A POSTERIORI ERROR ESTIMATION BY POSTPROCESSOR INDEPENDENT OF FLOWFIELD CALCULATION METHOD

A.K. Alekseev[a] and I. M. Navon[b]

a *Department of Aerodynamics and Heat Transfer, RSC ENERGIA, Korolev, Moscow Region 141070, Russian Federation*

b *Department of Mathematics and C.S.I.T., Florida State University, Tallahassee, FL 32306-4120, USA*

We consider a postprocessor that is able to analyze the flow-field generated by an external (unknown) code so as to determine the error of useful functionals. The residuals generated by the action of a high order finite-difference stencil on a numerically computed flow-field are used for adjoint based a-posteriori error estimation. The method requires information on the physical model (PDE system), flowfield parameters and corresponding grid and may be constructed without availability of detailed information on the numerical method used for the flow computation.

INTRODUCTION

The present paper is aimed at the quantitative estimation of approximation error in the verification of computational codes [1, 2 and 3]. The error in practically useful functionals due to the approximation error may be calculated using adjoint equations and different forms of the residual [4-13]. For example, the residual may be calculated for a differential approximation using a finite-difference scheme [11-13]. However, the differential approximation by finite-difference scheme may turn to be very cumbersome. Very often we have to deal with a commercial code. In this case the numerical method is provided without details and code descriptions are not available thus excluding an explicit formulation for the differential approximation. On other hand, the local approximation error may be estimated via the action of the main problem differential operator on an interpolation of the numerical solution [7-9]. In general, this provides the opportunity to develop a postprocessor able to analyze the flowfield calculated by some unknown numerical method. Such postprocessor is capable to determine the a posteriori error of practically useful functionals (drag, lift, etc) using information on the grid and flowfield parameters.

Herein we consider another (if compared with [7]) way for determining the local approximation error that enables us to avoid the interpolation stage. This should simplify treatments and avoid additional error of interpolation.

Let us consider a formal scheme of the algorithm. We are interested in properties of numerical solution of the following problem

$$N\tilde{f} = w \text{ in } \Omega \subset R^n, \; \tilde{f}(\partial\Omega) = \tilde{f}_B(x) \in L_2(\partial\Omega); \qquad (1)$$

Here N is a nonlinear differential operator ($H^k(\Omega)\times L_2(\partial\Omega) \to L_2(\Omega)$).

The numerical solution is provided by a finite-difference equation

$$N_h f_h = w \;, \; f_h = N_h^{-1} w \,. \qquad (2)$$

As a result we obtain a grid function f_k^n. We assume the existence of a smooth enough function $f \in H^{k+n}(\Omega)$ that coincides at the nodes with the grid function. Finite differences in $N_h f_h$ may be expanded using Taylor series in the Lagrange form. This provides us with a differential approximation of finite-difference scheme [14]

$$Nf + \delta_h(f) = w \; . \qquad (3)$$

Here $\delta_h(f)$ is the approximation error containing leading terms of Taylor expansion. Consider (1) as an exact equation and (3) as perturbed one. Exact and perturbed solutions are connected by the relation

$$f(t,x) = \tilde{f}(t,x) + \Delta f(t,x) \; . \qquad (4)$$

The operator N is assumed to be Frechet differentiable, the corresponding derivative being denoted as N_f. Then the expansion $N(\tilde{f} + \Delta f) = N(\tilde{f}) + N_f(f)\Delta f$ is valid with the tolerance of $O(\|\Delta f\|^2)$. The differential approximation (3) may be recast in a form

$$N\tilde{f} + N_f \Delta f + \delta_h(f) = w \; . \qquad (5)$$

By subtracting the exact equation (1) from (5) we obtain an equation for the perturbation

$$N_f \Delta f = -\delta_h(f) = q \, , \Omega \subset R^n \, , \Delta f(\partial\Omega) = 0; \qquad (6)$$

Consider Frechet-differentiable goal functional $\varepsilon : H^k(\Omega) \to R^1$. We are interested in the variation of this functional due to the truncation error of the finite-difference scheme. Its differential $\Delta\varepsilon = \varepsilon_f(f)\Delta f = \lim_{t\to 0}\frac{\varepsilon(f + t\Delta f) - \varepsilon(f)}{t}$ is a linear continuous functional that may be formulated as a Riesz-representation using an inner product in $L_2(\Omega)$

$$\Delta\varepsilon = (\varepsilon_f, \Delta f)_{L_2} = (g, \Delta f)_{L_2} \; . \qquad (7)$$

It may be recast as

$$\Delta\varepsilon = (\Delta f, g)_{L_2} = (N_f^{-1} q, g)_{L_2} = (q, N_f^{-1*} g)_{L_2} = (q, \Psi)_{L_2} \, , \qquad (8)$$

where $\Psi = N_f^{-1*} g$ is a formal solution of adjoint problem

$$N_f^* \Psi = g \; . \qquad (9)$$

The detailed form of the adjoint problem may be obtained according to [16] from the bilinear identity $(N_f^* \Psi, \Delta f)_{L_2} = (N_f \Delta f, \Psi)_{L_2}$ via integration by parts. Thus, the variation of the functional caused by the approximation error may be described by

$$\Delta\varepsilon(f) = \int_\Omega q\Psi \, d\Omega \, , \qquad (10)$$

Where $\Psi(f)$ is the solution of the adjoint problem

$$N_f^* \Psi - g = 0 \text{ in } \Omega \subset R^n \, , \Psi(\partial\Omega) = 0 \, . \qquad (11)$$

There are different ways for calculating the perturbation term *q*. For example, it may be explicitly calculated using finite-differences [11].

Herein we consider another option. Let us assume we do not know N_h exactly and are unable to display $\delta_h(f)$ explicitly. Let us use a known approximation of higher order $N_{1,h}$ and act with this stencil on the solution of system (2). Taking into account corresponding differential approximation, the following equation may be written as

$$N_{1,h} f = N\tilde{f} + N_f \Delta f + \delta_{1,h}(f) = \eta \; .$$

By subtracting the unperturbed equation we obtain

$$N_f \Delta f = \eta - w - \delta_{1,h}(f) \; .$$

According to (6) this equation determines the perturbation q .

If the truncation error $\delta_{1,h}(f)$ is known, or if it is known that this value is small compared to the error of the main scheme, we may estimate the value of disturbance as

$$q = \eta - w - \delta_{1,h} f \qquad (12)$$

or

$$q \approx \eta - w \ . \qquad (13)$$

The expression (13) serves as the basis for the postprocessor considered in present paper.

The perturbing term may be obtained as a residual engendered by the action of a differential operator on a cubic spline interpolation of a finite-dimensional solution [7]. As a matter of fact the approach discussed above may be considered as the implicit action of a differential operator on the natural interpolation of a solution performed using a Taylor series expansion. This approach simplifies the algorithm and enables avoidance of additional interpolation error.

1. TEST PROBLEM

Let us consider the approach discussed above for an example of supersonic inviscid flow. The following system of Euler equations and corresponding adjoint equations was used in numerical tests.

$$\frac{\partial\left(\rho U^k\right)}{\partial X^k} = 0 \qquad (14)$$

$$\frac{\partial\left(\rho U^k U^i + P\delta_{ik}\right)}{\partial X^k} = 0 \qquad (15)$$

$$\frac{\partial\left(\rho U^k h_0\right)}{\partial X^k} = 0\,; \qquad (16)$$

Herein $U^1 = U, U^2 = V$, $h(\rho, P) = \gamma e$ is the enthalpy, $h_0 = (U^2 + V^2)/2 + h$ is the total enthalpy.

The density at certain point $\rho(X^{est}, Y^{est})$ is used as an estimated parameter. We recast it as the goal functional.

$$\rho^{est} = \int_{\Omega} \rho(X,Y)\delta(Y - Y^{est})\delta(X - X^{est})dXdY \qquad (17)$$

and consider the variation of this functional as a function of local perturbations δf^i .

The corresponding adjoint system assumes the form :

$$U^k \frac{\partial \Psi_\rho}{\partial X^k} + U^k U^i \frac{\partial \Psi_i}{\partial X^k} + \frac{\gamma - 1}{\gamma}\frac{\partial \Psi_k}{\partial X^k}\left(h_0 - U_n U_n / 2\right) + U^k h_0 \frac{\partial \Psi_h}{\partial X^k} - \delta(X - X^{est})\delta(Y - Y^{est}) = 0 \qquad (18)$$

$$U^i \frac{\partial \Psi_i}{\partial X^k} + U^i \frac{\partial \Psi_k}{\partial X^i} + \frac{\partial \Psi_\rho}{\partial X^k} + \frac{\gamma - 1}{\gamma}\frac{\partial \Psi_n}{\partial X^n} U_k + h_0 \frac{\partial \Psi_h}{\partial X^k} = 0 \qquad (19)$$

$$U^k \frac{\partial \Psi_h}{\partial X^k} + \frac{\gamma - 1}{\gamma}\frac{\partial \Psi_k}{\partial X^k} = 0 \qquad (20)$$

where $\Psi_\rho, \Psi_1 = \Psi_U, \Psi_2 = \Psi_V, \Psi_h$ are the adjoint parameters. For a different goal functional the adjoint system would differ in as far as source terms are concerned.

According to (10) the functional variation as a function of the truncation error has a form:

$$\delta\varepsilon = \iint_{\Omega} \left(\delta\rho\Psi_\rho + \delta U\Psi_U + \delta V\Psi_V + \delta h\Psi_h\right)dXdY \qquad (21)$$

And according to (13) it may be estimated via

$$\delta\varepsilon \approx \sum_{k,n}^{N,Nx} \left(\Psi_{\rho,kn}\eta_{\rho,kn} + \Psi_{U,kn}\eta_{U,kn} + \Psi_{V,kn}\eta_{V,kn} + \Psi_{h,kn}\eta_{h,kn}\right)h_x h_y \qquad (22)$$

The parameters $\eta_{f,kn}$ are obtained by the action of a high order finite-difference stencil on the computed field.

As a heuristic example let us consider the equation $\frac{\partial \tilde{f}}{\partial x}+\frac{\partial \tilde{s}}{\partial y}=0$. Let the field be calculated using a first order finite-difference approximation.

$$\frac{f_k^{n+1}-f_k^n}{h_x}+\frac{s_{k+1}^n-s_k^n}{h_y}=0; \qquad (23)$$

Taylor series in Lagrange form yields a differential approximation [5] $\frac{\partial f}{\partial x}+\frac{\partial s}{\partial y}+\delta f+\delta s=0$, whose detailed form is:

$$\frac{\partial f}{\partial x}+\frac{\partial s}{\partial y}+\frac{1}{2}\left(h_x\frac{\partial^2 f(x_n,y_k)}{\partial x^2}+h_y\frac{\partial^2 s(x_n,y_k)}{\partial y^2}\right)+\frac{h_x^2}{6}\frac{\partial^3 f(x_n+\beta_k^n h_x,y_k)}{\partial x^3}+\frac{h_y^2}{6}\frac{\partial^3 s(x_n,y_k+\alpha_k^n h_y)}{\partial y^3}=0 \qquad (24)$$

(the parameters $\alpha_k^n\in(0,1),\beta_k^n\in(0,1)$, are unknown).

Let us assume we do not know the exact form of the truncation error in (24). It may be determined from the numerically calculated flowfield. For this purpose let us calculate the magnitude of residual η_k^n obtained as a result of action of a second order accurate stencil on the first order finite difference calculation.

$$\frac{f_k^{n+1}-f_k^{n-1}}{2h_x}+\frac{s_{k+1}^n-s_{k-1}^n}{2h_y}=\eta_k^n \qquad (25)$$

The Taylor expansion of (25) yields

$$\eta_k^n=\frac{f_k^{n+1}-f_k^{n-1}}{2h_x}+\frac{s_{k+1}^n-s_{k-1}^n}{2h_y}=\frac{\partial f}{\partial x}+\frac{h_x^2}{6}\frac{\partial^3 f(x_n+\gamma_k^n h_x,y_k)}{\partial x^3}+\frac{\partial s}{\partial y}+\frac{h_y^2}{6}\frac{\partial^3 s(x_n,y_k+\chi_k^n h_y)}{\partial y^3} \qquad (26)$$

The grid functions f_k^n and s_k^n are obtained by solving (23) and should satisfy (24). After substitution of (24) to (26) the residual may be expressed as

$$\begin{aligned}\eta_k^n=&\frac{h_x^2}{6}\frac{\partial^3 f(x_n+\gamma_k^n h_x,y_k)}{\partial x^3}+\frac{h_y^2}{6}\frac{\partial^3 s(x_n,y_k+\chi_k^n h_y)}{\partial y^3}-\\&-\frac{1}{2}\left(h_x\frac{\partial^2 f(x_n,y_k)}{\partial x^2}+h_y\frac{\partial^2 s(x_n,y_k)}{\partial y^2}\right)-\frac{h_x^2}{6}\frac{\partial^3 f(x_n+\beta_k^n h_x,y_k)}{\partial x^3}-\frac{h_y^2}{6}\frac{\partial^3 s(x_n,y_k+\alpha_k^n h_y)}{\partial y^3}\end{aligned} \qquad (27)$$

Correspondingly, the minimum order term of the truncation error (24) assumes the form

$$\begin{aligned}\frac{1}{2}\left(h_x\frac{\partial^2 f(x_n,y_k)}{\partial x^2}+h_y\frac{\partial^2 s(x_n,y_k)}{\partial y^2}\right)=&-\eta_k^n+\frac{h_x^2}{6}\frac{\partial^3 f(x_n+\gamma_k^n h_x,y_k)}{\partial x^3}-\frac{h_x^2}{6}\frac{\partial^3 f(x_n+\beta_k^n h_x,y_k)}{\partial x^3}+\\&+\frac{h_y^2}{6}\frac{\partial^3 s(x_n,y_k+\chi_k^n h_y)}{\partial y^3}-\frac{h_y^2}{6}\frac{\partial^3 s(x_n,y_k+\alpha_k^n h_y)}{\partial y^3}\end{aligned} \qquad (28)$$

Thus the residual may be used for estimatioing the main term of the differential approximation.

$$\eta_k^n\approx-\frac{1}{2}\left(h_x\frac{\partial^2 f(x_n,y_k)}{\partial x^2}+h_k\frac{\partial^2 s(x_n,y_k)}{\partial y^2}\right) \qquad (29)$$

By using a higher (fourth) order stencil we may estimate all truncation errors with an asymptotically small tolerance

$$\mu_k^n=-\frac{1}{2}\left(h_x\frac{\partial^2 f(x_n,y_k)}{\partial x^2}+h_y\frac{\partial^2 s(x_n,y_k)}{\partial y^2}\right)-\frac{h_x^2}{6}\frac{\partial^3 f(x_n+\beta_k^n h_x,y_k)}{\partial x^3}-\frac{h_y^2}{6}\frac{\partial^3 s(x_n,y_k+\alpha_k^n h_y)}{\partial y^3}+O(h_x^4)+O(h_y^4). \qquad (30)$$

So both the least order term of differential approximation (24) and the total approximation may be estimated by a residual obtained from the action of high order stencil on the numerical solution. These residuals may be considered as a field of truncation error perturbing an exact solution. Their influence on a goal functional may be accounted for by using adjoint parameters.

In comparison with the method of [11] the present approach does not require knowledge of the exact form of the differential approximation of the main numerical scheme. This may turn out to be useful if the differential approximation is very complicated (such as Godunov type schemes) or unknown (commercial code). Above all, this approach does not require calculation of high order derivatives of the differential approximation.

2. NUMERICAL TESTS

Several versions of first order finite-difference schemes were employed including donor cells [17] and the Roe scheme [18].

A symmetric second order stencil was used for residual calculation .

$$\frac{f_k^{n+1} - f_k^{n-1}}{2h_x} + \frac{s_{k+1}^n - s_{k-1}^n}{2h_y} = \eta_k^n. \qquad (31)$$

The adjoint problem was solved by a first order finite-difference scheme (donor cells [17]).

For comparison a fourth order approximation was used for estimation of residual

$$\frac{-f_{k+2}^n + 8f_{k+1}^n - 8f_{k-1}^n + f_{k-2}^n}{12h_x}. \qquad (32)$$

This stencil provided very similar results to those of (31).

2.1. Prandtl-Mayer flow.

The comparison of deviation of the numerical solution from analytical one $\frac{\rho - \rho_{exact}}{\rho}$ and error estimation (22) is performed for a rarefaction fan (freestream Mach number M=4, deflection angle $\alpha = 10°$). Fig. 1 displays the results of error estimation as a function of the inverse spatial step (number of nodes).

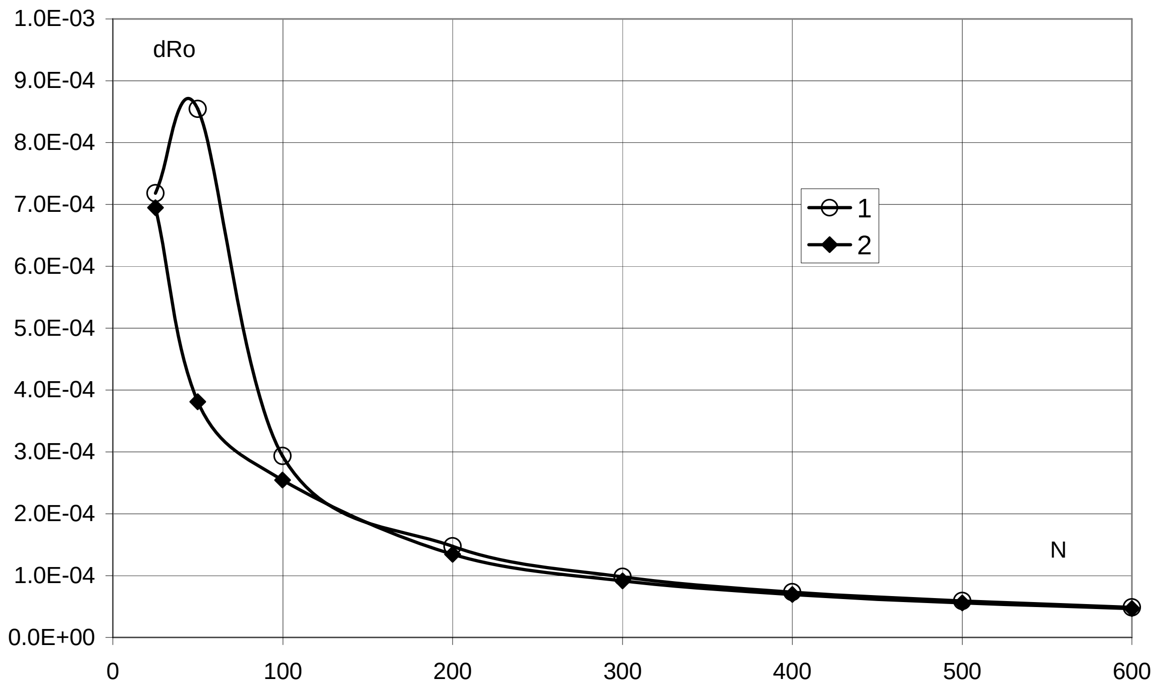

Fig. 1. 1-deviation of numerical solution from analytical value, 2- estimation of error using postprocessor.

The error of the target functional obtained from (22) is close to the discrepancy between the numerical result and the analytical value.

2.2. Shocked flow

The error in the density past two crossing shocks ($\alpha = \pm 22.23^{\circ}$, M=4) is calculated as an additional test. Figs. 2 and 3 display the isolines of density in flowfield and adjoint density (their concentration marks the location of estimated point).

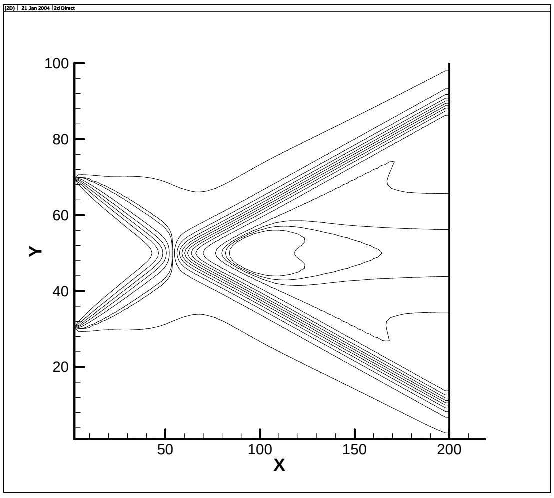

Fig. 2. Density isolines

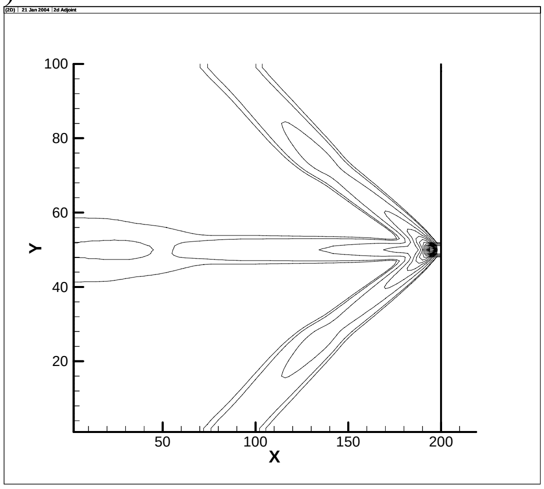

Fig.3 Adjoint density isolines

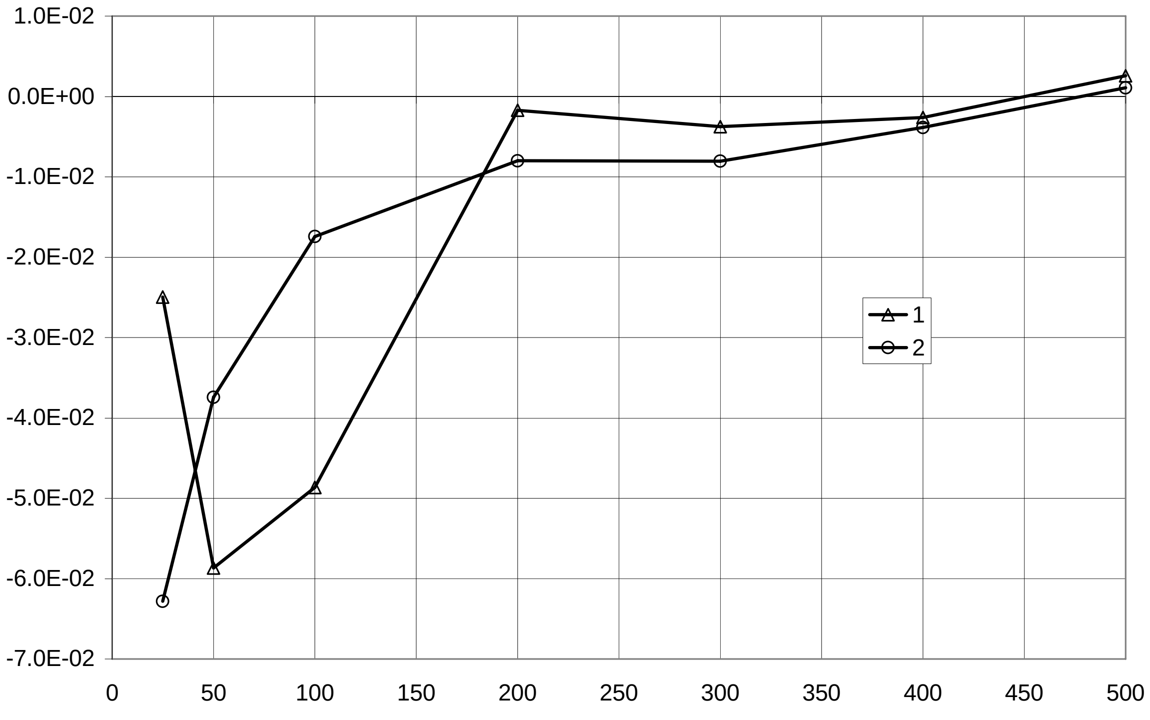

Fig. 4. The pointwise density error as a function of reciprocal spatial step. 1-deviation of numerical solution from analytical value, 2- error estimation by (22).

Fig. 4 presents the results for a flowfield calculated using the Roe scheme as a function of the spatial step.

Similar tests were performed for a flowfield calculated using the second order Godunov method [19], see Fig. 5. On smooth parts of the solution the second order stencil is not able to determine the approximation error. Only the first order components generated by the shocks [15] may be detected. However, these components dominate the solution of this problem since the results of second and fourth orders are rather close.

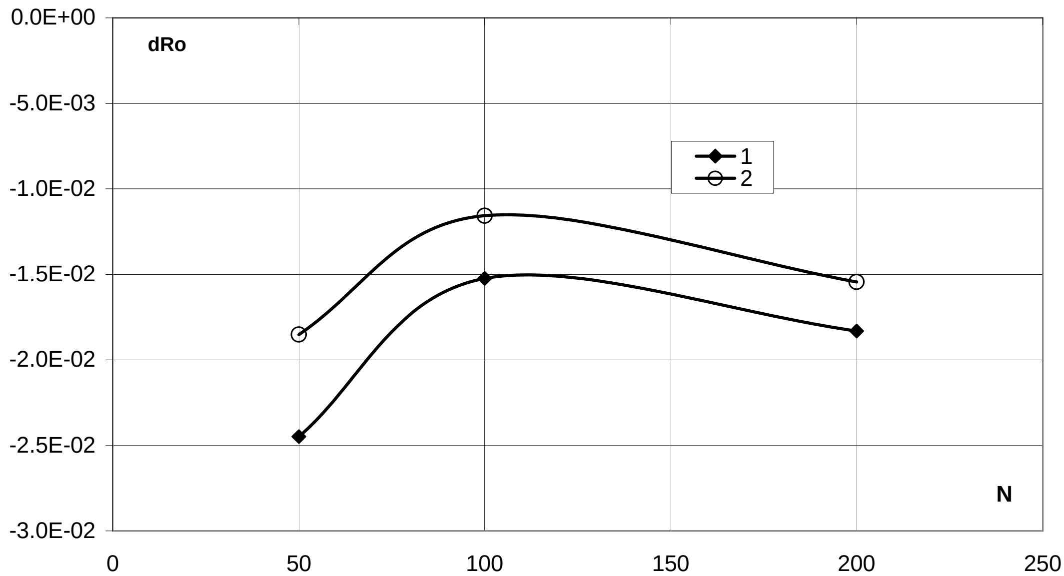

Fig. 5. Error as a function of reciprocal step (number of nodes) for second order Godunov [19]. 1-deviation of numerical solution from analytical values, 2- estimation of error by postprocessing.

3. CONCLUSION

The variation of the goal functional caused by the approximation error may be calculated via residuals obtained by the action of high order stencils on the numerical flowfield and adjoint parameters. This enables the development of a postprocessor using only the computed flowfield (and grid) information and connected with the analyzed code at the level of the respective PDE.

Numerical tests confirm validity of this methodology for the pointwise density estimation of a supersonic flow.

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Figure captions

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Fig. 2. Density isolines
Fig. 3. Adjoint density isolines
Fig. 4. The pointwise density error as a function of reciprocal spatial step. 1-deviation of numerical solution from analytical value, 2- error estimation by (22).
Fig. 5. Error as a function of reciprocal step (number of nodes) for second order Godunov [19]. 1- deviation of numerical solution from analytical values, 2- estimation of error by postprocessing.