parameter s are chosen as the basis operators then the flux-splitting is used to construct the semi-discretized scheme

$u_t + (L_M^+ f^+ + L_M^- f^-)/2h = 0$, $f^+ = f(u) + Cu$, $f^- = f(u) - Cu$, $C \geq 0$ where

$$L_M^+ = L_M(s_{\min}, s_{\max}) + L_M(-s_{\min}, -s_{\max}), \qquad (2)$$

$$L_M^- = L_M(s_{\min}, s_{\max}) - L_M(-s_{\min}, -s_{\max}).$$

In the same way, the left and right multioperators from the upwind-downwind pair can be used. It can be proved that the scheme belongs to the class of schemes with positive operators and hence is stable in the mean square root norm (in the frozen coefficients sense). Supposing that L_M is a centered multioperators, it can be used directly for approximating $f(u)_x$. In that case, the above described dissipation operator D_M should be added. Then the resulting scheme looks as

$$u_t + L_M f(u)/h + CD_M u = 0 \qquad (3)$$

where constant $C \geq 0$ can be used to control the dissipation level.

In multidimensional cases, schemes (2) and (3) are easily generalized by applying multioperators created independently for each spatial directions. Approximations to the viscous terms of the Navier-Stokes equations can be included to the schemes in different ways (for example, by using either compact or multioperators approximations).

The discretization of the time derivatives in Eqs.(2), (3) is a problem-dependent. We are interested mainly in unsteady problems so the natural choice is the Runge-Kutta time stepping of desired orders. Up to now, the fourth or the sixth-orders sufficed for our purposes.

2.3 Optimization

Once domains of admissible values of the multioperator's parameters are obtained, the $s_{\min}, s_{\max}$ or $c_{\min}, c_{\max}$ values from the domains can be used to control additional properties of the schemes. In particular, one can look for the values enlarging domains of wave numbers supported by meshes for which the phase and the amplitude errors are small. That problem is important in the case of aeroacoustics.

The phase errors can be characterized by the function of the dimensionless wave number $\alpha = kh$ defined by $r(\alpha) = a^*(\alpha)/a - 1$ where a and a^* are respectively actual and the numerical phase velocity in the case of Eq. (1) with

$$f(u) = au, \ \ a = const > 0.$$

Consider for example the tenth order scheme (3). Using the uniform parameters distribution between $c_{\min}$ and $c_{\max}$,. the optimal values of $c_{\min}, c_{\max}$ can be found. In the same way, it is possible also to enlarge the domain of small values of the dissipation function $d(\alpha)$ characterizing attenuations of harmonics. The examples of functions $r(\alpha)$ and $d(\alpha)$ for approximately optimal values of $c_{\min}, c_{\max}$ are presented in Fig.1. Judging from the Figure, the resolution of the scheme is close to the spectral one.

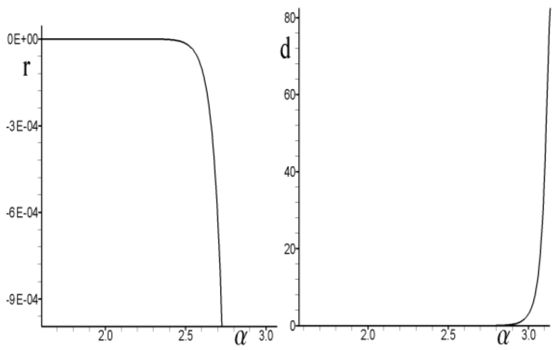

Fig.1. Phase errors $r(\alpha)$ and amplitude errors $d(\alpha)$ vs. dimensionless wave number α.

As to the dissipation, it damps only non-physical harmonics which are not resolved well by the scheme. Thus it plays the role of a built-in filter of spurious oscillations.

2.4 Benchmark calculations

Acoustic test.
To estimate resolution properties of the schemes, the following initial value problem was considered as a test problem:

$$u_t + u_x = 0,$$
$$u(0,x) = [2+\cos(\beta x)]\exp(-\ln(2)(x/10)^2),$$
$$\beta = 1.7$$

It should be discretized using the uniform mesh with $h=1$. The comparison of the exact solution and the obtained numerical solution at times $t=400$ and $t=800$ is needed. The problem was proposed by C.Tam in [8].
In our notations, the dimensionless wave number $\alpha=\beta=2.3>\pi/2$ approximately corresponds to the domain of phase and amplitude errors to be properly resolved. Fig.2 shows the comparison of the calculations at $t=800$. The solid line and the markers present the exact and numerical solutions respectively in the case of the 10th - order scheme. No deviation between the solutions is seen in the Figure.

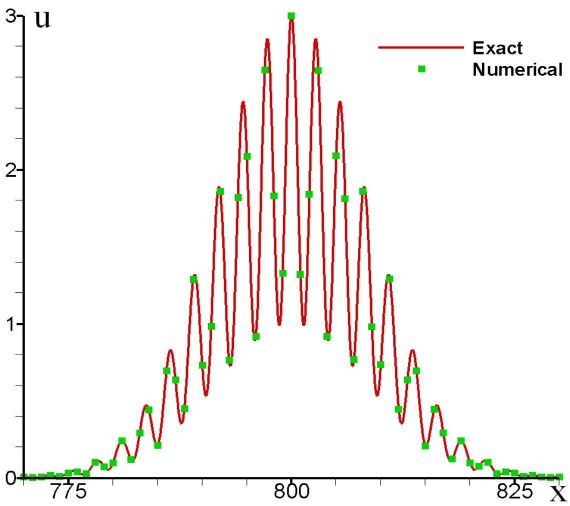

Fig.2. Acoustic test [6]. Comparison of the exact and numerical (markers)solutions

Periodic problem for Burger's equation.
The C-norm of the deviations or the numerical solutions from the exact solution of the periodic problem for the Burger's equation are shown in Table 1 for several numbers N of grid points. The time moment corresponds to the shock-free exact solution.

Table1.Solution errors for smooth exact solutions of the Burgers equations

N	WENO5	L59	L10	L18
16	1.3 E -2	1.3E-03	1.3E-3	1.3E-03
32	1.2 E -3	6.6E-06	6.6E-6	7.6E-06
64	9.5 E -5	5.4E-09	5.4E-9	1.4E-09
128	3.3 E -6	5.6E-12	4.9E-12	2.1E-14

In the table, WENO5, L59, L10.and L18 denote, respectively, the fifth-order well known WENO scheme, the 9th order multioperators scheme based on the fifth-order CUD operators, the above mentioned 10th and 18th order multioperators schemes. As seen, the accuracies and the convergence rates dramatically exceed those of the fifth-order scheme.

3 Examples of calculations.

3.1 Instability and sound radiation of hot subsonic jets

Possible target problems for multioperators-based schemes include direct numerical simulations in the cases requiring high accuracy and high resolution methods for long –term time integrations. An example in the aeroacoustics area is sound generation due to jet's instabilities. In [6], unstable behaviour of subsonic hot jets is calculated using the Navier-Stokes equations. Such type of jets under certain conditions exhibits several types of instabilities characterized by either non-synchronous rolling-up and vortex rings pairings or well synchronized regimes with or without pairings events. In all cases, the jets serve as sound generators, the source of radiation being unsteady motion of vortex rings.

The problem formulation was similar to that of [9] with jets specified by inflow conditions. The above described the tenth-order multioperators schemes were used with non-reflecting boundary conditions and outflow sponge zones. The Mach number, temperature ratio and shear layer thickness were varied in the calculations. Very high accuracy of the schemes allowed to detect small amplitude pressure fluctuations directly from the flow fields described by the Navier-Stokes equations without linearization or introduction deviations from base flows.

The snapshots of the flow field fragments with vortex rings at successive time moments in the case of synchronized (periodical regime) are shown in Fig.3. for the Mach number M_∞ = 0.1.. Calculations for $0.1 \le M_\infty \le 0.8$ showed stabilization effect of increasing M_∞ with the transition from synchronized regime to irregular one.

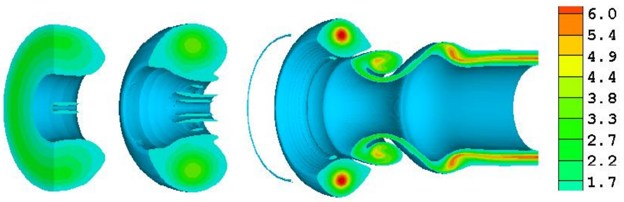

Fig.3 Instability of hot subsonic jets. Details of vorticity isosurfaces showing vortex rings.

3.2 Screech calculations

The scheme with the seventh- and ninth-order multioperators described in [3] was used for numerical simulation of unstable behavior of supersonic underexpanded jets. The calculations were carried out for the both 2D and 3D flow fields in the cases of narrow rectangular nozzles, the 2D calculations being reported in [7].. They allowed to obtain rather clear pictures of unsteady motions of shock cells and the resulting screech waves propagating upstream. Snapshots of the pressure, density and vorticity fields at two successive time moments calculated for the Mach number $M_j = 1.5$ of the perfectly expanded jet are presented in Fig.4. The red markers indicate the screech waves at both sides of the jet.. Fig. 5 shows the Strouhal numbers corresponding to the screech peaks in the spectra obtained for several values of M_j. For comparison, the theoretical estimates, experimental [9] and numerical data [10] are also shown in the Figure.

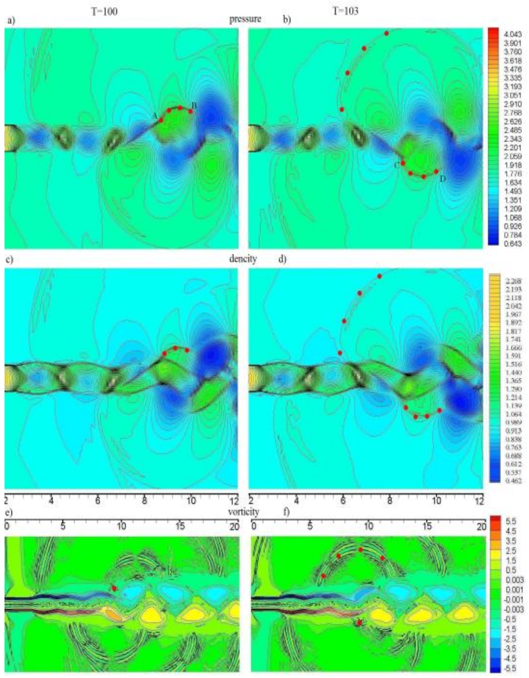

Fig. 4. Snapshots of the pressure, density and vorticity fields at two successive time moments.

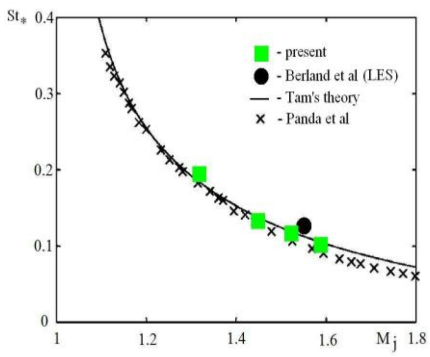

Fig. 5. Screech Strouhal number vs. Mach number. Comparison of calculated and existing data.

4. Hybrid multioperators schemes for strongly discontinuous solutions.

The above described way of using highly accurate multioperators approximations results in conservative schemes provided that governing equations are written in the forms of conservation laws. The schemes can be cast in the form of flux balances for control cells formed by meshes. Thus the schemes have the potential for using as shock capturing ones. Moreover, it can be proved that their solutions if converged are week approximations to the exact solutions. Clearly, the notion of approximation orders is meaningless in the vicinities of discontinuities. Thus the important question is whether the high-order convergence of the solutions .when refining meshes retains in the regions away from the shocks. The requirement is met in the case of multioperators schemes. In Table 2, the maximum norms of the numerical solutions errors is shown for the instance of time at which the exact solution of the above considered periodic problem for the Burgers equation is discontinuous. The calculations were carried out using the ninth-order L59 scheme, their errors being calculated for the nodes which lie exterior to the shock vicinity.

Table 2. Solution errors Er for discontinuous exact solutions of the Burgers equations away from the shock with the local convergence orders k.

N	64	128	256	512	1024
Er	2.8E-2	3.6E- 3	4.5E-5	2.7E-8	2.4E-14
k		2.9	6.3	10.7	20.1

As seen, the superconvergence holds when refining the meshes. The same fact was revealed when testing against the Riemann problems.

Another important point concerns the monotonicity problem. According to the well known Godunov's theorem, high order schemes formally are not monotone ones. It is the case of the multioperators-based scheme. However, the controlled high-order dissipation can damp noticeable spurious numerical oscillations in certain cases. An example is the flow fields shown in Fig.4. where the shocks are not accompanied by spurious oscillations. Thus the schemes have the potential for using in the cases of relatively small Mach numbers without special measures.

In the cases of strong discontinuities, the following ways to create robust shock capturing schemes with multioperators were investigated in [12]. The first one is using low-order monotone schemes and their fluxes for the flux correction described in [13]. Various options are possible when choosing monotone schemes as partners of high-order ones.. Numerical experiments were carried out using the monotone Lax-Friedrichs type of schemes. It was found that the device can kill or reduce spurious oscillations while reasonably accurate solutions can be obtained away from the shock. Unfortunately their convergence was found to be only first-order one. Nevertheless, the accuracy was an order of magnitude higher than that for the first order schemes.

An example of calculations with the flux-corrected ninth-order L59 scheme is shown in Fig.6 for the Riemann problem from [14] with extremely strong shocks.

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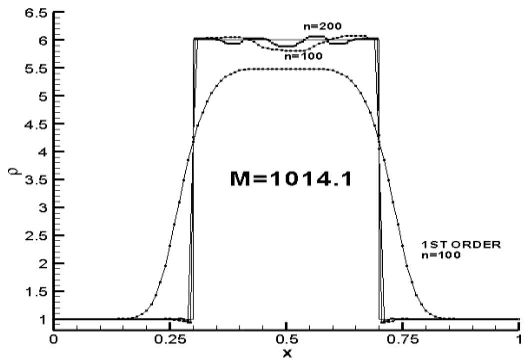

Fig. 6. Density distributions from numerical solutions of the Riemann problem [14]. The bold line indicates the exact solution

In the Figure, the density distribution showing two strong shocks (the Mach number M=1014.1) moving away from the center [14] are presented for two meshes (n=100,200). The solution obtained with the first-order partner of the L59 scheme is also displayed in the figure.

The second way to deal with strong discontinuities considered in [12] is to blend at each grid point j multioperators solutions u_j^M and solutions u_j^L of a monotone scheme in the form $u_j = r_j u_j^L + (1 - r_j) u_j^M$ where r_j is a grid function which is very small and is near unity respectively in domains of smooth and non-smooth solutions. Various types of the function can be used. In [12], it was a smooth function of the difference $u_j^L - u_j^M$. The monotone schemes are not supposed to be necessary first-order ones. For example, they can be high-order schemes with limiters. As an option, it is possible to blend u_j^M with the above described its flux-corrected solution considered as u_j^L. The hybrid scheme was constructed with the 16th order multioperator $L_M(c_{\min}, c_{\max})$ and 15th order dissipation multioperator $D_M(c'_{\min}, c'_{\max})$ in (3), the latter being tuned by choosing its free parameters to get an appropriate spectral content of the dissipation. The flux corrected scheme (3) was used to obtain monotone solutions u_j^L. The numerical example is presented in Fig.7. In the Figure, the details of the solutions of the Riemann problem from [15] obtained with the hybrid scheme and the scheme (3) without blending are shown for $n = 400$. The problem is characterized by rather strong contact and shock discontinuities, the Mach number being about 198.

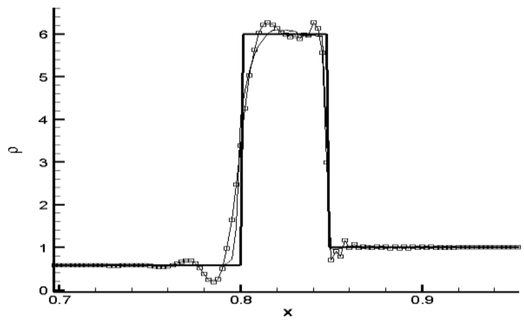

Fig. 7. Density distributions from numerical solutions of the Riemann problem[8] with the contact at $x = 0.8$.The bold line indicates the exact solution, solid line and line with markers correspond respectively to the blended and non-blended scheme with the 16th –order multioperators and the 15th –order dissipation.

As seen, the original scheme can work alone despite noticeable wiggles. It was found that blended multioperators schemes in contrast to flux-corrected ones can preserve high-order convergence away from discontinuities.

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