DEVELOPMENT OF SOLVER FOR MODELING COMPRESSIBLE FLOWS USING REGULARISED GAS DYNAMIC EQUATIONS (IN THE QUASI-HYDRODYNAMIC APPROXIMATION)

M. V. KRAPOSHIN[1], E.V SMIRNOVA[2] , T.G.ELIZAROVA[3], M.A.ISTOMINA[4]
[1]*Institute for System Programming RAS, os-cfd@yandex.ru*
[2]*Institute for System Programming RAS, ev_smir@mail.ru*
[3]*Keldysh Institute of Applied Mathematics RAS, telizar@mail.ru*
[4]*Keldysh Institute of Applied Mathematics RAS, m_ist@mail.ru*

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Introduction

In this work we announce the development of a new solver for numerical simulation of viscous compressible flows in the wide range of Mach numbers in the framework of OpenFOAM API. The new solver is based on the implementation of regularized, or quasi gas dynamic (QGD) equations. The mixed finite-volume and finite-difference approximation is constructed on unstructured space grids using the inherit in the OpenFOAM complex formalism.

Numerical methods for gas dynamic flow simulations based on QGD equations are known for more than 30 years - see for example [1], references given in the book, and the subsequent work of the authors. The advantages of the QGD algorithms consist in their uniformity in the modeling of the gas flows in a wide range of Mach numbers including subsonic flows and hypersonic flows with strong shock waves. Computational experience shows that the QGD algorithms are effective for modeling of oscillatory and rapidly varying flows including turbulent flow at low Reynolds numbers. In particular, in the number of problems the laminar-turbulent transition was obtained without the introducing of numerical turbulence models. These features of the QGD algorithms were confirmed by a number of test and practical calculations.

Previously, the QGD numerical algorithms were implemented for Cartesian and cylindrical coordinates for rectangular space-grids for three-dimensional flows. There were implementations of algorithms for regular and irregular non-orthogonal grids. A number of programs were implemented on multiprocessor computational systems with MPI standard.

Current implementation of the QGD algorithms on the basis of OpenFOAM would significantly expand the scope of their application and would give the possibilities to try it by a wide range of users.

1. Regularised, or quasi gas dynamic equations

A special feature of the QGD equations in comparison with the the Navier-Stokes system is the presence of additional terms in the constitutive relations, the contribution of which is determined by the smoothing parameter τ. These additional terms have a dissipative nature and ensure the conditional stability of the algorithm with the Courant time step and the central-difference second order approximation for all space derivatives, including convective terms. For viscous flows QGD equations have the following form:

continuity equation:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \vec{j}_m = 0, \qquad (1)$$

momentum equation:

$$\frac{\partial (\rho \vec{u})}{\partial t} + \nabla \cdot (\vec{j}_m \otimes \vec{u}) + \nabla p = \nabla \cdot \Pi, \qquad (2)$$

total energy equation:

$$\frac{\partial (\rho E)}{\partial t} + \nabla \cdot (\vec{j}_m H) + \nabla \cdot \vec{q} = \nabla \cdot (\Pi \cdot \vec{u}). \qquad (3)$$

Here, ρ is the gas density, $\vec{u}$ is the velocity, p is the pressure, T is the temperature, $\vec{j}_m = \rho\vec{u} - \tau(\nabla \cdot (\rho\vec{u}\otimes\vec{u}) + \nabla p)$ is the mass flux vector, $\tau = \alpha \frac{h}{c}$ is the smoothing parameter, h is the step of a space discretization, c is the sound speed, $\Pi = \Pi_{NS} + \tau\vec{u}\otimes(\rho(\vec{u}\cdot\nabla)\vec{u} + \nabla p) + \tau I\big((\vec{u}\cdot\nabla)p + \gamma p \nabla\cdot\vec{u}\big)$ is the shear stress tensor, I is the unit tensor of the second rank, γ is the specific heat ratio (adiabatic index), E is the total energy, H is the enthalpy, $\vec{q} = -\kappa\nabla T - \tau\rho\vec{u}\Big((\vec{u}\cdot\nabla)\varepsilon + pu\cdot\nabla 1\rho$ is the heat flux vector, κ is the heat conductivity coefficient, ε is the internal energy.

The system of equations (1)—(3) must be supplemented by an equation of state, as well as the necessary boundary conditions. In this paper we used the equation of state of an ideal polytrophic gas.

2. Implementation of quasi gas dynamic equations in OpenFOAM

We use the explicit finite-volume scheme with a second order approximation in space and first order approximation in time. For example, the continuity equation, in which the desired value ρ must be found, the scheme has the form

$$\rho_i^n = \rho_i^o - \sum_f F_{j_m,f}{}^o. \quad (4)$$

Here ρ_i is the density value in the center of the cell with the number i; $F_{j_m,f}$ is the density flux through the face f; index o means that the value is taken from the previous time step, index n means that the value is calculated in the new time step.

Flux calculations require to approximate the partial derivatives of gas dynamic quantities on the faces, for example, we must calculate the value of $\tau(\nabla\cdot(\rho\vec{u}\otimes\vec{u})+\nabla p)$, that is included in the mass flux vector. Derivatives must be calculated by the values in the cells nearest to the used face. To do this, the authors implement a module that allows to compute the gradients of scalar and vector fields, divergence of vector and tensor fields in the centers of the finite volumes. To calculate the gradient of the scalar field the method of least squares [3] is used. The value of the gradient at the faces is calculated using field values in the centers of the control volumes adjacent to the face through its nodes, by the formula

$$\nabla g|_f = \sum_{i=1}^N w_i^2 G^{-1}\overrightarrow{d_i}(g_i - g_f). \quad (5)$$

Here $g(\vec{x})$ is a salernitana (scalar) function, $\overrightarrow{d_i} = \overrightarrow{x_i} - \overrightarrow{x_f}$; $w_i = \frac{1}{|\overrightarrow{d_i}|}$ are the weights of the scheme, the summation is carried out using the adjacent to the face f cells. To calculate the weights of the schem, we use the data from all cells closest to the selected face (fig. 1).

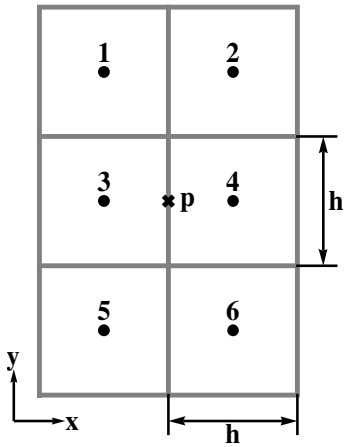

Figure Ошибка! Не указана последовательность.**: Template for calculation of the gradient of the field in the center of the face on a uniform two-dimensional grid.**

The proposed numerical scheme to calculate the derivatives on the cell faces and previously used one for solving the QGD equations [1] differ, but both schemes have the second order of approximation in space. The proposed scheme allows to approximate the required components on unstructured grids.

3. Testing of the solver on the Soda tests. Checking the grid convergence

The solver is tested on one-dimensional Soda problems of the decay of the discontinuities proposed in [2]. Consider the one-dimensional computational domain with a length $L = 1$. Adiabatic index is equal to $\gamma = 1.4$ (the heat capacity at constant pressure is $C_p = 1.4$, the heat capacity at constant volume is $C_v = 1.0$). Then, individual gas constant is $\frac{R}{\mu} = 0.4$, so the molar mass must be set equal to 20785. Initial field values are given in table 1.

Table 1. Parameters of test tasks

Test	ρ_L	u_L	p_L	T_L	ρ_R	u_R	p_R	T_R	t_{end}
1	1.0	0.0	1.0	2.5	0.125	0.0	0.1	2.0	0.25
2	1.0	-2.0	0.4	1.0	1.0	2.0	0.4	1.0	0.15

To check the grid convergence for test 1, case was solved on computational grids with number of cells 100, 200 and 400, test 2 problem additionally solved on grids with 800, 1600 and 3200 cells. In the first test numerical coefficient α in smoothing term is set equal to 0.5, for the test 2 it is equal to 0.1. The comparison of the numerical solution of the test problems with the analytical solutions are shown in fig.2-3. These graphs show the grid convergence of the solution with the decreasing the spatial step. The actual accuracy order for choosing tests is $O(\alpha h^{0.7} + \Delta t)$.

Conclusion

The solver based on regularized gas dynamic equations is implemented in OpenFOAM complex. Numerical scheme is explicit in time and has the second order centered space approximation. A module with the procedures for calculations of partial space derivatives on the faces of the finite volumes of unstructured grids is written. Testing of the solver on two Rieman problems shows the grid convergence of the numerical solution with decreasing space step.

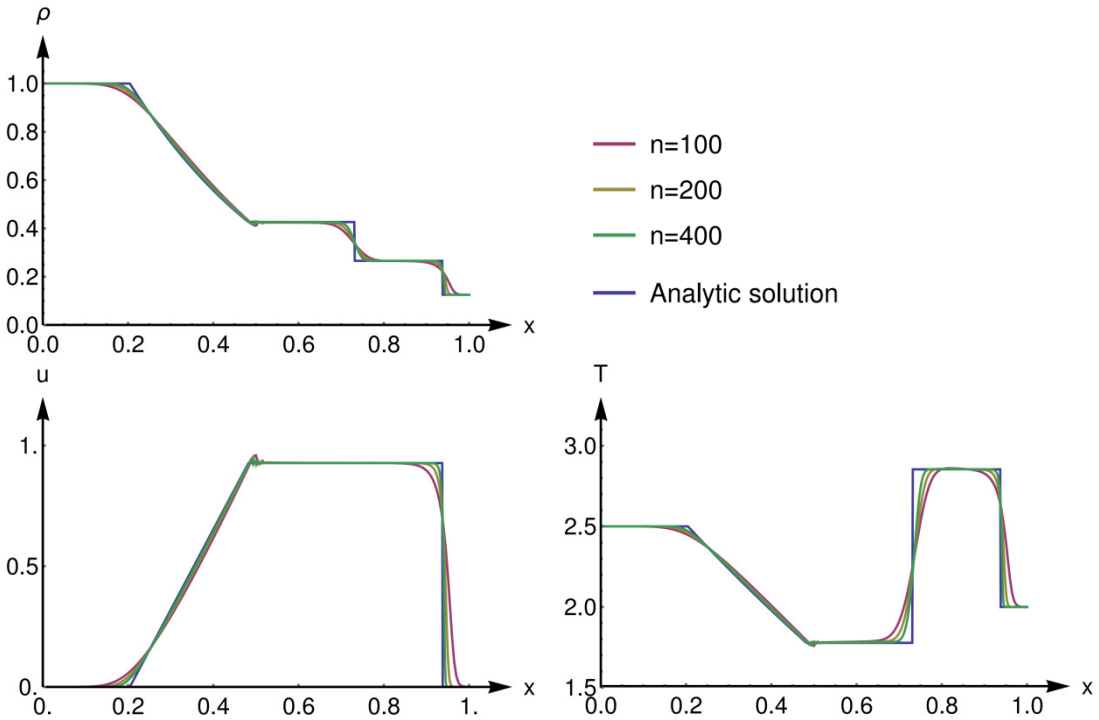

Figure 2: Comparison of the numerical solution on grids with 100, 200 and 400 cells with the analytical solution for test 1.

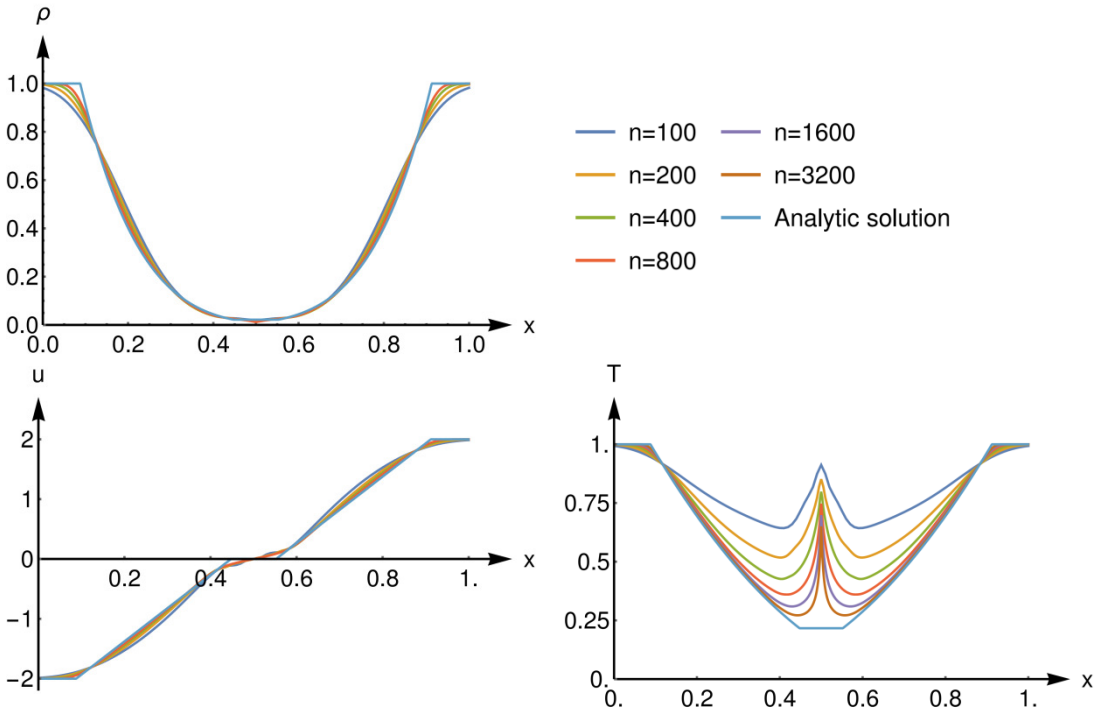

Figure 3: Comparison of the numerical solution on different grids with the analytical solution for test 2.

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