On Estimation of Discretization Error Norm via Ensemble of Approximate Solutions

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Abstract

The issue of single-grid discretization error estimator, operating in the postprocessor mode, is addressed in the paper. An ensemble of numerical solutions, obtained using solvers of different accuracy, is shown to provide an upper estimate for the norm of the discretization error.

Numerical tests for the supersonic flows, governed by two dimensional Euler equations, confirm the feasibility for the norm estimation, if the ensemble of numerical solutions is separated into clusters of “accurate” and “inaccurate” solutions.

Keywords: *truncation error, discretization error norm, ensemble of numerical solutions, Euler equations.*

1. Introduction

At present, CFD uses a wide selection of numerical methods that are characterized by a rich variety of properties such as monotonicity, conservativity, order of approximation etc. This is naturally caused by a search for more “accurate” numerical solutions. The abundance of numerical methods may provide some additional opportunities for quantitative analysis of CFD results, which we consider herein.

The “accurate” and “inaccurate” numerical schemes are often compared in terms such as the truncation error and the discretization error.

The truncation error δu is obtained via Taylor series decomposition of the discrete operator $A_h u_h = f_h$, which approximates a system of PDE, formally denoted herein as $Au = f$. The truncation error dependence on the spatial step h is usually presented as $\delta u = O(h^n)$, where the order n is equal to the minor order of series terms. On the next stage of analysis, the approximation error $\Delta u = u_h - u$ (of real practical interest) should be estimated. The approximation error may be described by the tangent linear equation $A\Delta u = \delta u$ whose formal solution is $\Delta u = A^{-1}\delta u$. For linear problems, the approximation error $\|\Delta u\| = O(h^n)$ tends to zero with the same order n (by Lax theorem, [1]), if the discrete operator is well-posed (i.e. the inverse operator is uniformly bounded $\|A_h^{-1}\| < C$).

The estimation of the error order is significantly more complicated for the case of nonlinear equations with discontinuities [2, 3, and 4]. In this event, the discretization error comprises the components of different orders, which occur at various elements of the flow structure (such as shock waves or expansion fans). So, the observed order of local convergence may be not equal to the nominal order of the approximation error even in the asymptotic range.

There are several general directions in the error estimation. A priori error estimation is the most widely used approach to the error analysis and may be expressed in the form $\|\Delta u\| < C \cdot h^n$, which contains the unknown constant independent of the current numerical solution. It is the theoretical basis both for the development of numerical algorithms and for the mesh refinement strategy commonly used in CFD. A posteriori error estimation [5, 6] has the form $\|\Delta u\| \le C_h e_h$, where C_h is the computable stability constant, which depends on the numerical solution, and e_h is the computable indicator of the truncation error. At present, the main successes in this direction are achieved for elliptic partial differential equations and finite element methods. In most of practical applications the stability constant is not estimated, while the error indicator is used for mesh adaptation. We consider herein only the single-grid approaches excluding the multigrid methods, such as the Richardson extrapolation.

The truncation error δu estimates may serve as the simplest computable error indicator. The truncation error δu may be computed by the action of the high order scheme stencil on the precomputed flowfield [7, 8], by the action of the differential operator on the interpolation of the numerical solution [9] or via the differential approximation [10, 11].

The application of the truncation error δu implies the calculation of the discretization (global) error $\Delta u = A^{-1}\delta u$. A survey of the error calculation methods may be found in [12]. In the simplest option, the estimation of this error may be performed using a defect correction [7, 13]. In the defect correction frame, the truncation error δu is used as the source term inserted in the discrete algorithm in order to correct the solution. However, the total subtraction of the error implies the elimination of the scheme viscosity that may cause oscillations in the vicinity of discontinuities or an activation of some additional dissipation sources, which engenders their own error. Also, the estimation of the error may be performed via a linearized problem [14], complex differentiation [15] or by adjoint equations [8, 9,11,16]. Usually, adjoint equations are applied to the estimation of the uncertainty of certain valuable functional (drag, lift coefficients etc.). Nevertheless, the approach by [11] enables to estimate the norm of the solution error. Unfortunately, it requires solving a number of adjoint problems, which is proportional to the number of grid nodes that implies an extremely high computational burden.

The presence of unknown components of the truncation error is the general disadvantage of above discussed residual-based error estimation methods. The differential approximation based methods use minor terms of Taylor series [11] and do not account for remaining higher terms. The postprocessor based methods do not account for the higher scheme truncation errors [8] or the interpolation errors [9].

The present paper considers the feasibility of finding the discretization error norm using the ensemble of calculations performed by solvers of different approximation order on the same mesh. We shall refer to this operation as the "*ensemble based error estimation*". Since the analysis is conducted in the space of numerical solutions, the truncation error is accounted for implicitly and completely. It is important that a mesh refinement is not used, thus requiring only moderate computational costs.

2. The estimate of error norm via the set of approximate solutions

Let's consider the ensemble of numerical solutions obtained using finite difference or finite volume schemes of different accuracy orders on the same grid. Let the relation of the approximation error of these schemes be known *a priori*.

We denote the numerical solution as the vector $u^{(i)} \in R^N$ (i is the scheme number, N is the number of grid points respectively), the values of unknown exact solution at nodes of this grid (further denoted as exact solution) as $\tilde{u} \in R^N$ and use a discrete L_2-equivalent norm. The unknown deviation of exact solution values at grid points $\tilde{u} \in R^N$ from the computed solution is assuming the form $\|u^{(k)} - \tilde{u}\|_{L_2} = r_k$. The numerical solutions $u^{(i)}$ are located at surfaces of concentric hyperspheres with the centre at $\tilde{u}$ and radii r_i (unknown).

In the simplest event of two numerical solutions $u^{(1)}$ and $u^{(2)}$ with *a priori* errors $r_1 \geq 2 \cdot r_2$ ($r_1 = \|\tilde{u} - u^{(1)}\|_{L_2}$, $r_2 = \|\tilde{u} - u^{(2)}\|_{L_2}$) the following theorem may be stated.

Theorem 1. *Let the norm of difference of two numerical solutions* $u^{(1)} \in R^N$ and $u^{(2)} \in R^N$

$$\|du_{1,2}\|_{L_2} = \|u^{(1)} - u^{(2)}\|_{L_2} \qquad (1)$$

be known from computations and there is the a priori information

$$\|\tilde{u} - u^{(1)}\|_{L_2} \geq 2 \cdot \|\tilde{u} - u^{(2)}\|_{L_2}\,, \qquad (2)$$

then the norm of approximate solution $u^{(2)}$ *error is less than the norm of difference of solutions:*

$$\|\tilde{u} - u^{(2)}\|_{L_2} \leq \|du_{1,2}\|_{L_2} \qquad (3)$$

Proof. The analysis is based on the triangle inequality [17] for $u^{(1)}$, $u^{(2)}$, and $\tilde{u}$. For our problem, it assumes the form $r_1 \leq r_2 + \|du_{1,2}\|_{L_2}$, which may be transformed to $r_1 - r_2 \leq \|du_{1,2}\|_{L_2}$. By accounting (2) as $r_1 - r_2 \geq r_2$ one obtains $r_2 \leq r_1 - r_2 \leq \|du_{1,2}\|_{L_2}$ and, finally, the desired expression $r_2 \leq \|du_{1,2}\|_{L_2}$.

3. A posteriori analysis of error norm rating

The widespread opinion that the schemes of higher order are more accurate has an asymptotic origin and, usually, is not supported by quantitative error norm estimates. So, the evident weakness of *Theorem 1* from the standpoint of applications is the assumption of the existence of solutions with *a priori* ranged error. Herein, we consider some options for *a posteriori* check of error ranging. The collection of distances between solutions $\|du_{i,j}\|_{L_2}$ (norms of difference of two numerical solutions) enables a detection of the nearby and distant solutions. For example, if $r_1 >> r_i$, the set $\|du_{i,j}\|_{L_2}$ is split into a cluster of inaccurate solutions with great values $\|du_{1,j}\|_{L_2}$ and a cluster of more accurate solutions $\|du_{i,j}\|_{L_2}\,(i \neq 1)$. This is caused by the asymptotics $\|du_{1,j}\|_{L_2} / r_1 \to 1$ and $\|du_{i,j}\|_{L_2} (i \neq 1)/r_1 \sim (r_i + r_j)/r_1 \to 0$ at $r_1/r_i \to \infty$.

The separation of distances between solutions into clusters may be considered as the evidence of existence of solutions with significantly different norms of error. The quantitative criterion, based on dimension of clusters and the distance between them, is of interest. Let us compare the set of distances $\|du_{1,j}\|_{L_2}$ and $\|du_{k,j}\|_{L_2}$, where $u^{(1)}$ denotes the maximally incorrect solution and $u^{(k)}$ is the certain accurate solution (the localization of the exact solution is performed in its vicinity), while $r_{i,\max}$ is the maximum error norm in the subset of accurate solutions.

We may state the following heuristic ***Criterion 1***:

The global error norm may be estimated if the distance between clusters is greater the size of the cluster of accurate solutions. Then the condition (2) is valid and $\|\tilde{u} - u^{(i)}\|_{L_2} \leq \|du_{i,k}\|_{L_2}$*, where* $u^{(i)}$ *belongs to the cluster of more accurate solutions and* $u^{(k)}$ *is the maximally inaccurate solution.*

This conjecture is based on the assumptions that the dimension of the accurate cluster is $r_{i,\max} + r_k$ and the cluster of inaccurate solutions belongs to the interval $(r_1 - r_{i,\max}, r_1 + r_{i,\max})$, so the relation of accurate cluster dimension and the distance between clusters assumes the form $r_1 - 2r_{i,\max} - r_k > r_{i,\max} + r_k$. This leads to the relation $r_1 > 2r_k$ that corresponds to condition (2). This criterion may be rigorous only in the limit of an infinite set of solutions, computed by independent methods. Nevertheless, the numerical check for this criterion confirmation or violation is of interest from the viewpoint of its applicability as heuristics.

4. Numerical Tests

The results of the error norm estimation using above mentioned criterion are presented below for several test flows governed by two dimensional unsteady Euler equations.

$$\frac{\partial \rho}{\partial t}+\frac{\partial\left(\rho U^k\right)}{\partial x^k}=0; \tag{4}$$

$$\frac{\partial\left(\rho U^i\right)}{\partial t}+\frac{\partial\left(\rho U^k U^i+P\delta_{ik}\right)}{\partial x^k}=0; \tag{5}$$

$$\frac{\partial(\rho E)}{\partial t}+\frac{\partial\left(\rho U^k h_0\right)}{\partial x^k}=0; \tag{6}$$

The single oblique shock wave, the interaction of shock waves of I and VI kinds according to Edney classification [18] were used as the test problems. Only steady-state solutions were considered, so only the spatial discretization error is addressed. An analytical solution was constructed for these problems and its values at grid points were considered as an “exact” solution. The flowfield contains undisturbed domains (nominal order of error is expected), shock waves (error order about $n=1$ [4]), contact discontinuity line (error order about $n=1/2$, [3]). In result, one may hope to obtain a nontrivial error composed of components with different error orders. The estimation of this error norm is the main purpose of the present paper.

The numerical computations were performed for Mach number range of $M=3\div 5$, flow deflection angles range of $\alpha=10-30^o$ and $C_p/C_v=1.4$. For example, Fig. 1 presents the density isolines for Edney I flow structure ($M=5$, flow deflection angles $\alpha_1=20^o$ and $\alpha_2=26^o$). The crossing shock waves and contact discontinuity line, engendered at the shocks crossing point, are the main elements of this flow structure. Fig. 2 presents the density distribution for Edney VI flow structure ($M=4$, two consequent flow deflection angles $\alpha_1=10^o$, $\alpha_2=15^o$). The flow is determined by the merging shock waves, the contact line and the expansion fan.

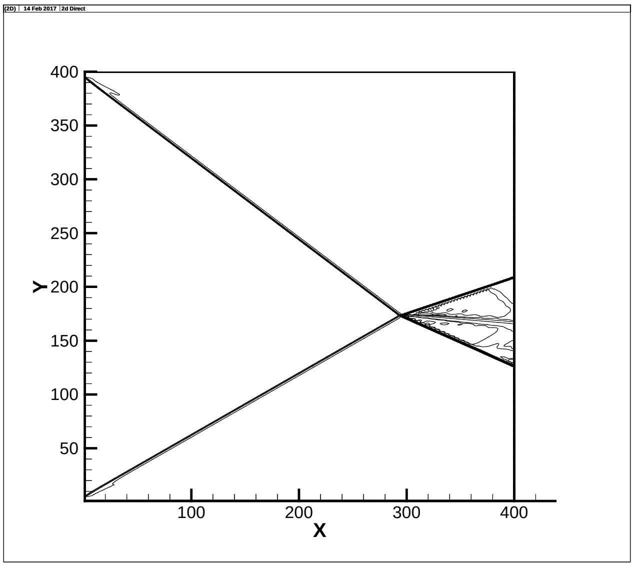

Fig. 1. Edney I density isolines.

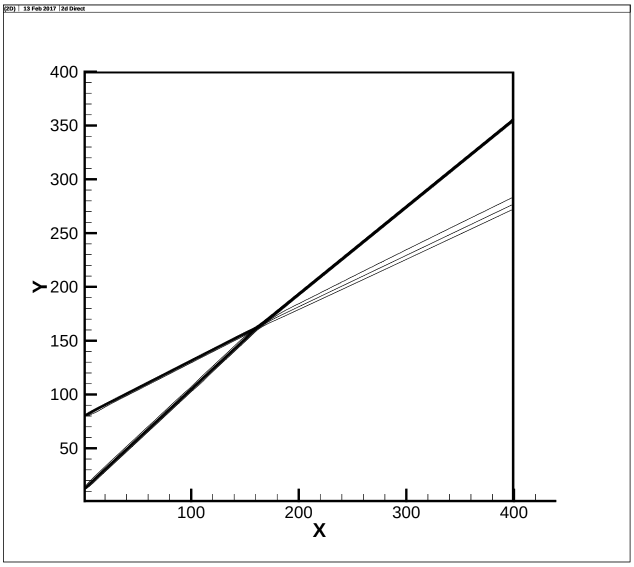

Fig. 2. Edney VI density isolines.

The paper contains an analysis of the ensemble of computations performed by methods listed below.

The first order scheme by Courant Isaacson Rees (CIR) [19] is referred to as $S1$.

The second order scheme using the MUSCL method [20] and algorithm by [21] at cell boundaries is denoted as $S2$.

Second order TVD scheme of relaxation type by [22] is referred to as $S2TVD$.

Third order modified Chakravarthy-Osher scheme [23, 24] is marked as $S3$.

Fourth order scheme by [25] is referred to as $S4$.

Computations were performed on uniform grids consisting of 100×100 or 400×400 nodes.

The total number of the test configurations (determined by Mach number, grid size, flow structure, deflection angles, respectively) was about 24. For every configuration the flowfield was computed using $S1, S2, S3, S4$ and S2TVD solvers, respectively.

The vector of solution of Eq. (4-6) contains four components $u^{(i)}=\{\rho^{(i)},U^{(i)},V^{(i)},E^{(i)}\}$. The norm

$$\left\|u^{(i)}-u^{(k)}\right\|_{L_2}=\left\|\{(\rho^{(i)}-\rho^{(k)}),(U^{(i)}-U^{(k)}),(V^{(i)}-V^{(k)}),(e^{(i)}-e^{(k)})\}\right\|_{L_2} \tag{7}$$

was used to calculate the distance between solutions in the following form

$$\|\Delta u\|_{L_2}=\left(\frac{1}{N}\left(\sum\Delta\rho_i^2+\sum\Delta U_i^2+...\right)\right)^{1/2}. \tag{8}$$

It should be noted that methods $S1, S2, S3, S4$ (1, 2, 3 and 4 nominal truncation orders) demonstrates the global order of convergence a bit below $n=1/2$ in norm L_2. The method S2TVD (nominal order 2) demonstrates the global order of about $n\sim 3/4$.

In numerical tests, we first check *Criterion 1* and, second, we verify the error norm estimation. We consider the $u^{(k)}$ error norm estimation to be successful, if the error estimate $\left\|u^{(1)}-u^{(k)}\right\|_{L_2}$ is greater than the true error norm $\left\|u^{(k)}-\tilde{u}\right\|_{L_2}$ ($\tilde{u}$ is the analytical solution, $u^{(1)}$ - "inaccurate" solution).

The comparison with the analytical solution permits us to conclude that scheme $S1$ (as "inaccurate") and schemes $S2$, $S3$ and $S4$ (as "accurate") enable one to find the upper bound of the error norm, if the *Criterion 1* is satisfied.

Second order $S2TVD$ scheme [22] from the standpoint of error norm is close to the first order scheme $S1$ for 100×100 grid and to the high order schemes for the grid of 400×400 nodes. When the clusters are detected, it also enables us to estimate the error norm of solutions generated by $S2, S3, S4$. The calculations on the grid 100×100 demonstrated the formation of clusters with "inaccurate" scheme $S2TVD$ and a successful error estimation. However, the scheme $S2TVD$ on the grid 400×400 does not form clusters. Paradoxically, the reason for this failure is due to the relatively rapid convergence of $S2TVD$ in comparison with schemes $S2, S3, S4$. As a result, the scheme $S2TVD$ on the grid 400×400 is close to "accurate" schemes $S2, S3, S4$.

The comparison of schemes $S2, S3, S4$ ($\left\|u^{(2)}-u^{(4)}\right\|_{L_2}$, $\left\|u^{(3)}-u^{(4)}\right\|_{L_2}$, $\left\|u^{(3)}-u^{(2)}\right\|_{L_2}$) does not enable the determination of the upper bound of the error norm. Similarly, the error norm estimation by pair $S2TVD, S1$ fails. A splitting into clusters is not observed for these schemes.

For all tests, if the *Criterion 1* is not satisfied (there are no clusters, or distance between them is less the dimension of the cluster of "accurate" solutions) the error norm estimation fails.

The numerical tests for the single oblique shock demonstrate the feasibility for the error norm estimation if the *Criterion 1* is satisfied. However, the set of distances between solutions splits into clusters in about half of tests, more frequently for finer meshes.

For Edney-I shock interaction (Fig. 1), the set of distances between solutions also splits into clusters in about half of the tests without dependence on the mesh size. However, for the distance between clusters, which approximately equals the dimension of the cluster, the error estimation may fail. The worst result over all tests, was obtained in calculations for $M=5$ and flow deflection angles $\alpha_1=20^o$, $\alpha_2=26^o$, and is presented in Figs. 3 and 4 (400×400 nodes). It should be noted that the data under the consideration are bulky, so for ease of visualization, the norm of error is laid out along both axes in Figs. 3-6, despite the fact that the data are one dimensional. The distances $d = \left\| u^{(i)} - u^{(k)} \right\|_{L_2}$ are marked as $SI - SK$.

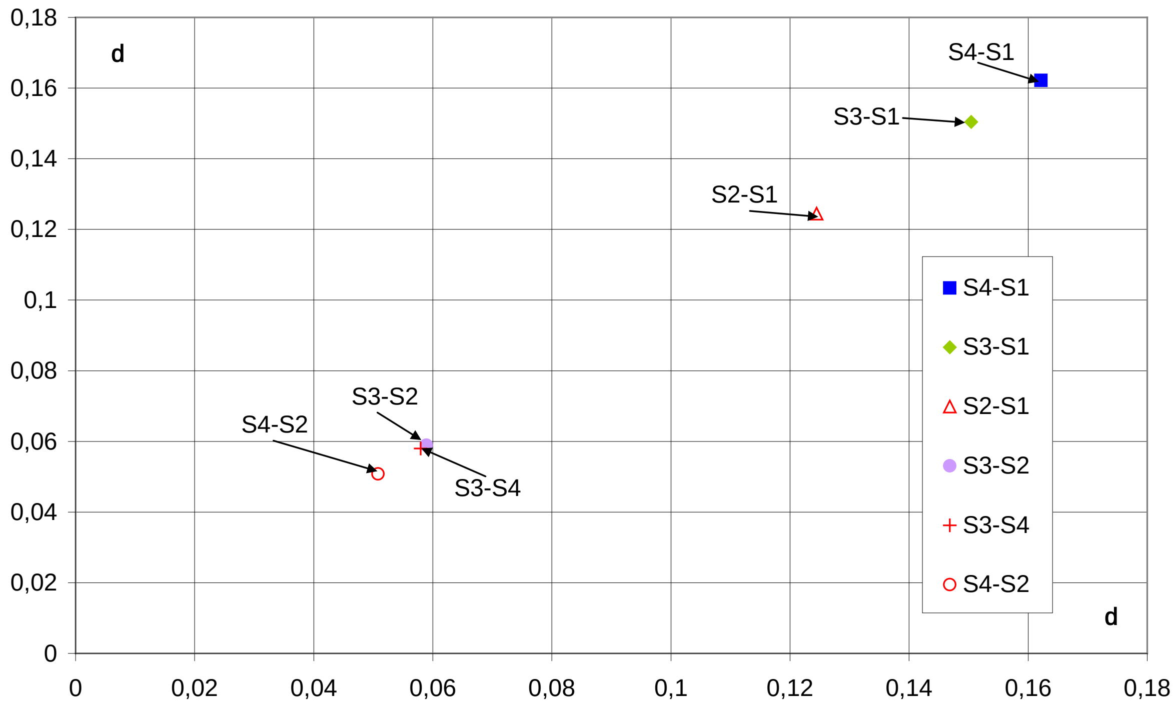

Fig. 3. Clusters (Edney-I)

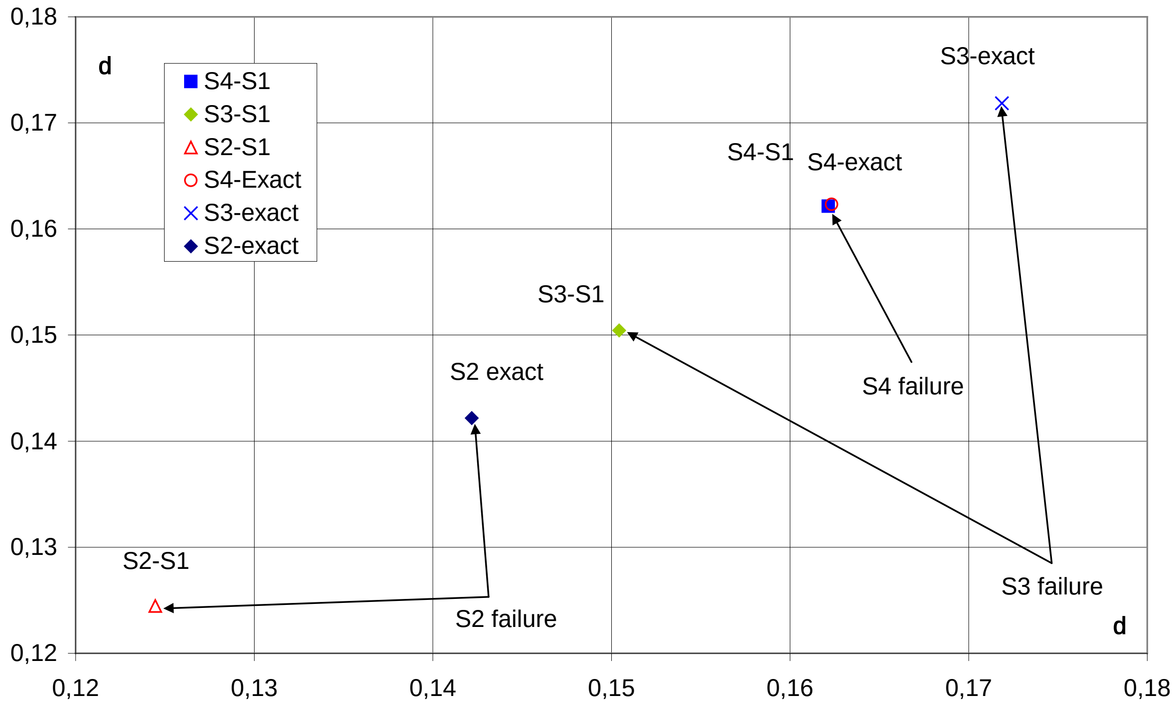

Fig. 4. Error norm estimation (Edney-I).

The maximum relative magnitude of capture condition violation

$\left\|\tilde{u}-u^{(2)}\right\|_{L_2}-\left\|du_{1,2}\right\|_{L_2}=\delta_{break}$ is about $\frac{\delta_{break}}{\left\|du_{1,2}\right\|_{L_2}}\approx 0.15$. This demonstrates the approximate nature of *Criterion 1*, however, the magnitude of the capture condition violation is not too great

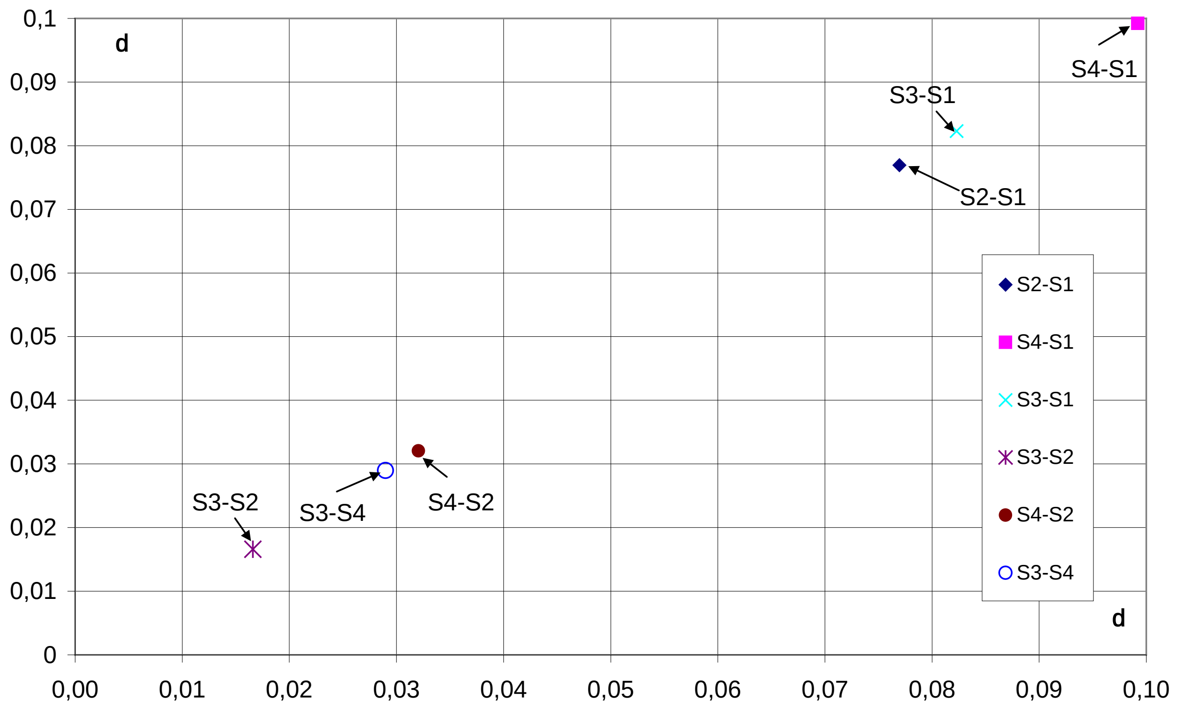

Fig. 5. Clusters (Edney-VI).

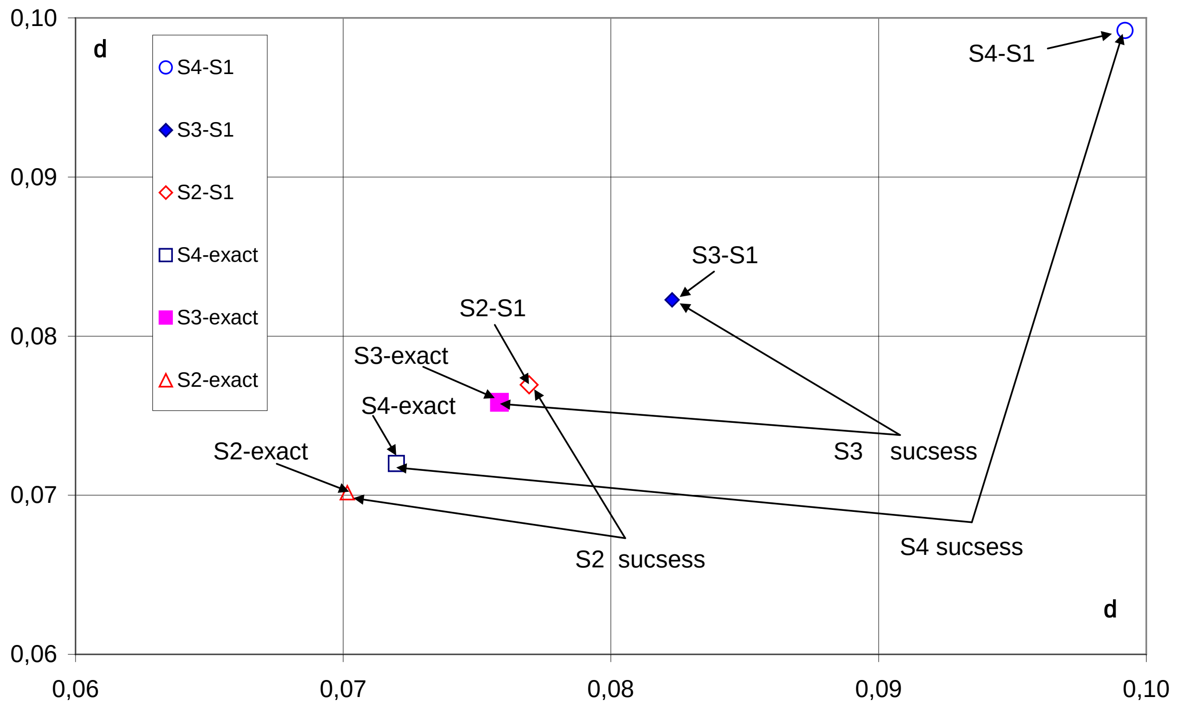

Fig. 6. Error norm estimation (Edney-VI).

For Edney-VI shock interaction (Fig. 2) the set of distances between solutions also splits into clusters in about half of numerical tests irrespective of the grid size. However, for the distance between clusters, which approximately equals the dimension of the cluster, the error estimation always performs correctly. The standard result, obtained in calculations for $M = 4$ and flow deflection angles $\alpha_1 = 10^o$, $\alpha_2 = 15^o$, is presented in Fig. 5,6 (400×400 nodes). Fig. 5 demonstrates the collection of distances between numerical solutions $\|du_{i,k}\|_{L_2} = \|u^{(i)} - u^{(k)}\|_{L_2}$ to break into two clusters, one of them being related to the "inaccurate" scheme $S1$. It enables the successful estimate of the error norm, Fig. 6. It should be noted that the distance between clusters in Fig. 5 is greater than such cluster distance in Fig. 3.

Thus, for the estimation of error norm upper bound, one should have a priori information regarding error rating (*Theorem 1*) or the ensemble of minimum three solutions with the distances between them split into two clusters. The distance between clusters should be greater than the dimension of the cluster of more accurate solutions (*Criterion 1*). Most of the numerical tests for two dimensional supersonic inviscid flows confirm the applicability of heuristic *Criterion 1*. The maximal observed violation of expression (3) is found to be about 15%.

The relation of errors obtained in the paper is not necessarily attributed to properties of the considered schemes. In the strict sense, it may be caused by the imperfections of numerical realization performed by the paper authors. So, authors do not pretend to provide a definitive assessment of the methods considered. Our purpose is rather to verify the single-grid error estimator based on the numerical results obtained by the solvers (algorithms realizations) of different accuracy.

5. Discussion

The standard grid convergence strategy is based on heuristic rule by C. Runge [6]. From this standpoint, if the difference of two approximate solutions on coarse grid T_h with step h and on the fine grid $T_{h,fine}$ with step h_{fine} is small, then $u_{h,fine}$ and u_h are close to exact solution. However, from a practical needs perspective one should desire the quantitative estimate of the form $\|u_h - \tilde{u}\| \le \delta$ with computable δ. Formally, the Richardson method [26] is close to this ideal. It enables us to determine the refined solution and the error estimate using a set of solutions computed on different meshes, which should belong to the asymptotic range of convergence. Two meshes are necessary if a single error order exists in flowfield. Unfortunately, in most CFD problems the error order on different flow structures varies, so the order should be determined additionally, requiring at least three consequent meshes. Thus, the Richardson method requires extremely high computer resources if applied in the CFD domain. The present paper addresses an alternative to the Richardson method. The set of solutions is collected at the same mesh using different solvers that provide the estimation of the global error norm. Calculations may be terminated if the preassigned error level $\|u_h - \tilde{u}\| \le \delta$ is attained.

The existence of "accurate" and "inaccurate" schemes is one of the main postulates of computational mathematics, although, rather often, it has a qualitative or asymptotic sense. The above results demonstrate the feasibility to distinguish "accurate" and "inaccurate" schemes in the sense of error norm rating. For example, for the events presented in Figs. 3,5, the distribution of distances between solutions $\|du_{i,j}\|_{L_2}$ shows the presence of two clusters corresponding to "accurate" and "inaccurate" schemes. This provides the possibility of finding the error norm only from observable values $\|du_{i,j}\|_{L_2}$ (without *a priori* information on errors ranging), that is confirmed by Fig. 6. The results presented in Fig. 6 demonstrate the standard quality of the error norm estimation obtained in most tests, if conditions by *Criterion 1* are satisfied. The violation of condition $\|\tilde{u} - u^{(2)}\|_{L_2} \le \|du_{1,2}\|_{L_2}$ above 15% (Fig. 4) is not detected in tests.

The above considered single-grid discretization error estimator operates with the total error including the discretization error in flowfield, initial and boundary condition error and round-off errors. It is used in a postprocessor mode similar to the Richardson extrapolation. However, it does not need any mesh refinement and may be used away from the asymptotic range.

The dependence on the set of numerical methods and analyzed solution is the drawback of the ensemble based estimator. The same set of methods may provide a segregation into clusters for one flow pattern and may not provide it for another. So, this approach cannot replace the mesh refinement and is aiming to supplement it by a non-expensive algorithm.

If there is no splitting in clusters, the distance between numerical solutions and analytical ones was observed to be 2-3 times greater than the maximum distance between approximate solutions. This feature provides some additional opportunity for a rough estimate of the numerical error.

6. Conclusions

It is feasible to estimate the discretization error norm using a collection of numerical solutions, obtained on the same grid.

If two numerical solutions with the error relating twice or more in L_2 norm are available, the norm of the error of the more accurate solution is majorized by the norm of the solutions difference.

If there is no *a priori* information on error norm ranging, the error norm estimation is feasible if the collection of solutions is split into separate clusters, corresponding to “accurate” and “inaccurate” schemes and the distance between clusters is greater than the dimension of the "accurate" cluster. Numerical tests demonstrated the efficiency of this heuristic rule in L_2 for two dimensional supersonic problems governed by the Euler equations.

The above considered single-grid discretization error estimator may be constructed using an ensemble of numerical solutions obtained by different solvers of various orders of accuracy. It is used in a non-intrusive postprocessor mode and does not require mesh refinement.

Acknowledgement

A.K. Alekseev and A.E. Bondarev acknowledge the partial support by grants of RFBR № 16-01-00553A and 17-01-444A.

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