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ON THE ESTIMATION OF APPROXIMATION ERROR IN COMPLEX VARIABLES

A.K. ALEXEEV[1], A.E. BONDAREV[2]

[1] Moscow Institute of Physics and Technology
Moscow, Russia
e-mail: aleksey.k.alekseev@gmail.com

[2] Keldysh Institute of Applied Mathematics Russian Academy of Sciences
Moscow, Russia
e-mail: bond@keldysh.ru

Summary. The feasibility for the approximation error estimation via the complex-valued solutions is demonstrated for the Euler equations describing the compressible inviscid flow. The comparison with the equations for disturbances is performed that demonstrates the distinction from the holomorphic case that caused the approximation error order reducing. The domains for Euler equations complex valued solutions are discussed.

1 INTRODUCTION

The approximation error estimation may be conducted by a great number of different methods [1] of specific advantages and demerits. The numerical computation of the problem for disturbances [2] needs for writing additional codes, close to the main problem from the viewpoint of laboriousness. The defect correction [3,4] method refines the numerical solution by deleting the impact of approximation error and leaves out the scheme or artificial viscosities having great significance for selecting “entropic” solutions. The Richardson extrapolation needs for significant number of grid levels [5] that causes significant computational burden (very high memory and time for computations). The ensemble based method [6,7] requires the computation on the set of independent numerical methods.

The “complex step” [8-11] method may be considered as “almost nonintrusive” (almost without change of codes) and computationally cheap alternative to above mentioned approaches. The main feature of this method is the expansion of the program code from real to complex numbers and inserting the truncation error to the right hand side of the imaginary part of equation. The imaginary part of solution is considered as the estimate of the approximation error.

Initially, the complex differentiation (complex step) method [8-11] was based on the Taylor expansion of holomorphic (having the complex derivative) function over imaginary disturbance

$$f(x+ih)-f(x)=ih\,df/dx-h^2d^2f/dx^2/2!-ih^3d^3f/dx^3/3!+\ldots \qquad (1)$$

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The imaginary part of this expansion provides the estimation of the disturbance (Gateau differential) with the third order of accuracy since the second order terms are left out (are in the real part).

For comparison, in real arithmetic the error has only second order.

$$f(x+h) - f(x) = hdf/dx + h^2 d^2 f/dx^2/2! + ... \qquad (2)$$

The main technical component of this approach is the transition from real numbers to complex ones in code (by declaring complex variables, the change of functions and input/output operators). These operations are nonexpensive that is one of reasons for this approach attractivity.

It is necessary to have a holomorphic function in order to obtain the third order accuracy. The Cauchy-Riemann condition should be meet that is, unfortunately, not valid for most equations of the interest. Nevertheless, the significant number of publications apply the complex step differentiation both for Euler and to Navier-Stokes equations. The paper [9] is addressed to the complex sensitivity of drag and lift coefficients to the variation of the aerodynamic profile for two-dimensional transonic turbulent flow. The sensitivity of the drag to Mach number for two-dimensional Euler equations and the sensitivity of the drag to chord length for three-dimensional flow are computed using complex step in [10]. The sensitivity of the drag and lift to geometry (profile thickness) are computed in [11] for compressible Euler and incompressible Navier-Stokes by both the complex step and adjoint method. We analyze herein the reasons for this (unexpected from the rigorous viewpoint) success and possible limitations by comparison of the imaginary part of complex valued solution and approximation of the equation for disturbances.

One of our purposes concerns the search for nonexpensive uncertainty quantification methods. Another goal is the expansion of the visualization means for multidimension problems by applying the imaginary component of the solution.

We consider the Gateau differential of the two dimensional compressible Euler equations along the direction defined by a source with the final purpose to estimate the approximation error via the local truncation error. The truncation error is estimated by a postprocessor acting on the numerical results according [12,13]. The comparison with the defect correction method is provided.

2 TEST PROBLEM

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

$$\frac{\partial \rho}{\partial t} + \frac{\partial \left(\rho u^k\right)}{\partial x^k} = 0 \qquad (3)$$

$$\frac{\partial\left(\rho u^m\right)}{\partial t}+\frac{\partial\left(\rho u^k u^m + P\delta_{mk}\right)}{\partial x^k}=0 \tag{4}$$

$$\frac{\partial(\rho E)}{\partial t}+\frac{\partial\left(\rho u^k h_0\right)}{\partial x^k}=0\,. \tag{5}$$

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

At the left boundary we accept the supersonic inflow conditions corresponding interactions of shock waves of VI kind according to Edney classification [14] (two shocks of the same family). At other boundaries we impose the outflow conditions by zero normal derivatives.

3 THE PROBLEM FOR DISTURBANCES

We consider equations (3-5) disturbed by some sources. The solutions are shifted by $\Delta\rho,\Delta u^k,\Delta E$.

$$\frac{\partial(\rho+\Delta\rho)}{\partial t}+\frac{\partial\left((\rho+\Delta\rho)(u^k+\Delta u^k)\right)}{\partial x^k}=q_\rho\,. \tag{6}$$

$$\frac{\partial\left((\rho+\Delta\rho)(u^m+\Delta u^m)\right)}{\partial t}+\frac{\partial\left((\rho+\Delta\rho)(u^k+\Delta u^k)(u^m+\Delta u^m)+(P+\Delta P)\delta_{mk}\right)}{\partial x^k}=q_{u_m}\,. \tag{7}$$

$$\frac{\partial((\rho+\Delta\rho)(E+\Delta E))}{\partial t}+\frac{\partial\left((\rho+\Delta\rho)(u^k+\Delta u^k)(h_0+\Delta h_0)\right)}{\partial x^k}=q_E\,. \tag{8}$$

In our tests we consider as the source terms the truncation error, estimated by postprocessor [13]. The estimation of the truncation error is obtained by the action of the high order stencil on the preliminary computed flow field. The forth order approximation was used for estimation of residual $\frac{-f_{k+2}^n+8f_{k+1}^n-8f_{k-1}^n+f_{k-2}^n}{12h}$. The residual, obtained by the action of this stencil on the numerical solution contains the sum of truncation errors of main scheme and the stencil, the former having the second order of approximation herein, the latter having the fourth order. The disturbance of solution is considered as an estimation of approximation.

4 COMPLEX-VALUED PROBLEM

We consider a complex-valued extension of the system (3-5) with an imaginary source term, corresponding to the above described estimate of the truncation error. The real and imaginary parts are compared with the main equations (3-5) and the equations for disturbances.

The complex continuity equation has the appearance:

$$\frac{\partial(\rho_r + i\rho_i)}{\partial t} + (u_r^k + iu_i^k)\frac{\partial(\rho_r + i\rho_i)}{\partial x^k} + (\rho_r + i\rho_i)\frac{\partial(u_r^k + iu_i^k)}{\partial x^k} = iq_\rho . \quad (9)$$

The real part:

$$\frac{\partial \rho_r}{\partial t} + u_r^k \frac{\partial \rho_r}{\partial x^k} - u_i^k \frac{\partial \rho_i}{\partial x^k} + \rho_r \frac{\partial u_r^k}{\partial x^k} - \rho_i \frac{\partial u_i^k}{\partial x^k} = 0 . \quad (10)$$

The imaginary part:

$$\frac{\partial \rho_i}{\partial t} + u_r^k \frac{\partial \rho_i}{\partial x^k} + u_i^k \frac{\partial \rho_r}{\partial x^k} + \rho_r \frac{\partial u_i}{\partial x^k} + \rho_i \frac{\partial u_r}{\partial x^k} = q_\rho . \quad (11)$$

The equations for undisturbed system (3-5) and disturbed one (6-8) engender the equations for disturbances. For density, the equation for disturbance has the form:

$$\frac{\partial \Delta\rho}{\partial t} + u^k \frac{\partial \Delta\rho}{\partial x^k} + \Delta u^k \frac{\partial \rho}{\partial x^k} + \rho \frac{\partial \Delta u^k}{\partial x^k} + \Delta\rho \frac{\partial u^k}{\partial x^k} + \frac{\partial(\Delta\rho \Delta u^k)}{\partial x^k} = q_\rho . \quad (12)$$

The comparison demonstrates that the real part (10) corresponds to the initial equation (3) disturbed by the second order term:

$$-u_i^k \frac{\partial \rho_i}{\partial x^k} - \rho_i \frac{\partial u_i^k}{\partial x^k} . \quad (13)$$

The imaginary part coincides with the equation for disturbances (12) without the second order term

$$\frac{\partial(\Delta\rho \Delta u^k)}{\partial x^k} . \quad (14)$$

Additionally, the imaginary part includes real coefficients that contain the second order disturbances caused by (13). This causes third order of disturbances in the imaginary part.

The complex equation for momentum

$$\frac{\partial((u_r^m + iu_i^m)(\rho_r + i\rho_i))}{\partial t} + \frac{\partial((\rho_r + i\rho_i)(u_r^m + iu_i^m)(u_r^k + iu_i^k))}{\partial x^k} + \\ + (\gamma - 1)\frac{\partial(e_r + ie_i)(\rho_r + i\rho_i)}{\partial x^k} = iq_{u^m} \quad (15)$$

has the real part, similar to Eq. (4) with the disturbances of the second and third order

$$\frac{\partial(\rho_r u_r^m)}{\partial t}-\frac{\partial(\rho_i u_i^m)}{\partial t}+\frac{\partial(\rho_r u_r^m u_r^k-\rho_r u_i^m u_i^k-\rho_i u_r^m u_i^k-\rho_i u_i^m u_r^k)}{\partial x^k}+(\gamma-1)\frac{\partial(e_r\rho_r-e_i\rho_i)}{\partial x^k}=0 \quad (16)$$

and the imaginary part

$$\frac{\partial(u_i^m\rho_r)}{\partial t}+\frac{\partial(u_r^m\rho_i)}{\partial t}+\frac{\partial(\rho_r u_r^m u_i^k+\rho_r u_r^k u_i^m+\rho_i u_r^m u_r^k-\rho_i u_i^m u_i^k)}{\partial x^k}+(\gamma-1)\frac{\partial(e_r\rho_i+e_i\rho_r)}{\partial x^k}=q_{u_m} \quad (17)$$

From the comparison one may see that the imaginary part is equivalent to the problem for disturbances

$$\frac{\partial(\Delta u^m\rho)}{\partial t}+\frac{\partial(u^m\Delta\rho)}{\partial t}+\frac{\partial(\rho u^m\Delta u^k+\rho u^k\Delta u^m+u^k u^m\Delta\rho+\Delta\rho\Delta u^k\Delta u^m)}{\partial x^k}+(\gamma-1)\frac{\partial(e\Delta\rho+\Delta e\rho)}{\partial x^k}=q_{u_m} \quad (18)$$

with different signs of the third order term.

The complex energy equation

$$\frac{\partial((\rho_r+i\rho_i)(E_r+iE_i))}{\partial t}+\frac{\partial\{(\rho_r+i\rho_i)(u_r^k+iu_i^k)(h_{0,r}+ih_{0,i})\}}{\partial x^k}=iq_e \quad (19)$$

contains real part

$$\frac{\partial(\rho_r E_r-\rho_i E_i)}{\partial t}+\frac{\partial(\rho_r u_r^k h_{0,r}-\rho_r u_i^k h_{0,i}-\rho_i u_r^k h_{0,i}-\rho_i u_i^k h_{0,r})}{\partial x^k}=0 \quad (20)$$

that is equivalent to Eq. (5) with the second order disturbances.

The imaginary part

$$\frac{\partial(\rho_i E_r+\rho_r E_i)}{\partial t}+\frac{\partial(\rho_r u_r^k h_{0,i}+\rho_r u_i^k h_{0,r}+\rho_i u_r^k h_{0,r}-\rho_i u_i^k h_{0,i})}{\partial x^k}=q_e \quad (21)$$

is close to the disturbances equation

$$\frac{\partial(\Delta\rho E+\rho\Delta E)}{\partial t}+\frac{\partial(\rho u^k\Delta h_0+\rho\Delta u^k h_0+\Delta\rho u^k h_0+\Delta\rho\Delta u^k\Delta h_0)}{\partial x^k}=q_e \quad (22)$$

with different signs of the third order term.

Thus, the transition to the complex valued solutions enables the computation of the density disturbance with the second order (not with the third order, as in [8-11]) and disturbances in the momentum and energy with the third order error. It is caused by the nonholomorphic properties of the system. However, the result is more optimistic, than one can predict from comparison of Eq. (1) and (2).

5 NUMERICAL TESTS

The interaction of shock waves of *VI* kind according to Edney classification [14] was used as the test problem. Only steady-state flow is considered, so only the spatial discretization error is addressed. The calculations are performed by the algorithm [15].

Fig. 1 demonstrates the flowfield (density isolines) for $M = 4$, $\alpha_1 = 10^o$, $\alpha_2 = 15^o$

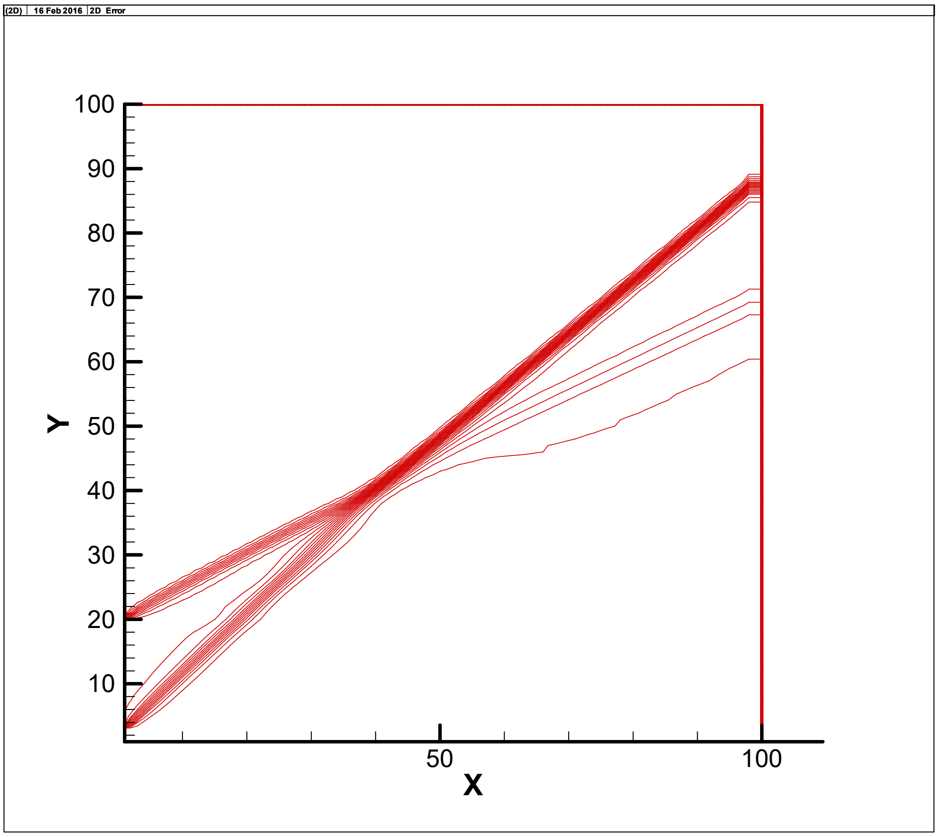

Fig. 1. Density isolines

Fig. 2 represents the field of the density disturbance caused by the truncation error used as a source in the real valued code variant.

The complex-valued code variant was run with the imaginary source term equal to the truncation error. The boundary conditions for real component are the same as for the real code variant. The inflow conditions for the imaginary component are zero. At other boundaries the imaginary outflow conditions are set by zero normal derivatives. Fig. 3 represents the imaginary part of the complex valued solution of the Euler equations.

The solutions in Fig. 2 and Fig. 3 are similar, however the complex valued solution seems to be more oscillating.

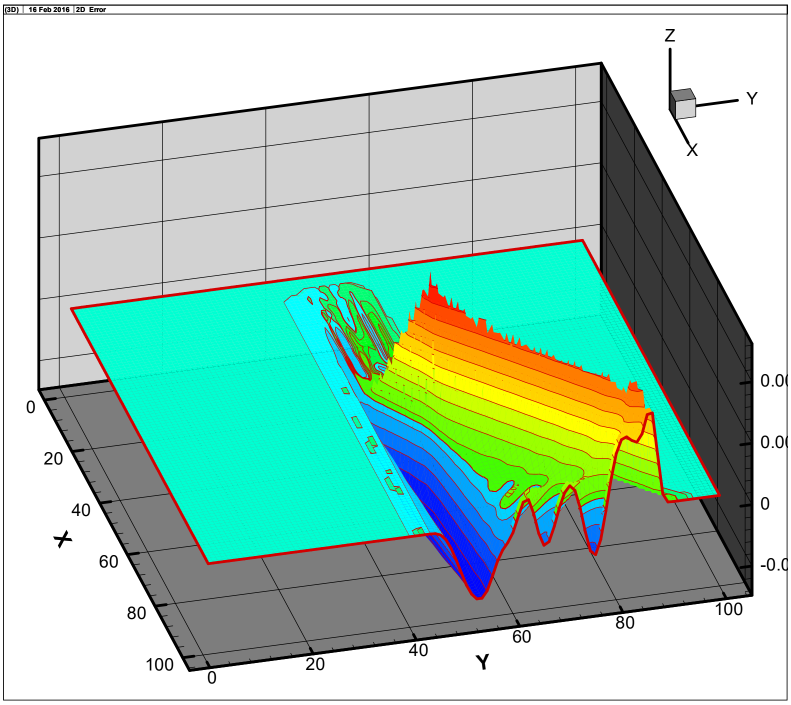

Fig. 2. Density disturbance caused by the truncation error used as a source in the real valued code variant

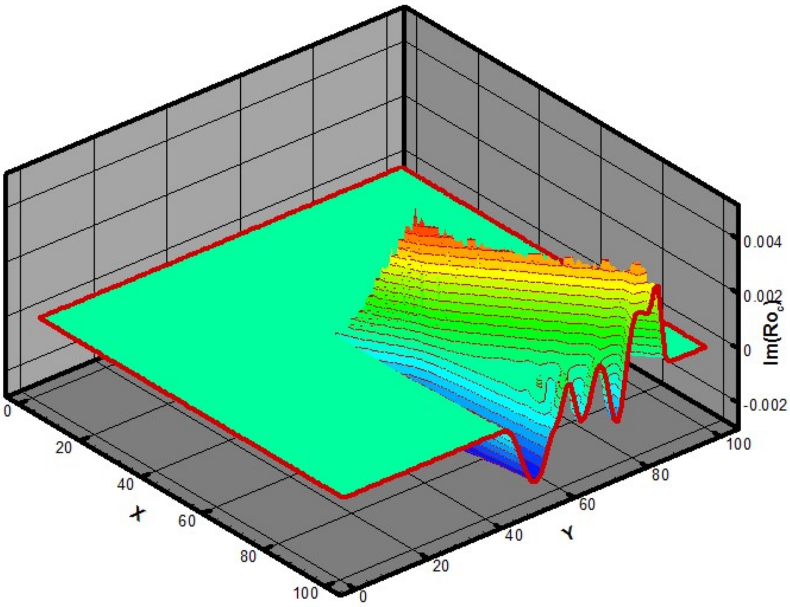

Fig. 3. Imaginary part of the complex valued solution

6 DISCUSSION

From the technical viewpoint, the defect correction may be rather easily implemented for the approximation error estimation. However, this approach for the Euler equations may cause oscillations and even deviation from the “entropic” solution, since the scheme and artificial viscosities are deleted.

The calculation of the problem for disturbances transfer may be more stable and reliable, however this approach requires coding and debugging.

The calculation of the disturbances by the complex valued problem is more reliable and need for a minimal coding efforts. Unfortunately, the range of applications for complex valued solutions for the equations, which satisfies Cauchy-Riemann conditions is strictly limited (potential two-dimensional flows). So, the Cauchy Riemann condition is not valid for the compressible Euler equations that restricts the order of accuracy for this estimation (but not prohibit it).

The expansion of CFD equations from the real to complex space seems to be of the interest from the algebraic viewpoint, since the complex numbers field is algebraically closed (by the fundamental theorem of algebra), in contrast to the real numbers. It may be important from the viewpoint of the search for coherent structures, disconnected solutions and a global structure of solutions by a smooth transformation (homotopy) of one solution to another [16,17]. In order to avoid singularities during the path tracking in real space, one may add a random complex number into the homotopy function [17]. For example, the homotopy continuation along viscosity coefficient in [17] is used to track the solution starting at the initial solution to obtain a steady state inviscous solution. So, CFD algorithms, enhanced for complex-valued solutions, may be of interest for - trick based homotopy methods.

On other hand, the singularities in real flow (if they exist) may be preceded by the formation of complex-space singularities [18]. It is another reason for interest to complex-valued solutions. There are papers [19-21] that demonstrates the blow-up solutions for 3D incompressible complex-valued Navier-Stokes for some class of complex initial data. The blow-up solutions for 3D incompressible complex-valued Euler equations are demonstrated by [22]. The present paper results and the papers using complex step differentiation algorithms [8-11] demonstrated the stable solutions for the complex-valued CFD problems that may be considered as an evidence of the blow-up being not the case of general position.

So, the search for the global structure of solutions including separated branches and domains of the blow-up is of the current interest and it provides the perspective application domain for complex-valued equations.

There are other domains for complex-valued fluid dynamics. Most popular one is the stability analysis based on the complex valued solutions for the linearized equations. Ref. [23] addresses a generalized form of the BGK-Boltzmann equation for complex-valued equilibrium distribution function. However, the real-valued Navier-Stokes equations are recovered, provided that the imaginary component of the macroscopic mass is neglected.

In general, the application of the complex-valued analogues of CFD equations is far away from the standard practice at present and needs for further analysis, especially, in topic concerning complex initial and boundary conditions and their physical meanings.

7 CONCLUSIONS

The complex valued extension of Euler equations enables the computation of the main problem and the problem for disturbances by the single program, obtained from standard CFD code by the change of variables and subroutines from real to complex ones. It requires the minor efforts in coding.

Fortunately, this approach is not restricted to holomorphic functions, and can be applied to the standard CFD codes, although with the lesser error order.

The real part of the complex-valued Euler equations corresponds to the main problem with the second order error.

The imaginary part of the problem corresponds to the problem for disturbances with the second (continuity) or third order (momentum and energy) errors.

The extension of the program codes from real numbers to complex ones provides additional possibilities for the computation and visualization of the disturbances in the flowfield including ones caused by the truncation errors.

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