Numerical Modelling of High-Speed Rarefied Gas Flows Using Supercomputers

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Introducton

- Development of new spacecraft, moving at high altitudes, is closely connected with the problems of their dynamic and thermal interaction with the surrounding gas. In order to reduce required time and cost, it is worthwhile to investigate aerodynamical characteristics using the approaches of computational physics.
- At present, the main computational tools for such studies are based on the direct simulation Monte Carlo (DSMC) approach, e.g. well known SMILE system developed at ITAM [Kashkovsky et al., 2004, Ivanov et al., 2010].
- An alternative to DSMC is the direct numerical solution of the Boltzmann kinetic equation for the velocity distribution function. The potential benefits of kinetic solvers include higher-order accuracy (typically at least 2nd order) and absence of statistical noise in the results.
- However, until recently the prohibitive computational cost of such methods did not allow applications to flows with high free-stream Mach numbers and complex geometries.
- The present talk will concentrate on the development of methods and parallel code to model hypersonic rarefied gas flows using the model kinetic equation of E.M. Shakhov (so-called S-model).

S-model in the dimensional form

- State of the gas is described by the velocity distribution function $f = f(t, \boldsymbol{x}, \boldsymbol{\xi})$.
- Macroscopic variables are defined as integrals with respect to molecular velocity:

$$n = \int f d\boldsymbol{\xi}, \quad n\boldsymbol{u} = \int \boldsymbol{\xi} f d\boldsymbol{\xi}, \quad \frac{3}{2} mnR_g T + \frac{1}{2} mnu^2 = \frac{1}{2} m \int \xi^2 f d\boldsymbol{\xi},$$
$$\boldsymbol{q} = \frac{1}{2} m \int \boldsymbol{v} v^2 f \, d\boldsymbol{\xi}, \quad \boldsymbol{v} = \boldsymbol{\xi} - \boldsymbol{u}, \quad \rho = mn, \quad p = \rho R_g T.$$

- Kinetic equation is written in the following form

$$\frac{\partial}{\partial t} f + \xi_\alpha \frac{\partial f}{\partial x_\alpha} = \frac{p}{\mu} (f^+ - f), \quad f^+ = f_M \left[1 + \frac{4}{5} (1 - \mathrm{Pr}) S_\alpha c_\alpha \left(c^2 - \frac{5}{2} \right) \right],$$
$$f_M = \frac{n}{(2\pi R_g T)^{3/2}} \exp(-c^2), \quad S_i = \frac{1}{n} \int c_i c^2 f d\boldsymbol{\xi}, \quad \boldsymbol{c} = \frac{\boldsymbol{v}}{\sqrt{2R_g T}}, \quad c^2 = c_\beta c_\beta.$$

  Here $\mathrm{Pr} = 2/3$ is Prandtl number, m – molecular mass, R_g - gas constant.
- Boundary condition of the diffusive reflection with complete thermal accommodation to the surface temperature T_w is given by

$$f_w = \frac{n_w}{(2\pi R_g T_\mathrm{w})^{3/2}} \exp\left(-\frac{\xi^2}{2R_g T_\mathrm{w}} \right), \quad n_w = \sqrt{\frac{2\pi}{R_g T_\mathrm{w}}} N_i, \quad N_i = -\int\limits_{\xi_n < 0} \xi_n f d\boldsymbol{\xi}.$$

Transformation to non-dimensional variables

- Introduce the following change of variables:

$$\boldsymbol{x}' = \frac{\boldsymbol{x}}{l_*}, \quad n' = \frac{n}{n_*}, \quad p' = \frac{p}{p_*}, \quad T' = \frac{T}{T_*},$$

$$\boldsymbol{u}' = \frac{\boldsymbol{u}}{v_*}, \quad \boldsymbol{\xi}' = \frac{\boldsymbol{\xi}}{v_*}, \quad \boldsymbol{q}' = \frac{\boldsymbol{q}}{m n_* \beta_*^3}, \quad f' = \frac{f}{n_* \beta_*^3}.$$

  where $p_* = m n_* R_g T_*$ – pressure, $\beta_* = \sqrt{2 R_g T_*}$ – most probable molecular speed.

- Degree of gas rarefaction is defined by the so-called rarefaction parameter δ, which is inversely proportional to the Knudsen number:

$$\delta = \frac{l_* p_*}{\mu(T_*)\beta_*} = \frac{8}{5\sqrt{\pi}} \frac{1}{\mathrm{Kn}}, \quad \mathrm{Kn} = \frac{\lambda_*}{l_*}.$$

  Here λ_* is the mean free path at reference conditions $*$.

- In the rest of the presentation non-dimensional variables will be denoted by the same symbols are dimensional ones.

S-model in the non-dimensional form

- The kinetic equation is re-written as

$$\frac{\partial f}{\partial t} + \xi_\alpha \frac{\partial f}{\partial x_\alpha} = J, \quad J = \nu(f^{(S)} - f), \quad \nu = \frac{nT}{\mu}\delta,$$

$$\delta = \frac{l_* p_*}{\mu(T_*)\sqrt{2R_g T_*}}, \quad \nu = T^\omega, \quad f^{(S)} = f_M\left(1 + \frac{4}{5}(1-\mathrm{Pr})\boldsymbol{Sc}(c^2 - \frac{5}{2})\right),$$

$$f_M = \frac{n}{(\pi T)^{3/2}}\exp(-c^2), \quad \boldsymbol{c} = \frac{\boldsymbol{v}}{\sqrt{T}}, \quad \boldsymbol{v} = \boldsymbol{\xi} - \boldsymbol{u}, \quad \boldsymbol{S} = \frac{2\boldsymbol{q}}{nT^{3/2}}.$$

- Macroscopic variables

$$\left(n, n\boldsymbol{u}, \frac{3}{2}nT + nu^2, \boldsymbol{q}\right) = \int \left(1, \boldsymbol{\xi}, \xi^2, \frac{1}{2}\boldsymbol{v}v^2\right) f d\boldsymbol{\xi}, \quad p = nT$$

- Boundary condition of diffuse reflection:

$$f(\boldsymbol{x}, \boldsymbol{\xi}) = f_w = \frac{n_w}{(\pi T_\mathrm{w})^{3/2}}\exp\left(-\frac{\xi^2}{T_\mathrm{w}}\right), \quad \xi_n = (\boldsymbol{\xi}, \mathbf{n}) > 0,$$

$$n_w = N_i/N_r, \quad N_i = -\int\limits_{\xi_n<0} \xi_n f d\boldsymbol{\xi}, \quad N_r = +\int\limits_{\xi_n>0} \xi_n \frac{1}{(\pi T_\mathrm{w})^{3/2}}\exp\left(-\frac{\xi^2}{T_\mathrm{w}}\right) d\boldsymbol{\xi}.$$

Conservative version of the discrete velocity method

- The improper integrals in the velocity space are replaced by proper integrals over some sufficiently large finite domain, e.g.

$$\frac{3}{2}nT + nu^2 = \int \xi^2 f d\xi \approx \int\limits_{0 \le \xi \le \xi_R} \xi^2 f d\xi, \quad \int\limits_{\xi > \xi_R} \xi^2 f d\xi \ll 1$$

- We introduce in the velocity domain (generally unstructured) mesh with N_ξ cells.

- Functions f, $f^{(S)}$ will be assigned to the centres of cells and interpreted as time-dependent matrices with components

$$f_j = f(t, \boldsymbol{x}, \boldsymbol{\xi}_j), \quad f_j^{(S)} = f^{(S)}(t, \boldsymbol{x}, \boldsymbol{\xi}_j), \quad \boldsymbol{\xi}_j = (\xi_{j1}, \xi_{j2}, \xi_{j3}), \quad j = 1, \dots N_\xi$$

- Kinetic equation is re-written as a system of N_ξ equations, written as a vector conservation law

$$\frac{\partial}{\partial t}\boldsymbol{f} + \frac{\partial}{\partial x_\alpha}\boldsymbol{F}_\alpha = \boldsymbol{J}, \quad \boldsymbol{J} = \nu(\boldsymbol{f}^{(S)} - \boldsymbol{f}), \quad \alpha = 1, 2, 3$$

- Here the components of "advection" fluxes are given by $F_{j\alpha} = \xi_{j\alpha} f_j$.

General form of the semi-discrete method

- Integration over the spatial cell V_i and fairly standard approximation of flux integrals and the right hand side leads to the following

$$\frac{\partial \boldsymbol{f}_i}{\partial t} = \boldsymbol{R}_i = -\frac{1}{|V_i|}\sum_{l=1} \boldsymbol{\Phi}_{li} + \boldsymbol{J}_i, \quad \boldsymbol{\Phi}_{li} = \int\limits_{A_{li}} (n_1 \boldsymbol{F}_1 + n_2 \boldsymbol{F}_2 + n_3 \boldsymbol{F}_3)) \, dS$$

- The second order of spatial accuracy is achieved by computing numerical fluxes $\boldsymbol{\Phi}_{li}$ using an upwind TVD method on arbitrary mesh:
- For the so-called boundary extrapolated value $\boldsymbol{f}_{li}$ for face l of cell i:

$$\boldsymbol{f}_{li} = \boldsymbol{f}_i + \boldsymbol{f}_{li}^{\text{correction}}$$

  For $\boldsymbol{f}_{li}^{\text{correction}}$ we use either general 3D method or directional method.
- The upwind flux function is written as follows:

$$\boldsymbol{\Phi}_{li} = \frac{1}{2}\boldsymbol{\xi}_{nli} \circ \left[\boldsymbol{f}^- + \boldsymbol{f}^+ - \text{sign}(\boldsymbol{\xi}_{nli}) \circ (\boldsymbol{f}^+ - \boldsymbol{f}^-)\right] |A_{li}|.$$

- Rusanov-type solver is also possible.

Calculation of macroscopic variables and time advance

- The main idea in computing macroscopic data introduced in [Titarev, 2017]) is to discretize directly approximation conditions of the S-model equation. The vector of primitive variables $\boldsymbol{W} = (n, u_1, u_2, u_3, T, q_1, q_2, q_3)^T$ is found from the following system:

$$\boldsymbol{H}(\boldsymbol{W}) = \sum_{j=1}^{N_\xi} \begin{pmatrix} 1 \\ \boldsymbol{\xi} \\ \xi^2 \\ \boldsymbol{v}v^2 \end{pmatrix}_j (f^{(S)} - f)_j \omega_j + \begin{pmatrix} 0 \\ \mathbf{0} \\ 0 \\ 2\,\mathrm{Pr}\,\boldsymbol{q} \end{pmatrix} = \mathbf{0}.$$

- For time advance we use implicit Euler method in time:

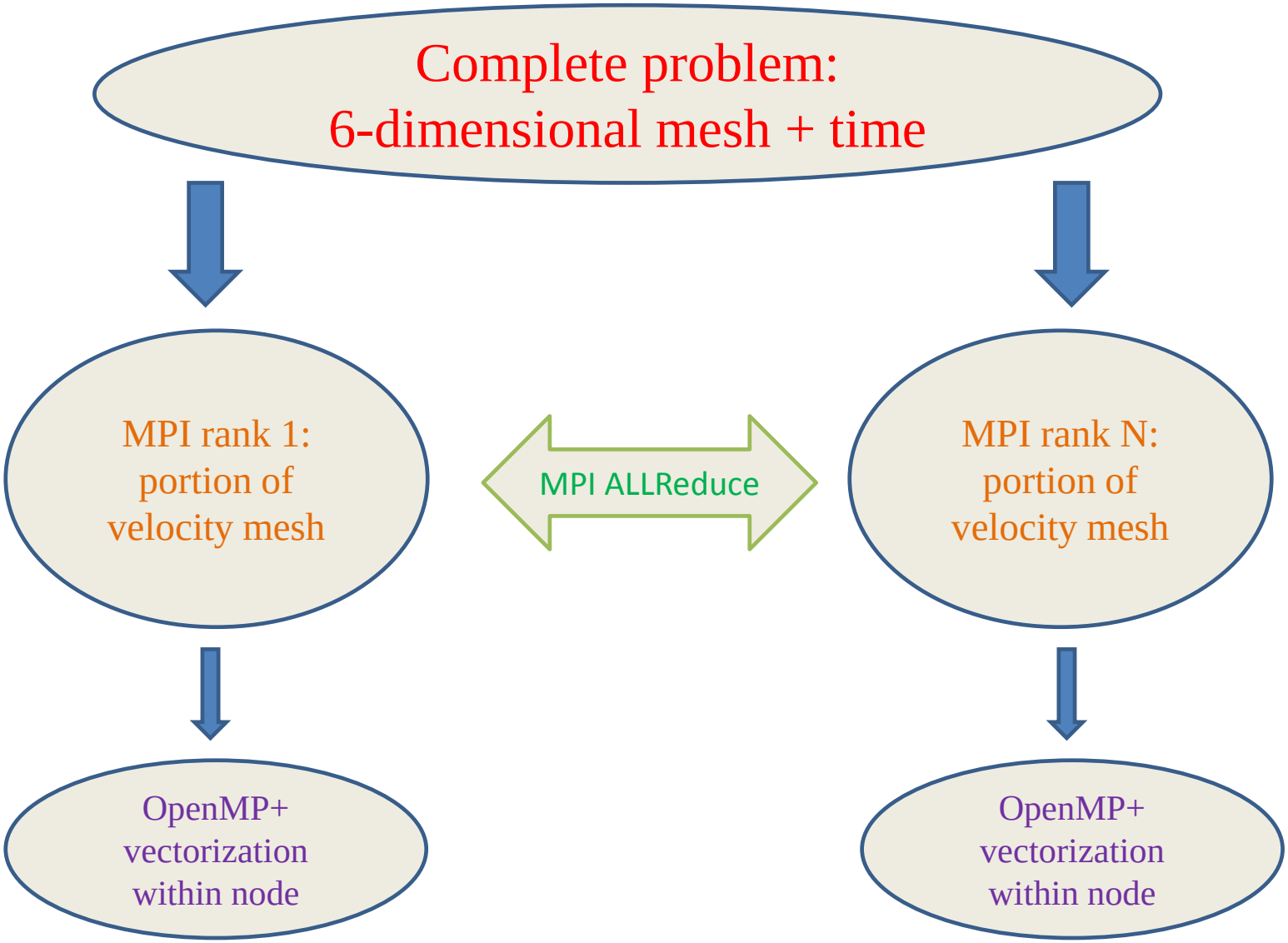
$$\frac{\Delta \boldsymbol{f}_i}{\Delta t} = \boldsymbol{R}_i^{n+1}, \quad \Delta \boldsymbol{f}_i = \boldsymbol{f}_i^{n+1} - \boldsymbol{f}_i^n, \quad \rightarrow \frac{\Delta \boldsymbol{f}_i}{\Delta t} = \boldsymbol{R}_i^n + \left(\frac{\partial \boldsymbol{R}}{\partial \boldsymbol{f}}\right) \Delta \boldsymbol{f}_i.$$

- After all usual linearisations and manipulations of terms the solution of the resulting huge system is constructed using an approximate LU-SGS factorization proposed for Euler equations in
  [Jameson and Yoon, 1987, Men'shov and Nakamura, 1995]
- The resulting procedure is matrix-free and computationally very fast.
- Details are omitted

Organization of parallel computations

- 3D kinetic calculations require the use of very large meshes
- Typical 6-dimensional mesh size is at the order of 10^9 nodes/cells
- General idea is to use geometrical mesh decomposition in
  - physical space - traditional in CFD
  - velocity space - specific to model kinetic equations
  - in both spaces
- Standard approach: use message passing (MPI) for parallel computations
  - for decomposition in physical space all ideas from general CFD apply
  - for velocity space decomposition each MPI rank performs calculations for its set (or range) of velocity nodes + sums up integral sums for computing macroscopic data
  - in general, velocity decomposition method is much easier to implement, but may be not applicable to the exact BKE
- However, pure MPI has its limitations - it does not scale well on systems with too many multi/many-core nodes, e.g. modern Xeon /Xeon Phi processors.

Schematic of two-level parallel model



Software package "Nesvetay-3D"

- "Nesvetay-3D" consists of
  - computing core - library to read mesh, establish connectivity, implement various TVD reconstruction, single-block and multi-block output into Tecplot format
  - three-dimensional kinetic solver for BGK and Shakhov models, including implicit/explicit solvers, macroparameter calculations, boundary conditions
  - spatial/velocity mesh preprocessor for parallel computation, including adaptive mesh for hypersonic flows
- 20000 lines of Fortran 2003 code with elements of object-oriented programming.
- Two-level OpenMP + MPI model of parallel computations is used on computers with large core count per node.
- Development tools are Microsoft Visual Studio and Intel Fortran Compiler v. 17.
- "Nesvetay-3D" has been successfully run on the HPC systems of Cranfield University, Lomonosov Moscow State University, MIPT, Joint Supercomputing Center of RAS as well as SCC and Peter the Great Saint-Petersburg Polytechnic University.
- Current version is tested on up to 256 nodes (61440 hyperthreads)

Velocity mesh construction for high-speed external flows

- If we use integration of a Maxwellian function

$$f = n(2\pi T)^{-3/2}\exp(-(\boldsymbol{\xi} - \boldsymbol{u})^2/T)$$

  as a guide for choosing the cell size and domain size, than we have

$$\Delta\xi \leq (0.5 \ldots 1)\sqrt{T}, \quad |\xi| \leq 3.5\sqrt{T_{sw}},$$

  where T_{sw} is after shock temperature and is proportional to M_∞^2.
- Naive velocity mesh construction is not useful for calculations as $N_\xi \approx M_\infty^3$.
- In the existing literature an octree-type velocity mesh is proposed, e.g. [Arslanbekov et al., 2013, Baranger et al., 2014]
- In the present work we advocate a much simpler approach to the creation of non-uniform velocity mesh, suitable for external flows with $M_\infty \gg 1$:
  - Near $\boldsymbol{\xi} = 0$ and $\boldsymbol{\xi} = \boldsymbol{u}_\infty$ we use cubical subdomains with $\Delta\xi = \sqrt{T_w}$, $\Delta\xi = 1$, respectively.
  - The rest of the domain is filled by tetrahedrons; their size grows up to $\approx 0.5\sqrt{T_{sw}}$.
- As a result, N_ξ dependence on M_∞ is close to linear.

Verification study: flow over 6-inch cylinder

- We compare our results with one of the leading DSMC code "Monaco", published in Ph.D. thesis of Lofthouse, 2008.
- We consider argon and free-stream Mach number $M_\infty = 25$:
  - Dimensional velocity $U_\infty = 6585$ m/s, temperature $T_\infty = 200$K, $T_w = 1500$K,
  - Two values of free-stream density: $\rho_\infty = 1.127 \times 10^{-6}$ kg/m^3 so that $\delta = 1.6$ and $\rho_\infty = 2.818 \times 10^{-5}$ kg/m^3 so that $\delta = 40$
  - Here δ is computed using cylinder radius $R = .0762$m.
- Viscosity law $\mu = T^{0.734}$.
- We use the pressure, friction and heat transfer coefficients for comparison:

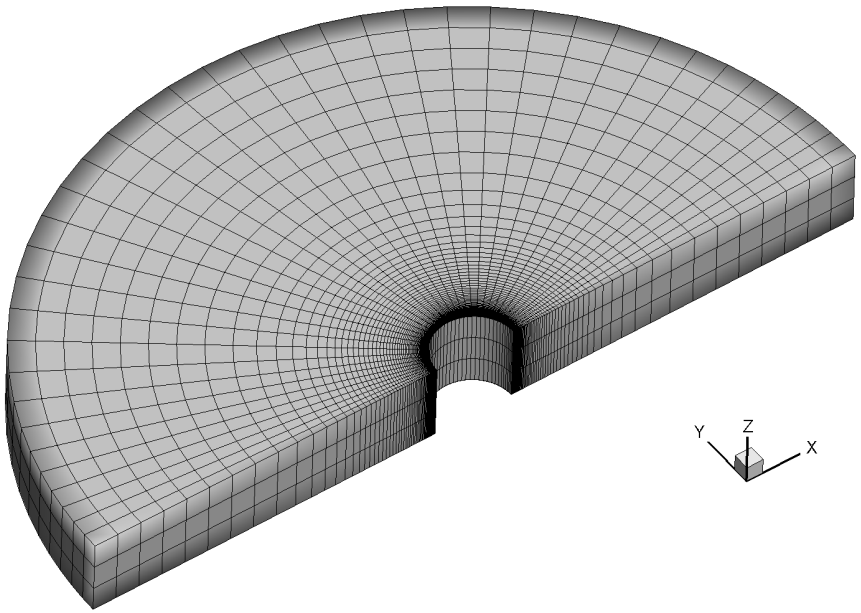
$$c_p = \frac{\boldsymbol{P} \cdot \boldsymbol{n} - p_\infty}{S_\infty^2}, \quad c_f = \frac{\boldsymbol{P} - (\boldsymbol{P} \cdot \boldsymbol{n})\boldsymbol{n}}{S_\infty^2}, \quad c_h = 2\frac{\boldsymbol{M} \cdot \boldsymbol{n}}{S_\infty^3},$$

where force acting on an unit surface with normal vector $\boldsymbol{n}$ and energy flux vector given by

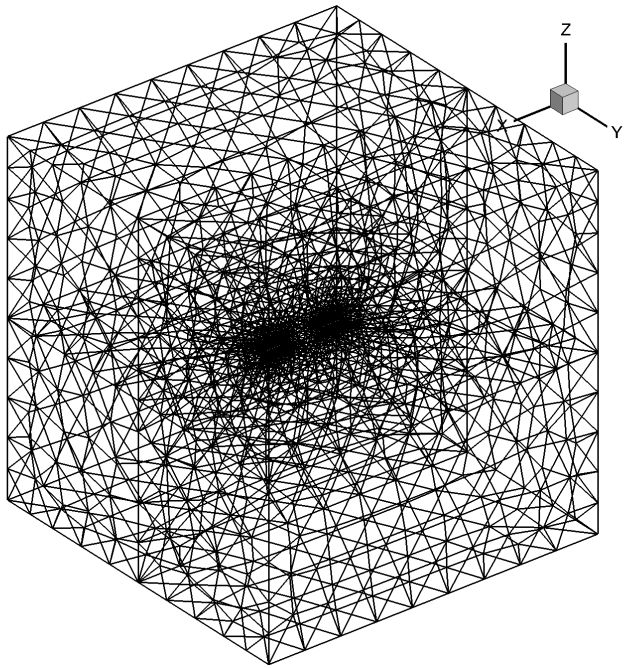
$$\boldsymbol{P} = 2\int \xi_n \boldsymbol{\xi} f d\xi, \quad \boldsymbol{M} = \frac{1}{2}\int \boldsymbol{\xi}\xi^2 f d\xi.$$

Computational mesh

- We use hexa mesh, with 115×40 cells in x-y plane and 3 cells along z axis.
- Velocity mesh consisted of 35720 cells.



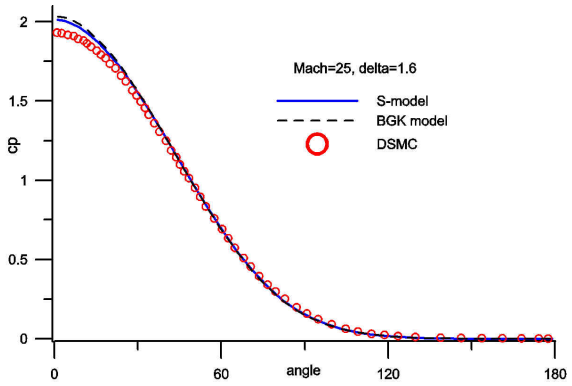
(a) Spatial mesh



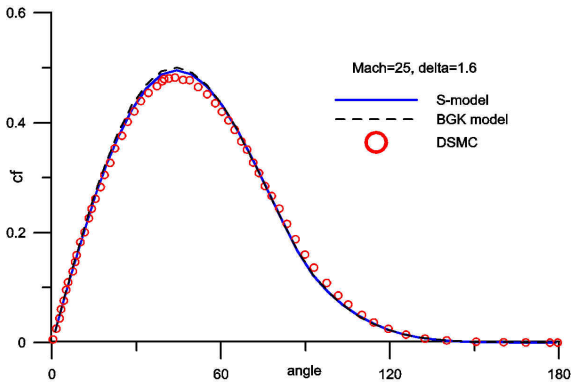
(b) Velocity mesh

Pressure c_p, friction c_f and heat transfer c_h coeffs for argon

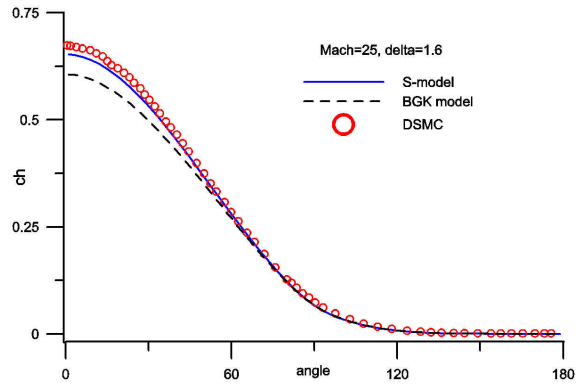
Results for $\delta = 1.6$



(a) c_p

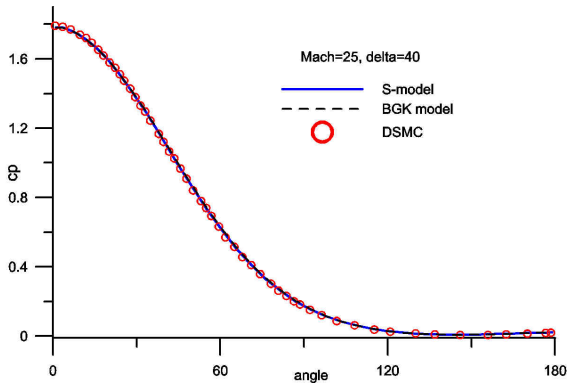


(b) c_f

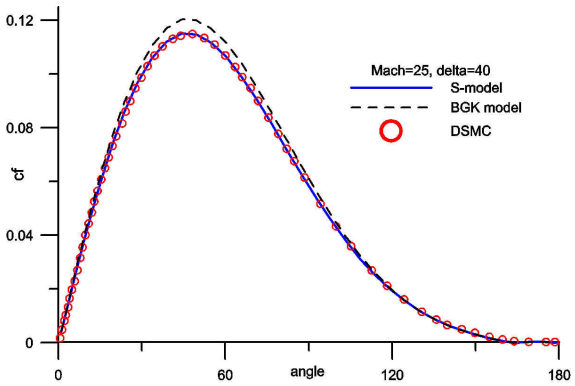


(c) c_h

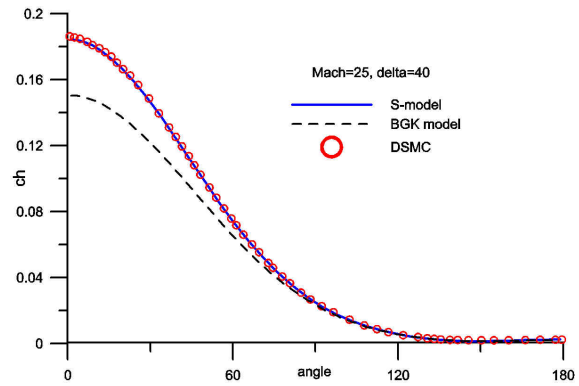
Results for $\delta = 40$



(a) c_p



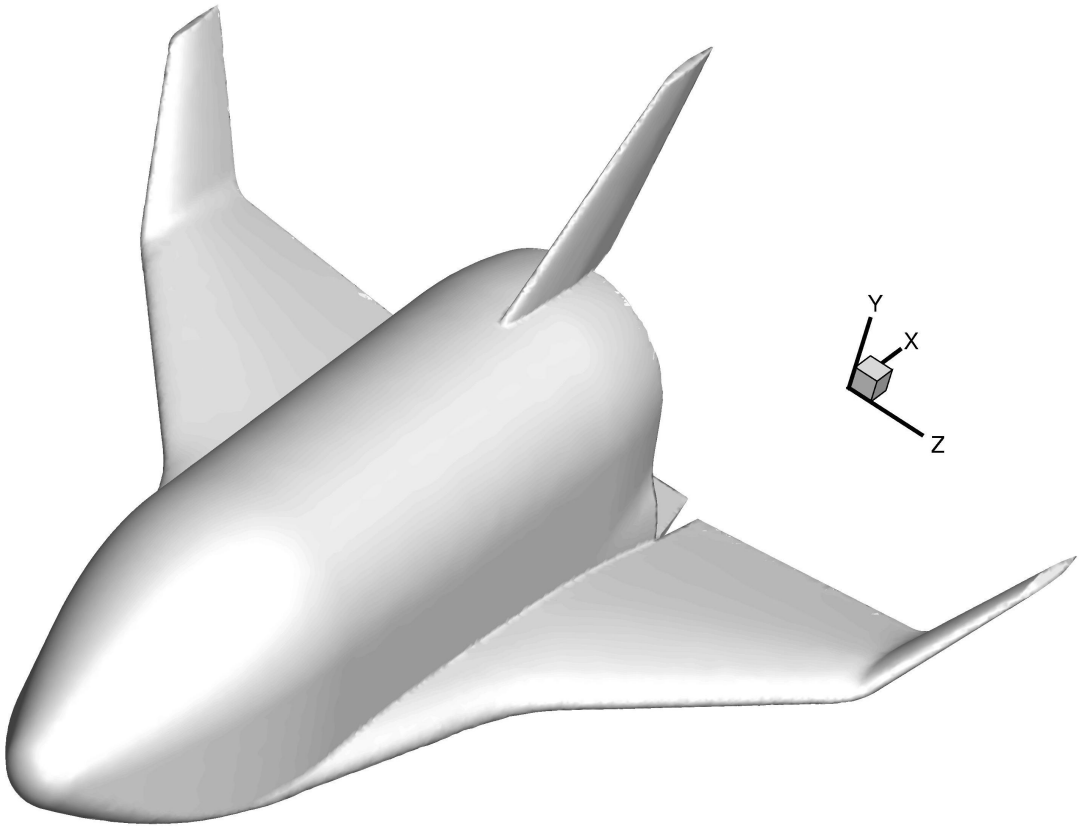
(b) c_f



(c) c_h

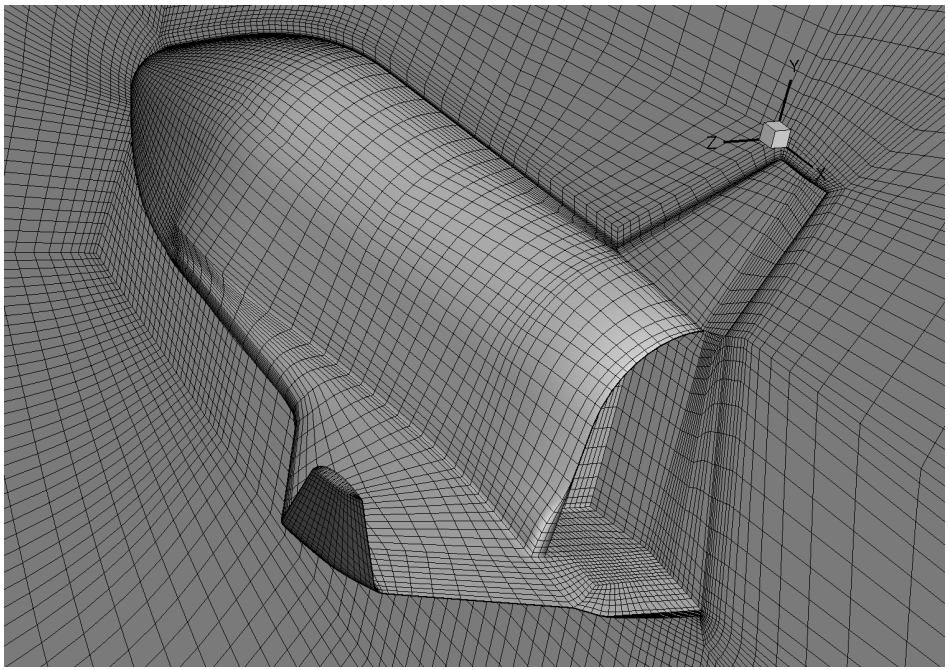
Test problem: external supersonic flow

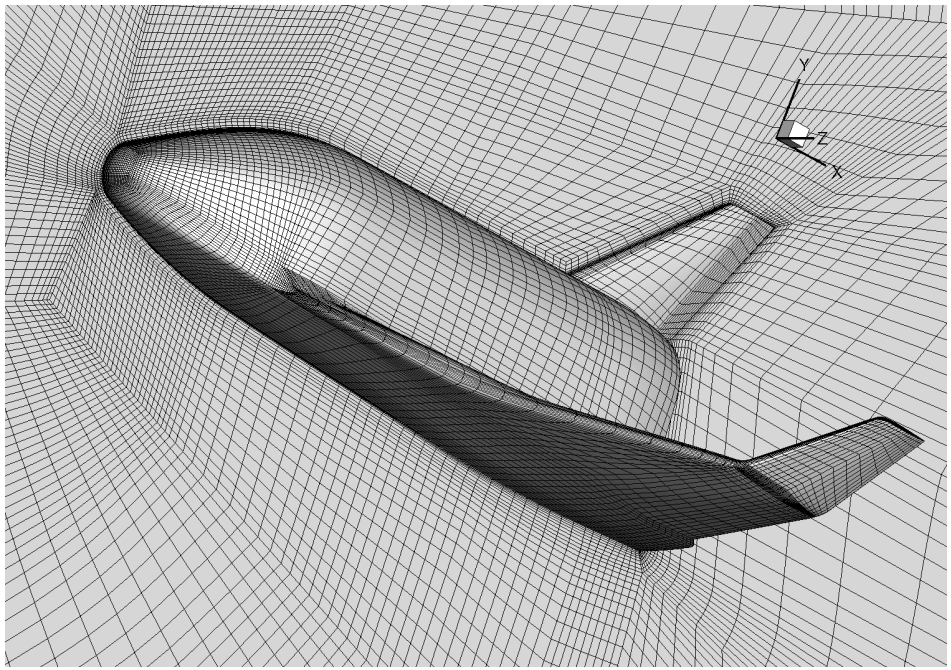
- We consider external supersonic flow over the TsaGI re-entry vehicle model, which consists of fuselage with blunted nose, wings, vertical keel and flap.
- The total length of the model is 10 meters.
- The aim is to compare S-model results with the DSMC data.



Multi-block spatial mesh for kinetic equation

- Half-domain with symmetry plane
- 159 blocks
- 436 thousand hexa cells with near-surface layer
- Some cells of low quality so that an implicit solver is a must

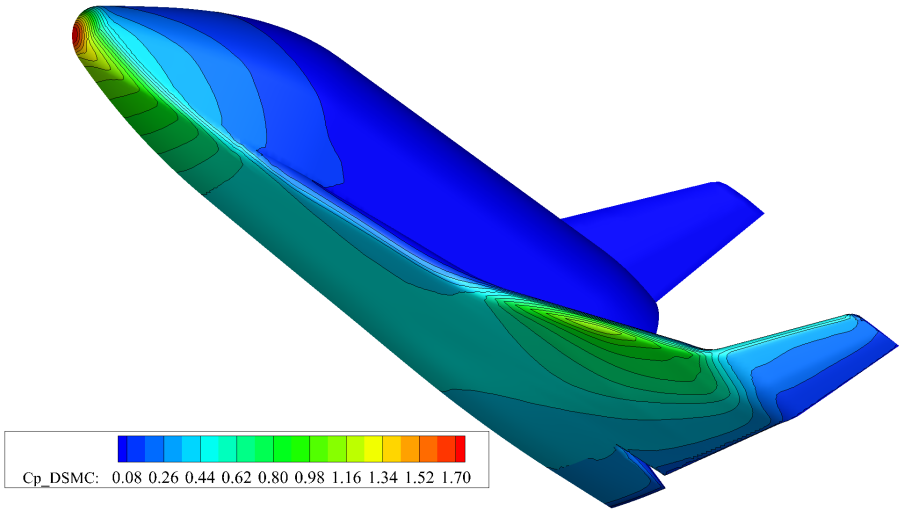


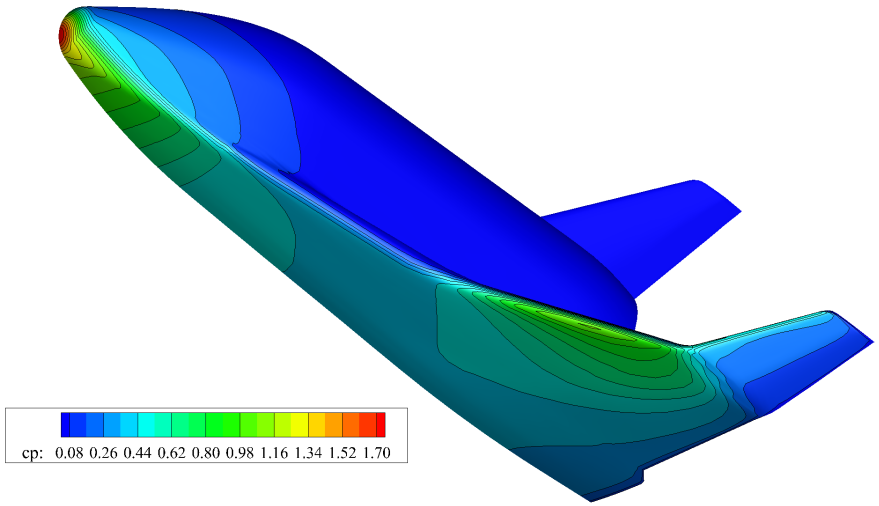


S-model vs DSMC: setup details

- The calculations were carried out for the altitude $H = 90$ km, $M_\infty = 10$ and $\alpha = 25$, $T_w/T_\infty = 5$
- The DSMC computations were performed using the SMILE software system [Kashkovsky et al., 2004, Ivanov et al., 2010] by a team from ITAM SB RAS: Ye.A. Bondar, P.V. Vashchenkov, A.A. Shevyrin
- For the sake of comparison, air was treated as a monatomic gas, in other words, internal degrees of freedom were ignored in both kinetic and DSMC calculations.
- Below, results are studied in the non-dimensional variables, in which the free-stream values of pressure and temperature are set as scales of pressure and temperature. The characteristic length scale was set to 1 meter.
- The rarefaction parameter is then $\delta_\infty = \dfrac{1 \cdot p_\infty}{\mu(T_\infty)\sqrt{2R_g T_\infty}} = 38.$
- The power-law intermolecular interaction $\mu = T^\omega$ is assumed, with $\omega = 0.734$.
- "Nesvetay-3D" calculations were run on PetaStream system at Peter the Great Saint-Petersburg Polytechnic University

Comparison of pressure coefficient c_p



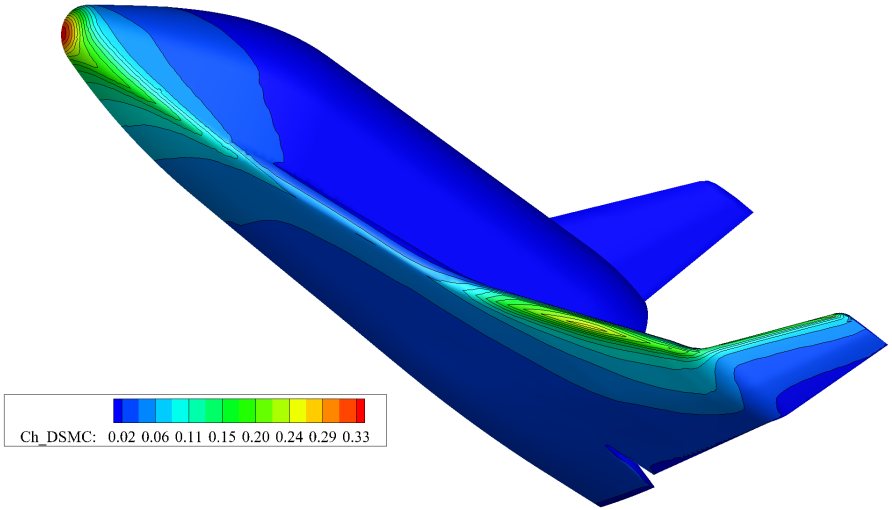


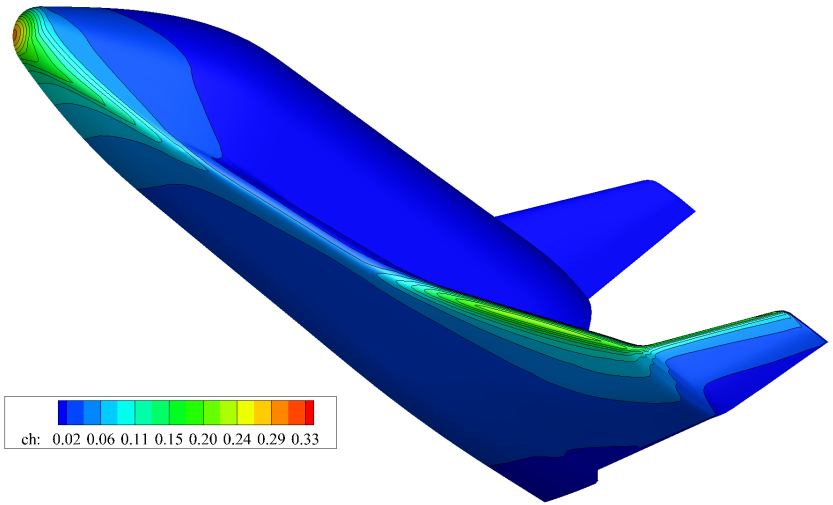
Left - SMILE

right - "Nesvetay-3D"

Overall, we see the excellent agreement for pressure coefficient c_p.

Comparison of heat transfer coefficient c_h



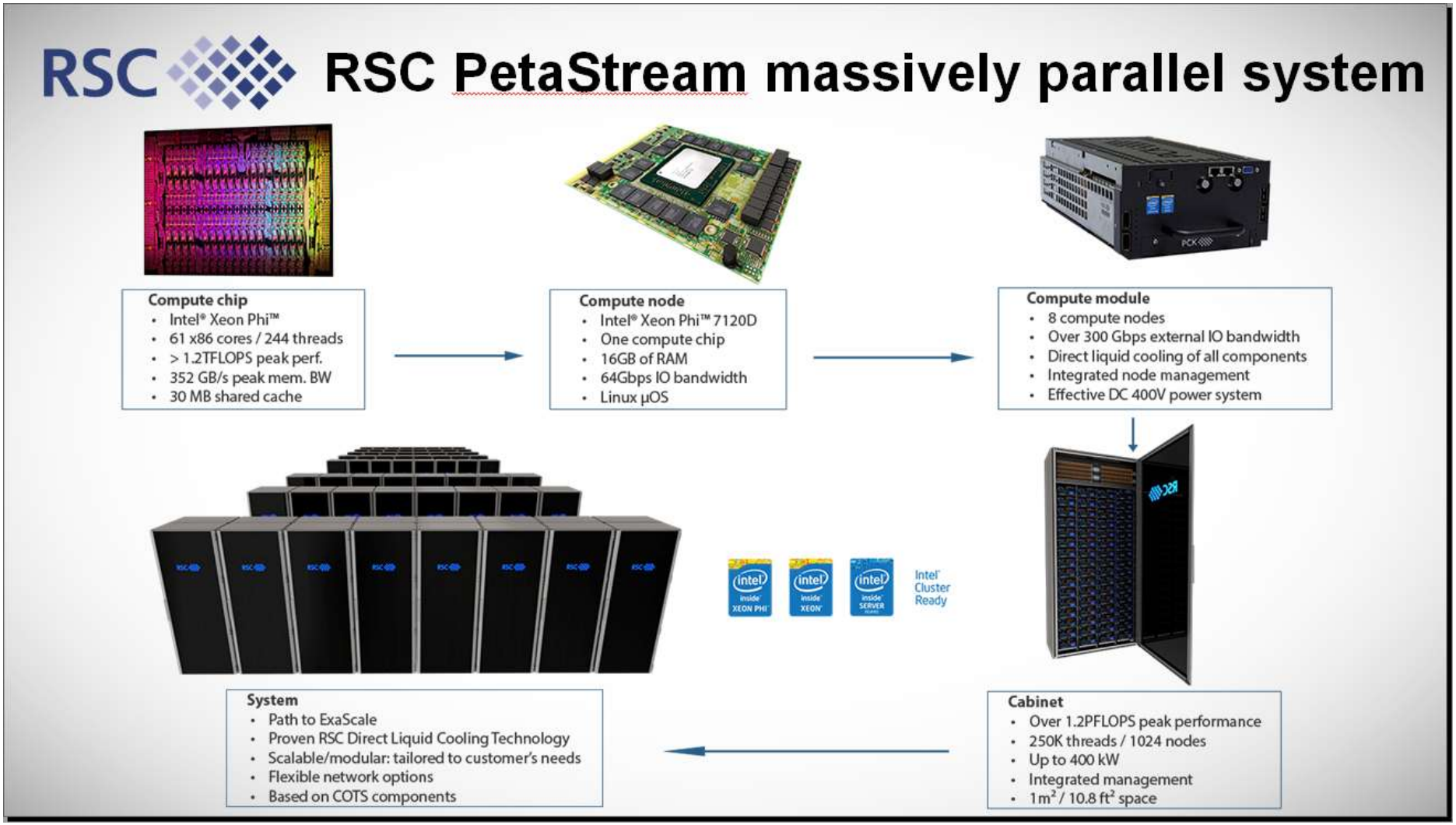


Left - SMILE

right - "Nesvetay-3D"

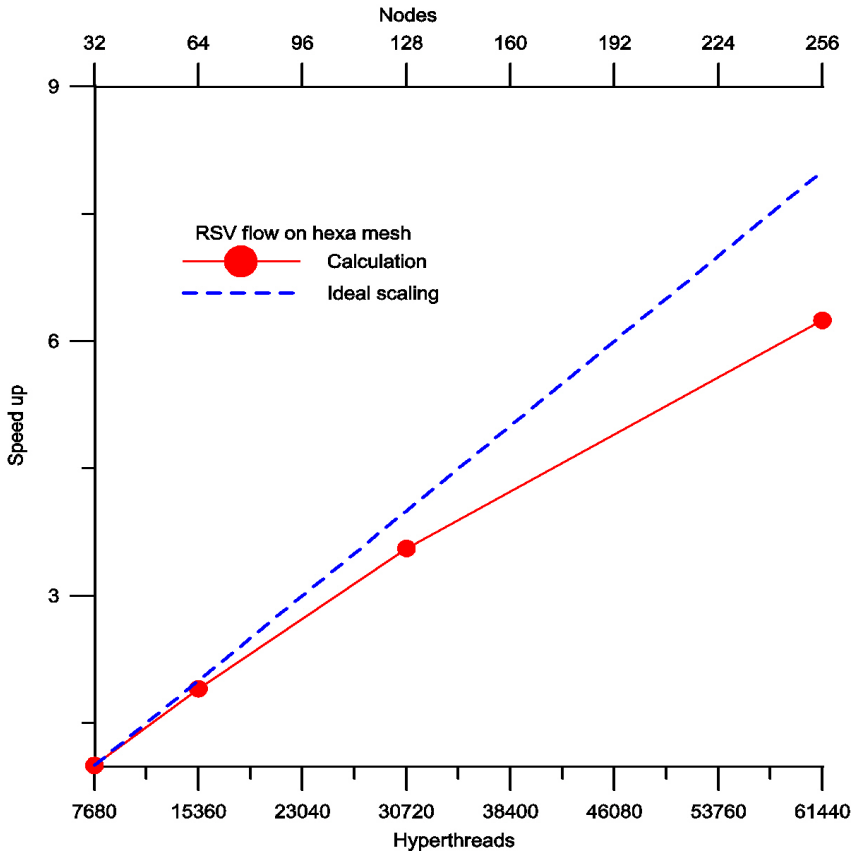
- The most difficult quantity to compute is the heat transfer coefficient c_H.
- As expected, the highest heating takes place on the blunt nose of the RSV.
- The tail of the RSV is in the shadow of the fuselage hence the energy flux there is much lower.
- We in general observe satisfactory agreement, with the largest difference on the nose around 10%.

RSC "PetaStream" family of supercomputers

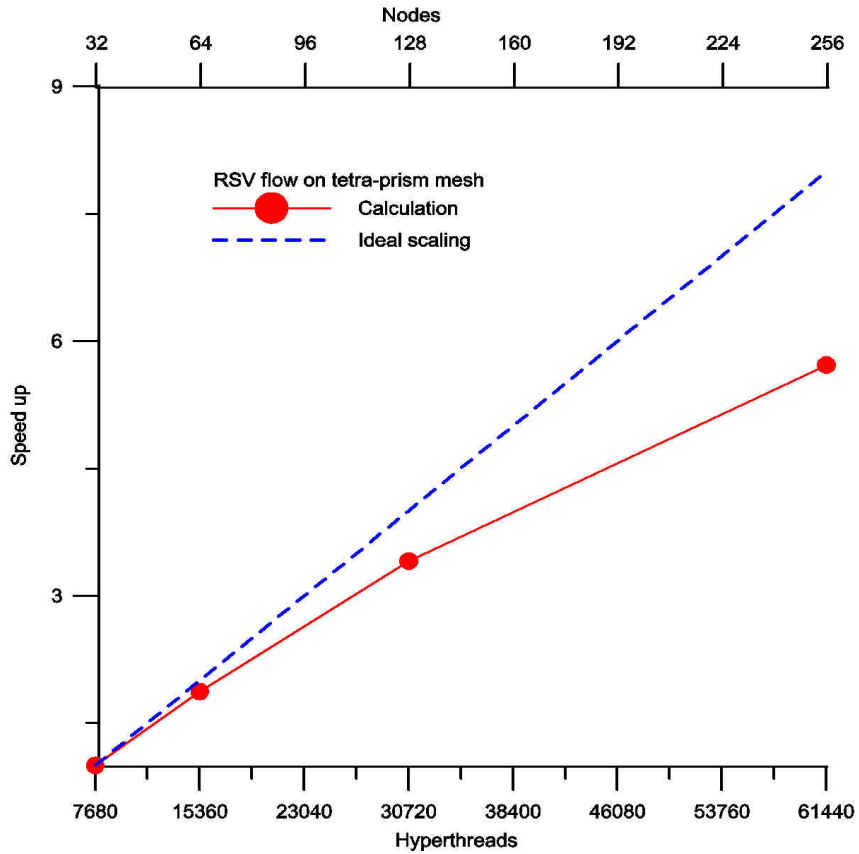


VKA flow on "Polytechnic RSK PetaStream" of SPbPU

- Flow regime: $U_\infty = 1500$ m/s, 100 km altitude
- Hexa va tetra-prism spatial mesh, up to 256 nodes (61140 hyperthreads)
- Parallel efficiency around 73%



(a) Hexa, 6D mesh 9.5 bln cells



(b) Tetra-prism, 6D mesh 8.7 bln cells

Conclusions

- We have developed a parallel software package to model three-dimensional monatomic rarefied gas flows
- A two-level model of parallel computations is implemented, which allows to run on tens of thousands of cores/hyperthreads.
- A comparison study shows good accuracy of kinetic model for high-Mach number flows.
- The capabilities are demonstrated by computing rarefied gas flow over 3D model under angle of attack.
- The work is supported by Russian Foundation for Basic Research project 18-08-00501
- Computing resources are from Joint Super Computing Center of Russian Academy of Sciences and Polytechnic Supercomputing Center of Saint-Petersburg Polytechnic University.
- The author would like to thank Dr. A. Frolova (Computing Center) for many fruitful discussions.