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Quasi-gasdynamic numerical algorithm for gas flow simulations

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SUMMARY

Numerical algorithm for calculation of non-stationary viscous gasdynamic flows is presented. Algorithm is based on a special form of regularization in Navier-Stokes equations that includes additional dissipative terms and forms quasi-gasdynamic equation system. Finite-different approximations and numerical examples are presented. Copyright © 2007 John Wiley & Sons, Ltd.

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Quasi-gasdynamic equations

This paper is devoted to a contemporary mathematical model for gas flow and to the related numerical methods for flow simulation. Algorithm is based on a mathematical model, that generalize 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 quasi-gasdynamic (QGD) system of equations. The first variant of QGD system is presented in [1] and developed later in, e.g., [2] – [5]. QGD system has a form of conservation laws and in common notations writes

$$\frac{\partial \rho}{\partial t} + div\vec{j}_m = 0, \tag{1}$$

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

$$\frac{\partial}{\partial t}\Big[\rho\Big(\frac{\vec{u}^2}{2} + \varepsilon\Big)\Big] + div\Big[\vec{j}_m\Big(\frac{\vec{u}^2}{2} + \varepsilon + \frac{p}{\rho}\Big)\Big] + div\vec{q} = div(\Pi \cdot \vec{u}), \tag{3}$$

with the closing relations

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

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$$\Pi = \Pi_{NS} + \tau\vec{u}\otimes\Big[\rho(\vec{u}\cdot\vec{\nabla})\vec{u} + \vec{\nabla}p\Big] + \tau I\Big[(\vec{u}\cdot\vec{\nabla})p + \gamma p div\vec{u}\Big], \tag{5}$$

$$\vec{q} = \vec{q}_{NS} - \tau\rho\vec{u}\Big[(\vec{u}\cdot\vec{\nabla})\varepsilon + p(\vec{u}\cdot\vec{\nabla})\Big(\frac{1}{\rho}\Big)\Big]. \tag{6}$$

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

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

$$X = \kappa\Big(\frac{\vec{\nabla}T}{T}\Big)^2 + \frac{(\Pi_{NS}:\Pi_{NS})}{2\eta T} + \frac{p\tau}{\rho^2 T}\Big[div(\rho\vec{u})\Big]^2 + \\ + \frac{\tau}{\rho T}\Big[\rho(\vec{u}\cdot\vec{\nabla})\vec{u} + \vec{\nabla}p\Big]^2 + \frac{\tau}{\rho\varepsilon T}\Big[\rho(\vec{u}\cdot\vec{\nabla})\varepsilon + p div\vec{u}\Big]^2. \tag{7}$$

Above equation proves a dissipative nature of the additional τ-terms.

QGD sistem differs from NS one 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 $\tau \to 0$. In a boundary layer limit both QGD and NS equations reduce to Prandtl equation system.

Terms in τ allow to construct a family of novel efficient numerical algorithms for simulation nonstationary supersonic and subsonic gasdynamic flows. QGD algorithms inherit mathematical properties of QGD system.

Finite-difference approximation

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

As an example we show a finite-volume algorithm for two-dimensional Cartesian coordinate system. In this case QGD system writes as

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

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

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

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

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

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

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

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

where

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

Components of Π are determined by formula, convenient for a programme realization:

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

where

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

Components of the heat flux $\vec{q}$ are:

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

Heat conductivity coefficient κ and coefficient τ are connected with a viscosity coefficient μ by:

$$\kappa = \frac{\gamma \mathcal{R}}{(\gamma - 1)Pr}\ \mu, \qquad \tau = \frac{1}{p\ Sc}\ \mu, \qquad \mu = \mu_0 \Big(\frac{T}{T_0}\Big)^{\omega}, \tag{17}$$

where Pr is Prandtl number, Sc is Schmidt number, $\mathcal{R}$ ia a gas constant, γ is a specific heat ratio.

Equation system (8) - (11) is completed by initial and boundary conditions. In contrast to NS system, continuity equation (8) in QGD system is an equation of a second order in space. So QGD system must be completed by an additional boundary condition. This condition for pressure p is obtained by imposing appropriate boundary condition for mass flux vector $\vec{j}_m$.

To solve the problem numerically, a grid in space and in time is introduced in a computational domain. Gasdynamic parameters – density ρ, pressure p and velocity $\vec{u}$ are determined at the nodes of the grid. The values of 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. A finite-difference approximation of QGD system (1) – (6) is constructed using control volume method. The similar approximations are used for rectangular structural grids and for unstructured three-cornered grids.

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

Numerical algorithm for supersonic flows

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

$$\tau = \frac{\mu_0}{pSc}\Big(\frac{T}{T_0}\Big)^{\omega} + \alpha\frac{h}{c}, \quad \mu = \tau pSc, \quad \kappa = \frac{\tau pSc}{Pr(\gamma-1)}, \tag{18}$$

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

As an example of application we consider a strong discontinuity step evolution problem in non-viscous gas without heat conductivity. It means that we solve Euler equations with artificial dissipation that is introduced as $\tau = \alpha h/c$. The problem is solved in the space interval $0 \le x \le 200$ for the time period $0 \le t \le 4$ with Courant stability condition $\Delta t = \beta h/c_{max}$, where β is a factor of unity order. We take $Sc = 1.$, $Pr = 2/3$ and $\gamma = 5/3$. Initial conditions form a discontinuity at $x = 100$. The values to the left and to the right from the break look as follows:

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

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

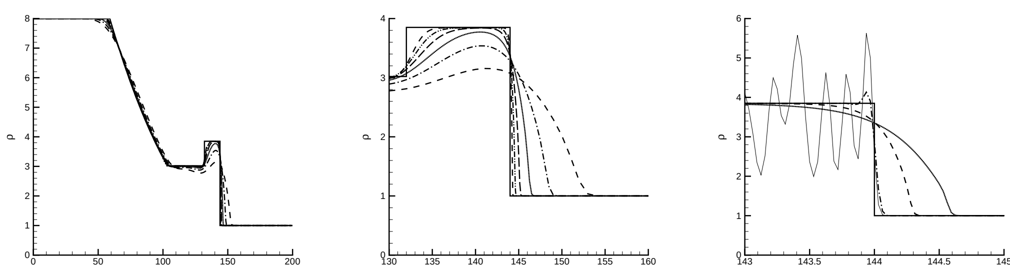

Figure 1. Density distribution along x (left - whole computational domain, right - fragments)

three variants, and $\Delta t = 0.0002$ for the last three ones. Convergency of the numerical results to analytical solution with reducing h for $t = 4$ is seen in Fig. 1 for $\alpha = 0.5$ (left figures). The dependence of the solution from parameter α ($h = 0.03125$) 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 numerical instability is clearly seen. The best solution is attained for $\alpha \sim 0.2 - 0.5$, $\beta \sim 0.1$.

Numerical algorithm for subsonic flows

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

$$\tau = \frac{\mu_0}{pSc}\Big(\frac{T}{T_0}\Big)^{\omega} + \alpha\frac{h}{c}, \quad \mu = \mu_0\Big(\frac{T}{T_0}\Big)^{\omega}, \quad \kappa = \frac{\mu}{Pr(\gamma-1)}.$$

Here a heat flux and a shear-stress tensor are not affected by a grid dissipation.

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

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

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

$$\frac{\partial \rho}{\partial n} = 0, \quad \frac{\partial \vec{u}}{\partial n} = 0, \quad p = p_{out}.$$

As an example a numerical simulation of a flow in a vicinity of a circular cylinder for Mach number $Ma = 0.1$ and Reynolds number $Re = 90$ is presented. Calculations were made for air flow ($\gamma = 1.4, Pr = 0.72, Sc = 0.746$, and $\omega = 0.74$) using unstructured grid consisting from 2191 points. Here $\alpha = 0.1$. In Fig. 2 time dependence of the velocity is shown. Calculated Strouhal number is Sh=0.147. Rayleigh formula for incompressible flow gives $Sh = 0.212(1 - 21.2/Re) = 0.162$.

In Fig.3 Karman street in the wake is plotted using isolines for $\vec{u}^2$ in dimensional form ($u_{in} = 35,31$ m/sec).

Conclusions

Contemporary mathematical model for gas flow simulations, named quasi-gasdynamic (QGD) equation system, is presented. QGD equations differ from Navier–Stokes system in additional dissipative terms with a small parameter. Basing on QGD model a family of new robust algorithms for non-stationary viscous flow simulations are constructed and verified. Universality, efficiency and accuracy of these algorithms are provided by a validity of conservation laws and entropy balance for QGD system.

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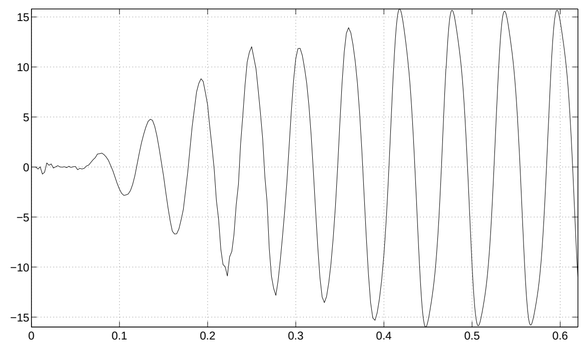

Figure 2. Time-dependence for u_y in a cylinder wake.

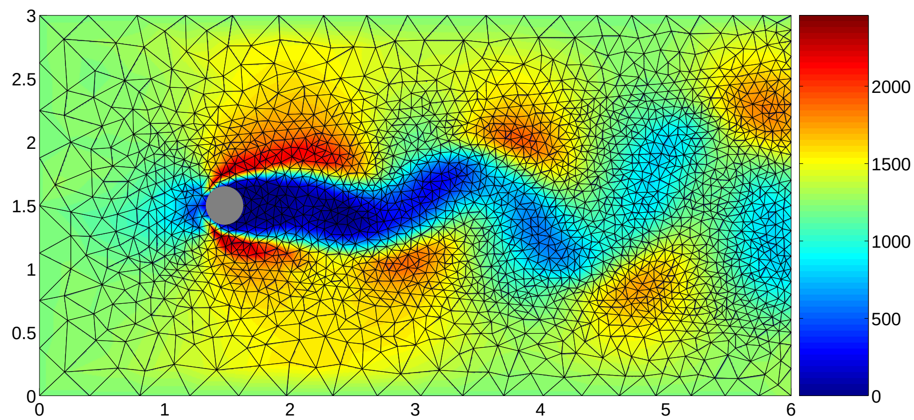

Figure 3. Mesh and flow picture for non-stationary flow near a cylinder, $Re = 90$.

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