Hybrid Parallel Algorithm for Nonequilibrium Viscous Reaction Gas Mixture Numerical Simulation

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Hybrid parallel algorithm for nonequilibrium viscous reaction gas mixture numerical simulation is presented. This approach is used for the 3D hypersonic multicomponent nonequilibrium dissociated air flow over catalytic surface and for the flow in the chemical reactors. High level of the parallel algorithms efficiency is demonstrated.

Problem description

Two problem of the reaction gas mixture numerical simulation are considered:

- 3D hypersonic multicomponent nonequilibrium dissociated air flow over catalytic surface of blunt complex bodies, moving at attack and slipping angles along prescribed aerodynamic reentry trajectory.
- Reaction gas mixture flow in the chemical reactors.

For the first problem the thin (hypersonic) viscous shock layer theory (TVSL) including nonequilibrium chemical reactions, multicomponent diffusion and excluding barodiffusion, thermodiffusion, diffusion thermoeffect is used as initial mathematical model. Today this model is widely applied because it has a correct asymptotical character and it is relatively simple in comparison with solutions of full Navier-Stokes equations. Comparisons with solutions obtained for more complete flow models and experimental data demonstrate that the TVSL model has rather high accuracy and it may be used for investigations of hypersonic viscous gas flow over smooth blunt bodies.

The initial system of equations written in curvilinear coordinate system (x^i) is

$$D_i(\rho u^i a^{1/2} a_{(ii)}^{-1/2}) = 0, \quad D_3 P = -\rho A^3_{\alpha\beta} u^\alpha u^\beta, \tag{1}$$

$$\rho(Du^\alpha + A^\alpha_{\beta\delta} u^\beta u^\delta) = -a^{\alpha\beta} a^{1/2}_{(\alpha\alpha)} D_\beta P + D_3(\mu Re^{-1} D_3 u^\alpha),$$

$$\rho c_p DT = 2D^* P + D_3(\mu c_p (\sigma Re)^{-1} D_3 T) + 2\mu Re^{-1} B_{\alpha\beta} D_3 u^\alpha D_3 u^\beta - D_3 T \sum_{k=1}^{N} c_{pk} I_k - \sum_{k=1}^{N} h_k \dot{W}_k,$$

$$\rho D c_k + D_3 I_k = \dot{W}_k, \quad P = \rho RT \sum_{k=1}^{N} \frac{c_k}{m_k},$$

$$D_i = \frac{\partial}{\partial x_i}, \quad D^* = u^\alpha a^{-1/2}_{(\alpha\alpha)} D_\alpha, \quad D = D^* + u^3 D_3,$$

$$\mu \frac{\partial c_i}{\partial x^3} = \sum_{j=1}^{N} \frac{m}{m_j S_{ij}} \left(c_i I_j - c_j I_i \right) - c_i \sum_{k=1}^{N} \sum_{j=1}^{N} \frac{m}{m_j S_{kj}} \left(c_k I_j - c_j I_k \right).$$

The system (1) is solved with boundary conditions on the shock wave and on body surfaces. On the shock wave the hypersonic approximation of generalized conditions of Renkine - Hugoniot is used, which take into account the effects of molecular transfer into the shock wave. On the body surface heterogeneous chemical reactions are taken into account and heat discharge inward of body is leaved out of account.

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Flow in the chemical reactors is described by NS equations.

$$\frac{d\rho}{dt} = -\rho\nabla\mathbf{V}, \quad \rho = m(1+\gamma M^2 p)/T, \tag{2}$$

$$\rho\frac{d\mathbf{V}}{dt} = -\nabla p + \frac{1}{Re}(2\,\mathrm{Div}(\mu\dot{S}) + \frac{2}{3}\nabla(\mu\nabla\mathbf{V}),$$

$$\rho\frac{dc_k}{dt} = -\frac{1}{ReSc}(\rho D_k\nabla c_k) + w_{1k} - w_{2k}c_k, \quad k = 1,2,...,N,$$

$$\rho\frac{de}{dt} + (\gamma-1)\nabla\mathbf{V} = -\frac{1}{RePr}\nabla\left[\gamma\frac{\lambda}{c_v}\left(\nabla e - \sum_{i=1}^{N} e_i\nabla c_i\right) + Le\rho\sum_{i=1}^{N} h_i D_i\nabla c_i\right] +$$

$$+M^2\gamma(\gamma-1)\left[\frac{2\mu}{Re}\left(\dot{S}^2 - \frac{1}{3}(\nabla\mathbf{V})^2\right) - p\nabla\mathbf{V}\right].$$

Hybrid parallel algorithm

This approach is consist of two decomposition level

- All processors set is divided to some subsets number and all calculation region is partitioned to the same subdomain number.
- In the each subset only processor is used for the solutions of numerical problem in appropriate subdomain, but of processors from this set used only for transport coefficient calculations.

Numerical calculation are shown, that this approach is very sutable for clusters with comparatively low interprocessors data exchange rate.

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