ON SOME FEATURES OF RICHARDSON EXTRAPOLATION FOR COMPRESSIBLE INVISCID FLOWS

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Summary. The estimation of the discretization error via the Richardson extrapolation (RE) is considered for problems with discontinuities (shock waves and contact lines) having the variable order of accuracy. The computation of the local order of convergence is addressed. The numerical tests for the supersonic flows, governed by two dimensional Euler equations, demonstrate the feasibility and troubles for discretization error estimation via the Richardson extrapolation. The need for the great number of grid space levels is the main obstacle for practical applications of RE for compressible flows that may be partly relaxed by the mixed order RE.

1 INTRODUCTION

The grid convergence strategy, based on heuristic rule by C. Runge [1] is the foundation of significant part of modern numerical methods (excluding finite element p-refinement). From this standpoint, if the difference between 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. The Richardson extrapolation (RE) method [2-11] enables us to determine the refined solution and the discretization error estimate using a set of solutions computed on different meshes. Formally, two meshes are necessary for the Richardson method application, if the solution is in the asymptotic range of the convergence. The check of this condition requires one or more additional levels of mesh refinement.

RE achieves most success for elliptic and parabolic problems with smooth enough solutions. However, the significant current interest exists in the application of RE to CFD problems of hyperbolic or mixed types. The Ref. [4] describes calculation of the observed order of accuracy for the solution of RANS (subsonic and supersonic) for smooth enough flows. The paper [5] considers the multi-dimensional advection equation under the condition that the coefficients before the spatial derivatives are continuously differentiable. The paper [6] states, that behavior of Richardson extrapolation error estimates for simulations of solutions with jumps, such as shock and contact lines for fluid mechanics, is known to be problematic. One of the reasons is caused by the fact that the error order is local and depends

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on the type of flow structure for CFD problems of inviscid compressible fluid containing shock waves and contact lines [6, 10, 12-15].

Since the value of the convergence order on different flow structures varies, the RE should be modified to estimate the local order of convergence in the flowfield. This problem requires at least three consequent meshes in the asymptotic range of the convergence. The check for this condition causes the need for additional grid, so, four consequent meshes are necessary as a minimum. Thus, the Richardson method requires rather high computer resources if applied in the CFD domain. The additional computational problems are related to the instabilities at the local order estimation. To circumvent this problem, some part of publications [6] concerns the averaged order of convergence. The work [10] compare the generalized RE (accounting for the local order of convergence) and mixed-order RE. The mixed-order analysis [10] provides the best results for inviscid problems with strong shocks if the nonmonotonic convergence is manifested. Formally, nonmonotoniticy should disappear in the asymptotic range (where the minor order term governs the error), however, it may require so fine grids, which are prohibitive from the computer memory standpoint.

The present paper is addressed to the application of Richardson method for two dimensional compressible Euler equations with discontinuities (shock waves and contact lines). The emphasis is made on the estimation of the local order of convergence in comparison with the mixed-order RE, the single grid postprocessor by [22], and exact error (obtained by comparison with analytic solutions).

2 TEST PROBLEM

The results of the a posteriori error estimation are presented below for test flows governed by two dimensional unsteady Euler equations.

$$\frac{\partial \rho}{\partial t} + \frac{\partial \left(\rho U^k\right)}{\partial x^k} = 0 \tag{1}$$

$$\frac{\partial \left(\rho U^i\right)}{\partial t} + \frac{\partial \left(\rho U^k U^i + P\delta_{ik}\right)}{\partial x^k} = 0 \tag{2}$$

$$\frac{\partial (\rho E)}{\partial t} + \frac{\partial \left(\rho U^k h_0\right)}{\partial x^k} = 0 \tag{3}$$

Here the summation over repeating indexes is assumed, $i,k = 1,2$, $U^1 = U, U^2 = V$ are the velocity components, $h_0 = (U^2 + V^2)/2 + h$, $h = \frac{\gamma}{\gamma - 1}\frac{P}{\rho} = \gamma e$, $e = \frac{RT}{\gamma - 1}$, $E = \left(e + \frac{1}{2}(U^2 + V^2)\right)$ are enthalpies and energies, $P = \rho RT$ is the state equation and $\gamma = C_p / C_v$ is the specific heat ratio.

The interactions of shock waves *of VI* kind according to Edney classification [16] were used as the test problems. Only steady-state flows were considered, so only the spatial discretization error is addressed. The analytical solution was constructed for this problem.

3 ESTIMATION OF LOCAL ORDER OF CONVERGENCE (GENERALIZED RE)

Let's consider the RE approach for estimation of the local order of convergence. The results of computation for three meshes of different steps h_i (related to nodes of most coarse grid) may be presented as (k is the grid point index):

$$u_k^{(1)} = \tilde{u}_k + C_k h_1^{\alpha_k}$$
$$u_k^{(2)} = \tilde{u}_k + C_k h_2^{\alpha_k} \qquad (4)$$
$$u_k^{(3)} = \tilde{u}_k + C_k h_3^{\alpha_k}.$$

These relations are valid if C_k is independent on h and higher order terms may be neglected, that is the solution is in the asymptotic range. The system (4) can be solved by several formally very close variants. For example, one may obtain expression

$$C_k = (u_k^{(2)} - u_k^{(3)})/(h_2^{\alpha_k} - h_3^{\alpha_k}), \qquad (5)$$

that engender the relation

$$(u_k^{(3)} - u_k^{(1)})(h_2^{\alpha_k} - h_3^{\alpha_k}) - (u_k^{(2)} - u_k^{(3)})(h_3^{\alpha_k} - h_1^{\alpha_k}) = 0, \quad \alpha_k \in (0, \alpha_{\max}) \qquad (6)$$

In order to determine α_k we should resolve (6) at every grid cell k. This expression contains small values that diverges at $h \to 0$, so, it is not convenient from the numerical viewpoint. For grid relation by factor 2 ($h_2 = h/2, h_3 = h/4$) one may transfer (6) to the expression without small values

$$\varphi_1(\alpha_k) = \frac{(u_k^{(3)} - u_k^{(1)})}{(u_k^{(3)} - u_k^{(2)})}. \qquad (7)$$

The function $\varphi_1(\alpha_k) = (4^{\alpha_k} - 1)/(2^{\alpha_k} - 1)$ has the asymptotic $\varphi_1(\alpha) \sim 2^{\alpha_k}$ at great α_k. There are three simplest options for estimation of α_k in dependence on data combinations: $\varphi_1(\alpha) = \frac{(u_k^{(3)} - u_k^{(1)})}{(u_k^{(3)} - u_k^{(2)})}$, $\varphi_2(\alpha) = \frac{u_k^{(3)} - u_k^{(1)}}{u_k^{(2)} - u_k^{(1)}}$, $\varphi_3(\alpha) = \frac{u_k^{(3)} - u_k^{(2)}}{u_k^{(2)} - u_k^{(1)}}$. The corresponding functions have the appearance

$$\varphi_2(\alpha_k) = \frac{(4)^{\alpha_k} - 1}{(4)^{\alpha_k} - (2)^{\alpha_k}}, \qquad (8)$$

and

$$\varphi_3(\alpha_k) = \frac{(1/2)^{\alpha_k} - (1/4)^{\alpha_k}}{1 - (1/2)^{\alpha_k}}. \qquad (9)$$

The functions $\varphi_1(\alpha), \varphi_2, \varphi_3$ are presented in Fig. 1. The solution of (9) (φ_3) corresponds to expression $\alpha_k = \frac{\ln(\frac{u_3 - u_2}{u_2 - u_1})}{\ln(2)}$ used by [4, 10]. The function $\varphi_3(\alpha_k)$ has the asymptotic

$\varphi_3(\alpha_k) \sim (1/2)^{\alpha_k}$. The low sensitivity of $\varphi_3(\alpha_k)$ visible in Fig.1 at the great α_k may be one of reasons for high level of α_k oscillations observed in [10].

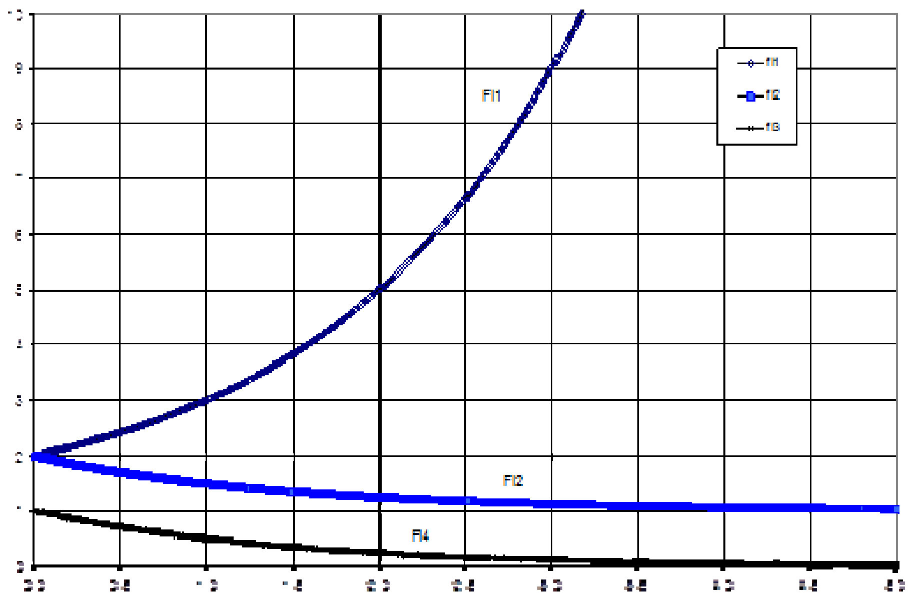

Fig. 1. Sensitivity functions in dependence on the order α_k

One may see in Fig. 1 that the sensitivity of φ_2, φ_3 decreases as α_k increases that should cause the oscillations for high α_k. From this viewpoint, φ_1 is the best choice and it is used in presented tests.

Solving the equation (7) is equivalent to the search of the minimum of the functional

$$\varepsilon(\alpha_k) = \{(u_k^{(3)} - u_k^{(1)}) - (u_k^{(3)} - u_k^{(2)}) \cdot (4^{\alpha_k} - 1)/(2^{\alpha_k} - 1)\}^2 . \qquad (10)$$

Due to observed oscillations, we consider herein the regularized version of (10)

$$\varepsilon(\alpha_k) = \{(u_k^{(3)} - u_k^{(1)}) - (u_k^{(3)} - u_k^{(2)}) \cdot (4^{\alpha_k} - 1)/(2^{\alpha_k} - 1)\}^2 + reg \cdot \alpha_k^2 . \qquad (11)$$

The one dimensional minimization problem was solved by sorting for every cell, the regularization coefficient value $reg = 10^{-4}$ provides the regularization without a visible distortion of the solution.

The estimation of the real local convergence order may provide the additional information on the generation and transfer of the discretization error.

The approximation error may be provided as

$$\Delta u_k = u_k^{(1)} - \widetilde{u}_k = C_k h_1^{\alpha_k} . \qquad (12)$$

Herein, the approximation error is defined for coarse grid. The approach by [11] enables the estimation of the error for the fine grid, however it requires the interpolation from the coarse to fine meshes that engender an additional error, which complicates the analysis. Herein, we avoid this procedure for brevity and lucidity.

It should be noted, that all expressions (7-9) demonstrate singularity at $\alpha_k \to 0$. The paper [4] recommends restriction for the minimum values of α_k. The main problem with small values of α_k occurs for undisturbed domains of flow (before shock waves, for example), where no convergence exists. In these domains the estimation of error via RE is not limited.

4 MIXED-ORDER ANALYSIS

The problem under the consideration contains errors of several different orders emerged at different flow structures. In the standard RE, the asymptotic grid convergence range is considered as the condition that permits neglecting all Taylor expansion terms of higher order. In mixed order analysis [10], the asymptotic range means saving two different low orders and dropping higher terms. It is useful for the nonmomotonic convergence caused by the different signs of two leading terms of expansion.

The influence of the shock wave (first order error) engender the series $u_k = \widetilde{u}_k + C_k^1 h^1 + C_k^2 h^n \ldots$ (n is the formal order for the considered numerical method). The availability of both shock waves and contact lines causes the form of expansion $u_k = \widetilde{u}_k + C_k^1 h^{1/2} + C_k^2 h + C_k^3 h^n \ldots$. The asymptotic range means, herein, the small influence of higher order terms and one may obtain the form, which seems to be most suitable for compressible flows:

$$\begin{aligned}
u_k^{(1)} &= \widetilde{u}_k + C_k^1 h_1^{1/2} + C_k^2 h_1 + C_k^3 h_1^n \\
u_k^{(2)} &= \widetilde{u}_k + C_k^1 h_2^{1/2} + C_k^2 h_2 + C_k^3 h_2^n \\
u_k^{(3)} &= \widetilde{u}_k + C_k^1 h_3^{1/2} + C_k^2 h_3 + C_k^3 h_3^n \\
u_k^{(4)} &= \widetilde{u}_k + C_k^1 h_4^{1/2} + C_k^2 h_4 + C_k^3 h_4^n
\end{aligned} \tag{13}$$

This system is potentially suitable for extraction of the main sources of errors, including shock waves, contact lines and undisturbed field. However, this statement needs four grid levels at the asymptotic range (considered herein, as the absence of influence from the higher orders of error). We consider several simplified versions of the system (13). The expressions for error on the coarse grid are presented. The notation $\varepsilon_{im} = u_k^{(i)} - u_k^{(m)}$ is used.

The first order component of error is related with the shock wave and (for the first order scheme) with the nominal error in the total flowfield. In order to account for first order we consider the RE version that follows:

$$\begin{aligned}
u_k^{(1)} &= \widetilde{u}_k + C_k^1 h_1 \\
u_k^{(2)} &= \widetilde{u}_k + C_k^1 h_2
\end{aligned} \tag{14}$$

and

$$\Delta u_k = u_k^{(1)} - \widetilde{u}_k = 2(u_k^{(1)} - u_k^{(2)}) \,. \tag{15}$$

In order to account for contact discontinuity we consider another RE version:

$$u_k^{(1)} = \widetilde{u}_k + C_k^1 h_1^{1/2},$$
$$u_k^{(2)} = \widetilde{u}_k + C_k^1 h_2^{1/2}. \qquad (16)$$

Assuming according [10] $h_2 = 1$ for finest grid

$$u_k^{(1)} = \widetilde{u}_k + \sqrt{2} C_k^1$$
$$u_k^{(2)} = \widetilde{u}_k + C_k^1. \qquad (17)$$

The expression for error

$$\Delta u_k = u_k^{(1)} - \widetilde{u}_k = \sqrt{2}(u_k^{(1)} - u_k^{(2)})/(\sqrt{2}-1). \qquad (18)$$

In order to account for both shock wave and contact discontinuity we consider the RE:

$$u_k^{(1)} = \widetilde{u}_k + C_k^1 h_1^{1/2} + C_k^2 h_1$$
$$u_k^{(2)} = \widetilde{u}_k + C_k^1 h_2^{1/2} + C_k^2 h_2 \qquad (19)$$
$$u_k^{(3)} = \widetilde{u}_k + C_k^1 h_3^{1/2} + C_k^2 h_3.$$

Assuming $h_3 = 1$ for finest grid and binary relations between grid levels, one obtains

$$u_k^{(1)} = \widetilde{u}_k + 2C_k^1 + 4C_k^2$$
$$u_k^{(2)} = \widetilde{u}_k + \sqrt{2} C_k^1 + 2C_k^2 \qquad (20)$$
$$u_k^{(3)} = \widetilde{u}_k + C_k^1 + C_k^2.$$

The error is:

$$\Delta u_k = u_k^{(1)} - \widetilde{u}_k = 2\{(5-4\sqrt{2})(u_k^{(3)} - u_k^{(1)}) - 2(u_k^{(3)} - u_k^{(2)})\}/(4-3\sqrt{2}). \qquad (21)$$

Another set of expressions may be obtained for the second order scheme if the contact discontinuity effect is neglected:

$$u_k^{(1)} = \widetilde{u}_k + C_k^1 h_1^1 + C_k^2 h_1^2 = \widetilde{u}_k + 4C_k^1 + 16C_k^2$$
$$u_k^{(2)} = \widetilde{u}_k + C_k^1 h_2^1 + C_k^2 h_2^2 = \widetilde{u}_k + 2C_k^1 + 4C_k^2 \qquad (22)$$
$$u_k^{(3)} = \widetilde{u}_k + C_k^1 h_3^1 + C_k^2 h_3^2 = \widetilde{u}_k + C_k^1 + C_k^2.$$

The corresponding error is:

$$\Delta u_k = u_k^{(1)} - \widetilde{u}_k = -2/3\varepsilon_{31} - 2\varepsilon_{32} = -2/3(u_k^{(3)} - u_k^{(1)}) - 2(u_k^{(3)} - u_k^{(2)}) = -8/3u_k^{(3)} + 2u_k^{(2)} + 2/3u \qquad (23)$$

The general form for the second order scheme and solution, containing shock wave and contact discontinuity is

$$u_k^{(1)} = \tilde{u}_k + 2\sqrt{2}C_k^1 + 8C_k^2 + 64C_k^3 ,$$
$$u_k^{(2)} = \tilde{u}_k + 2C_k^1 + 4C_k^2 + 16C_k^3 ,$$
$$u_k^{(3)} = \tilde{u}_k + \sqrt{2}C_k^1 + 2C_k^2 + 4C_k^3 ,$$
$$u_k^{(4)} = \tilde{u}_k + C_k^1 + C_k^2 + C_k^3 . \tag{24}$$

The coefficients may be expressed as:

$$C_k^1 = u_k^{(2)} - u_k^{(4)} - 3C_k^2 - 15C_k^3 = \varepsilon_{2,4} - 3C_k^2 - 15C_k^3 , \tag{25}$$

$$C_k^2 = \{\varepsilon_{1,4} - (2\sqrt{2}-1)\varepsilon_{2,4} + (30\sqrt{2}-78)C_k^3)\}/(10-6\sqrt{2}) , \tag{26}$$

$$C_k^3 = -\frac{\varepsilon_{3,4} + (3\sqrt{2}-4)\varepsilon_{1,4} - (15-10\sqrt{2})\varepsilon_{2,4}}{(3\sqrt{2}-4)(30\sqrt{2}-78)/(10-6\sqrt{2}) - 15\sqrt{2} + 18} \tag{27}$$

And the error has the appearance:

$$\Delta u_k = u_k^{(1)} - \tilde{u}_k = 2\sqrt{2}C_k^1 + 8C_k^2 + 64C_k^3 . \tag{28}$$

The mixed-order RE expressions (15), (18), (21), (23), (28) provide results of acceptable quality if the order of the error is known a priori. The results of the error norm computation performed using artificially generated data with the error order $1/2$ are presented in the Table 1 in comparison with the results by generalized Richardson (12) and the exact error norm. The mixed-order RE provides acceptable results only if terms with $h^{1/2}$ are available. Since the order at such flow structures as shock waves and shear layers is not known precisely [6,15], the uncertainty of the results may be significant.

		$\lVert \Delta\rho_k \rVert_{L_2}$
1	generalized Richardson (12)	1.000026
2	$u_k = \tilde{u}_k + C_k^1 h^{1/2}$	1.000021
3	$u_k = \tilde{u}_k + C_k^1 h^1$	0.5857704
4	$u_k = \tilde{u}_k + C_k^1 h^{1/2} + C_k^2 h$	1.050285
5	$u_k = \tilde{u}_k + C_k^1 h + C_k^2 h^2$	0.7475487
6	$u_k = \tilde{u}_k + C_k^1 h^{1/2} + C_k^2 h + C_k^3 h^2$	1.000028
7	Exact error norm	1

Table 1. The results of the error norm computation

5 NUMERICAL TESTS

Values $\alpha_{k,j}$ и $C_{k,j}$ were calculated for Edney VI flow pattern. The first order method [17,18], second order method [19], and third order method [20,21] were used in tests. The mesh is uniform (100×100, 200×200, 400×400, 800×800 nodes) and it is not aligned to the shock wave, so the errors at the shock exhibit an oscillatory behavior.

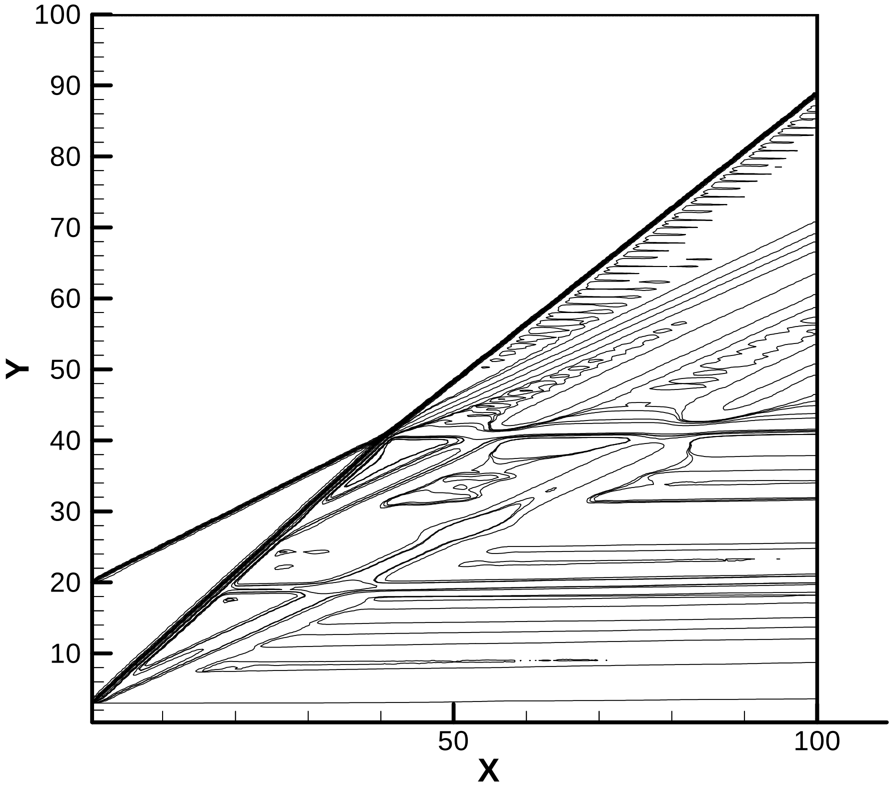

Fig. 2. The density isolines

Fig. 2 presents the density distribution for Edney-IV flow structure ($M = 4$, two consequent flow deflection angles $\alpha_1 = 10^o$, $\alpha_2 = 15^o$) computed using [19]. The flow is determined by the merging shock waves, the contact line and the expansion fan.

The distribution of $\alpha_{k,j}$ is presented in Fig. 3 in three dimensional form. The order $\alpha_{k,j} \sim 10$ at the shock wave and at some points is visible, contamination error order ($\alpha_{k,j} \sim 1, \alpha_{k,j} \sim 1/2$) past shock wave is visible also.

One may compare RE error and true error (the difference between the exact (analytic) and numerical solutions) in Figs. 4,5. The oscillations in RE are visible, this may be a trouble for the error analysis even if the comparison of the error norms demonstrate the asymptotic range.

The results of mixed-order analysis [10] are presented for the first order scheme [17], the second order scheme [19], and the third order scheme [20,21]. The comparison of the Richardson method and the single grid ensemble based approach [22] is conducted. The set of solutions obtained by different solvers [17-21] are used for this purpose. The feasibility for the estimations of the discretization error norm without mesh refinement is the significant merit of approach [22]. This is another way if compare with the standard mesh refinement approach, the Richardson extrapolation and a multigrid approach, presented, for example, by [23].

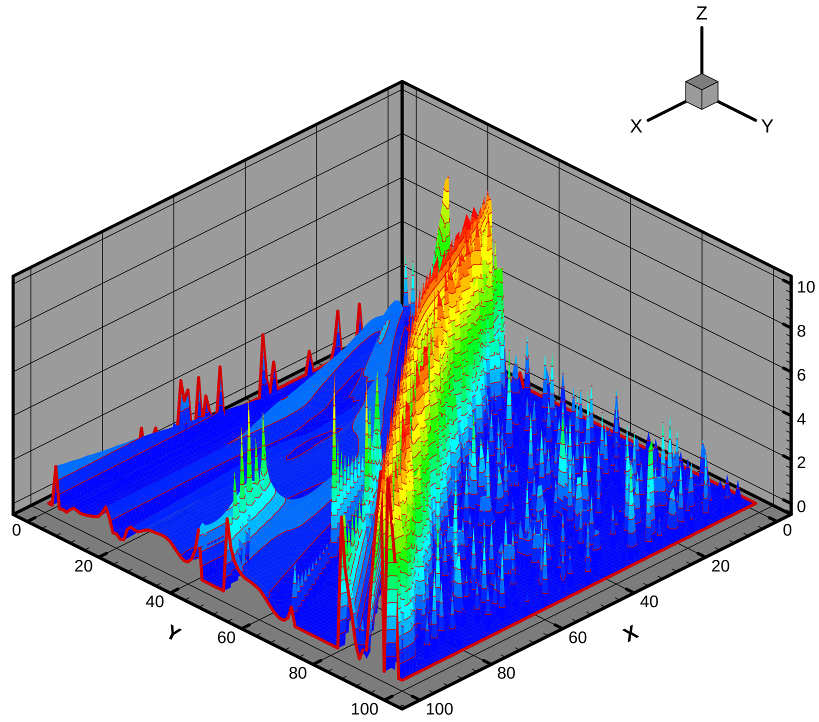

Fig. 3 The distribution of $\alpha_{k,j}$.

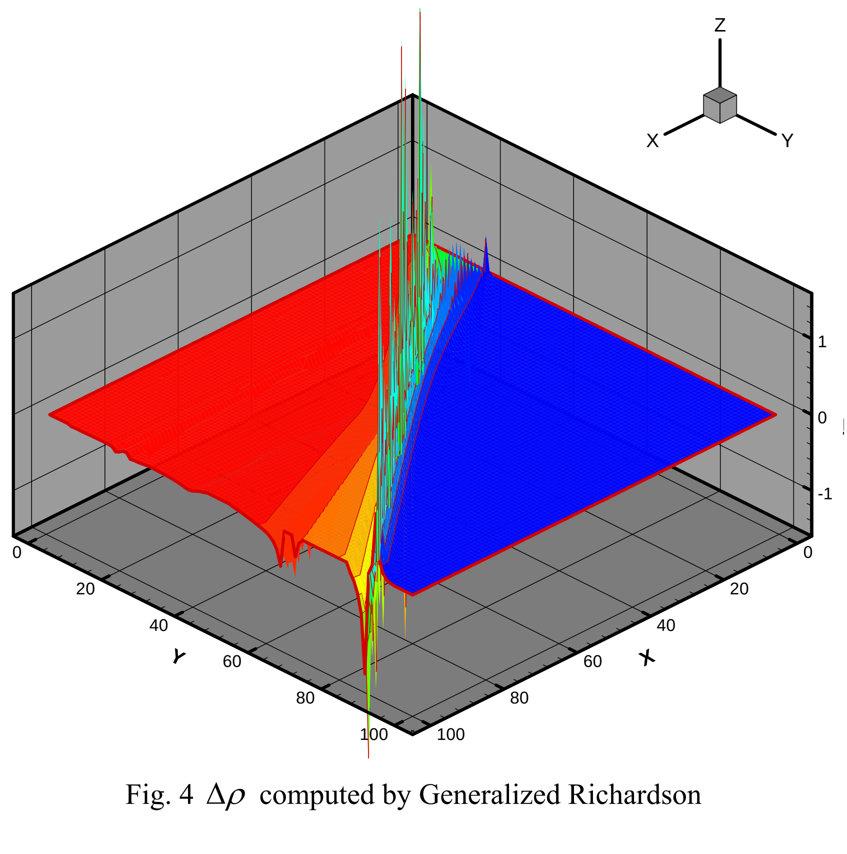

Fig. 4 $\Delta\rho$ computed by Generalized Richardson

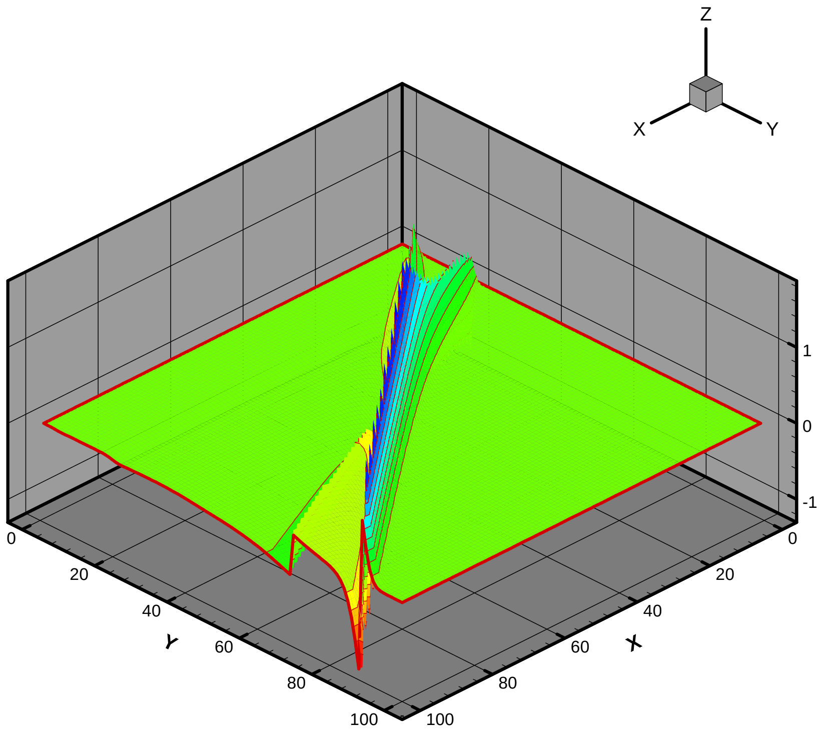

Fig. 5. The difference of densities $\Delta\rho$ between numerical and analytical solutions.

The estimations of the error norm via generalized Richardson extrapolation, the mixed-order RE, and by [22] in comparison with the true error are presented in Table 2 for Edney-VI test. The norms of errors corresponding expressions (12), (15), (18), (21), (23), (28) are computed and presented below. The order of convergence evaluated by the norms of difference between numerical and analytical solutions was about 1/2. The mixed-order RE, governed by the orders, specific for the shock wave and contact discontinuities, also provides the acceptable estimation of the error norm.

	First order scheme [17]		Second order scheme [19]		Third order scheme [20,21]	
	$\|\Delta\rho_k\|_{L_1}$	$\|\Delta\rho_k\|_{L_2}$	$\|\Delta\rho_k\|_{L_1}$	$\|\Delta\rho_k\|_{L_2}$	$\|\Delta\rho_k\|_{L_1}$	$\|\Delta\rho_k\|_{L_2}$
generalized Richardson	0.0672	0.226	0.0394	0.139	0.0398	0.137
$u_k = \tilde{u}_k + C_k^1 h^{1/2}$	0.1271	0.320	0.0585	0.192	0.0627	0.234
$u_k = \tilde{u}_k + C_k^1 h^1$	0.0748	0.187	0.0348	0.113	0.0365	0.135
$u_k = \tilde{u}_k + C_k^1 h^{1/2} + C_k^2 h$	0.1224	0.387	0.0470	0.215	0.0611	0.281
$u_k = \tilde{u}_k + C_k^1 h + C_k^2 h^2$	0.0834	0.229	0.0355	0.134	0.0360	0.159
$u_k = \tilde{u}_k + C_k^1 h^{1/2} + C_k^2 h + C_k^3 h^2$	0.0969	0.287	0.0926	0.481	0.0389	0.195
Error norm bound by [22]	-	-	0.0563	0.146	0.0585	0.157
Exact error norm	0.0876	0.216	0.0391	0.126	0.0392	0.137

Table 2. Comparative estimations of the error norm

The Table 2 demonstrates that generalized Richardson extrapolation provides estimation of the error norm, which is closest to the exact error norm. The approach by [2] provides reasonable estimation of the error norm with minor requirement to computer resources (several runs of solvers on the coarse grid).

6 DISCUSSION

The present numerical tests illustrate the Richardson method application for two dimensional compressible Euler equations with discontinuities (shock waves and contact lines).

Three consequent grids enable the discretization error and the local order α_k estimation in the asymptotic range.

The estimation of the local error order α_k demonstrates the oscillations. The great values $\alpha_k \sim 10$ are observed in vicinity of shocks and may be caused by the misalignment of grid and shocks or an accidental compensation of errors [10] of different signs at nonasymptotic mode. The high α_k produces relatively small impact to error Δu_k and especially to its norm estimation.

The small values limit $\alpha_k \to 0$ contains singularity that causes the divergence of the error estimation. So, GRE needs for a posteriori information regarding minimal order of convergence, it does not operate in the domains of non-monotonic convergence and in domains of undisturbed flow.

The non-monotonic behaviour is generic for discontinuous solutions away the asymptotic range (for example, for *S*-shape solutions, the terms $h\dfrac{\partial^2 u}{\partial x^2} + h^2\dfrac{\partial^3 u}{\partial x^3}$ in truncation error demonstrates the feasibility for error cancellation).

The estimation of the asymptotic range by the error norm analysis [6] may not coincide with the local error analysis.

The verification of the order requires that all three grid solutions be in the asymptotic grid convergence range. The additional grid levels are necessary to check the asymptotic range. For example, the paper [10] used ***eight*** grid levels for complete RE analysis. So, the Richardson extrapolation for flows with discontinuities requires the extremely high computer memory. The need for the asymptotic grid convergence range may be partly relaxed using the mixed-order approach [10]. However, the mixed-order RE requires the precise a priori information on the order of convergence.

The estimation of the error norm by RE provides results close to approach by [22] and the true error. The RE provides more detailed information, if compare with [22], however, it require much more computer resources.

7 CONCLUSIONS

The estimation of the discretization error using generalized Richardson extrapolation is feasible for the problems with local variable error order, such as compressible fluid flows, containing shocks and contact discontinuities.

The correct choice of the sensitivity function is important for the local error order estimation.

The Richardson extrapolation for flows with discontinuities needs for abundant computer resources. The local error order should be estimated that demands three consequent grids. The additional grid levels are necessary to verify the asymptotic range correctness.

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