

Quasi-gasdynamics numerical algorithm for gas flow simulations

T. G. Elizarova^{1,*}, A. A. Khokhlov² and Yu. V. Sheretov³

¹*Institute for Mathematical Modeling, Russian Academy of Sciences, Miusskaya pl. 4a, Moscow 125047, Russia*

²*Faculty of Physics, M. V. Lomonosov Moscow State University, Leninskie Gory, Moscow 119992, Russia*

³*Tver State University, ul. Zhebyabova 33, Tver, Russia*

SUMMARY

The quasi-gasdynamics equation system and the numerical algorithm for non-stationary viscous gasdynamic flow calculations are presented. The quasi-gasdynamics equation system generalizes the Navier–Stokes equations and differs from it by the additional dissipative terms. The numerical examples are presented. Copyright © 2007 John Wiley & Sons, Ltd.

Received 16 April 2007; Revised 6 October 2007; Accepted 8 October 2007

KEY WORDS: quasi-gasdynamics equations; numerical algorithm; compressible flows

QUASI-GASDYNAMIC EQUATIONS

The paper is devoted to the contemporary mathematical model for gas flows and to the related numerical methods for flow simulations. The mathematical model generalizes the Navier–Stokes (NS) system of equations. This model is different from the NS system in additional dissipative terms with a small parameter in τ . The new model is named the quasi-gasdynamics (QGD) system of equations. The first variant of the QGD system was presented in [1] and developed later in, e.g. [2–5]. The QGD system has a form of the conservation laws and in common notations is expressed as

$$\frac{\partial \rho}{\partial t} + \text{div } \mathbf{j}_m = 0 \quad (1)$$

$$\frac{\partial(\rho \mathbf{u})}{\partial t} + \text{div}(\mathbf{j}_m \otimes \mathbf{u}) + \nabla p = \text{div } \Pi \quad (2)$$

$$\frac{\partial}{\partial t} \left[\rho \left(\frac{\mathbf{u}^2}{2} + \varepsilon \right) \right] + \text{div} \left[\mathbf{j}_m \left(\frac{\mathbf{u}^2}{2} + \varepsilon + \frac{p}{\rho} \right) \right] + \text{div } \mathbf{q} = \text{div}(\Pi \cdot \mathbf{u}) \quad (3)$$

*Correspondence to: T. G. Elizarova, Institute for Mathematical Modeling, Russian Academy of Sciences, Miusskaya pl. 4a, Moscow 125047, Russia.

†E-mail: telizar@yahoo.com

with the closing relations

$$\mathbf{j}_m = \rho(\mathbf{u} - \mathbf{w}) \quad \text{where } \mathbf{w} = \frac{\tau}{\rho} [\text{div}(\rho \mathbf{u} \otimes \mathbf{u}) + \nabla p] \quad (4)$$

$$\Pi = \Pi_{\text{NS}} + \tau \mathbf{u} \otimes [\rho(\mathbf{u} \cdot \nabla) \mathbf{u} + \nabla p] + \tau I[(\mathbf{u} \cdot \nabla) p + \gamma p \text{div } \mathbf{u}] \quad (5)$$

$$\mathbf{q} = \mathbf{q}_{\text{NS}} - \tau \rho \mathbf{u} \left[(\mathbf{u} \cdot \nabla) \varepsilon + p(\mathbf{u} \cdot \nabla) \left(\frac{1}{\rho} \right) \right] \quad (6)$$

Here, Π_{NS} and \mathbf{q}_{NS} are the NS shear-stress tensor and heat flux vector, respectively, τ is a small parameter with dimension of time. System (1)–(6) is completed by the state equations for a perfect gas and the expressions for the coefficients of viscosity, heat conductivity and τ coefficient.

The entropy production X for the QGD system is the entropy production for the NS system completed by the additional terms in τ that are squared left-hand sides of the classical stationary Euler equations with positive coefficients:

$$\begin{aligned} X = & \kappa \left(\frac{\nabla T}{T} \right)^2 + \frac{(\Pi_{\text{NS}} : \Pi_{\text{NS}})}{2\mu T} + \frac{p\tau}{\rho^2 T} [\text{div}(\rho \mathbf{u})]^2 \\ & + \frac{\tau}{\rho T} [\rho(\mathbf{u} \cdot \nabla) \mathbf{u} + \nabla p]^2 + \frac{\tau}{\rho \varepsilon T} [\rho(\mathbf{u} \cdot \nabla) \varepsilon + p \text{div } \mathbf{u}]^2 \end{aligned} \quad (7)$$

in which $(\Pi_{\text{NS}} : \Pi_{\text{NS}})$ is the double scalar product of two identical tensors. Equation (7) proves the dissipative nature of the additional τ -terms and the correctness of the QGD model with respect to the second law of thermodynamics.

The QGD system differs from the NS equations by the second space derivative terms of an order $O(\tau)$. For stationary flows, the dissipative terms (terms in τ) in the QGD equations have the asymptotic order of $O(\tau^2)$ for $\tau \rightarrow 0$. In a boundary layer limit both QGD and NS equations reduce to the Prandtl equation system.

The terms in τ allow one to construct the family of the novel efficient numerical algorithms for the simulation of non-stationary supersonic and subsonic gasdynamic flows. The QGD algorithms inherit the mathematical properties of the QGD system.

Others gasdynamic models with non-classical continuity equation are presented in, e.g. [6–11]. Models [6–10] do not include the velocity derivatives in mass flux vector. The system [11] includes the second time derivatives that do not appear in the QGD model.

FINITE-DIFFERENCE APPROXIMATION

Finite-difference approximations of the QGD system are constructed in a flux form directly using the mass flux vector \mathbf{j}_m , the shear-stress tensor Π and the heat flux vector \mathbf{q} that correspond to the conservation laws for the QGD equations (1)–(6). Invariant form of the QGD system allows one to construct numerical methods for any orthogonal coordinate system for the structured and unstructured space grids.

As an example below we present the finite-volume algorithm for the two-dimensional Cartesian coordinate system. In this case, the QGD system is expressed as

$$\frac{\partial \rho}{\partial t} + \frac{\partial j_{mx}}{\partial x} + \frac{\partial j_{my}}{\partial y} = 0 \tag{8}$$

$$\frac{\partial(\rho u_x)}{\partial t} + \frac{\partial(j_{mx}u_x)}{\partial x} + \frac{\partial(j_{my}u_x)}{\partial y} + \frac{\partial p}{\partial x} = \frac{\partial \Pi_{xx}}{\partial x} + \frac{\partial \Pi_{yx}}{\partial y} \tag{9}$$

$$\frac{\partial(\rho u_y)}{\partial t} + \frac{\partial(j_{mx}u_y)}{\partial x} + \frac{\partial(j_{my}u_y)}{\partial y} + \frac{\partial p}{\partial y} = \frac{\partial \Pi_{xy}}{\partial x} + \frac{\partial \Pi_{yy}}{\partial y} \tag{10}$$

$$\begin{aligned} \frac{\partial E}{\partial t} + \frac{\partial(j_{mx}H)}{\partial x} + \frac{\partial(j_{my}H)}{\partial y} + \frac{\partial q_x}{\partial x} + \frac{\partial q_y}{\partial y} \\ = \frac{\partial}{\partial x}(\Pi_{xx}u_x + \Pi_{xy}u_y) + \frac{\partial}{\partial y}(\Pi_{yx}u_x + \Pi_{yy}u_y) \end{aligned} \tag{11}$$

Here u_x and u_y are the projections of the velocity \mathbf{u} onto the x - and y -axes, respectively, E is the total energy of a unit volume and H is the total specific enthalpy. The last two quantities are calculated as

$$E = \rho \frac{u_x^2 + u_y^2}{2} + \frac{p}{\gamma - 1}, \quad H = \frac{(E + p)}{\rho} \quad \text{with } p = \rho \mathcal{R}T, \quad \varepsilon = \frac{p}{\rho(\gamma - 1)} \tag{12}$$

The components of the mass flux vector \mathbf{j}_m are

$$j_{mx} = \rho(u_x - w_x), \quad j_{my} = \rho(u_y - w_y) \tag{13}$$

where

$$w_x = \frac{\tau}{\rho} \left[\frac{\partial(\rho u_x^2)}{\partial x} + \frac{\partial(\rho u_x u_y)}{\partial y} + \frac{\partial p}{\partial x} \right], \quad w_y = \frac{\tau}{\rho} \left[\frac{\partial(\rho u_x u_y)}{\partial x} + \frac{\partial(\rho u_y^2)}{\partial y} + \frac{\partial p}{\partial y} \right]$$

The components of Π are determined by the following formula, convenient for a programme realization:

$$\begin{aligned} \Pi_{xx} &= \Pi_{xx}^{NS} + u_x w_x^* + R^*, & \Pi_{xx}^{NS} &= 2\mu \frac{\partial u_x}{\partial x} - \frac{2}{3}\mu \operatorname{div} \mathbf{u} \\ \Pi_{xy} &= \Pi_{xy}^{NS} + u_x w_y^*, & \Pi_{xy}^{NS} = \Pi_{yx}^{NS} &= \mu \left(\frac{\partial u_y}{\partial x} + \frac{\partial u_x}{\partial y} \right) \\ \Pi_{yx} &= \Pi_{yx}^{NS} + u_y w_x^* \\ \Pi_{yy} &= \Pi_{yy}^{NS} + u_y w_y^* + R^*, & \Pi_{yy}^{NS} &= 2\mu \frac{\partial u_y}{\partial y} - \frac{2}{3}\mu \operatorname{div} \mathbf{u} \end{aligned} \tag{14}$$

where

$$\begin{aligned} w_x^* &= \tau \left[\rho u_x \frac{\partial u_x}{\partial x} + \rho u_y \frac{\partial u_x}{\partial y} + \frac{\partial p}{\partial x} \right], & w_y^* &= \tau \left[\rho u_x \frac{\partial u_y}{\partial x} + \rho u_y \frac{\partial u_y}{\partial y} + \frac{\partial p}{\partial y} \right] \\ R^* &= \tau \left[u_x \frac{\partial p}{\partial x} + u_y \frac{\partial p}{\partial y} + \gamma p \operatorname{div} \mathbf{u} \right] \end{aligned} \quad (15)$$

The components of the heat flux \mathbf{q} are

$$\begin{aligned} q_x &= q_x^{\text{NS}} - u_x R^q, & q_y &= q_y^{\text{NS}} - u_y R^q \\ R^q &= \tau \rho \left[\frac{u_x}{\gamma-1} \frac{\partial}{\partial x} \left(\frac{p}{\rho} \right) + \frac{u_y}{\gamma-1} \frac{\partial}{\partial y} \left(\frac{p}{\rho} \right) + p u_x \frac{\partial}{\partial x} \left(\frac{1}{\rho} \right) + p u_y \frac{\partial}{\partial y} \left(\frac{1}{\rho} \right) \right] \end{aligned} \quad (16)$$

The heat conductivity coefficient κ and the coefficient τ are connected with the viscosity coefficient μ by

$$\kappa = \frac{\gamma \mathcal{R}}{(\gamma-1) Pr} \mu, \quad \tau = \frac{1}{p Sc} \mu \quad \text{where } \mu = \mu_0 \left(\frac{T}{T_0} \right)^\omega \quad (17)$$

and Pr is the Prandtl number, Sc is the Schmidt number, \mathcal{R} is the gas constant and γ is the specific heat ratio.

The equation system (8)–(11) must be completed by the initial and boundary conditions. In contrast to the NS system, the continuity equation (1) in the QGD system is an equation of a second order in space. Thus, the QGD system must be completed by an additional boundary condition. This condition for the pressure p is obtained by imposing appropriate boundary condition for the mass flux vector \mathbf{j}_m . For example, for unpenetrated wall with $\mathbf{u} = \mathbf{0}$ and $\mathbf{j}_m = \mathbf{0}$, according to (4), the additional boundary condition for the pressure has the form $\partial p / \partial n = 0$, where n is the normal vector to the wall.

To solve the problem numerically, the space and time grids are introduced in a computational domain. The gasdynamic parameters—density ρ , pressure p and velocity \mathbf{u} —are determined at the nodes of the grid. The values of the gasdynamic parameters at the nodes with half-integer indices and at the cell's centers are determined as the arithmetic mean of their values at the adjacent nodes. The finite-difference approximation of the QGD system (1)–(6) is constructed using the control volume method. The similar approximations are used for rectangular structural grids and unstructured three-cornered grids.

An initial boundary value problem is solved by applying an explicit finite-difference scheme in time. The spatial derivatives are approximated by the central differences with a second-order accuracy, and the time derivatives are approximated by the forward differences with a first-order accuracy. The stability of the numerical algorithm is provided by the QGD terms in τ .

NUMERICAL ALGORITHM FOR SUPERSONIC FLOWS

To ensure stability of a numerical solution for the supersonic flows, the term proportional to the grid step h is added to τ . Then, the coefficient τ , viscosity and heat conductivity are calculated as

$$\tau = \frac{\mu_0}{p Sc} \left(\frac{T}{T_0} \right)^\omega + \alpha \frac{h}{c}, \quad \mu = \tau p Sc, \quad \kappa = \frac{\gamma \mathcal{R} \tau p Sc}{Pr(\gamma-1)} \quad (18)$$

where $c = \sqrt{\gamma \mathcal{R} T}$ is a local sound velocity and α is a numerical factor $0 \leq \alpha \leq 1$.

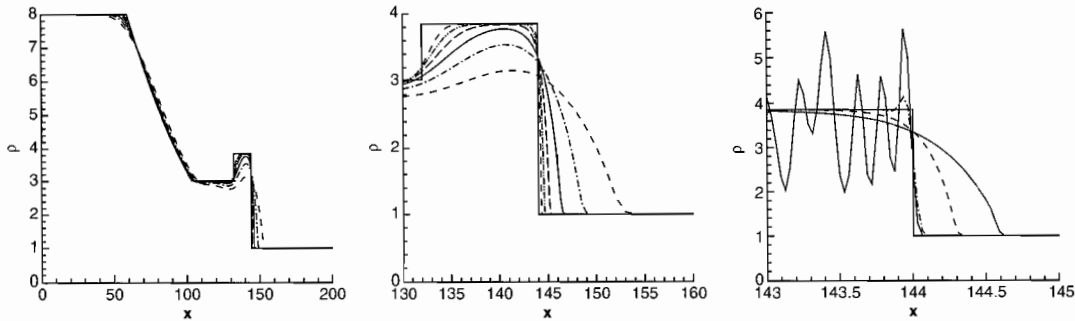


Figure 1. Density distribution along x (left—whole computational domain, right—fragments).

As an example of application we present here the strong discontinuity step evolution problem in non-viscous gas without heat conductivity ($1/Re=0$). To solve Euler equations all terms proportional to $\tau = \alpha h/c$ are regarded as the artificial dissipation.

The problem is solved in the space interval $0 \leq x \leq 200$ for the time $0 \leq t \leq 8$ with Courant stability condition $\Delta t = \beta h/c_{\max}$. We take $Sc = 1$, $Pr = \frac{2}{3}$ and $\gamma = \frac{5}{3}$. Initial conditions form a discontinuity at $x = 100$. The values to the left and to the right from the break are as follows:

$$\rho(x, 0) = \begin{cases} 8, & x \leq 100 \\ 1, & x > 100 \end{cases}, \quad p(x, 0) = \begin{cases} 480, & x \leq 100 \\ 1, & x > 100 \end{cases}, \quad u(x, 0) = 0$$

We used grid steps $h = 1, 0.5, 0.25, 0.125, 0.0625$ and 0.03125 with $\Delta t = 0.002$ for the first three variants, and $\Delta t = 0.0002$ for the last three ones. The convergence of the numerical results to analytical solution with reducing h for $t = 4$ is shown in Figure 1 for $\alpha = 0.5$ (two left figures). The dependence of the solution from parameter α for $h = 0.03125$ is shown on the right figure for $\alpha = 1, 0.1, 0.5, 0.1$ and 0.02 . The last value corresponds to the ‘saw’ solution, where the beginning of the numerical instability is clearly seen. Best solutions are attained for $\alpha \sim 0.2-0.5$, $\beta \sim 0.1$.

NUMERICAL ALGORITHM FOR SUBSONIC FLOWS

In contrast to the previous case (18), here the additional stabilizing term $\alpha h/c$ is introduced only in τ coefficient as

$$\tau = \frac{\mu_0}{p Sc} \left(\frac{T}{T_0} \right)^\omega + \alpha \frac{h}{c}, \quad \mu = \mu_0 \left(\frac{T}{T_0} \right)^\omega, \quad \kappa = \frac{\gamma \mathcal{R} \mu}{Pr(\gamma - 1)}$$

Thus, the heat flux and the shear-stress tensor are not affected by the grid dissipation.

Within the framework of the QGD model the simple unreflecting boundary conditions may be applied on the free subsonic boundaries. These conditions are similar to those used for viscous incompressible flows. For inlet boundary (in) they have the form

$$\frac{\partial p}{\partial n} = \alpha_{in}, \quad \mathbf{u} = \mathbf{u}_{in}, \quad \rho = \rho_{in}$$

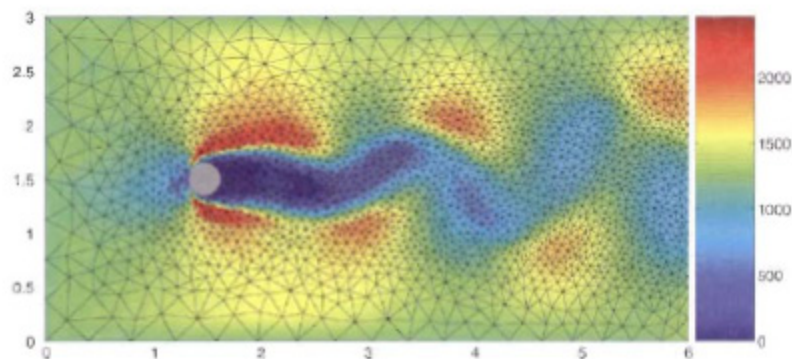


Figure 2. Mesh and flow picture for non-stationary flow near a cylinder, $Re=90$.

where $z_{in} \sim 1/Re$ is a small constant and n is a unit vector normal to the boundary. At the outlet boundary ($_{out}$) soft boundary conditions are imposed for the density and velocity, but the outlet pressure is supposed to be a constant:

$$\frac{\partial p}{\partial n} = 0, \quad \frac{\partial \mathbf{u}}{\partial n} = 0, \quad p = p_{out}$$

As an example, the numerical simulation of a flow in a vicinity of a circular cylinder for the Mach number $Ma=0.1$ and the Reynolds number $Re=90$ is presented. This problem is a well-known test, e.g. [12] and citations therein. Our calculations were done for air flow, $\gamma=1.4$, $Pr=0.72$, $Sc=0.746$ and $\omega=0.74$ using unstructured grid consisting of 2191 points with $\alpha=0.1$. For $Re=20$, the stationary flow regime was obtained. For $Re=90$ and 100, the Karman street flow was formed. For $Re=90$, the calculated Strouhal number is $Sh=0.147$. The Rayleigh formula for incompressible flow gives $Sh=0.212(1-21.2/Re)=0.162$. With h decreasing the numerical frequency tends to the empirical result.

In Figure 2, the Karman street in the wake is plotted using isolines for \mathbf{u}^2 in the dimensional form ($u_{in} = 35.31$ m/s, $D=0.3$ m).

CONCLUSIONS

The novel mathematical model for the gas flow simulations, named the quasi-gasdynamics (QGD) equation system, is presented. The QGD equations differ from the NS system by the additional dissipative terms with a small multiplicative parameter. Based on the QGD model, the new robust algorithms for non-stationary viscous flow simulations are constructed and verified. Universality, efficiency and accuracy of these algorithms are provided by the validity of the conservation laws and the entropy balance theorem for the QGD system.

REFERENCES

1. Elizarova TG, Chetverushkin BN. Kinetic algorithms for calculating gasdynamic flows. *Computational Mathematics and Mathematical Physics* 1985; **25**:164–169.

2. Sheretov YuV. *Mathematical Modeling of Liquid and Gas Flows based on Quasi-hydrodynamic and Quasi-gasdynamical Equations*. Publishing house of Tver State University: Russia, Tver, 2000 (in russian).
3. Elizarova TG, Sheretov YuV. Theoretical and numerical investigation of quasi-gasdynamical and quasi-hydrodynamic equations. *Computational Mathematics and Mathematical Physics* 2001; **41**:219–234.
4. Elizarova TG, Sokolova ME, Sheretov YuV. Quasi-gasdynamical equations and numerical simulation of viscous gas flows. *Computational Mathematics and Mathematical Physics* 2005; **45**:524–534.
5. Elizarova TG. *Quasi-gasdynamical Equations and Numerical Methods for Viscous Flow Computations*. Scientific World: Moscow, 2007 (in russian).
6. Slezkin NA. About a differential equations of a gas motion. *Doklady of USSR Academy of Science* 1951; **77**:205–208.
7. Vallander SV. Equations of viscose gas motion. *Doklady of USSR Academy of Science* 1951; **58**:25–27.
8. Klimontovich YuL. About the necessity and possibility of unified description of kinetical and hydrodynamical processes. *Theoretical and Mathematical Physics* 1992; **92**:312–330.
9. Brenner H. Navier–Stokes revisited. *Physica A* 2005; **349**:60–132; **370**:190–224.
10. Ottinger HC. *Beyond Equilibrium Thermodynamics*. Wiley: Hoboken, 2005.
11. Alexeev BV. *Generalized Boltzmann Physical Kinetics*. Elsevier: Amsterdam, 2004.
12. Roushan P, Wu XL. Universal wake structures of Karman vortex streets in two-dimensional flows. *Physics of Fluids* 2005; **17**:073601.