Комплекс программ SMILE: инструмент для расчетов разреженных течений методом прямого статистического моделирования

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CFD Weekend

Институт прикладной математики им. М.В. Келдыша РАН, г. Москва

28-29 ноября, 2015

Введение

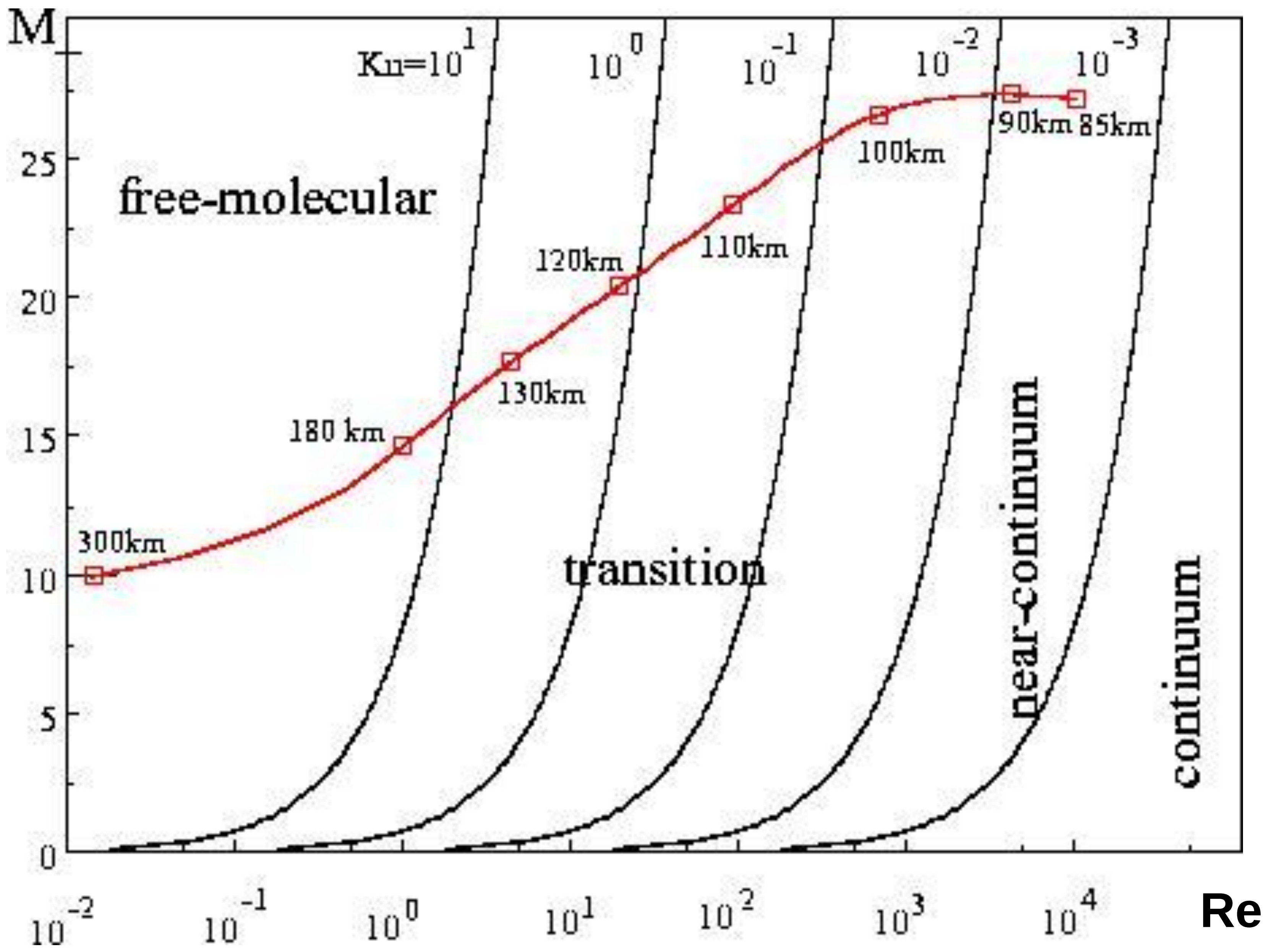
- Актуальность исследования гиперзвуковых разреженных течений обусловлена необходимостью анализа аэротермодинамики орбитального и высотного полета перспективных космических аппаратов (КА).

- Экспериментальное моделирование разреженных неравновесных высокоэнтальпийных течений затруднительно как с технической, так и с экономической точки зрения.

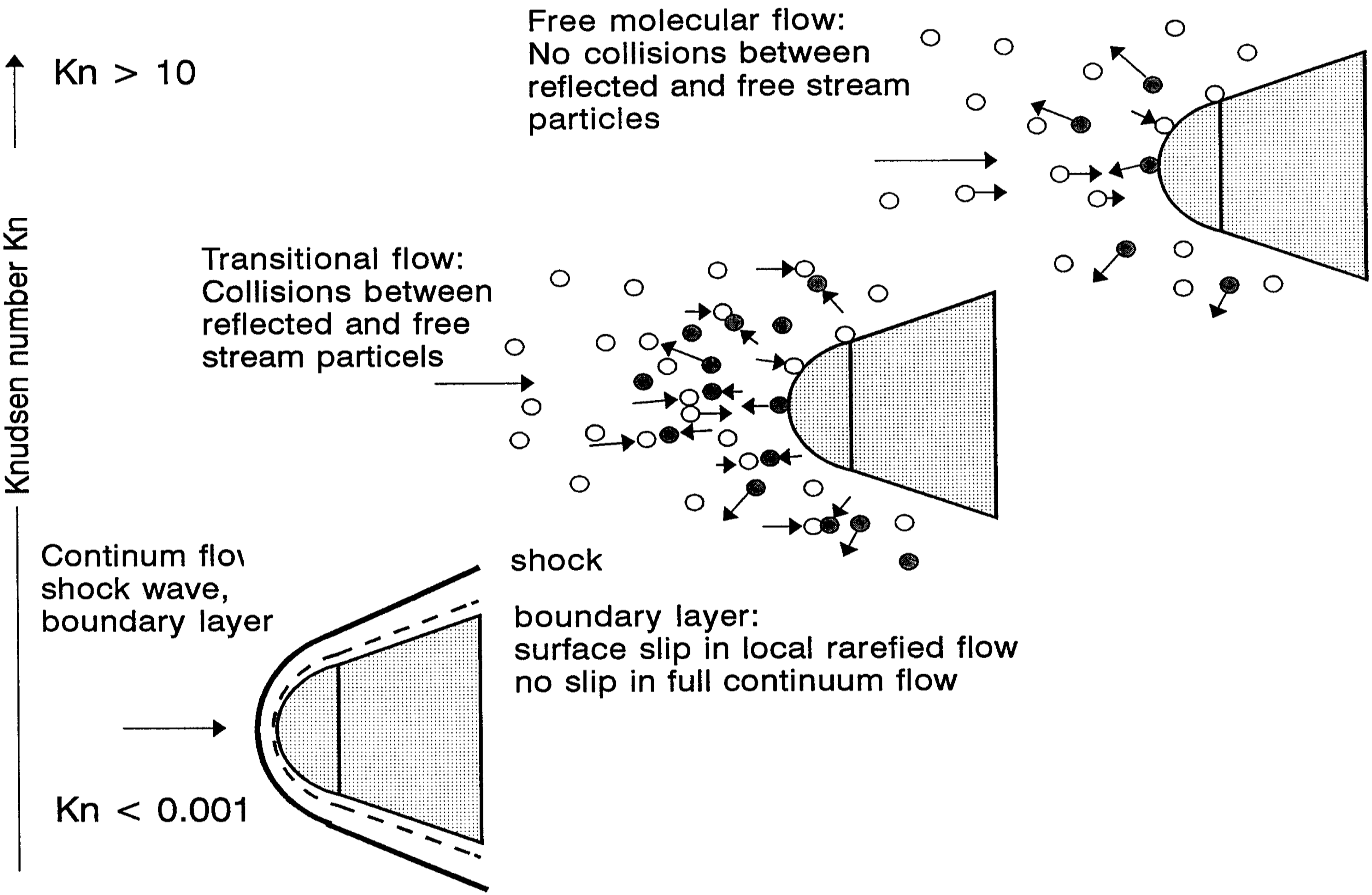
- Степень разреженности течения характеризуется числом Кнудсена Kn = λ / L, где λ – длина свободного пробега, а L – характерный размер.

- Численные методы динамики разреженного газа в настоящее время фактически являются основным инструментом для исследования многомерных течений разреженного газа в областях со сложной геометрией в свободномолекулярном (Kn>10), переходном (10>Kn>0,01) и около-континуальном режимах (0,01>Kn>0,001).

FLOW REGIMES



FLOW REGIMES

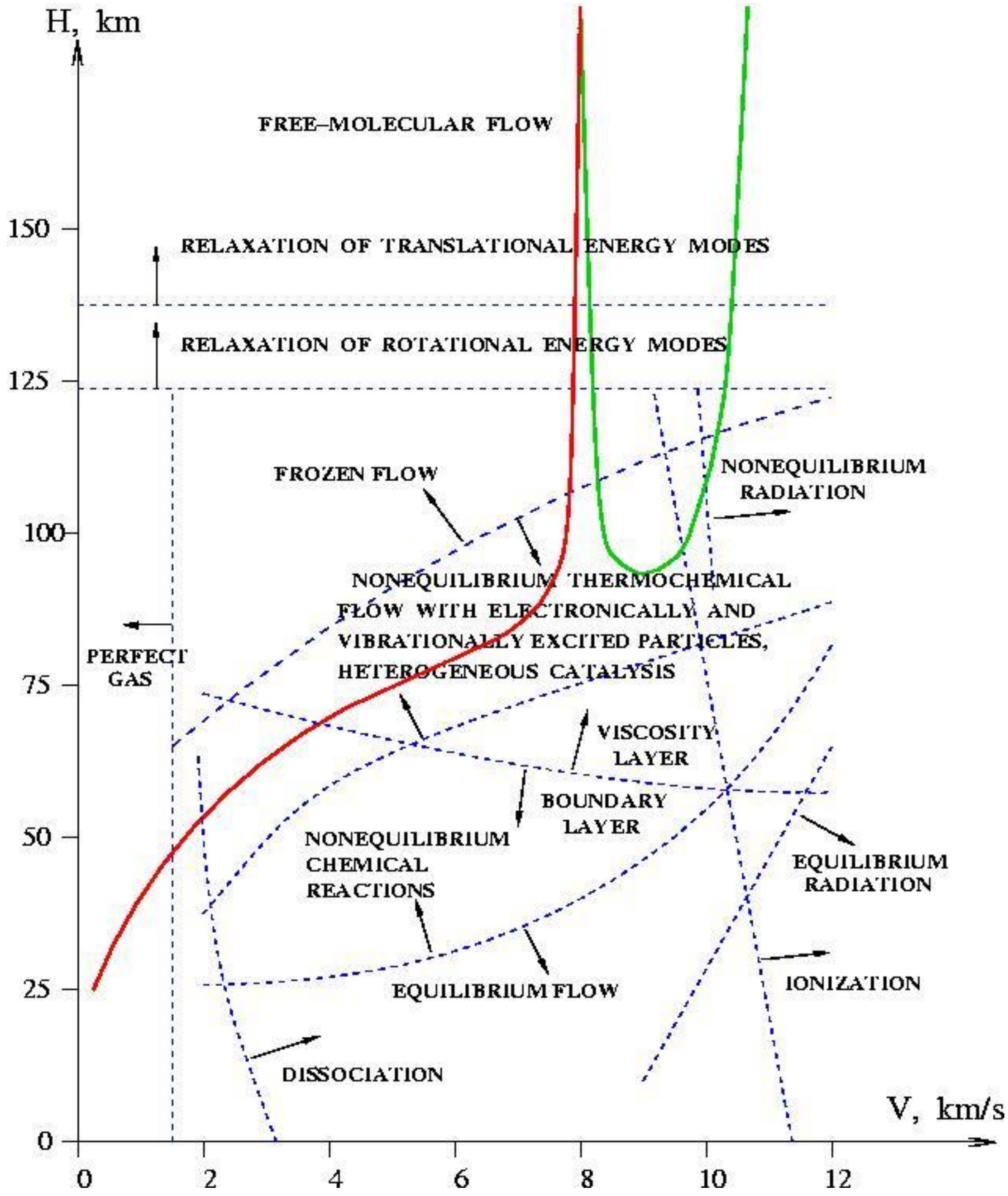


Mathematical Models of Gas Flows

$$Kn = \frac{\lambda}{L}$$

Knudsen number	Flow regime	Mathematical model	
$Kn \to 0$	continuum (inviscid)	Euler equations	Boltzmann equation, DSMC
$Kn \le 10^{-3}$	continuum	Navier-Stokes equations (without slip on the wall)	
$10^{-3} \le Kn \le 10^{-2}$	near-continuum	Navier-Stokes equations (1st order slip on the wall)	
$10^{-2} \le Kn \le 10$	transition	Burnett equations Moment equations (Grad equations, R13 and etc.) Model equations (BGK, ES-BGK, Shakhov model)	
$Kn > 10$	free molecular flow	Free-molecular Boltzmann equation	

Flow regimes and physico-chemical processes



Пакеты прикладных аэродинамических программ
М.С. Иванов (1945-2013)

AEROTHERMODYNAMICS

Theory | Numerical modeling | Experiment

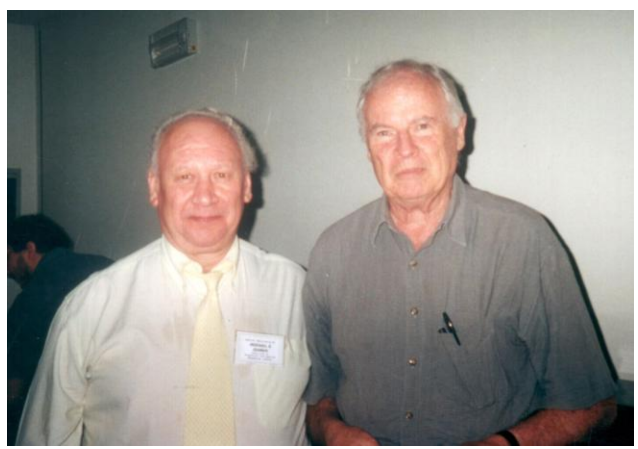
↓

Orbital and high-altitude re-entry modeling systems

↓

AEROSPACE APPLICATIONS

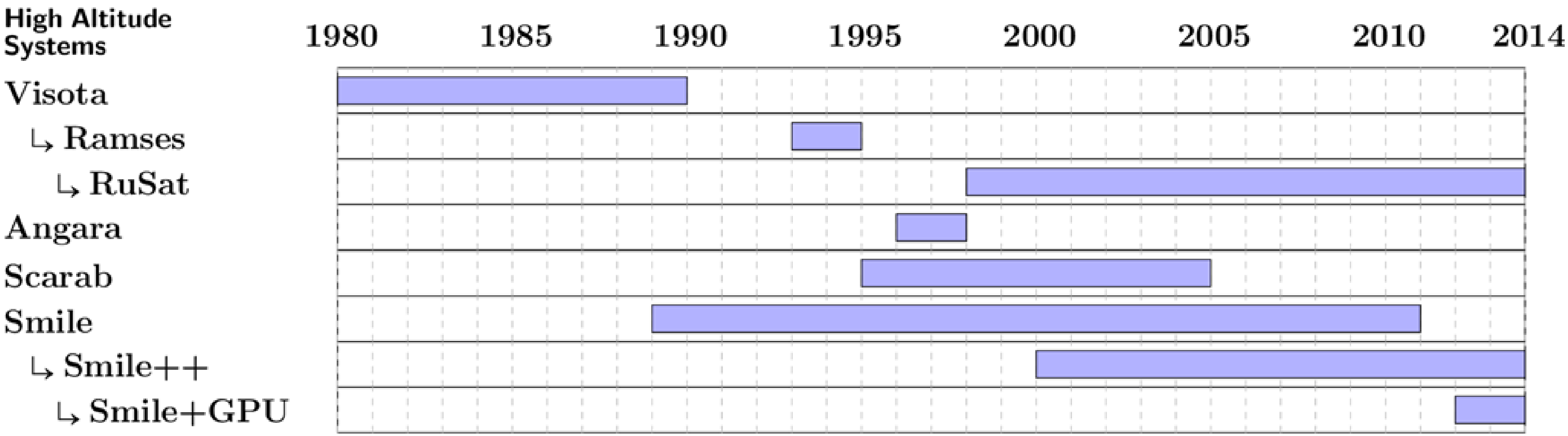
С академиком В.В. Струминским

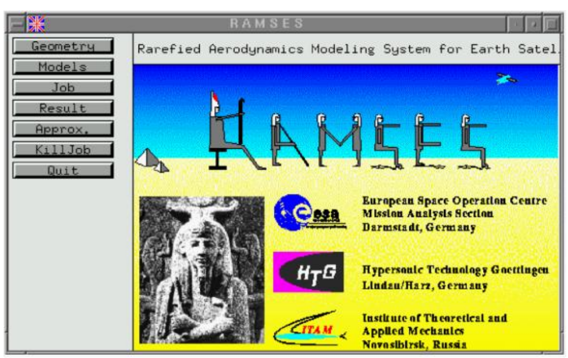


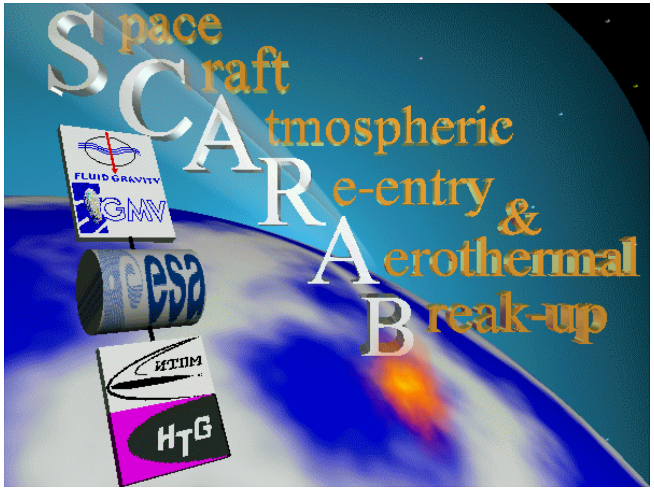
С проф. Г. Бёрдом

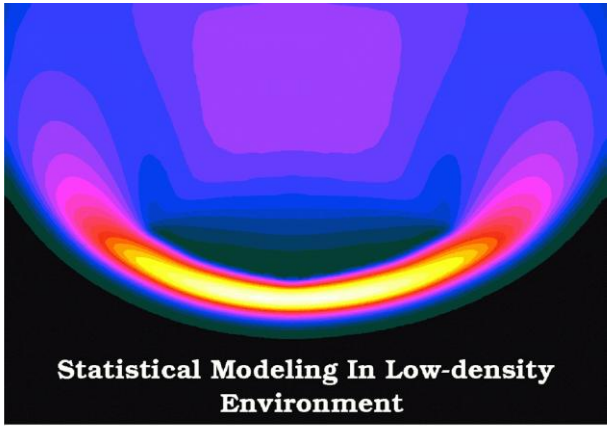
С проф. Х. Хорнунгом

Пакеты программ для решения аэрокосмических задач, разрабатываемые в ИТПМ СО РАН









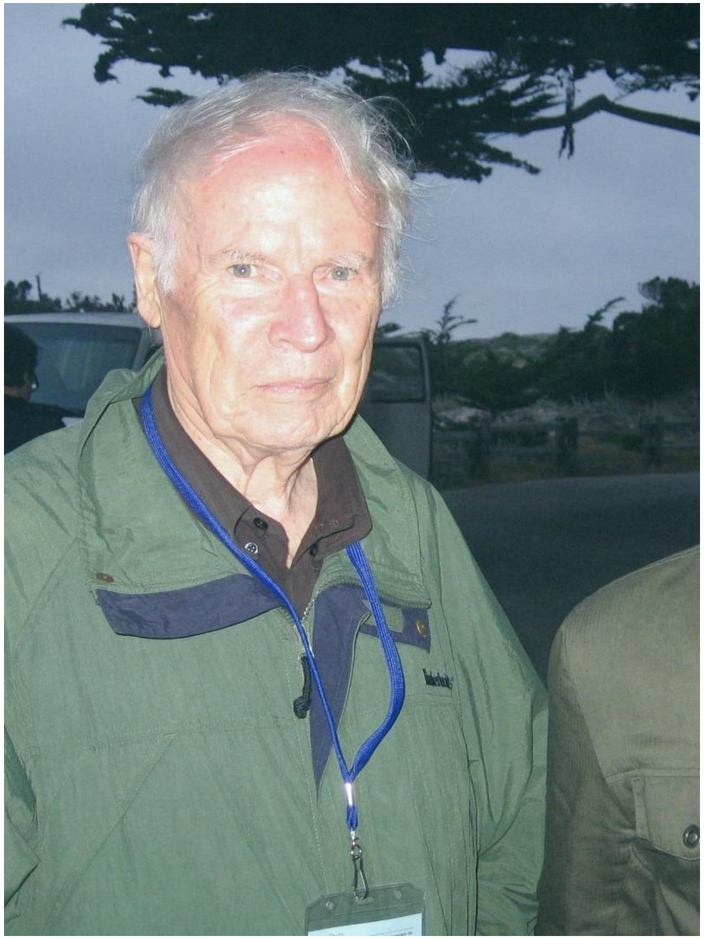
DSMC method

The Direct Simulation Monte Carlo (DSMC) method was introduced by G. A. Bird (1963) and first applied to the problem of translational relaxation in a homogeneous gas.

The method was originally based on physical concepts of rarefied gas and on physical assumptions which form the basis for the phenomenological derivation of the Boltzmann equation.

It has since been extended to multidimensional flows, gas mixtures, flows with internal degrees of freedom, and chemically reacting gas ionized flows. In principle, it can contain all of the physics needed for any problem.

In practice, the technique is computationally intensive compared with its continuum counterparts. However, with appearance of up-to-date parallel computers, this method acquires new areas of application.



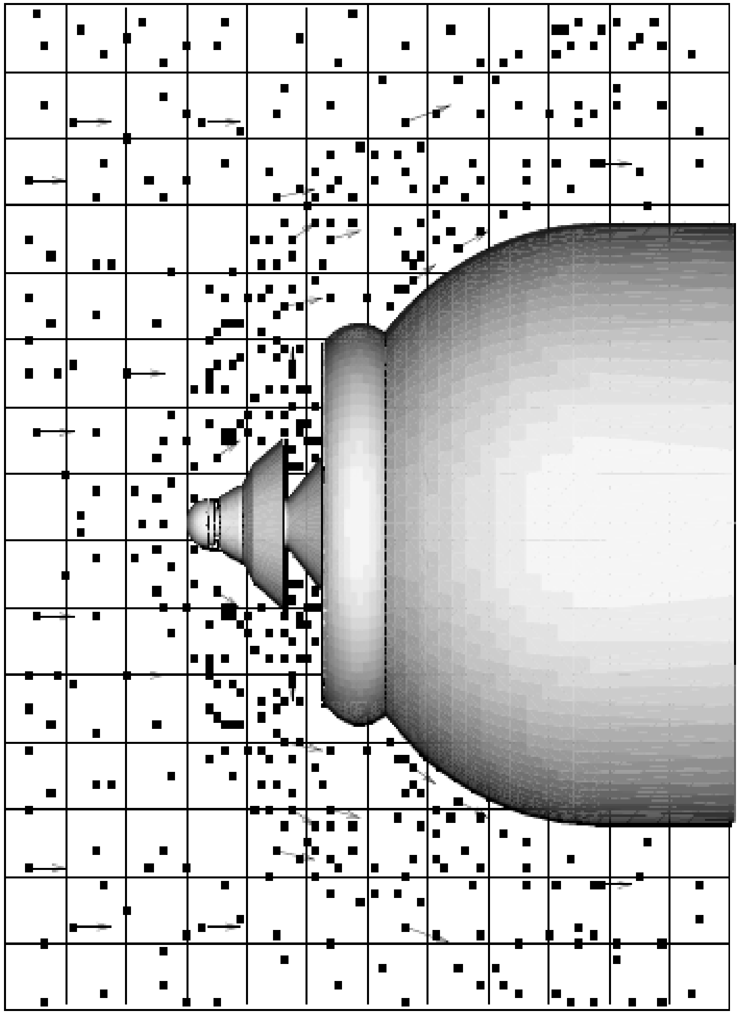
Prof. Graeme Bird

DSMC method

The DSMC method has become de facto the main tool for the study of complex flows of rarefied hypersonic aerothermodynamics.

The conventional treatment of the DSMC method is based on considering the rarefied gas flow as a set of 10^5-10^9 particles (each of them represents a large number of gas molecules) and on the principle of splitting of permanent motion and collisions of gas molecules within a small time step Δt into two consecutive stages:

- free-molecular transfer;
- binary collisions in cells.



Considered as a numerical solution of the system of generalized Boltzmann equations

$$\frac{\partial f_{cij}}{\partial t} + \overline{\xi}\frac{\partial f_{cij}}{\partial \overline{x}} = J_{cij}^{el} + J_{cij}^{\mathrm{int}} + J_{cij}^{reac}$$

DSMC Method

Master **K**inetic **E**quation (MKE)

$$\frac{\partial f_N}{\partial t}+\sum_{i=1}^{N}\mathbf{v}_i\frac{\partial f_N}{\partial \mathbf{r}_i}=\sum_{i<j}\delta(\mathbf{r}_i-\mathbf{r}_j)\int_0^{2\pi}d\varepsilon_{ij}\int_0^{\infty}b_{ij}db_{ij}\,|\mathbf{v}_i-\mathbf{v}_j|\left\{f_N(t,V_{ij}^{'})-f_N(t,V)\right\}$$

Linear MKE for N-particle DF $f_N\,(\mathrm{t},R,V)$ may be transformed into *nonlinear* BE for the one-particle DF $f\,(\mathrm{t},\mathbf{r}_\mathrm{i},\mathbf{v}_\mathrm{i})$ when $\mathrm{N} \Rightarrow \infty$ and molecular chaos holds

Boltzmann **E**quation

$$\frac{\partial f}{\partial t}+\mathbf{v}_i\frac{\partial f_N}{\partial \mathbf{r}_i}=\int_0^{2\pi}d\varepsilon_{ij}\int_0^{\infty}b_{ij}db_{ij}\int_0^{\infty}|\mathbf{v}_i-\mathbf{v}_j|\left\{f_N(t,\mathbf{v}_i^{'})f_N(t,\mathbf{v}_j^{'})-f_N(t,\mathbf{v}_i)f_N(t,\mathbf{v}_j)\right\}d\mathbf{v}_j$$

- Many researchers applied mathematical approach to development of DSMC numerical schemes (**Belotserkovsky, Yanitsky, Deshpande, Kondurin, Hisamutdinov, Nanbu, Koura,…**)
- DSMC uses a finite number of simulated particles, which prompted **M. Ivanov and S. Rogasinsky** to construct DSMC schemes directly from MKE
- They also showed that one can use DSMC without splitting free molecular motion and collisions
- Starting from MKE also allows assessment of statistical errors and also provides connection between the N-particle gas model and the solution of BE
- ***Majorant Collision Frequency Schemes*** are mathematically strictly derived from the MKE, in contrast to traditional phenomenological DSMC schemes.

SMILE Software System

- To solve basic and applied problems of high-altitude spacecraft aerothermodynamics, a software system Statistical Modeling In Low-density Environment (SMILE) was developed at ITAM SB RAS.
- The objective of SMILE software system was – and still is, to provide scientists and engineers with a modern, easy to use implementation of efficient and accurate numerical schemes of the DSMC method that can be applied to a wide range of challenging high-altitude aerodynamic problems in 2D, axisymmetric, and 3D

SMILE uses the modern theory of DSMC and features innovative developments in numerical algorithms and physical models

SMILE is a multi-purpose tool used for simulations ranging from spacecraft/space station aerodynamics to microscale flows

SMILE is a monolithic self-consistent system for DSMC computations, designed to be easily used even by a person not familiar with DSMC

РОССИЙСКАЯ ФЕДЕРАЦИЯ

СВИДЕТЕЛЬСТВО

о государственной регистрации программы для ЭВМ

№ 2008611184

Программный комплекс SMILE «Statistical Modeling in Low-Density Environment» (статистическое моделирование в средах с низкой плотностью)

Правообладатель(ли): *Государственное учреждение «Институт теоретической и прикладной механики имени С.А. Христиановича Сибирского отделения Российской академии наук» (ИТПМ СО РАН) (RU)*

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Заявка № 2008610035

Дата поступления 9 января 2008 г.

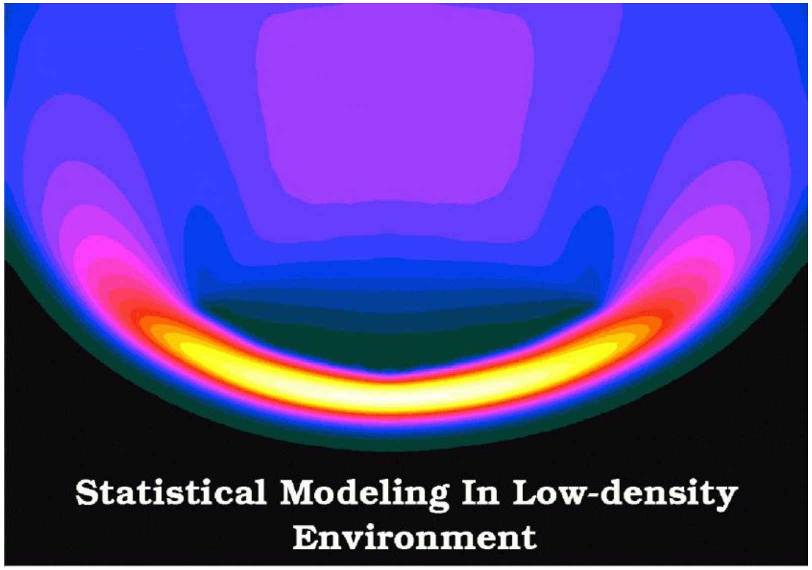
Зарегистрировано в Реестре программ для ЭВМ

6 марта 2008 г.

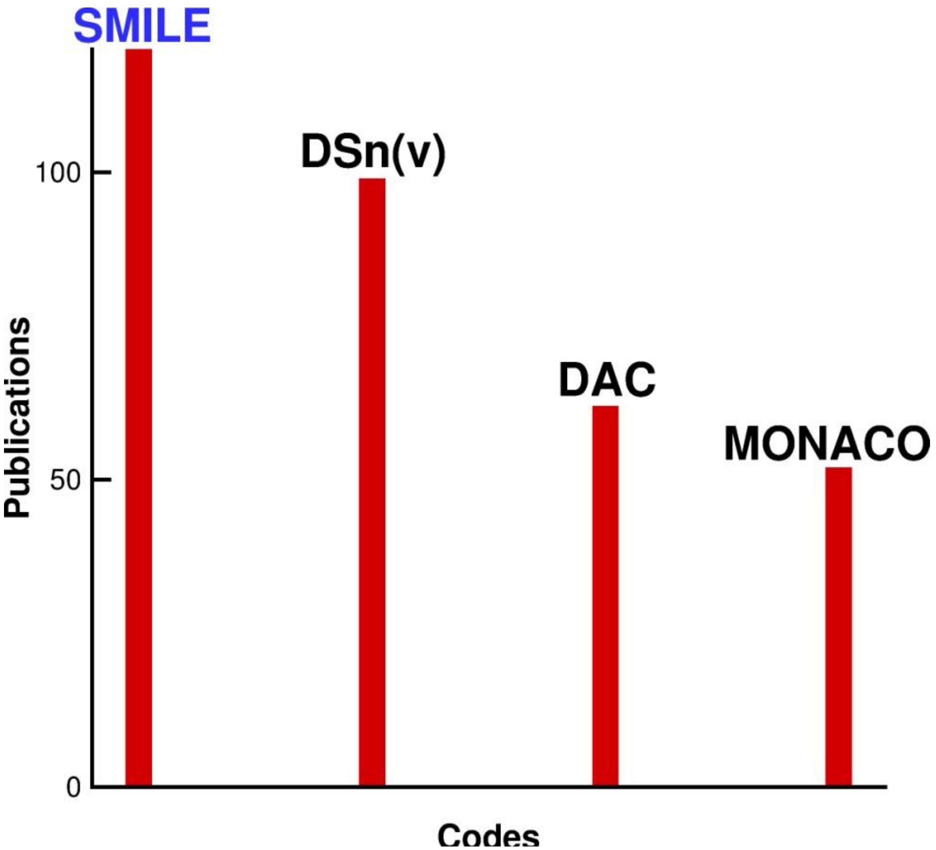
Руководитель Федеральной службы по интеллектуальной собственности, патентам и товарным знакам

Б.П. Симонов

SMILE Software System



Number of publications for most popular DSMC codes since 2010



Installed and used at

- RSC «Energia» (Russia)
- Makeyev (Russia)
- MIPT (Russia)
- KARI (Korea)
- PSU (USA)
- ESTEC (The Netherlands)
- VKI (Belgium)

and other space institutions and universities

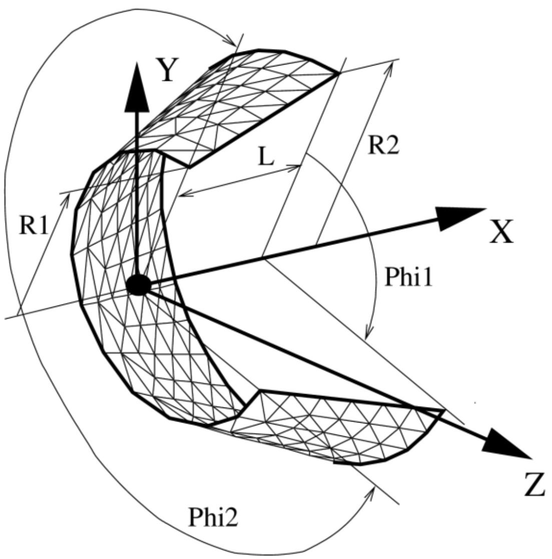
SMILE Subsystems

SMILE is split into several systems to simplify user interface

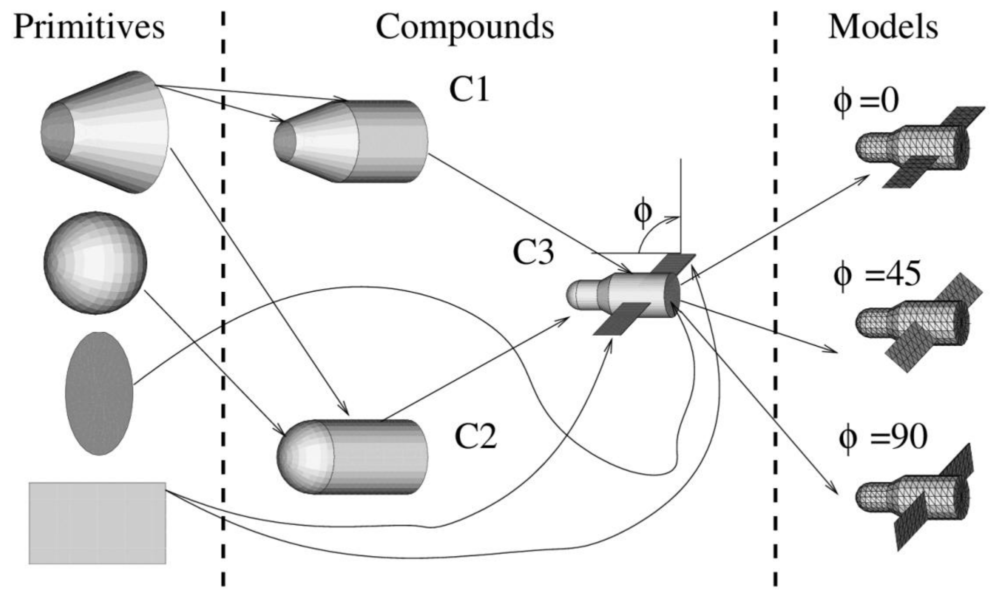
- **3D Geometry modeling system**
  - Contains a set of predefined geometry primitives (cylinder, sphere, cone, etc.)
  - Combines primitives into one compound object
  - Generates complex 3D geometry models from primitives and compounds (MIR station, ISS)
  - Has CAD Interface: STL import capability
- **Interactive GUI pre-processing system** (sets-up new computations)
  - Subsystems to define, manipulate, and store the geometry
  - Advisor which gives recommended values of DSMC method parameters
  - Elements (atoms and molecules) and collision properties (includes reactions)
  - Saves current computation and imports previous computations
  - Interface to couple Navier-Stokes and DSMC computations
  - Online help support
- **Interactive GUI post-processing system** (processes computation results)
  - Internal visualization tools for 3D and 2D plots
  - Visualization of surface properties and flow fields
  - Output for Tecplot and VTK
  - Online help support
- **High-performance computation subsystem** (DSMC computation core)
  - 2D/AS/3D, single / multiprocessor
  - Runs on a variety of CPUs (both 32-bit and 64-bit families)
  - Runs on remote clusters

Geometry Modeling Subsystem

- Element-by-element description
- Parametrized model, such as rotation of solar arrays)

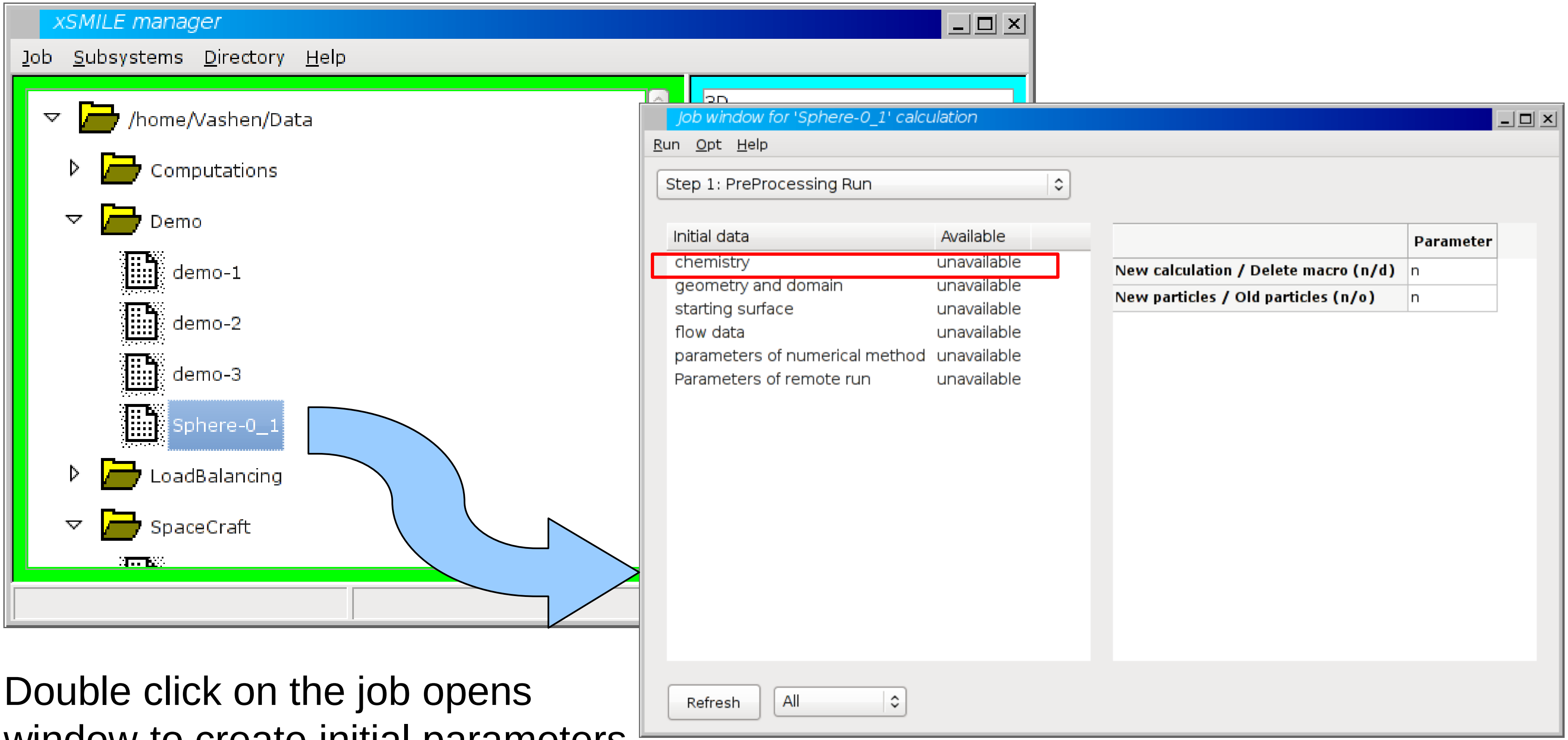


Primitive ***Cone***



Hierarchy of modeling

Pre-processing Subsystem Window



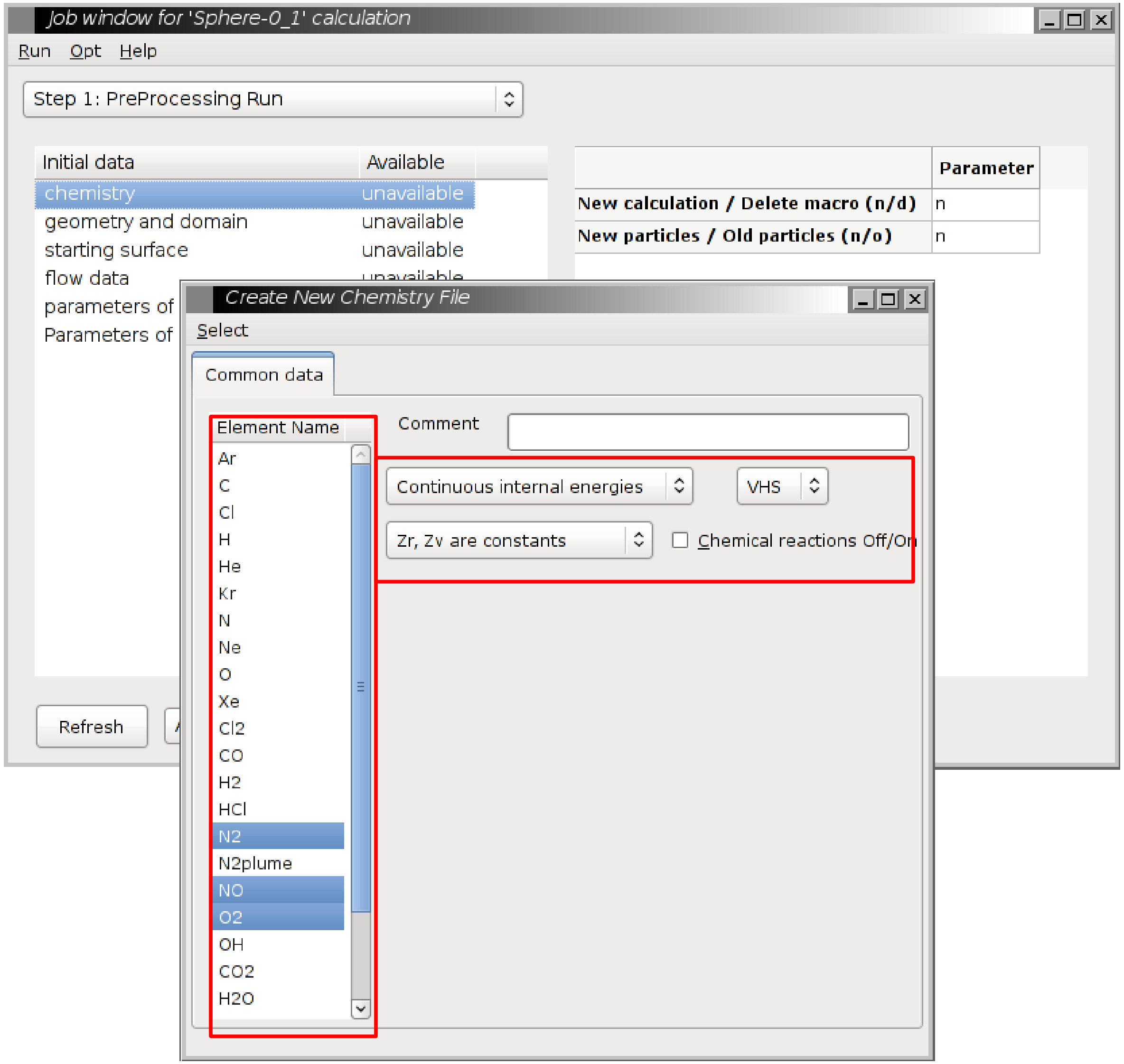
Double click on the job opens window to create initial parameters

Chemistry Window

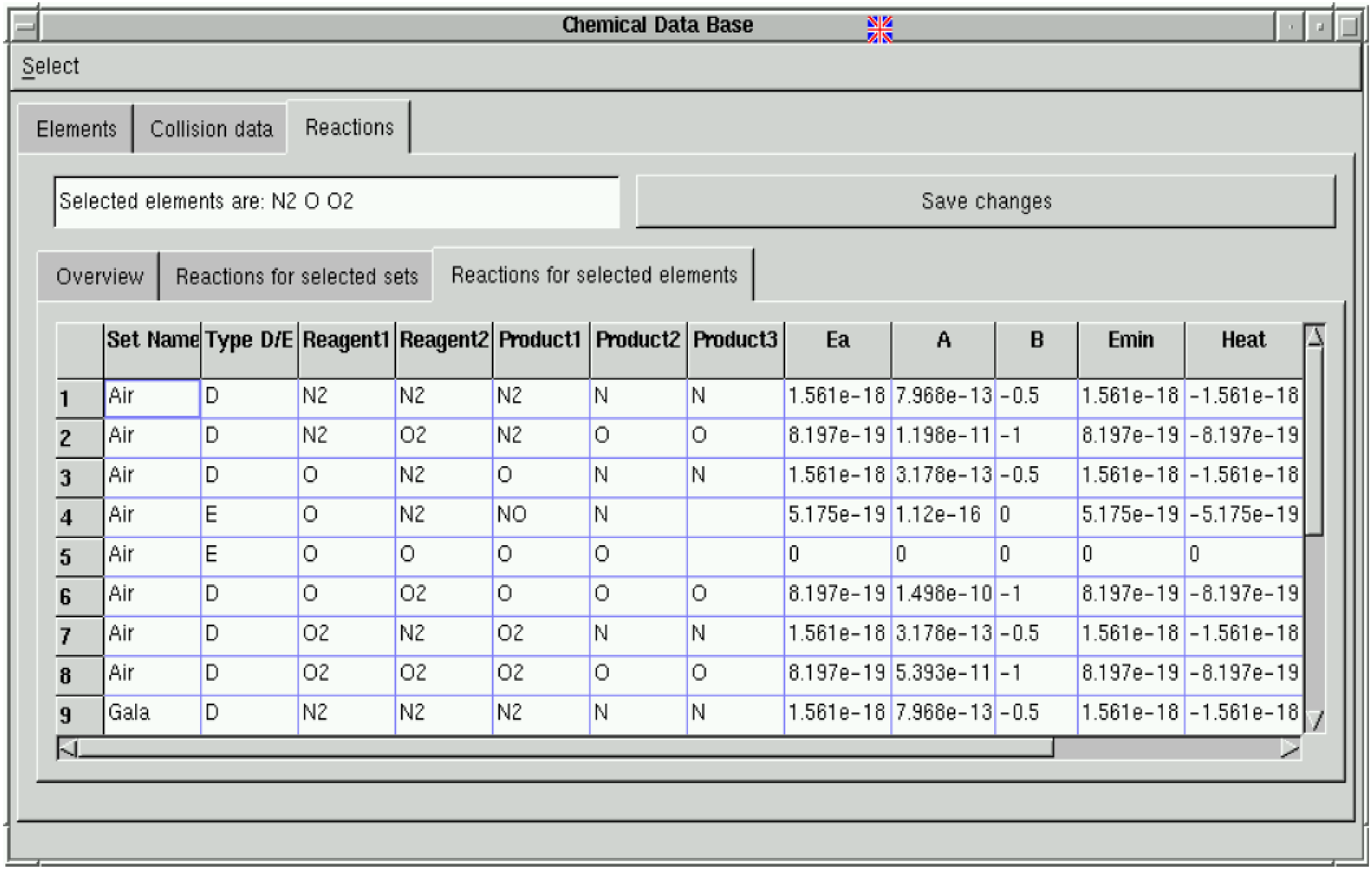
Species, collision models and chemical reaction sets are selected here.

Molecural properties and chemical reactions sets are stored in Chemistry database.

This database can be expanded by experts.

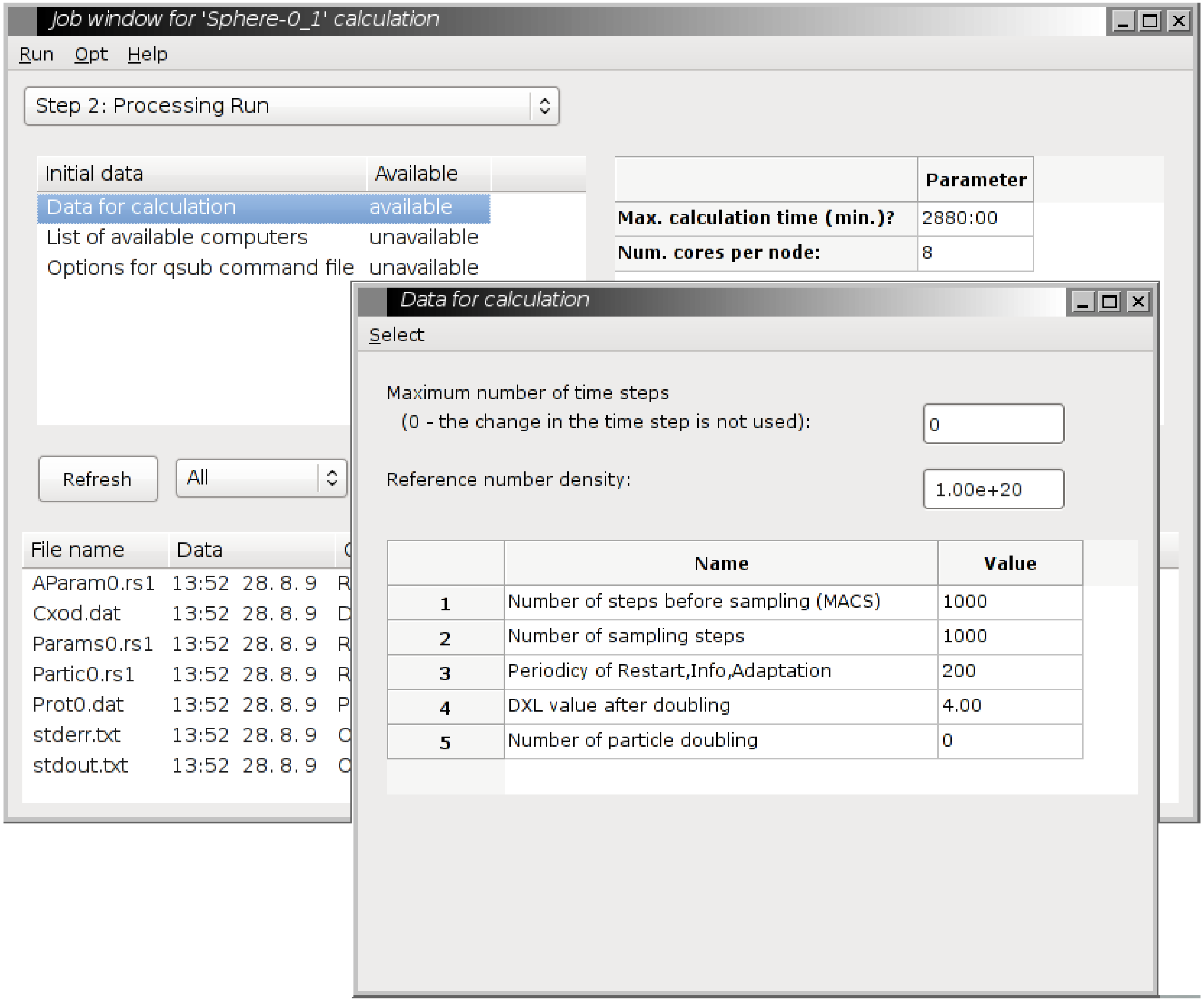


Chemical Data Base

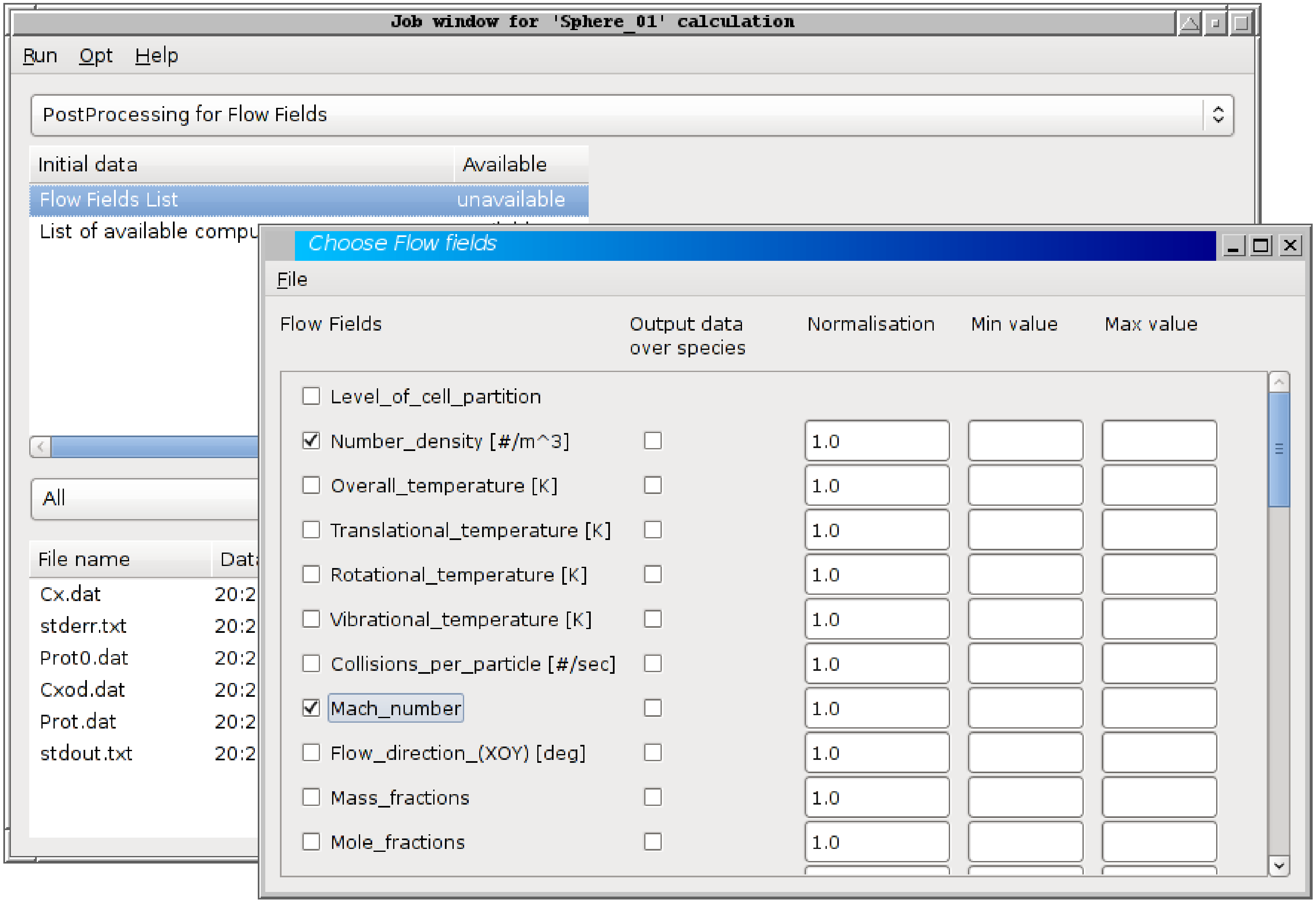


	Set Name	Type D/E	Reagent1	Reagent2	Product1	Product2	Product3	Ea	A	B	Emin	Heat
1	Air	D	N2	N2	N2	N	N	1.561e-18	7.968e-13	-0.5	1.561e-18	-1.561e-18
2	Air	D	N2	O2	N2	O	O	8.197e-19	1.198e-11	-1	8.197e-19	-8.197e-19
3	Air	D	O	N2	O	N	N	1.561e-18	3.178e-13	-0.5	1.561e-18	-1.561e-18
4	Air	E	O	N2	NO	N		5.175e-19	1.12e-16	0	5.175e-19	-5.175e-19
5	Air	E	O	O	O	O		0	0	0	0	0
6	Air	D	O	O2	O	O	O	8.197e-19	1.498e-10	-1	8.197e-19	-8.197e-19
7	Air	D	O2	N2	O2	N	N	1.561e-18	3.178e-13	-0.5	1.561e-18	-1.561e-18
8	Air	D	O2	O2	O2	O	O	8.197e-19	5.393e-11	-1	8.197e-19	-8.197e-19
9	Gala	D	N2	N2	N2	N	N	1.561e-18	7.968e-13	-0.5	1.561e-18	-1.561e-18

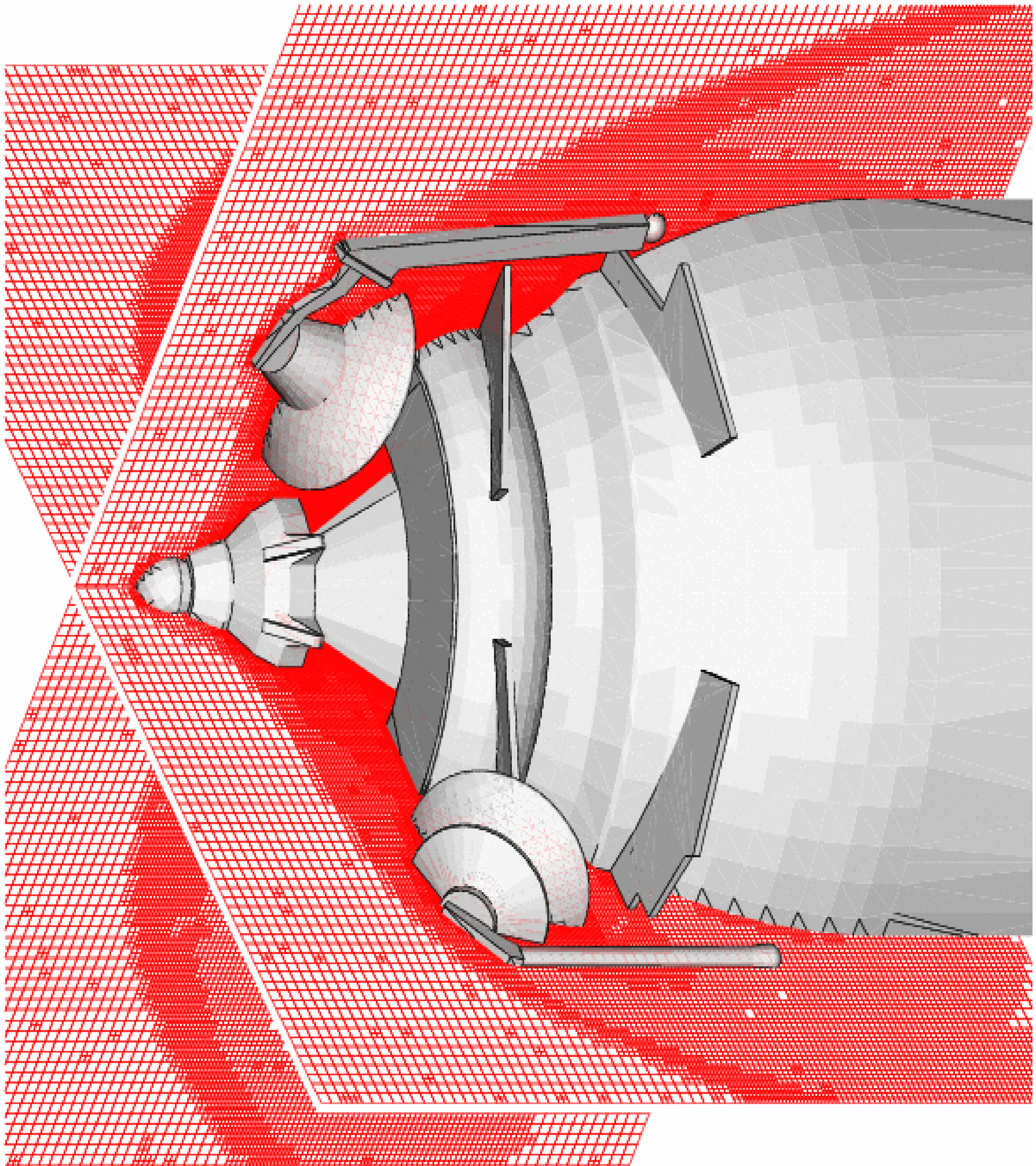
Processing Subsystem Window



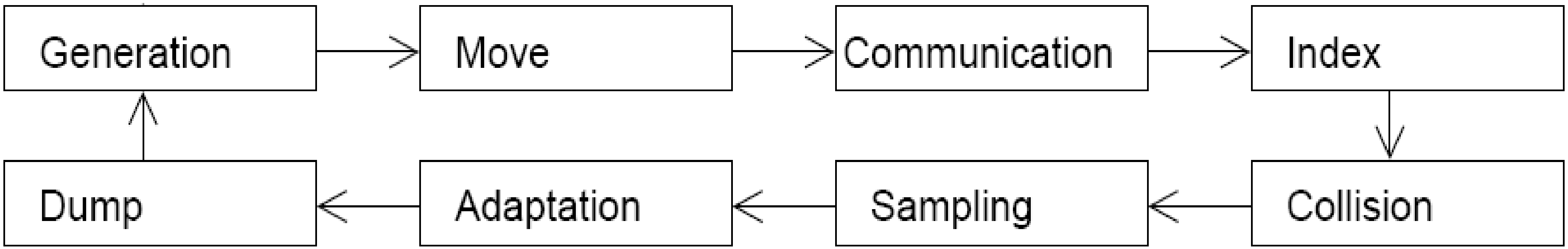
Post-processing Subsystem Window



Adaptive rectangular mesh

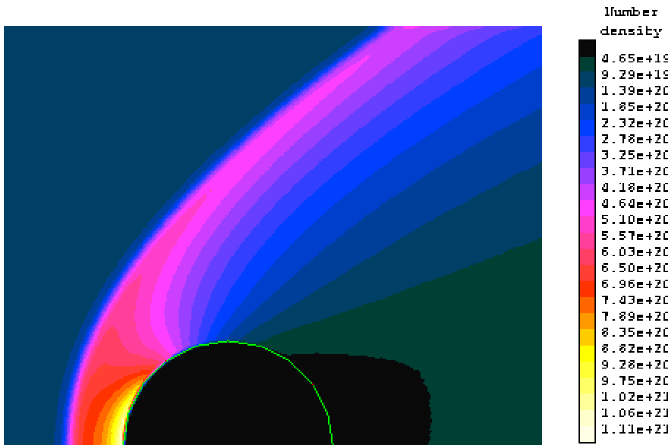


Structure of the DSMC Computation

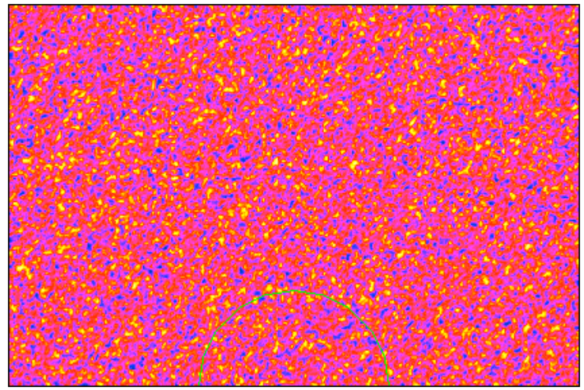


Generation: initialize new model particles on the domain boundaries (Flow) or on the starting surface (Jet)
Move: move all particles (including interaction with the geometry model and deleting molecules leaving the domain)
Communication: exchange particles between computational nodes in multiprocessor computations
Index: localization of particles in cells (determination which particles belong to a given cell)
Collision: collide particles in each cell (including elastic collisions and various inelastic processes)
Sampling : collect statistical information on molecular properties over cells and geometry surface panels
Adaptation : adapt cells according to the local mean free path
Dump : write computational data (particles, cell, etc.) and sampled properties to back-up files

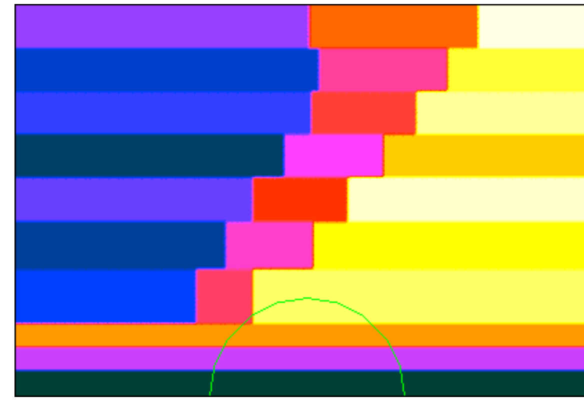
Примеры декомпозиции расчётной области при работе различных алгоритмов



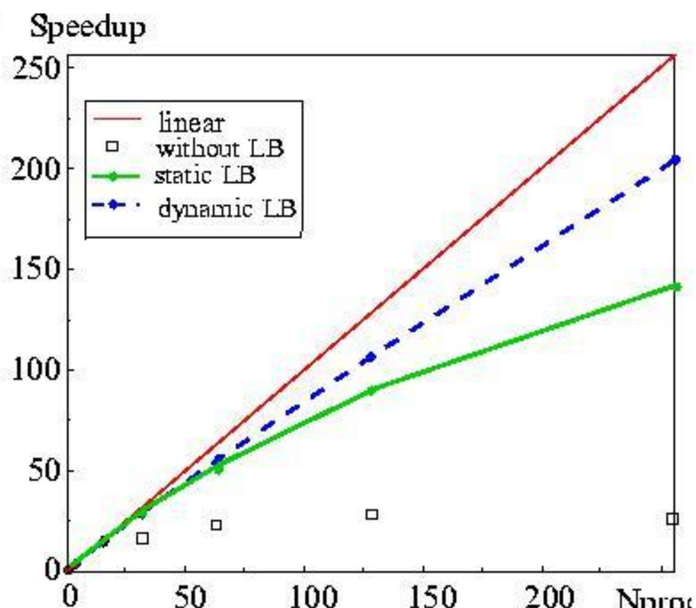
Числовая плотность

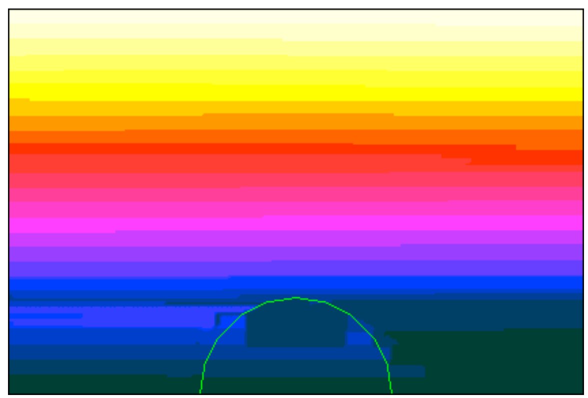


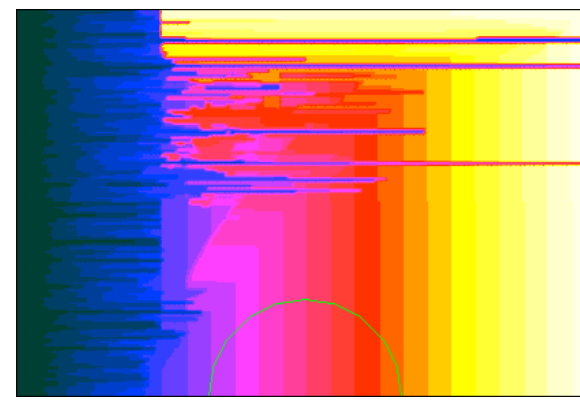
Вероятностный



Деление на равные части





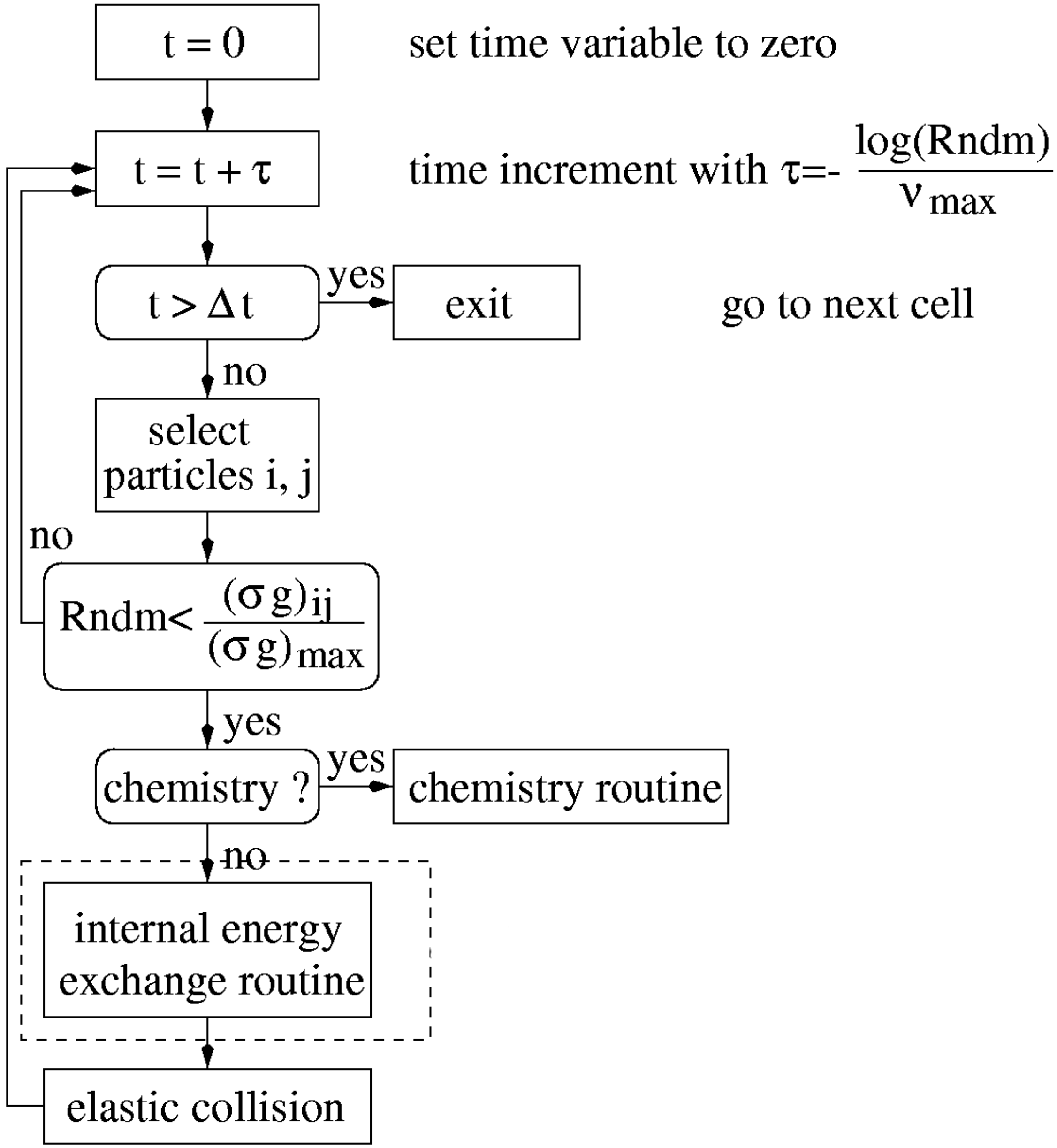


Алгоритм с подвижными границами

Начальное разбиение вдоль потока

Начальное разбиение поперёк потока

MFS DSMC collision algorithm



Столкновительные модели физико-химических процессов для ПСМ

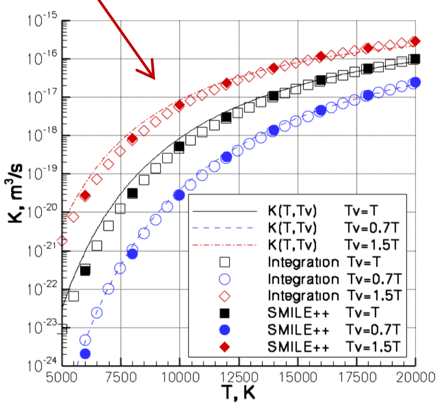
Система обобщенных уравнений Больцмана:

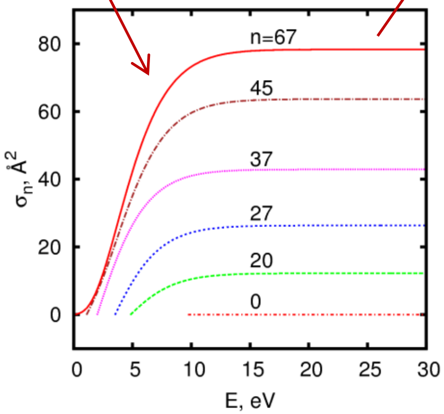
$$\frac{\partial f_{cij}}{\partial t} + \bar{\xi}\frac{\partial f_{cij}}{\partial \bar{x}} = J_{cij}^{el} + J_{cij}^{\text{int}} + J_{cij}^{reac}$$

Столкновительный алгоритм метода ПСМ

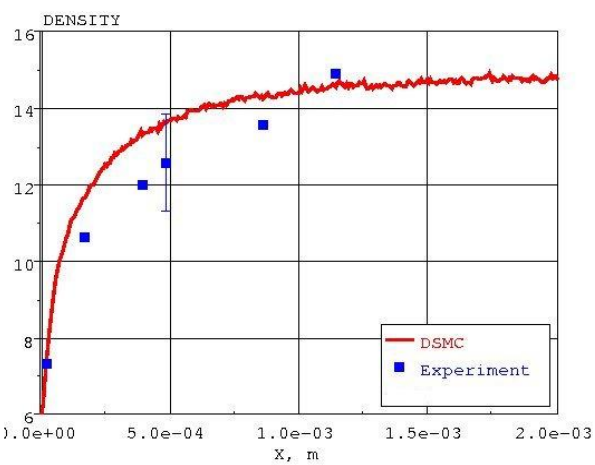
Двухтемпературная константа диссоциации:

$$K(T,T_v) = \frac{C(T)}{Q(T_v)}\sum_{n=0}^{N_{\max}}\exp\left(-\frac{E_v(n)}{kT_v}\right)\int_{E_d-E_n}^{\infty}\sigma_n(E)\left(\frac{E}{kT}\right)^{\frac{\xi_r}{2}+1}\exp\left(-\frac{E}{kT}\right)dE$$



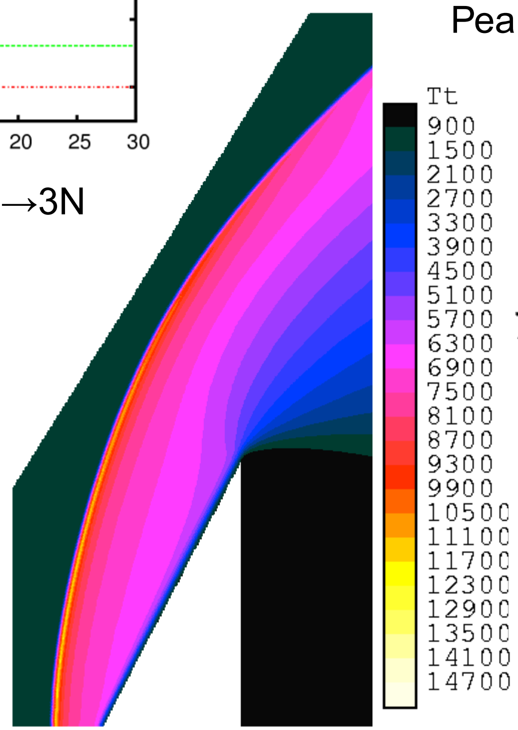


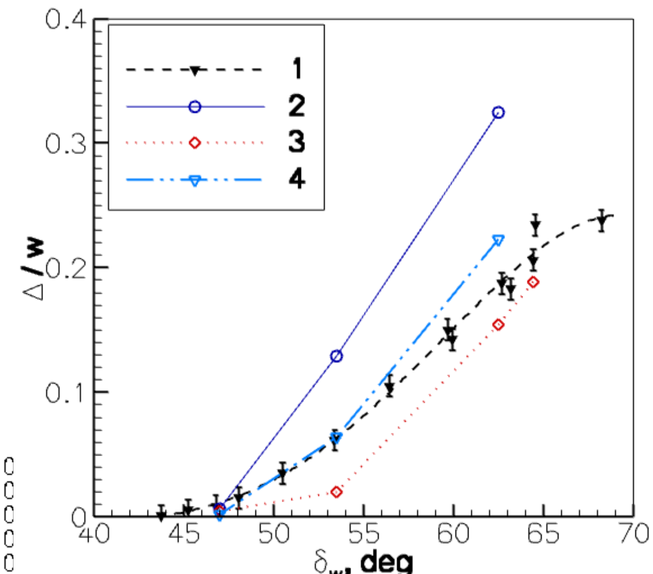
Константа и сечения реакции N2+N→3N



Структура ударной волны в азоте M=21

Реагирующее течение азота около клина



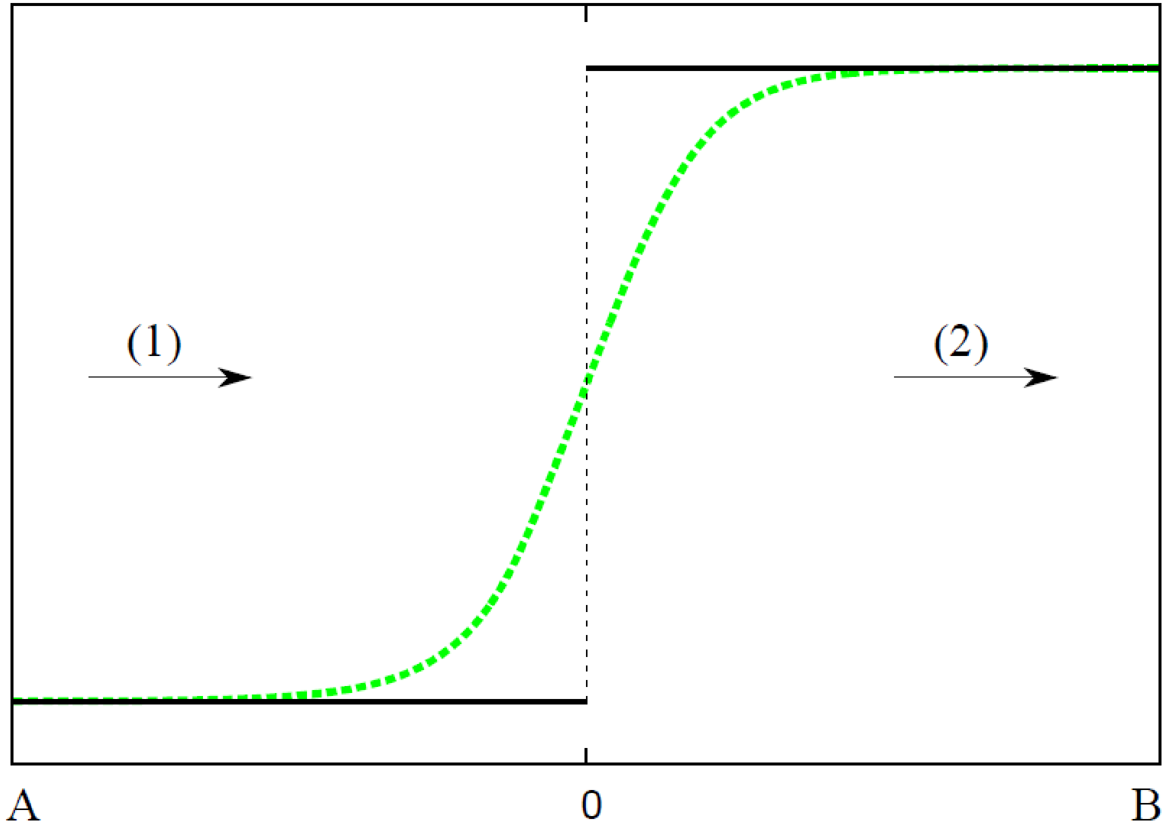


1 – эксперимент,

2 – нерегирующий газ,

3 – TCE, **4** – KSS

Shock wave structure: formulation of the problem



$$Kn = \frac{\lambda}{\delta} \sim 0.1$$

Boundary conditions at the upstream and downstream boundaries:

Maxwell distribution of incoming molecules, Rankine-Hugoniot relations

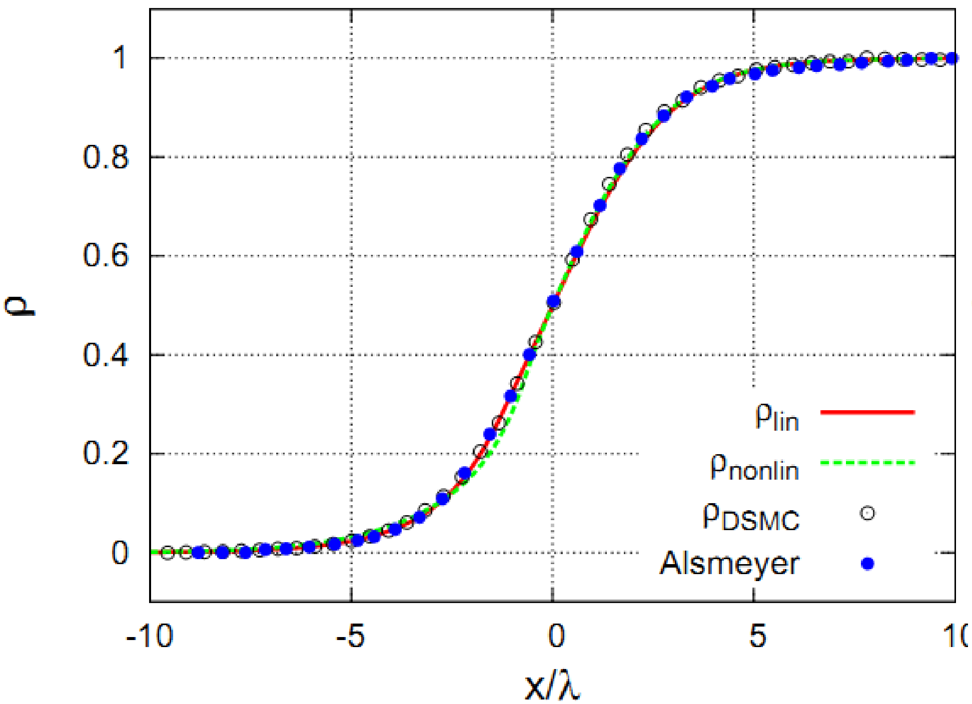
Density profile: initial conditions (black line) and DSMC solution (green line)

Parameters of the problem in case of monatomic gas:

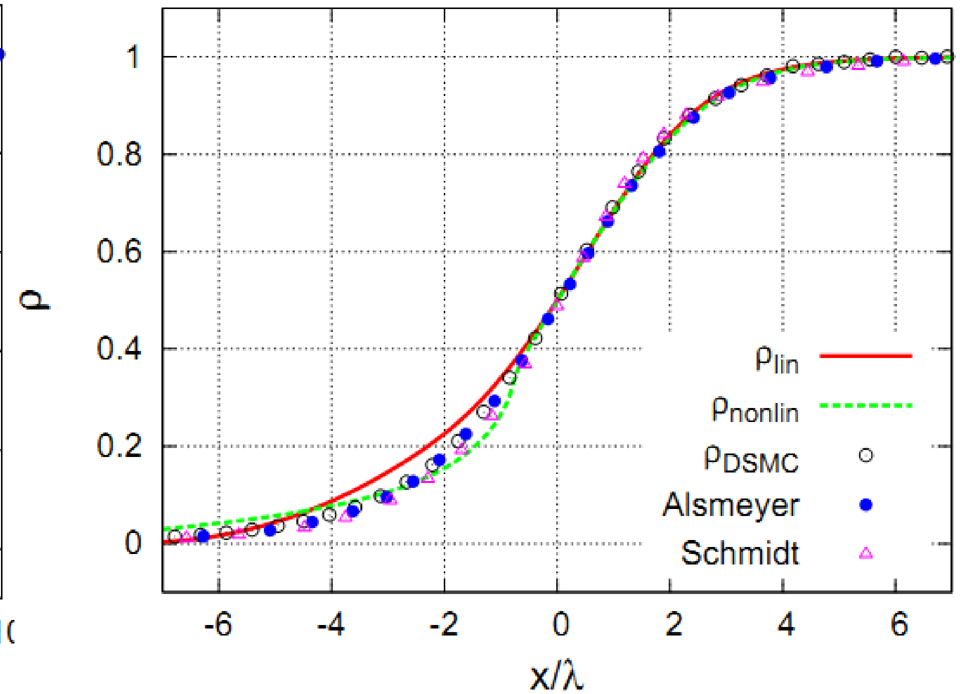
• Mach number of the shock

• Molecular interaction law (hard spheres, Maxwell molecules, VHS/VSS, inverse power law potential, Lennard-Jones ….).

Shock Wave Structure in Argon

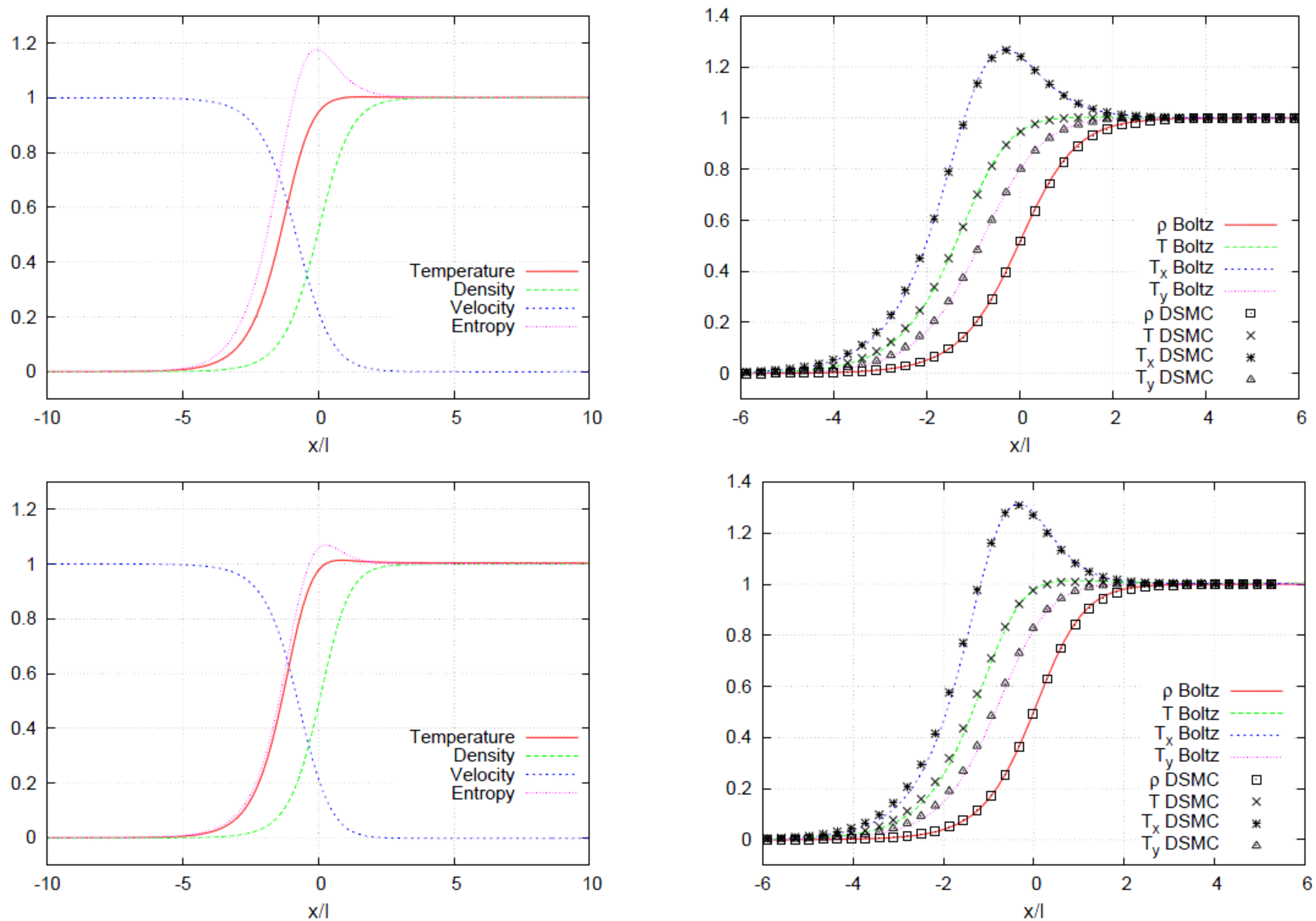


Density for M=2.05



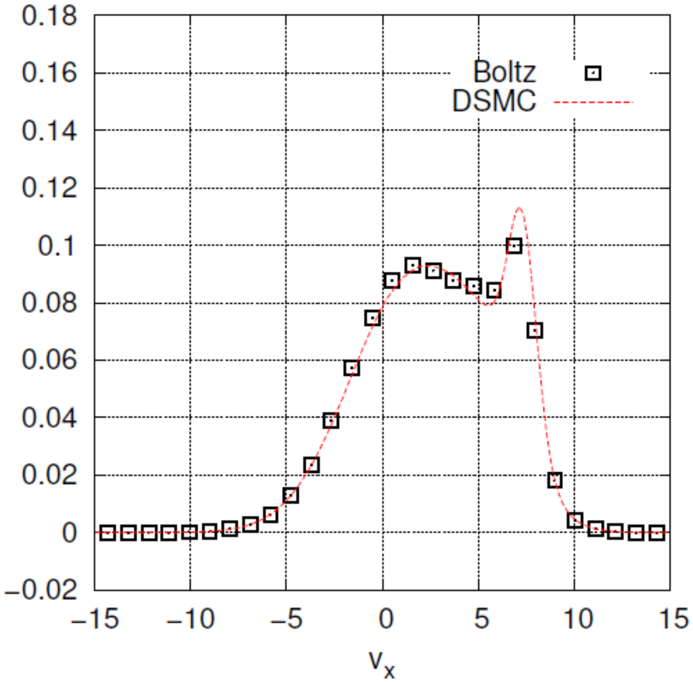
Density for M=8.0

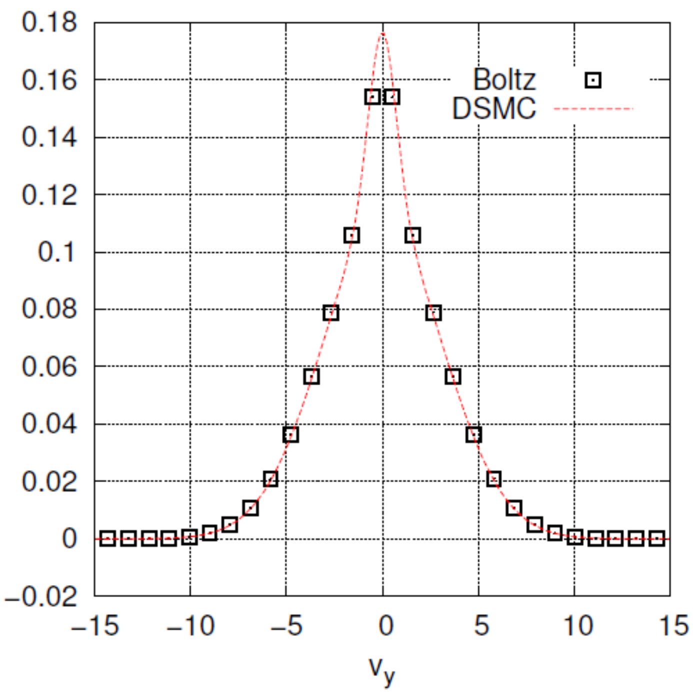
Shock wave structure

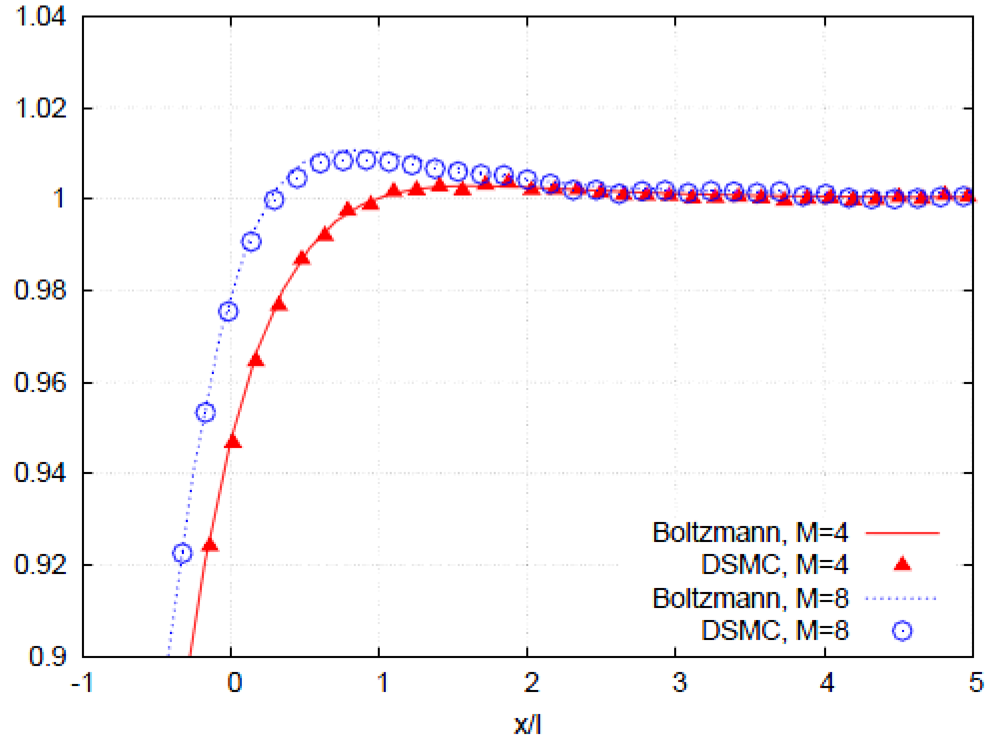


Comparison of the profiles of temperature components obtained on the basis of the deterministic solution of the Boltzmann equation and by the DSMC method, M=4 (top) and M=8 (bottom).

The fine structure of the shock wave

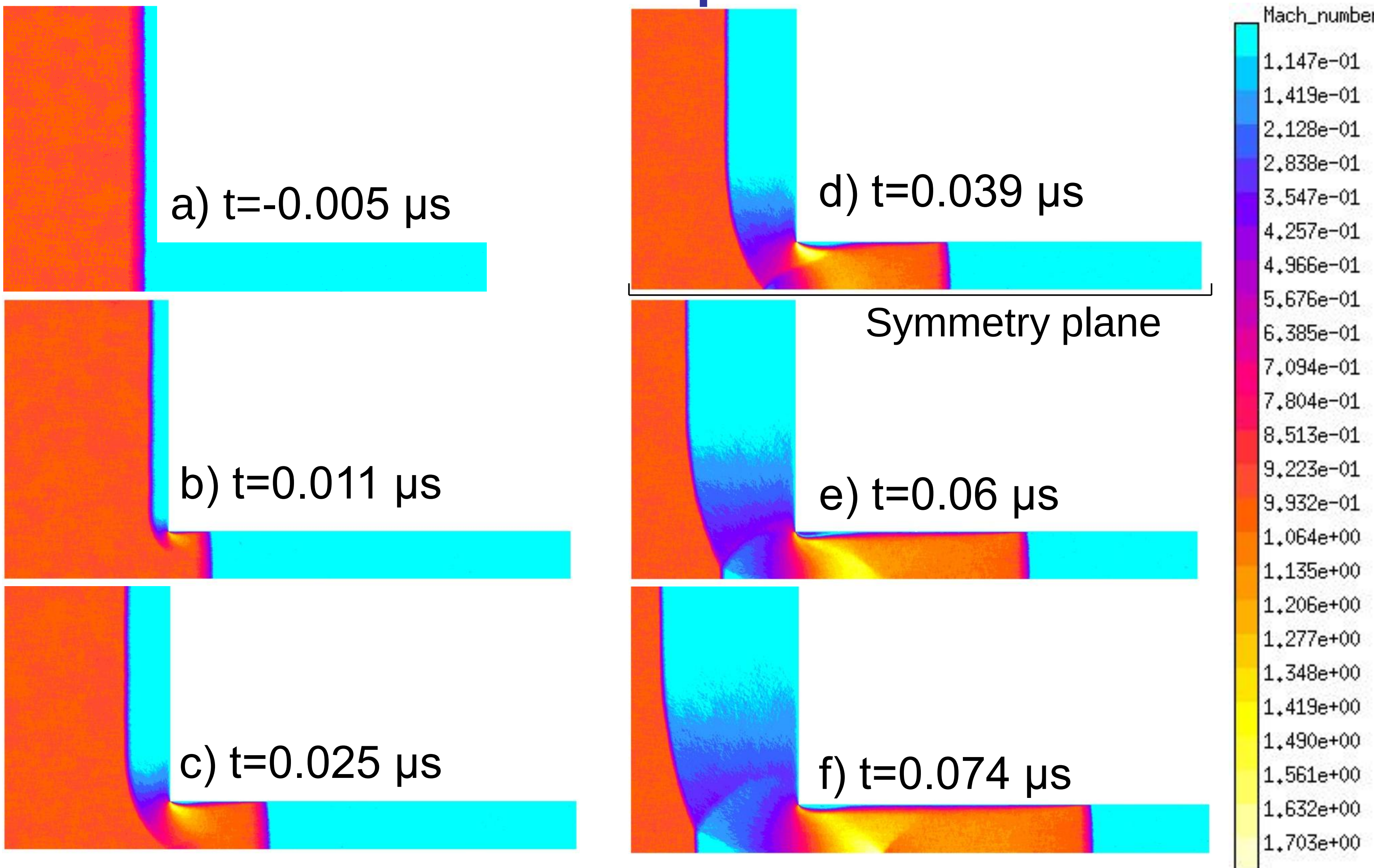






Velocity distribution function inside the shock (M=8) and temperature profiles in the vicinity of temperature overshoot

Mach number flow fields at different times DSMC computations

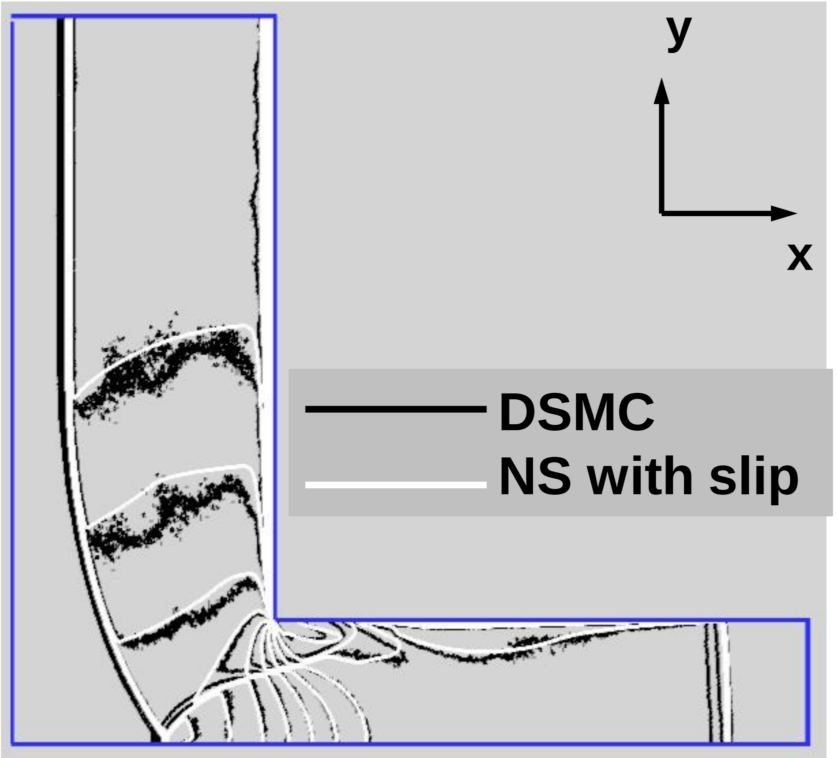


Initial parameters: M_{is}=2.03, γ=1.4, P_0=1 atm, T_0=293 K, Kn=8.2×10^{-3}

P_0, T_0 - the quiescent gas pressure and temperature.

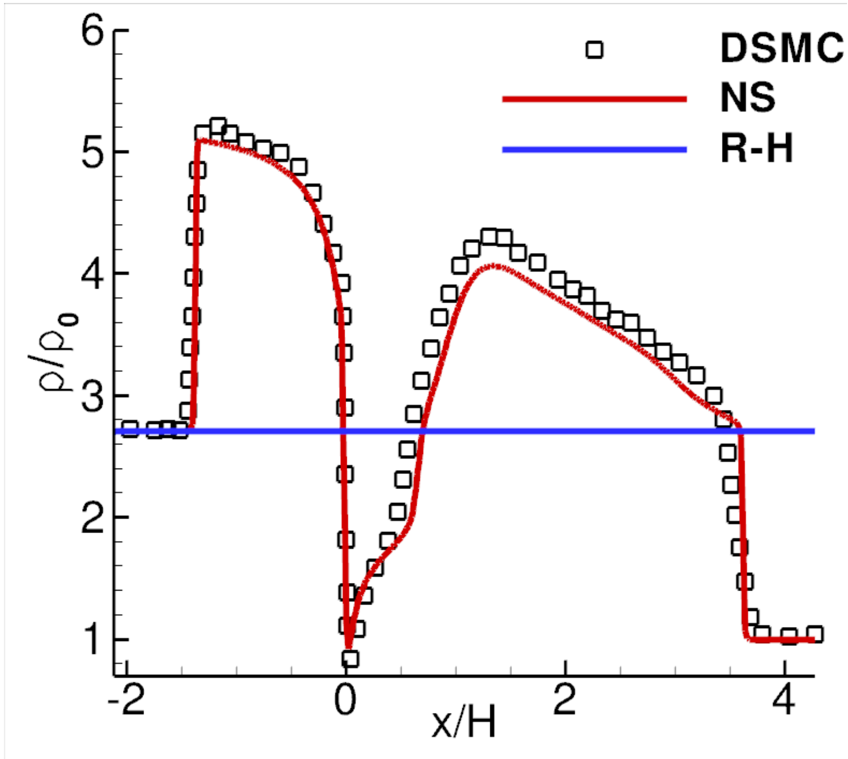
t=0 corresponds to the instant when the incident shock wave enters the microchannel.

Comparison of NS and DSMC computations



Symmetry plane

Density contours



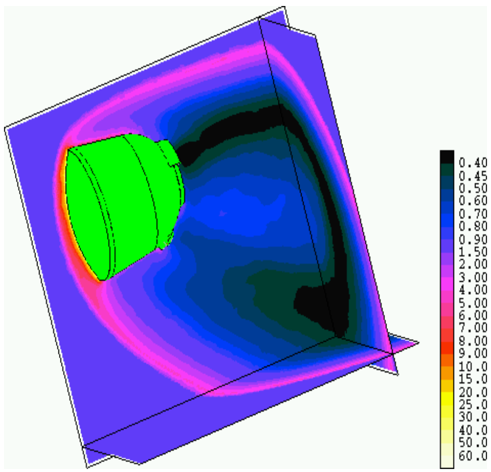
Density distribution near the upper wall of the microchannel

Initial parameters: M_{is}=2.03, γ=1.4, P_0=1 atm, T_0=293 K, Kn=8.2×10^{-3}

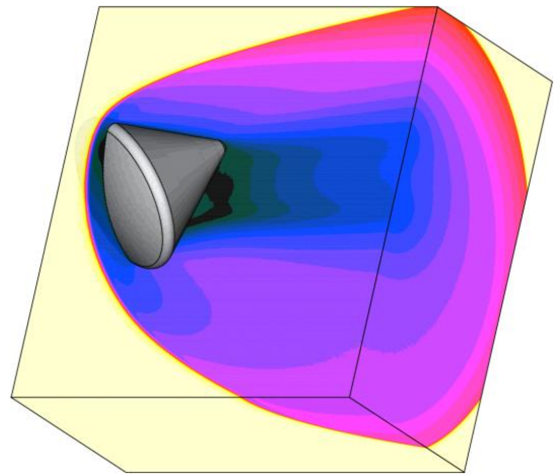
P_0, T_0 - the quiescent gas pressure and temperature.

t=0 corresponds to the instant when the incident shock wave enters the microchannel.

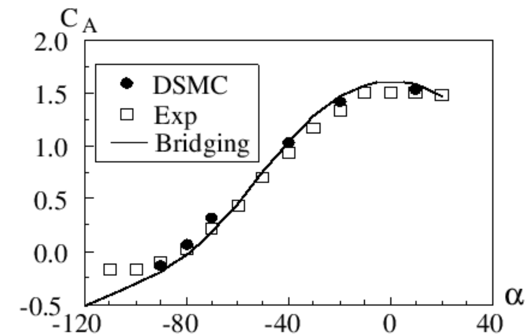
Examples: Re-entry Aerodynamics

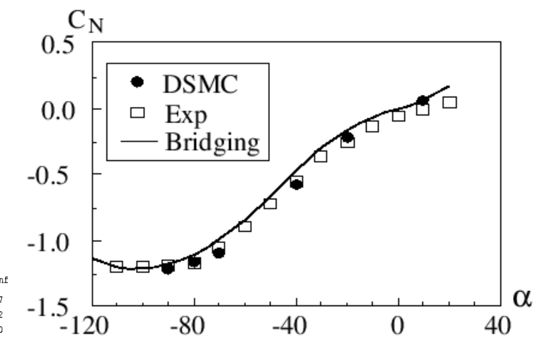


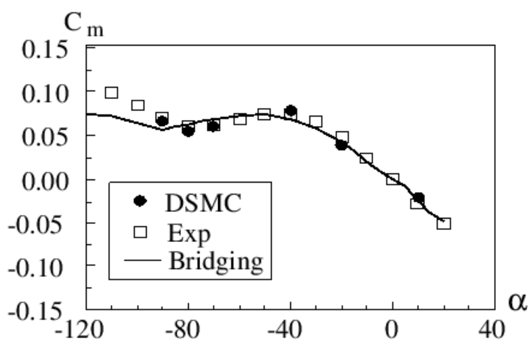
Soyuz

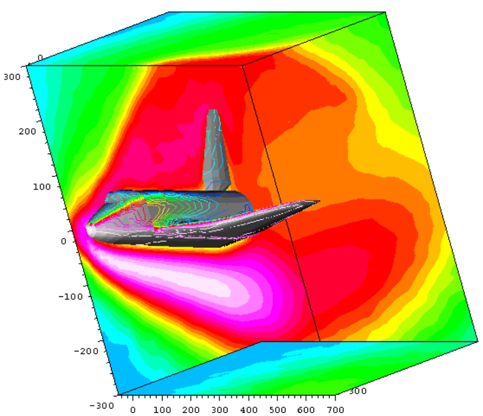


Apollo

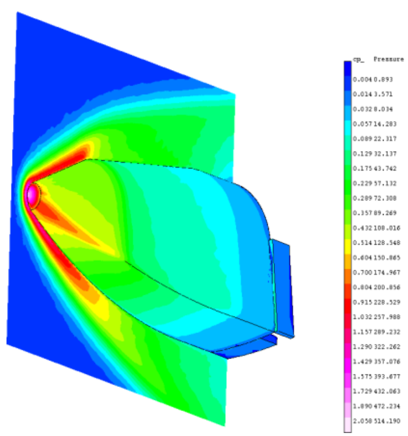




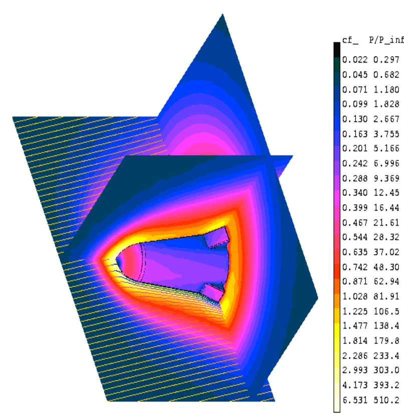




Buran

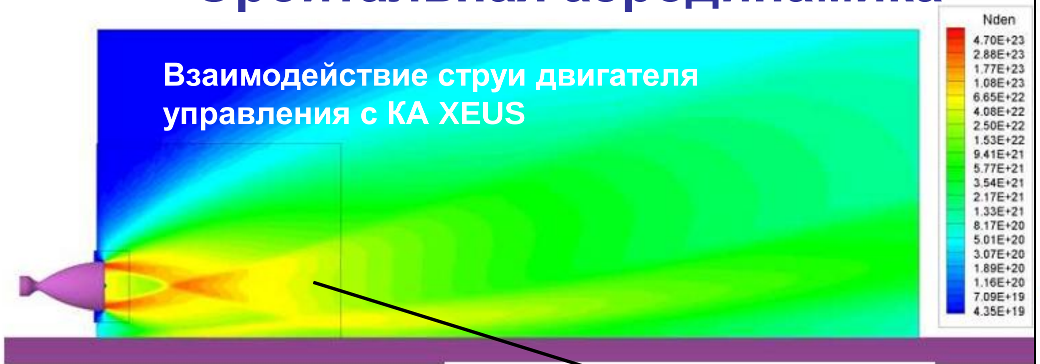


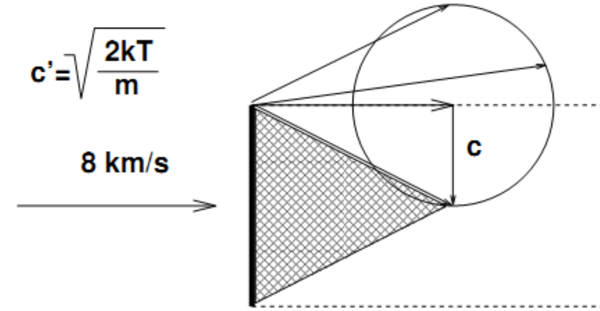
Clipper



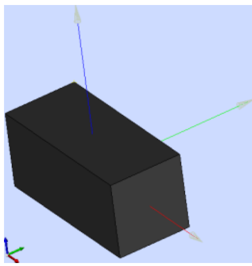
Kheops

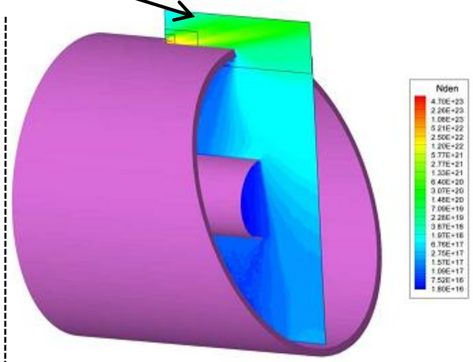
Орбитальная аэродинамика



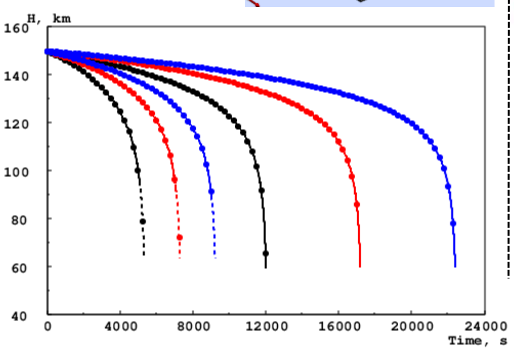


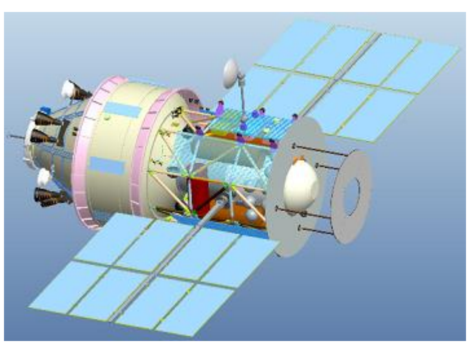
Спутник
QubeSat



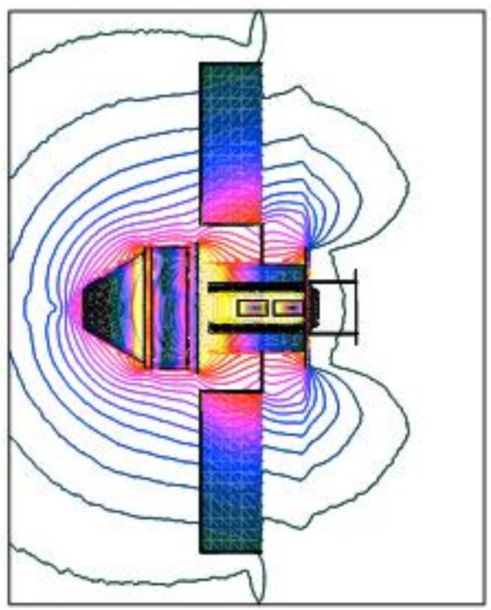


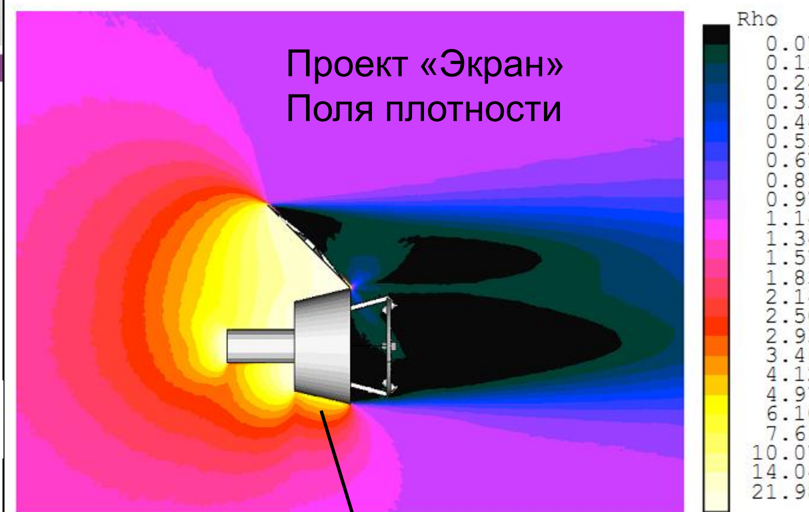
Траектории

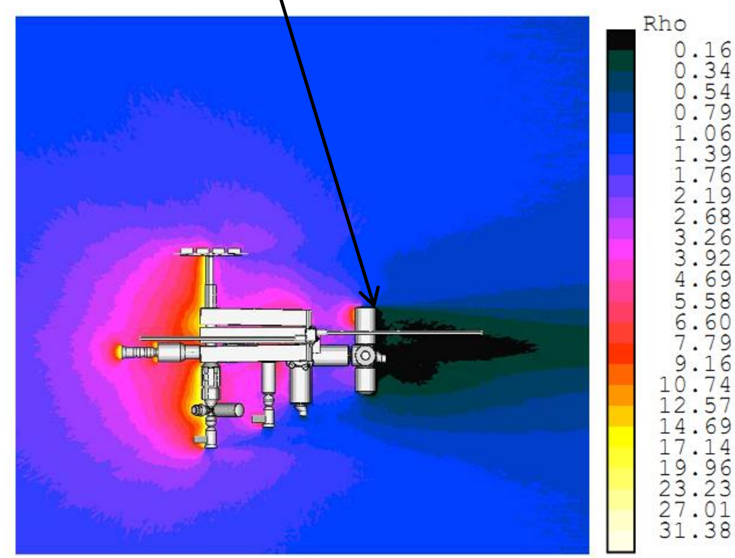




КА «Ока-Т». Поле плотности

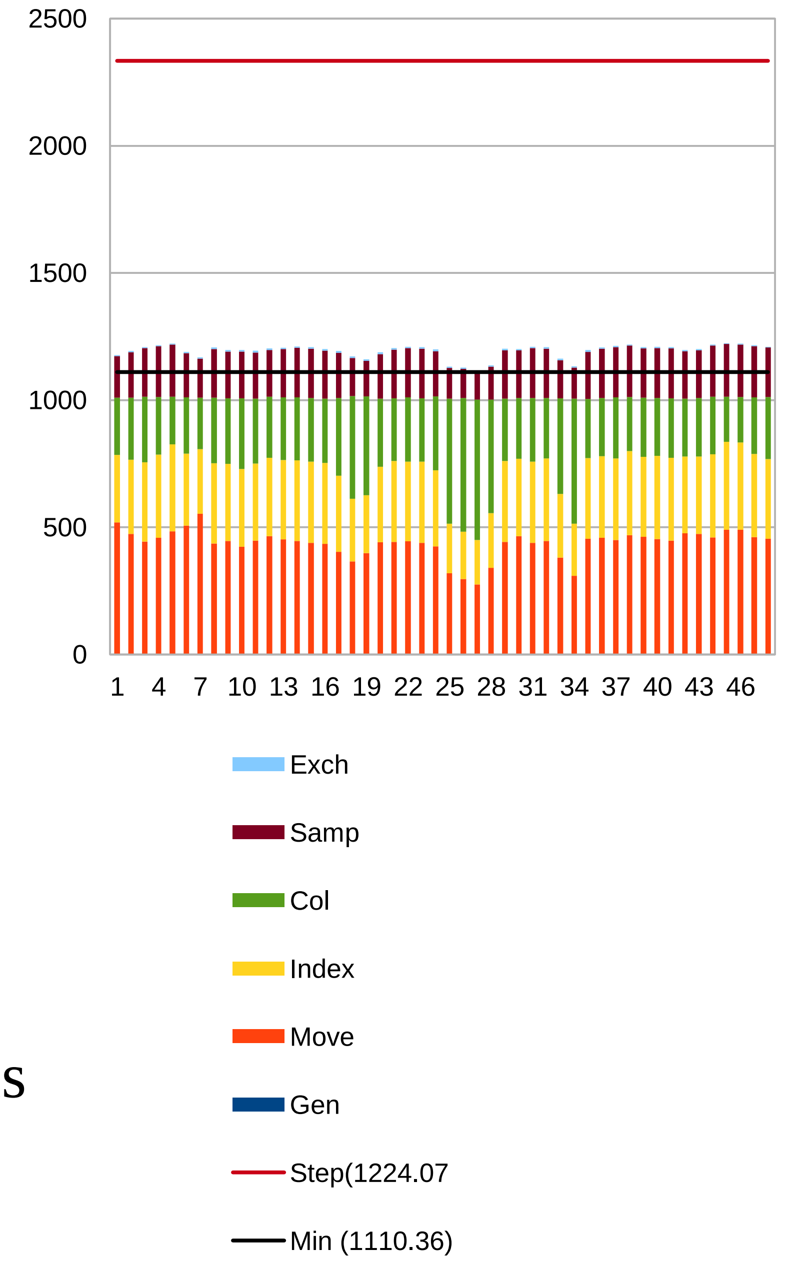






SMILE Future

- **SMILE++**
  - Object-oriented version for implementation and testing of new models and algorithms
  - Flexibility



- **SMILE+GPU**
  - Multi-GPU (CUDA) implementation
  - Optimization for huge computations: many billions of cells and particles

SMILE++ software system

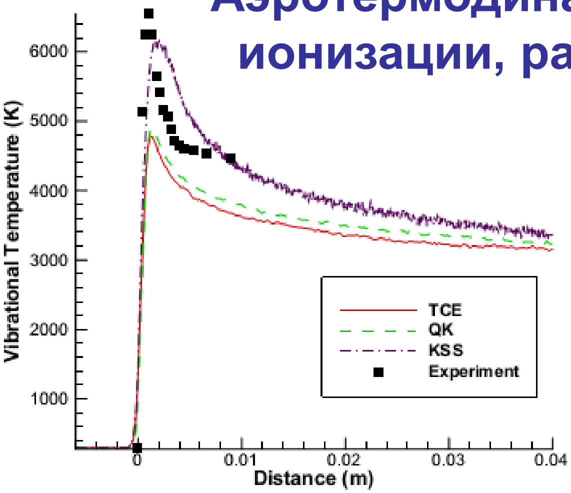
Our experience achieved during development of the SMILE software system clearly demonstrates the fact that the greater the capabilities of the DSMC system are, the harder it is to modify the system by implementation of new models, methods and algorithms. The necessity of creation of the DSMC software system of the new generation based on the OOP approach became evident to us more than a decade ago.

As a result the **SMILE++** software system has been developed at the Computational Aerodynamics Lab of ITAM (the main developer: **A.V. Kashkovsky**). The **SMILE++** is based on the OOP approach and completely written in C++. It is the descendant of SMILE and incorporates most of the capabilities of the latter. At the same time, it has new capabilities and significant advantages offered by OOP.

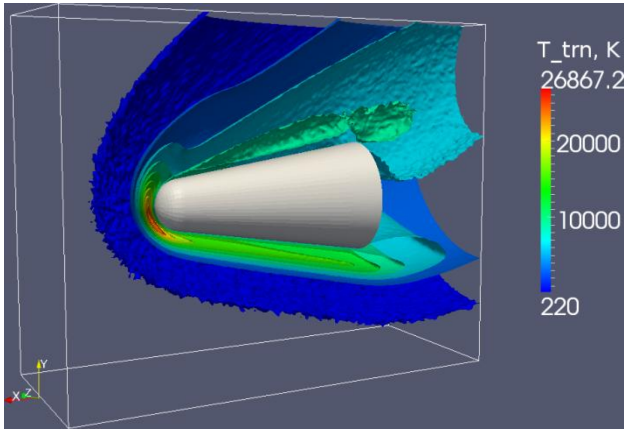
The **SMILE++** system provides a complete lifecycle of computations starting from a geometry model, pre-processing, going through the computation, and finishing with post-processing and presentation of results.

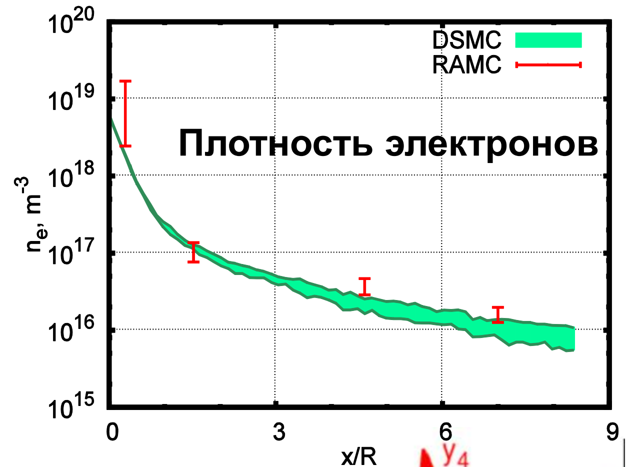
M.S. Ivanov, A.V. Kashkovsky, P.V. Vashchenkov and Ye.A. Bondar. Parallel Object-Oriented Software System for DSMC Modeling of High-Altitude Aerothermodynamic Problems (INVITED), AIP Conference Proceedings Volume 1333, Proc. of **RGD27**, pp. 211-218 (2011).

Аэротермодинамика космических аппаратов с учетом процессов ионизации, радиации и гетерогенной рекомбинации (SMILE++)

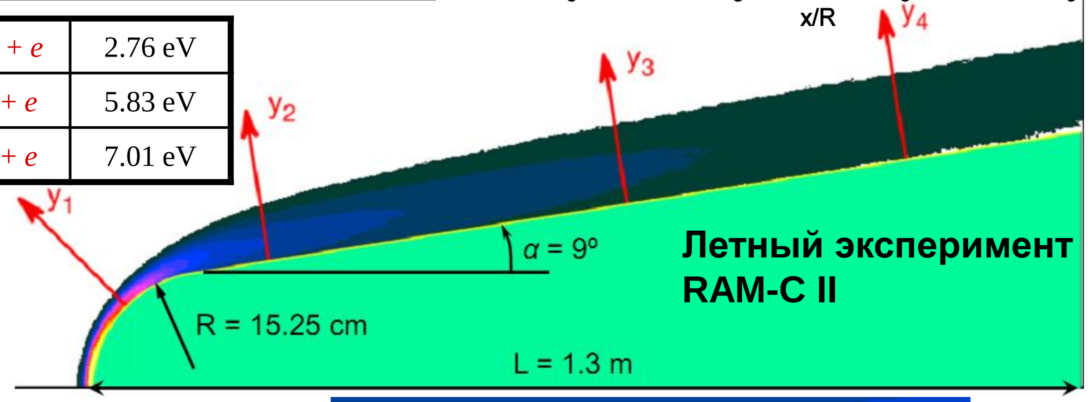


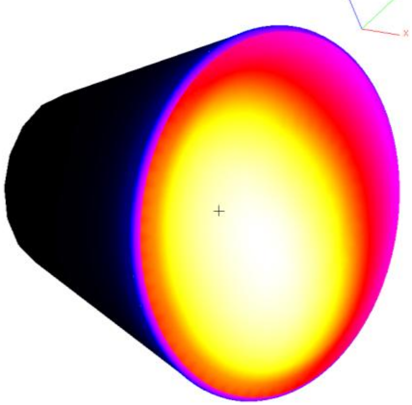
Сравнение с экспериментальными данными Шаталова и др. (2013) по структуре ударной волны в кислороде для M=13.4

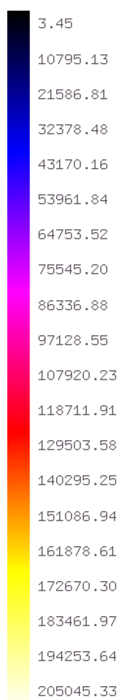




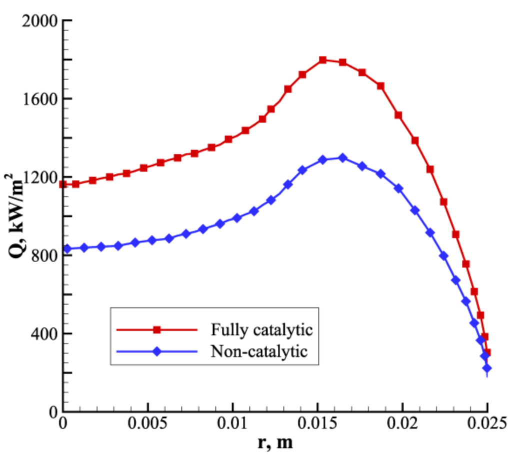
$N + O \leftrightarrow NO^+ + e$	2.76 eV
$N + N \leftrightarrow N_2^+ + e$	5.83 eV
$O + O \leftrightarrow O_2^+ + e$	7.01 eV





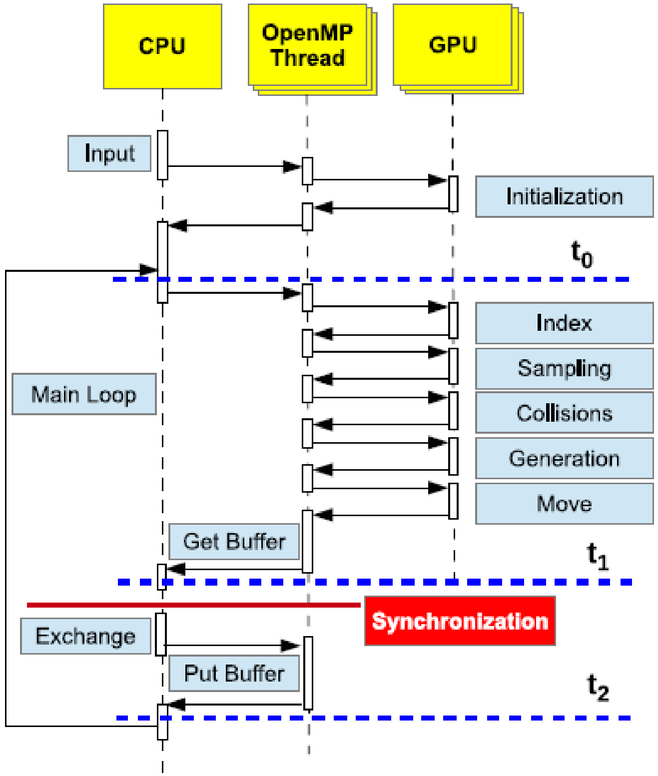


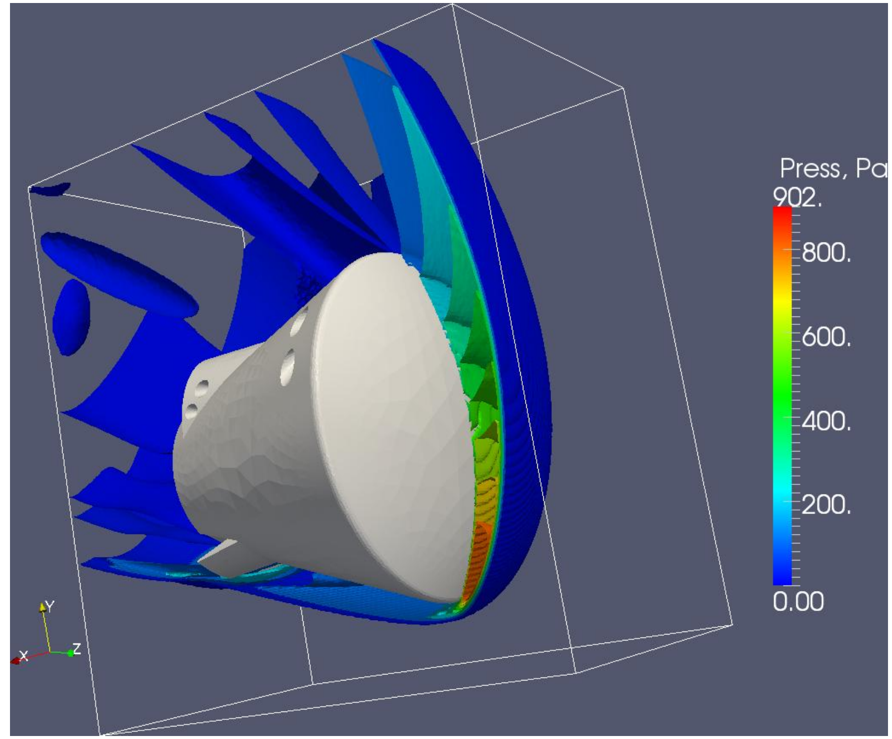
Радиационный тепловой поток на поверхность КА ORION, H=80 км



Влияние поверхностной рекомбинации на аэротермодинамику входа в атмосферу Марса

Создание комплексов аэродинамических программ для расчетов на гетерогенных (CPU/GPU) суперкомпьютерах





Обтекание ППТС на высоте 85 км. Давление

2,1 миллиарда молекул. 120 GPU, 12 часов

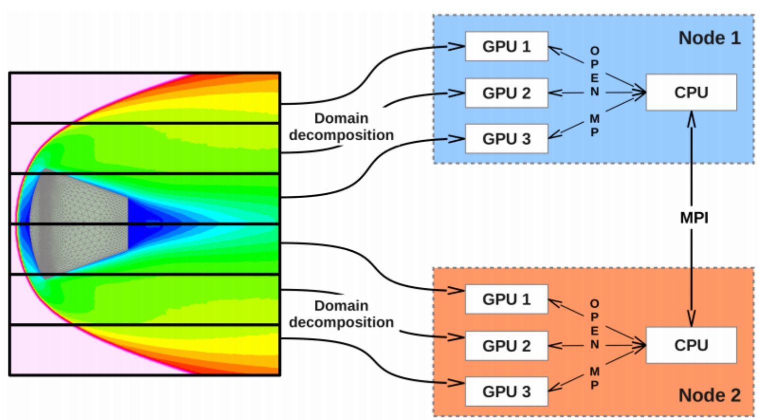
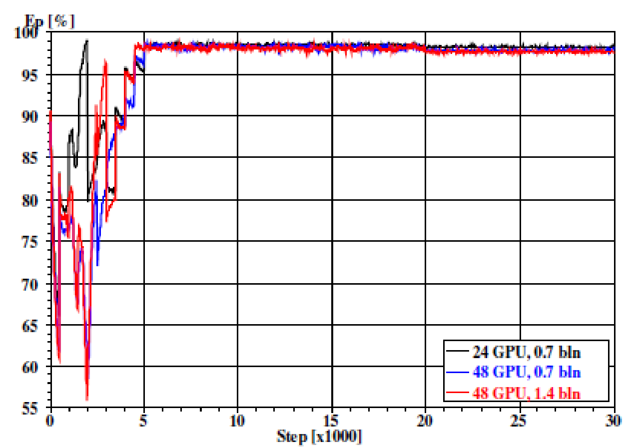


Схема параллелизации системы для расчетов методом ПСМ



Эффективность параллелизации

Thank you
for your attention!