Construction and Comparison of Parallel Implicit Kinetic Solvers in Three Spatial Dimensions

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FlowModellium Lab at MIPT

1. The laboratory was created at MIPT in 2011 as part of the work in the framework of the Russian government under grant *Measures to Attract Leading Scientists to Russian Educational Institutions* (contract No. 11.G34.31.0072).
2. Research interests of the laboratory include hypersonic flows and computational fluid dynamics, among other things
3. Leading staff of the laboratory:
   - Head: Sergey Utyuzhnikov, PhD, DSc, FIMA, Professor of Computational Mathematics
   - Deputy Head: V.A. Titarev, Ph.D.
   - Deputy Head: S.S. Simakov, PhD, Docent
   - Leader of FALT branch of the laboratory: I.V. Egorov, DSc, Professor, Corresponding member of RAS
4. Vladimir Titarev is a leading researcher at Computing Center, Moscow; previous positions held at Cranfield University (UK) and University of Trento (Italy)

   Sergei Utyuzhnikov's main position is at University of Manchester, UK.
5. Laboratory consists of more than 40 researchers
6. Web page http://www.flowmodellium.ru/en/

Motivation: why to use BKE?

At present, the Monte-Carlo statistical simulation method (DSMC) is the computational method of choice. However,

- Due to statistical fluctuations and 1st order not very suitable for unsteady flows, transitional and near-continuum flows, slow flows
- Computational efficiency may not be optimal for some flows due to explicit time evolution

The Boltzmann kinetic equation (BKE) is free of these limitations of the DSMC:

- The equation is applicable across all flow regimes, i.e. from free molecular to near-continuum flows
- Unsteady flows can be treated in a straightforward manner.
- The deterministic nature of the equation allows the development of efficient high-order accurate methods, including methods with implicit time evolution
- It is possible to use special properties of the flow problem (e.g. asymptotic solution) in construction of numerical methods

BKE with the Shakhov model collision integral (1968)

- In the non-dimensional variables the kinetic equation takes the form:

$$\frac{\partial f}{\partial t} + \xi_x \frac{\partial f}{\partial x} + \xi_y \frac{\partial f}{\partial y} + \xi_z \frac{\partial f}{\partial z} = \nu(f^{(S)} - f), \quad \nu = \frac{nT}{\mu}\delta,$$

$$\delta = \frac{l_* p_*}{\mu(T_*)\sqrt{2RT_*}} \sim \frac{1}{\mathrm{Kn}}, \quad f^{(S)} = f_M\left(1 + \frac{4}{5}(1-\mathrm{Pr})\mathbf{Sc}(c^2 - \frac{5}{2})\right),$$

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

- Macroscopic quantities defined as

$$\left(n, n\mathbf{u}, n(\frac{3}{2}T + u^2), \mathbf{q}\right) = \int \left(1, \boldsymbol{\xi}, \xi^2, \frac{1}{2}\mathbf{v}v^2\right) f d\boldsymbol{\xi}.$$

- Boundary condition on the surface:

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

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

Computational challenges in solving model kinetic equation

Although the equation is linear it is still very challenging to numerical solution:

- Equation is six dimensional (3 physical and 3 velocity coordinates) and temporal dependence.
- Solutions are discontinuous in both physical and velocity spaces
- For transitional flows $\delta \gg 1$ the equation becomes stiff
- The solution procedure needs to be conservative with respect to the model collision integral

Conservative discrete velocity framework

- March in time to steady state:

$$\frac{\partial}{\partial t} f = -\boldsymbol{\xi} \nabla f + J(f), \quad J = \nu(f^{(S)} - f),$$

- Replace the infinite domain of integration in the molecular velocity space $\boldsymbol{\xi}$ by a finite computational domain.
- The kinetic equation is replaced by a system of N_ξ advection equations for each of $f_\alpha = f(t, \mathbf{x}, \boldsymbol{\xi}_\alpha)$:

$$\frac{\partial}{\partial t} f_\alpha = -\boldsymbol{\xi}_\alpha \nabla f_\alpha + J(f_\alpha),$$

which are connected by the macroscopic parameters in the function $f^{(S)}$ from the model collision integral J.

Calculation of macroscopic quantities (Titarev 2003,2007)

Primitive variables

$$\mathbf{W} = (n, u_1, u_2, u_3, T, q_1, q_2, q_3)^T$$

are found from the following system of equations

$$\mathbf{R}(\mathbf{W}) = \sum_{\alpha} \begin{pmatrix} 1 \\ \boldsymbol{\xi} \\ \xi^2 \\ \mathbf{v}v^2 \end{pmatrix}_{\alpha} (f_\alpha^+ - f_\alpha)\omega_\alpha + \begin{pmatrix} 0 \\ \mathbf{0} \\ 0 \\ 2\,\mathrm{Pr}\,\mathbf{q} \end{pmatrix} = \mathbf{0}.$$

Here subscripts i are n are omitted for simplicity.
These eight equations are solved using the Newton iterations For each cell the system of eight equations is solved using Newton iterations:

$$\mathbf{W}^s = \mathbf{W}^{s-1} - J^{s-1} \cdot \mathbf{R}^{s-1}, \quad s = 1, 2, \ldots, \quad J = \frac{\partial \mathbf{R}}{\partial \mathbf{W}}.$$

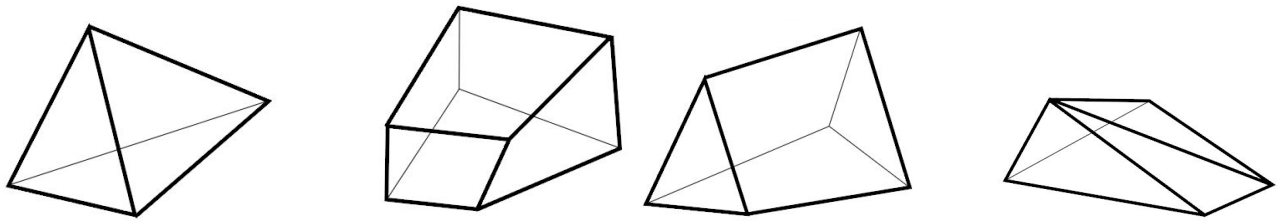
The initial guess for which is provided by the direct (non-conservative) approximation.

Remark 1: the method applies to virtually any model kinetic equation, even if the H-theorem for it is not proven.

Remark 2: for $\mathrm{Pr} = 1$ the method reduces to method from Mieussens, 2000.

Fully discrete advection scheme

- Consider cells of various shapes.



- Denote by $|V_i|$ the cell volume, $|A|_{il}$ area of face l.
- Omit subscript α for simplicity. Let $\Delta t = t^{n+1} - t^n$, $f^n = f(t^n, \mathbf{x}, \boldsymbol{\xi})$. The implicit one-step method has the following form:

$$(1 + \Delta t \nu^n + \Delta t \boldsymbol{\xi} \nabla) \frac{f^{n+1} - f^n}{\Delta t} = -\boldsymbol{\xi} \nabla f^n + J^n.$$

- After integration we get a system of linear equations for $\phi^n = f^{n+1} - f^n$:

$$(1 + \nu_i^n \Delta t)\phi_i^n + \frac{\Delta t}{|V_i|} \sum_l \xi_{nl} F_l(\phi_i^n, \phi_{\sigma_l(i)}^n)|A_{il}| = \{-(\boldsymbol{\xi} \nabla f^n)_i + J_i^n\} \Delta t$$

$$F_l = \frac{1}{2}(\phi_i^n + \phi_{\sigma_l(i)}^n) - \frac{1}{2}\mathrm{sign}(\xi_{nl}) \cdot (\phi_{\sigma_l(i)}^n - \phi_i^n).$$

- The values at the next time level are given by $f_i^{n+1} = f_i^n + \phi_i^n$.

Flux calculation

Using divergence theorem $\rightarrow$ sum of face fluxes:

$$(\xi \nabla g^n)_i = \frac{1}{|V_i|} \sum_l \Phi^n_{il},$$

$$\Phi^n_{il} = \frac{\xi_{nl}}{2} \left(f^- + f^+ + \mathrm{sign}(\xi_{nl})(f^- - f^+) \right) |A_{il}|,$$

$$f^- = f^n_{il}, \quad f^+ = f^n_{\sigma_l(i) l_1}.$$

Here l_1 is the number of the face of the cell $\sigma_l(i)$, adjacent to the face l of the cell i, the face averages f^n_{il} of the function f for each cell i.

Reconstruction of face values

Possible choices for face values f_{il}^n:

- First-order accurate method: $f_{il}^n = f_i^n$.
- Second-order accurate TVD method: use a piece-wise linear reconstruction of the solution in each spatial cell

$$f_i(x) = f_i^n + a_{i1} e_1(\hat{\mathbf{x}}) + a_{i2} e_2(\hat{\mathbf{x}}) + a_{i3} e_3(\hat{\mathbf{x}}),$$

  where e_k are the basis functions with zero mean, in local coordinate system $\hat{\mathbf{x}}$.
- Third and higher-order: weighted essentially non-oscillatory (WENO) method on mixed-element meshes.
- For hexa elements only: quasi one-dimensional reconstruction along mesh directions:

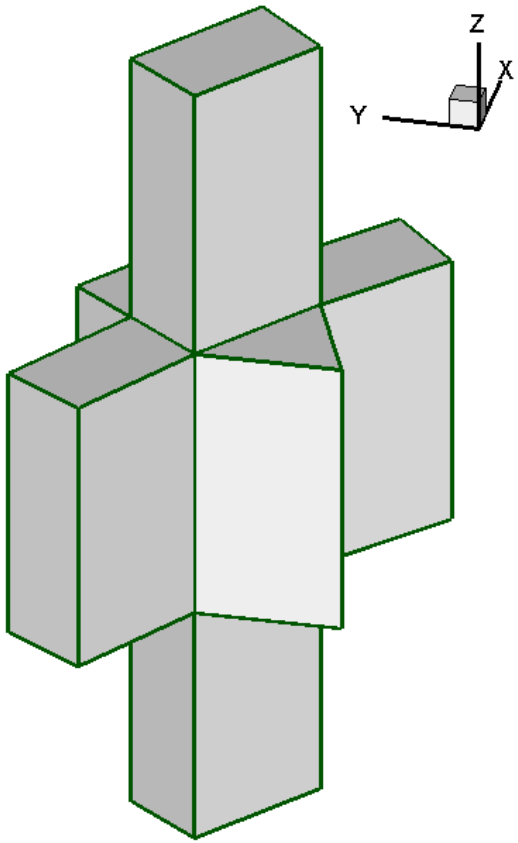
$$f_{il}^n = f_i^n + \phi(S_L, S_R)\Delta_l,$$

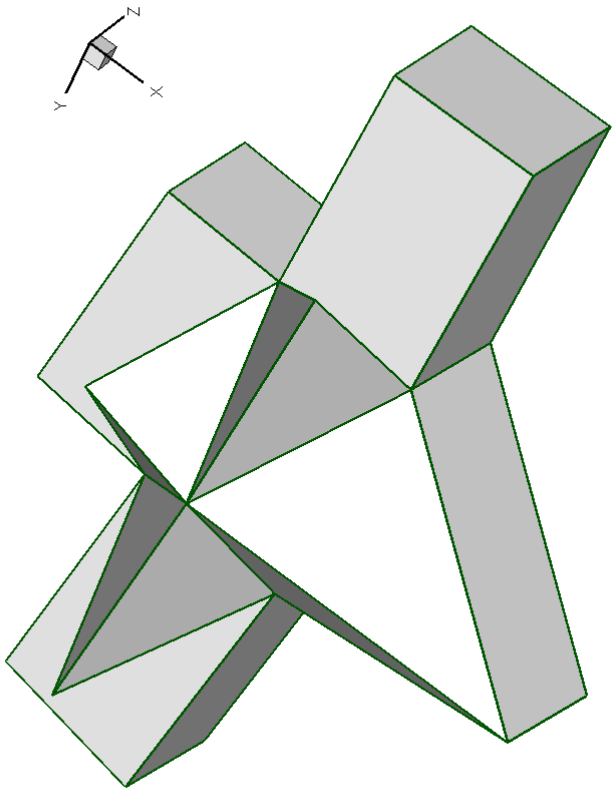
  where Δ_l is the distance from cell centre to face centre, S_L, S_R are left and right estimates of solution slope, $\phi(a, b)$ is the slope limiter.

Note that method (4) is most efficient out of second-order reconstructions.

Construction of 2nd order reconstruction polynomial

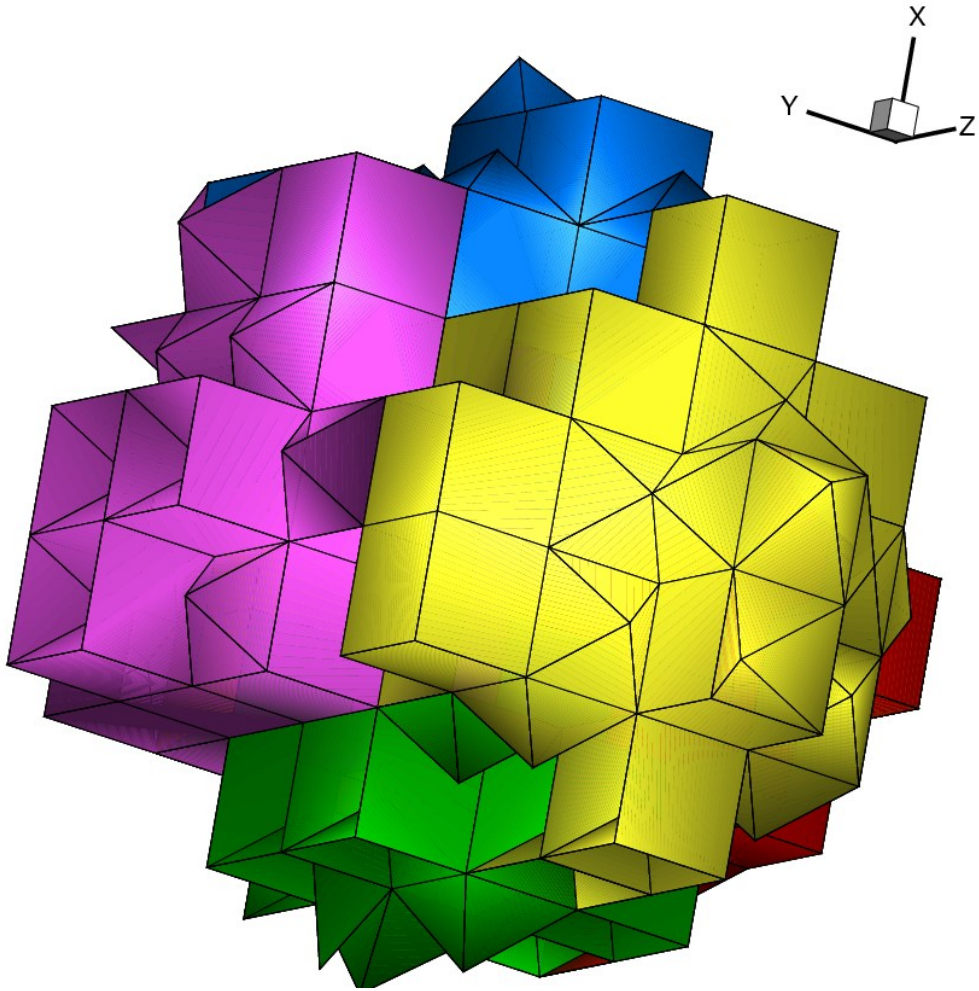
Velocity distribution function is represented by a piece-wise linear function in each cell. Coefficients of the function are computed using values in the reconstruction stencils.





Uniformly high order of spatial accuracy

One can use some version of Weighted Essentially Non-Oscillatory (WENO) method with multiple stencils for each spatial cell.



Time evolution

- Re-grouping, we can obtain:

$$(1 + \Delta t \nu_i^n + \Delta t b_i)\phi_i^n + \Delta t \sum_l c_{i,\sigma_l(i)} \phi_{\sigma_l(i)}^n = \left\{ -\frac{1}{|V_i|} \sum_l \Phi_{il}^n + J_i^n \right\} \Delta t$$

$$b_i = \sum_l \xi_{nl}(1 + \mathrm{sign}\xi_{nl}) \frac{|A_{il}|}{2|V_i|}, \quad c_{i,\sigma_l(i)} = \xi_{nl}(1 - \mathrm{sign}\xi_{nl}) \frac{|A_{il}|}{2|V_i|}.$$

- An approximate LU SGS factorization of the system is carried out using the approach suggested in Men'shov & Nakamura 1995, 2000
- As a result, the computational cost of one time step of the implicit method is only 25% larger than the computational cost of a one-step explicit method.
- In calculations, the value of the time step Δt is evaluated according to the expression

$$\Delta t = C \min_i d_i / \xi_0,$$

  where C is the prescribed CFL number, d_i the characteristic linear size of V_i.
- $C \leq \frac{1}{3}$ corresponds to the conventional explicit method

Parallel version of implicit method

Spatially single-block parallel implementation

Pros:

- transient identical to single-block implicit method
- relatively simple to code
- convenient for special versions

Cons:

- relatively high memory requirements per core
- does not scale well above 128 cores for $N_{space} > 10^5$

Spatially multi-block parallel implementation

Pros:

- excellent scaling
- can handle spatial meshes of arbitrary size

Cons:

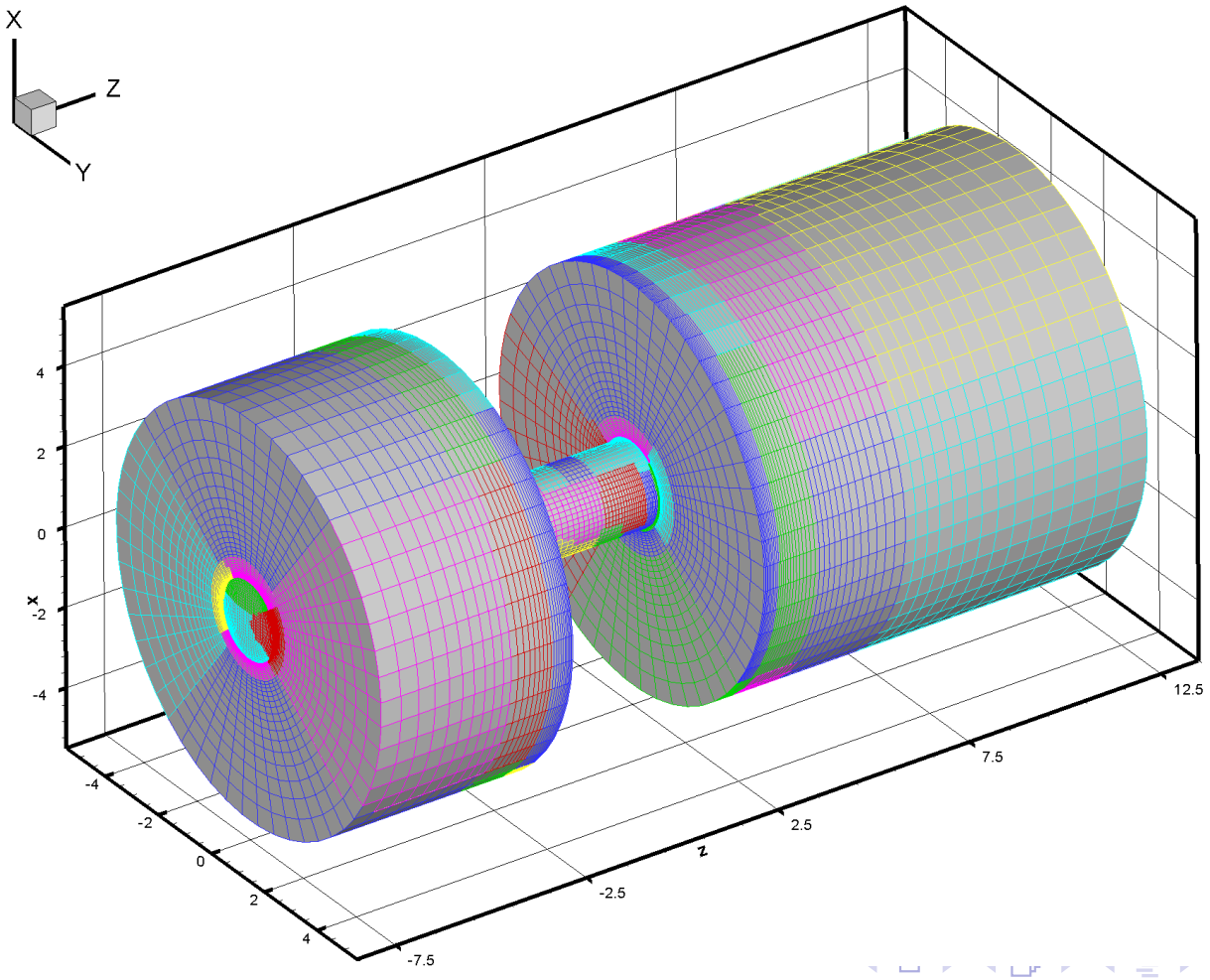
- requires complicated coding (to be done once)
- steady-state convergence slower than for single-block version

Results

1. Calculations are run for both 2D and 3D versions, but only 3D results will be shown
2. Efficiency of implicit time evolution is assessed
3. Parallel scalability tests are carried out for both single-block and multiple-block versions
4. Calculations are run on 'Lomonosov' HPC of Lomonosov Moscow State University, Russia. This is a T-Platforms machine, made in 2009. A total peak performance of the computer system 1.37 Pflops, and Linpack performance 674 Tflops. 'Lomonosov' was ranked 13th in the June 2011 edition of Top500 list.

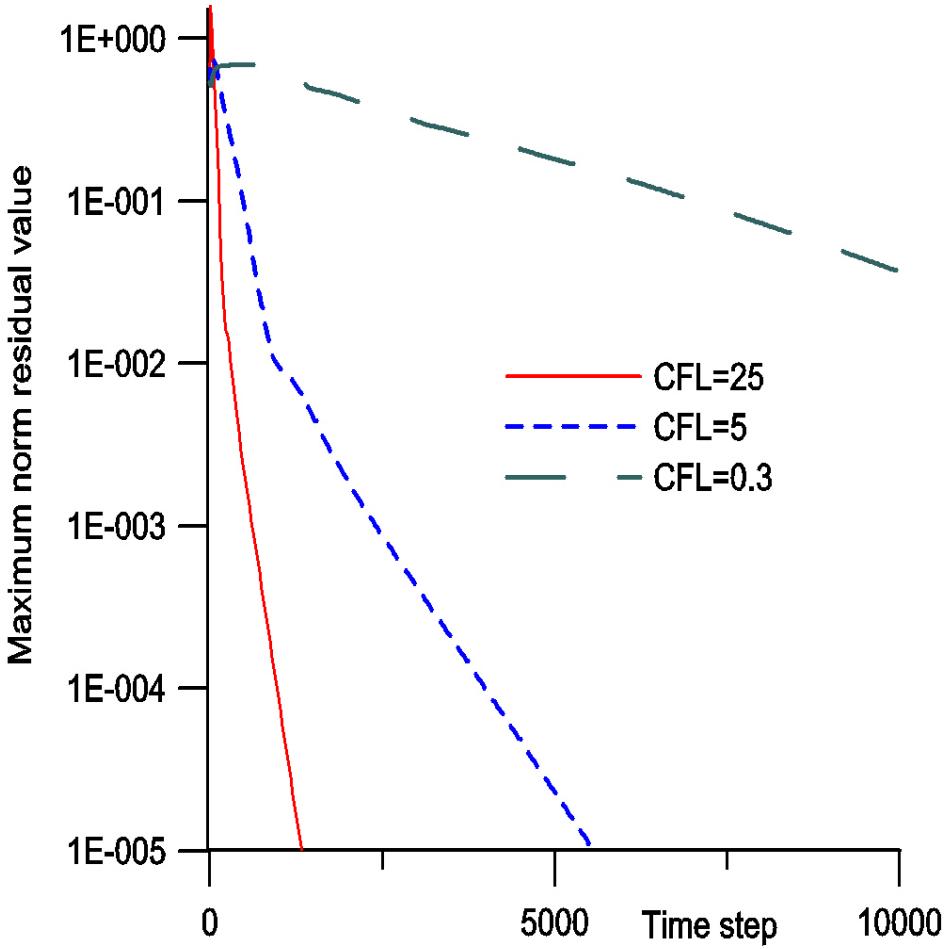
Flow in a circular pipe

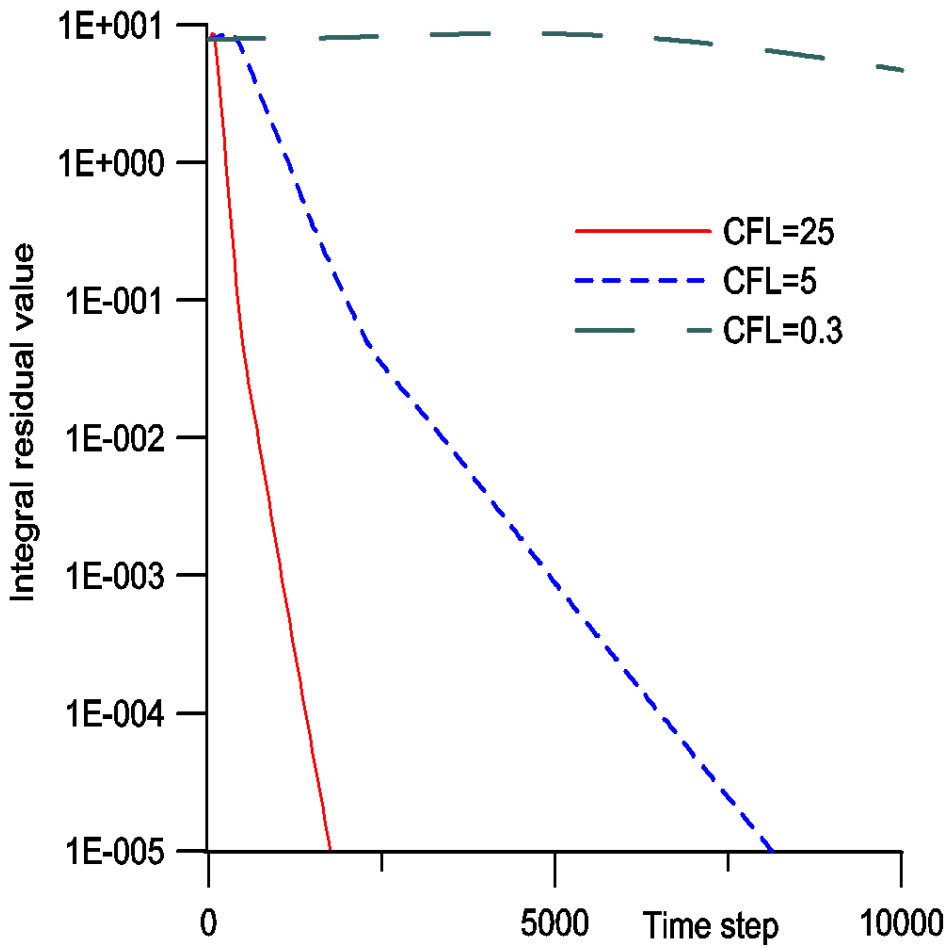
Consider two large reservoirs filled with the same monatomic gas and connected by a pipe of length L and radius R. Inside the reservoirs away from the pipe the gas is at rest with pressures p_1, $p_2 = p_1/2$ and equal temperatures $T_1 = T_2 = T_0$.
Use L/R=5 and spatial mesh of 267×10^3 hexas. Shown are 128 blocks.



Efficiency of implicit time evolution in 3D

The solution of the nonlinear problem is computed for $\delta_1 = 1$.

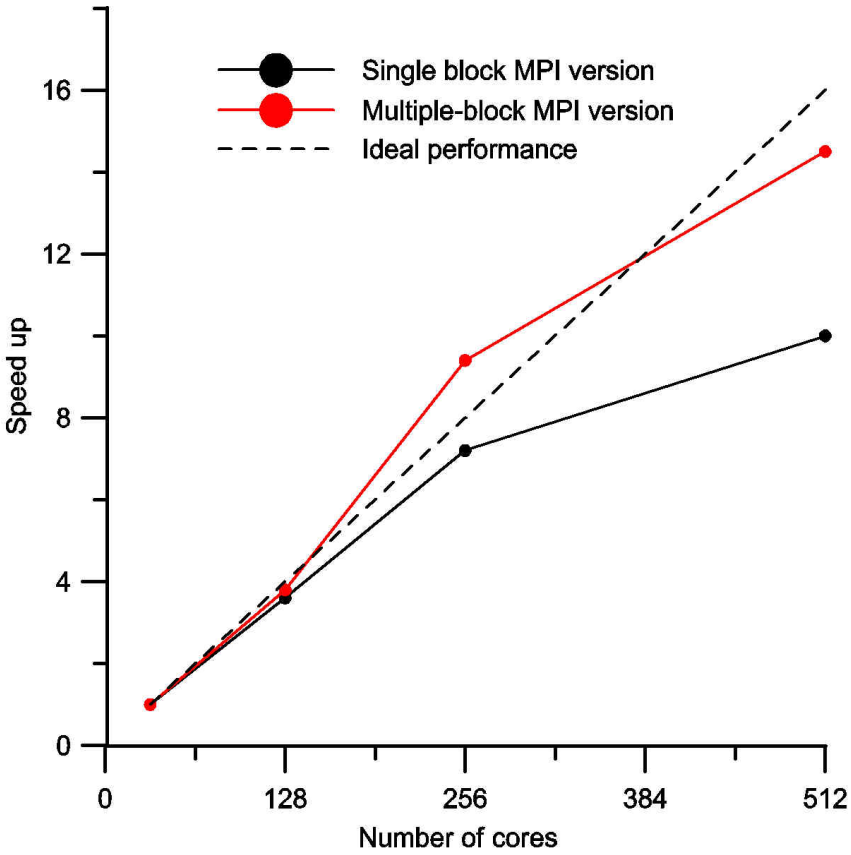




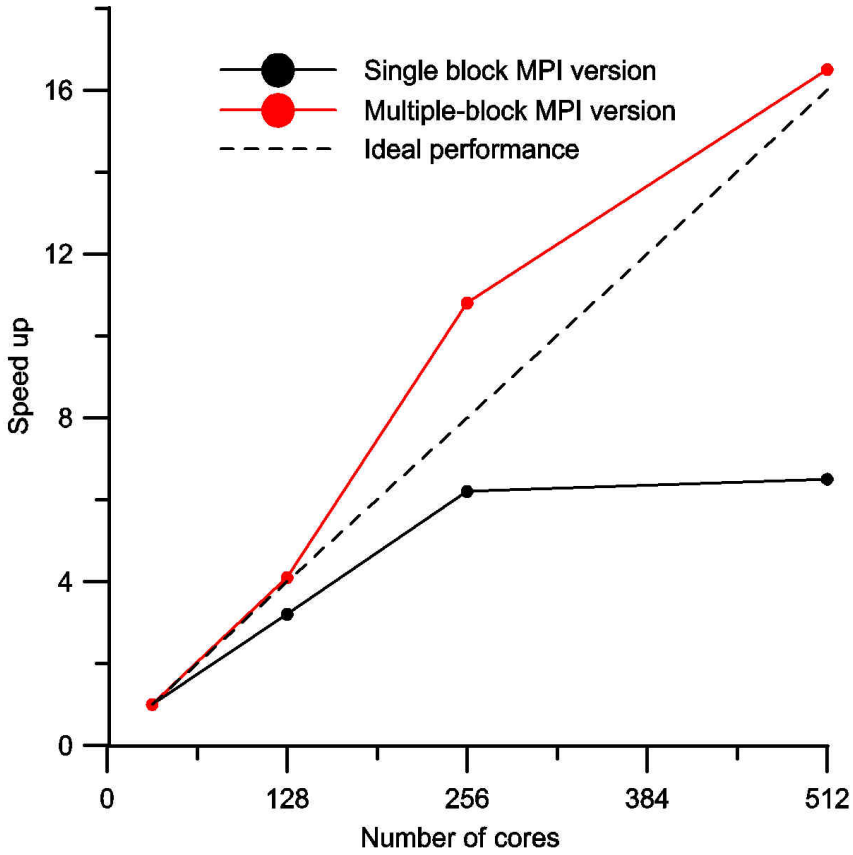
Implicit time marching method converges significantly faster, than its explicit counterpart.

Scalability on 'Lomonosov'

Unstructured 2nd order method



Quasi one-dimensional 2nd order method

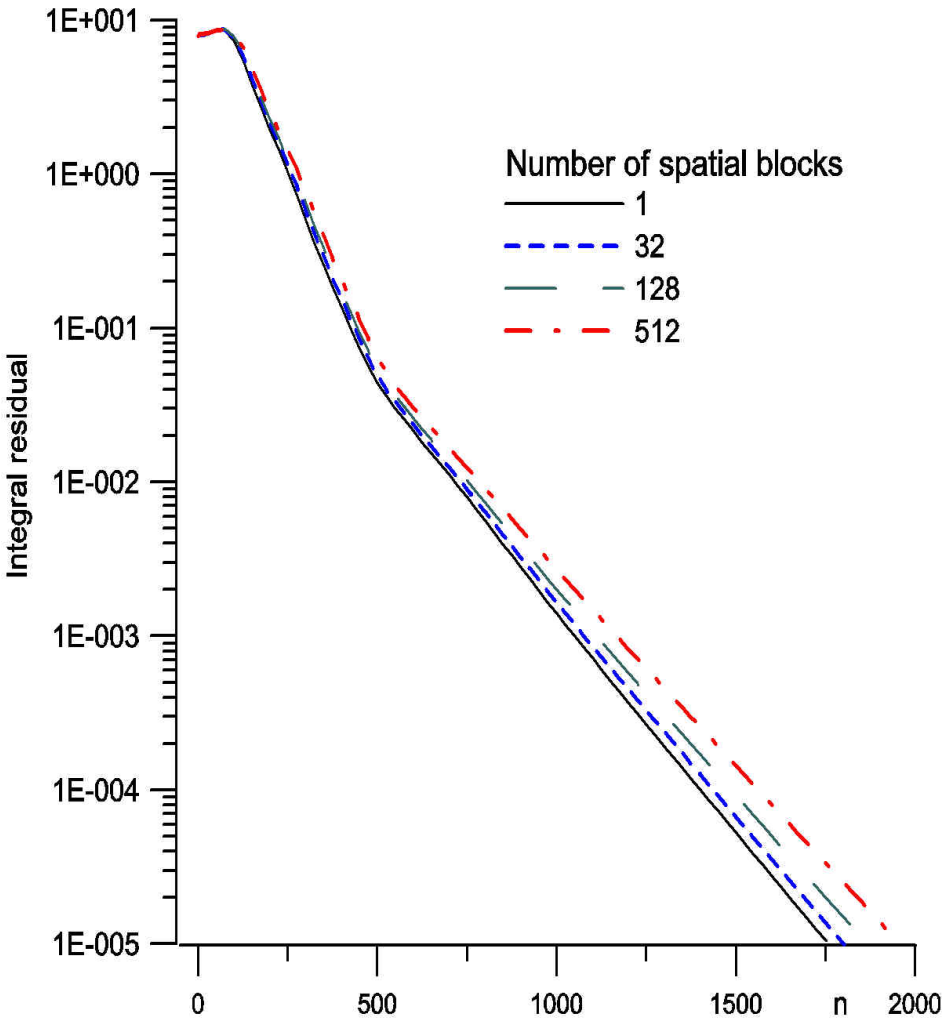


Purely unstructured version is around 40% slower and hence scales better for single-block MPI version.

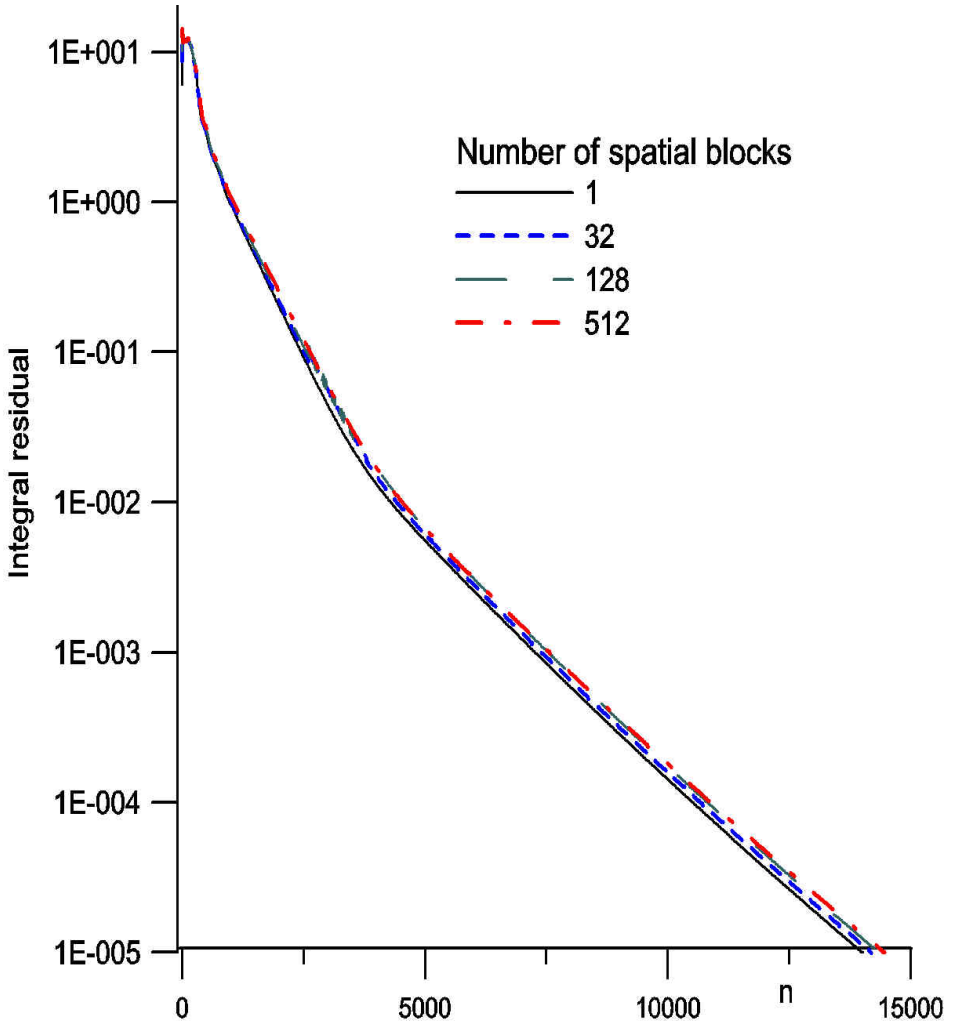
Convergence properties

All data for quasi one-dimensional 2nd order method with limiters.

$\delta = 1$

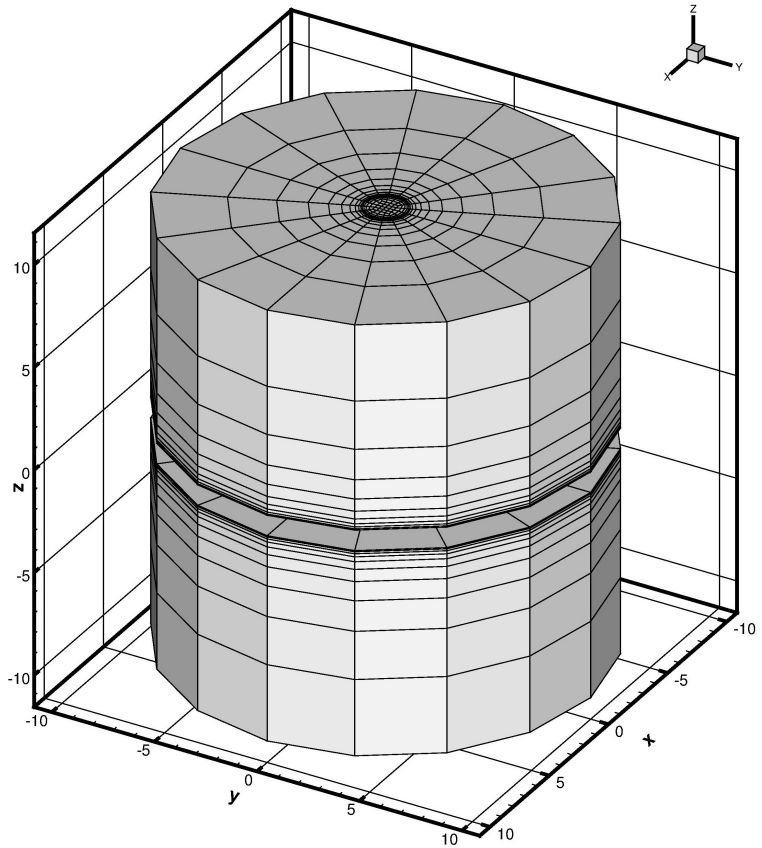


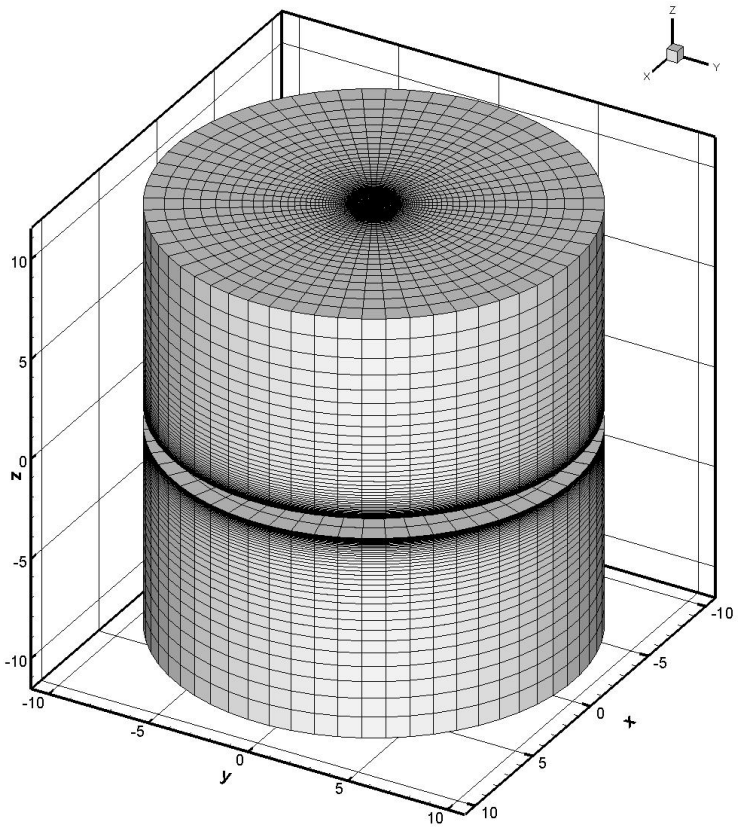
$\delta = 20$



Flow into vacuum for $L/R = 1$

Formal convergence study: three spatial meshes: 5.6×10^3, 41×10^3 & 350×10^3 spatial cells and various velocity meshes.
Solution method: TVD1D scheme (quasi one-dimensional).
Shown meshes with 5.6 and 350 thousands cells.





Flow into vacuum for $L/R = 1$: results

This is a benchmark problem from *Sharipov, F., 2012. Benchmark problems in rarefied gas dynamics. Vacuum, 86 (11), 1697–1700.*

Data provided for $0 \leq \delta_1 \leq 500$: from free-molecular to continuum regime. This is wider range than suggested in the original benchmark.

δ_1	Mesh 1	Mesh 2	Mesh 3	DSMC	Experiment
0.	0.666	0.670	0.672	0.672	
0.1	0.678	0.683	0.684	0.680	0.675
1.	0.758	0.766	0.768	0.754	0.743
10.	1.035	1.061	1.066	1.062	1.06
100.	1.290	1.351	1.367	1.358	1.33
200.	1.331	1.406	1.425	1.412	
500.	1.331	1.454	1.474	1.449	

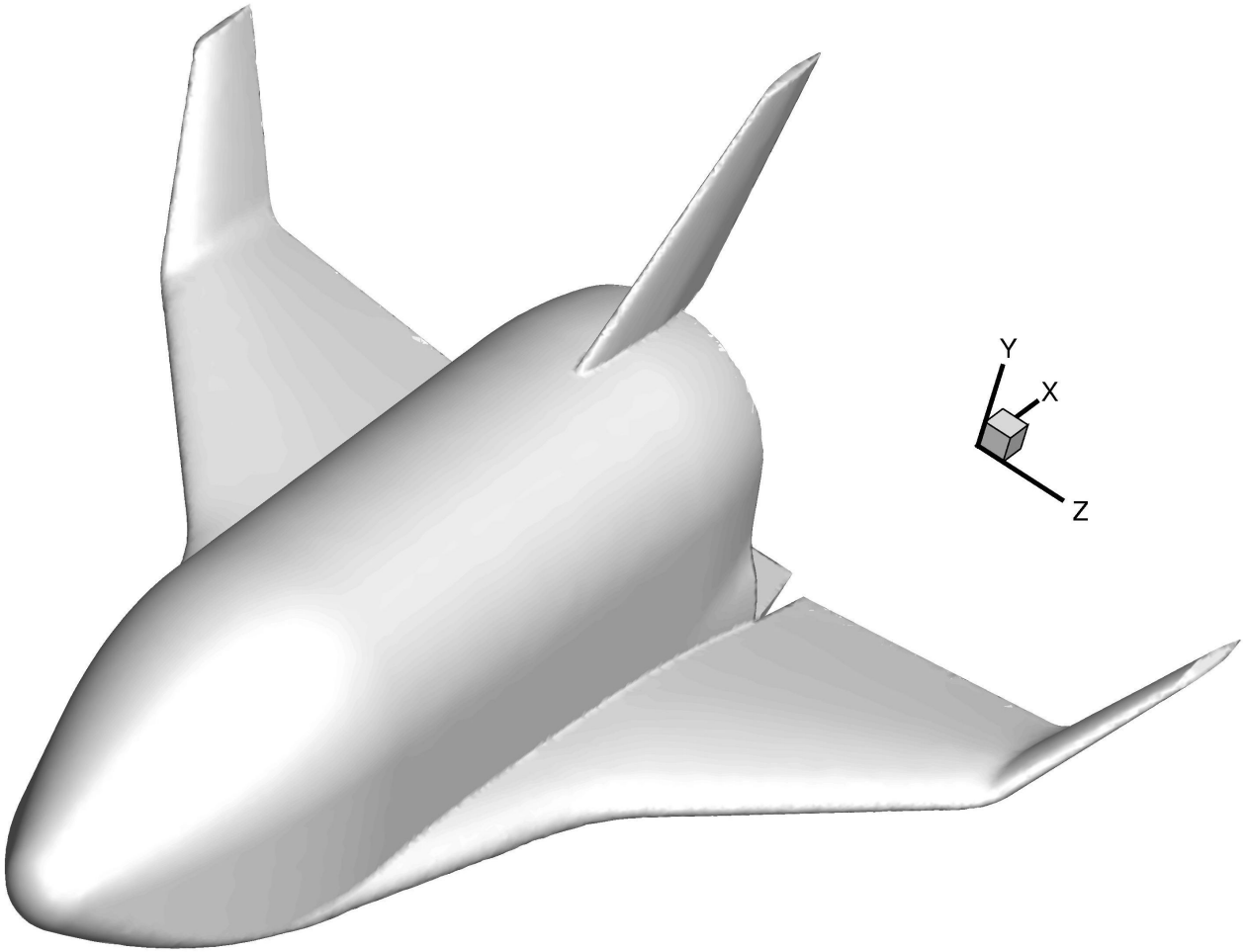
DSMC data: *Varoutis et al, 2008, J. Vac. Sci. Technol. V. 26*

Experimental data: *T. Fujimoto and M. Usami , 1984. J. Fluids Eng Tran ASME V. 106.*

Convergence rate above 1 is observed.

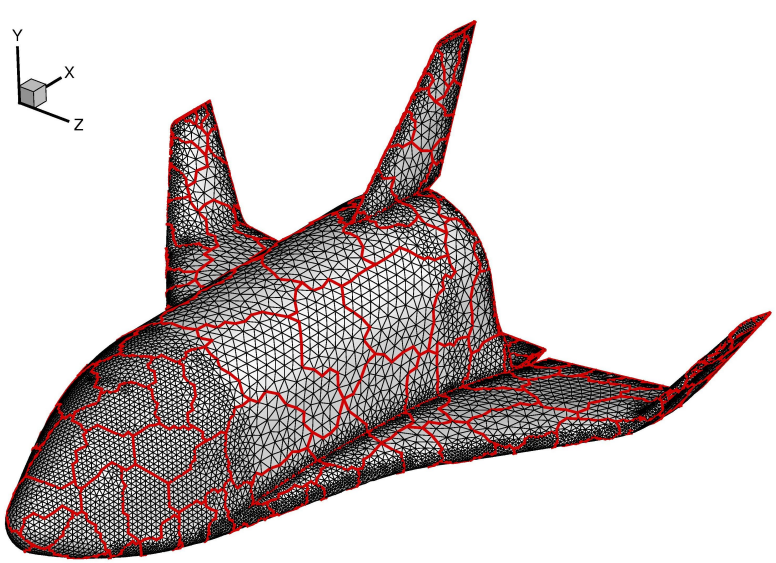
Supersonic flow over a model re-entry space vehicle (RVS).

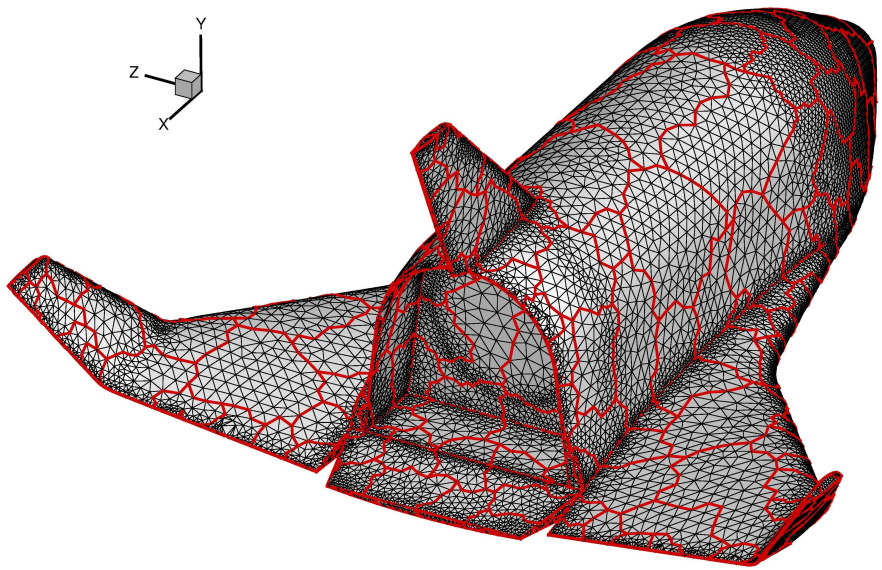
The aerodynamic shape of the RSV consist of a fuselage with spherical nose bluntness, two wings with dogtooth extension and end edges, and a vertical keel and fuselage flap. The length of the fuselage is 9000mm, the radius of the nose is 450mm, the upper surface diameter is 2600mm. The total length of the RVS with the flap is 10000mm.



Computational mesh

- The four layers of prismatic cells of 20mm heights are used near the surface of the RVS, whereas the rest of the computational domain is filled with tetrahedrons.
- The total number of spatial cells is $N_{space} \approx 533 \times 10^3$, including approximately 386×10^3 tetrahedrons, 147×10^3 prisms and 551 pyramids.
- The mesh is split into 256 blocks with approximately 2100 internal cells each and between 900 and 2800 so-called ghost cells, required by the second-order TVD method.
- The velocity mesh consisted of 24^3 nodes. The total number of cells in the 6-dimensional mesh is thus approximately 6.9×10^9.





Calculation data and solution procedure

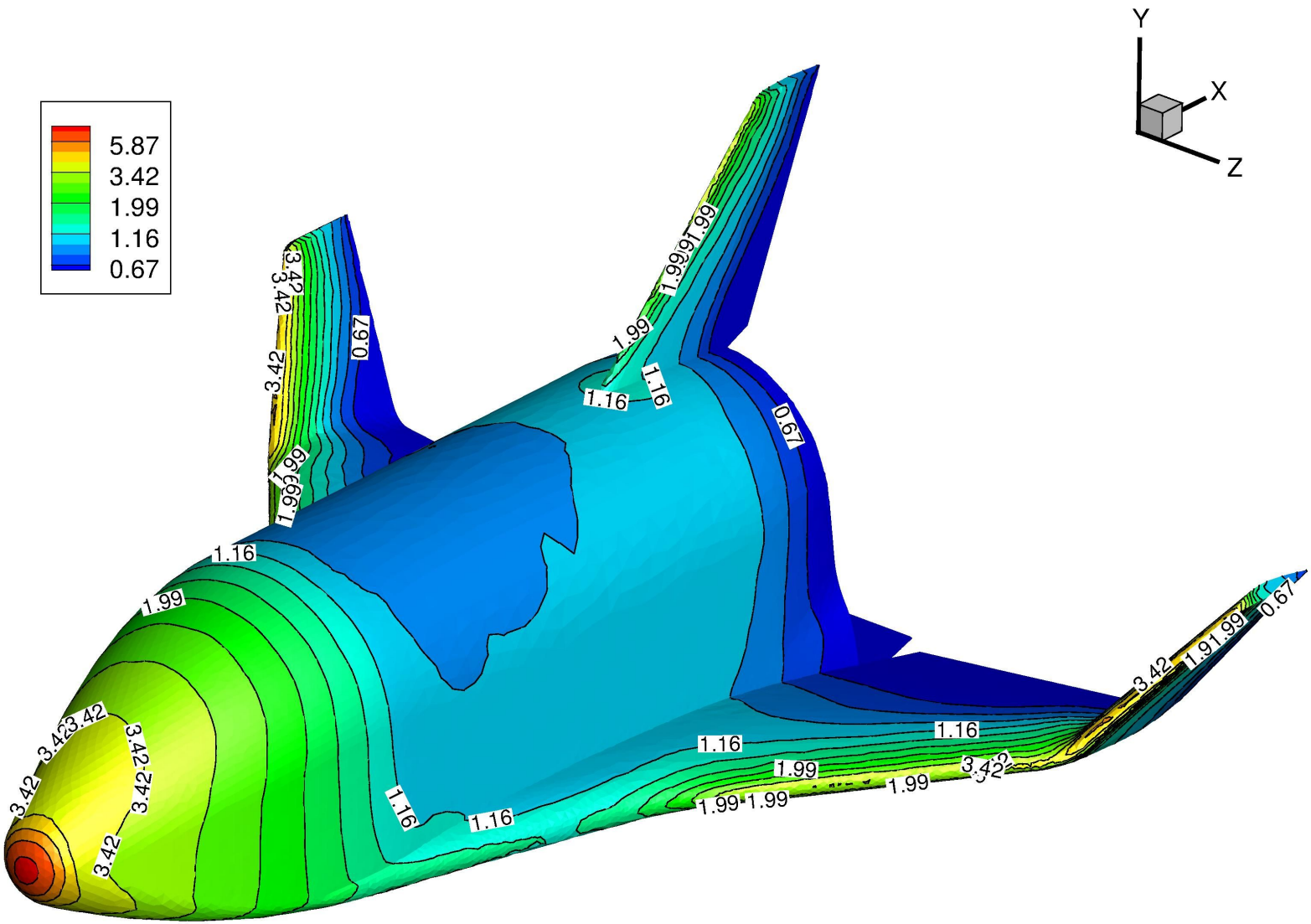
Flow data:

- The total length of the vehicle is chosen as the spatial scale l_*, whereas the free-stream values of pressure and temperature are set as p_*, T_*.
- The surface temperature was fixed and equal to the free-stream temperature.
- The non-dimensional spatial mesh is obtained from the initial dimensional mesh by dividing over l_*. Calculations were carried out for the non-dimensional free-stream velocity number $u_\infty = 2$.
- The rarefaction parameter is set to $\delta_\infty = 1000$, which approximately corresponds to the altitude of 100 km (1cm mean free path).

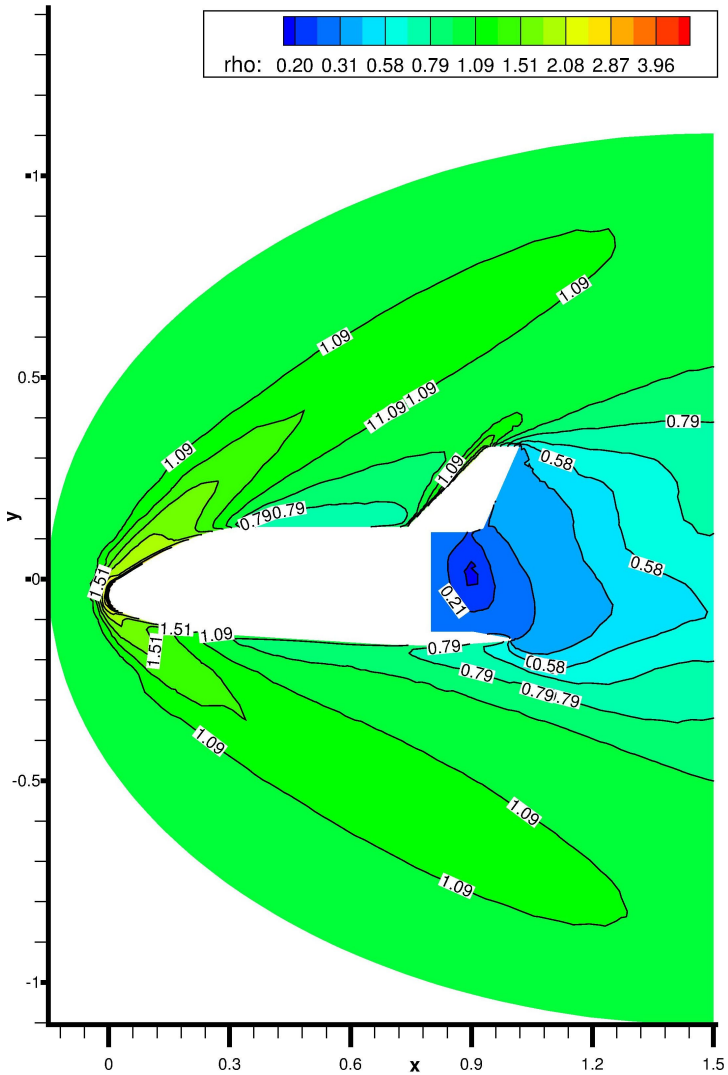
The calculation process is organized as follows:

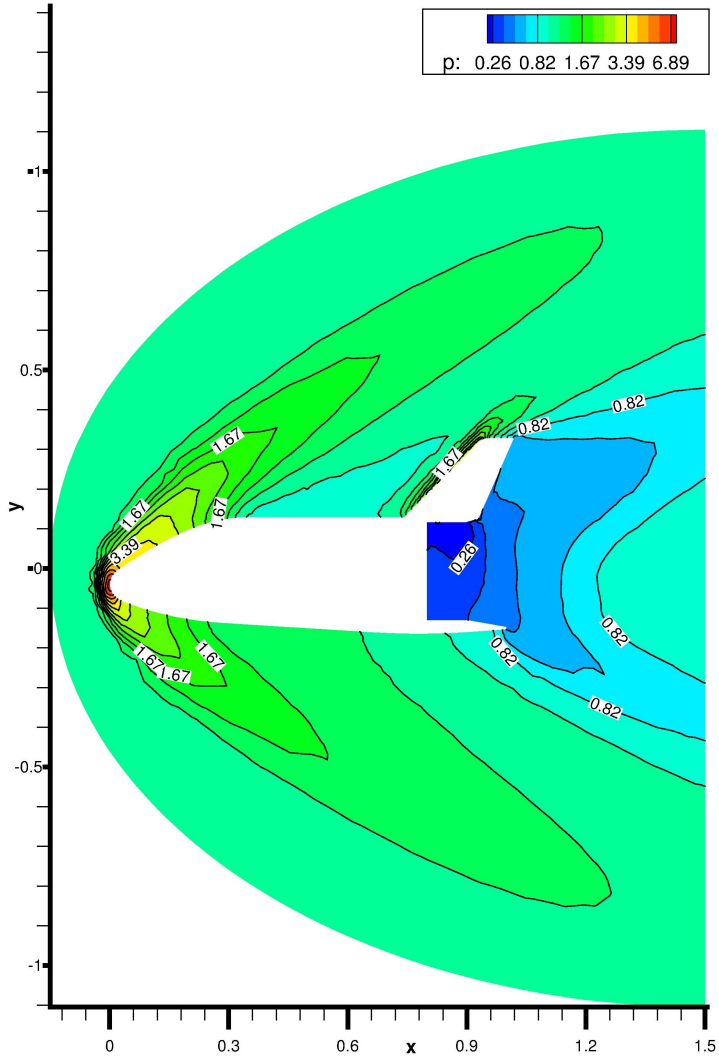
- The free-stream values of all macroscopic variables are used as the initial guess.
- The first-order solution is constructed, using CFL number of 25.
- Then, the second-order solution is computed using first-order solution as the initial guess.
- One time step of the TVD scheme takes approximately 120 seconds. The complete steady-state convergence requires several thousand iterations.

Surface pressure distribution



Density (left) and pressure (right) in x-y plane





Recent publications

1. V.A. Titarev. Implicit numerical method for computing three-dimensional rarefied gas flows using unstructured meshes // *Comput. Math. & Math. Phys.*, 2010, 50(10):1719–1733.
2. V.A. Titarev. Efficient deterministic modelling of three-dimensional rarefied gas flows // *Comm. Comp. Phys.*, 2012, 12(1):162-192.
3. V.A. Titarev and E.M. Shakhov. Computational study of a rarefied gas flow through a long circular pipe into vacuum //*Vacuum, Special Issua "Vacuum Gas Dynamics"*, 2012, 86(11):1709-1716.
4. M. Dumbser, V.A. Titarev, S.V. Utyuzhnikov. Implicit multiblock method for solving a kinetic equation on unstructured meshes // *Comput. Math. & Math. Phys.*, 2013, V. 53, N. 5, p. 601-615.
5. V.A. Titarev, E.M. Shakhov and S.V. Utyuzhnikov. Rarefied gas flow through a diverging conical pipe into vacuum // *Vacuum*, 2014, V. 101. P. 10-17
6. V.A. Titarev, M. Dumbser, S.V. Utyuzhnikov. Construction and comparison of parallel implicit kinetic solvers in three spatial dimensions, *J. Comput. Phys., 2013, in press*, http://dx.doi.org/10.1016/j.jcp.2013.08.051.