Enhanced theoretical models and numerical methods for hypersonic flows

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Collaborations

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Objective and Outline

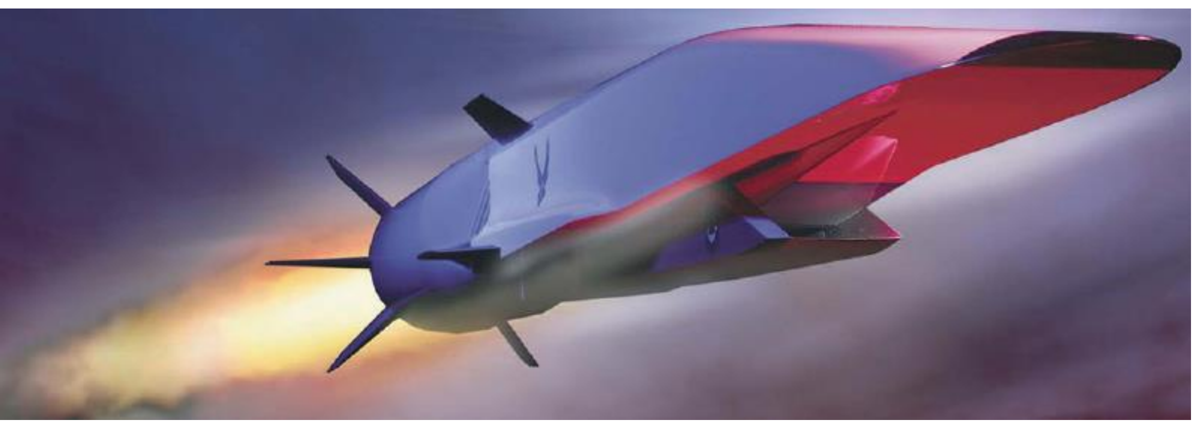
Objective:
Development of a High Performance Computing (HPC) CFD code for investigating high enthalpy flows

Outline:

- **Governing equations and numerical method**
- **Thermochemical non-equilibrium models**
- **multi-GPU code performance**
- **Immersed boundary approach**
- **Results**
- **Conclusions**

Hypersonic Flight

Transcontinental civil flights: LAPCAT, FAST20xx (source: esa website)

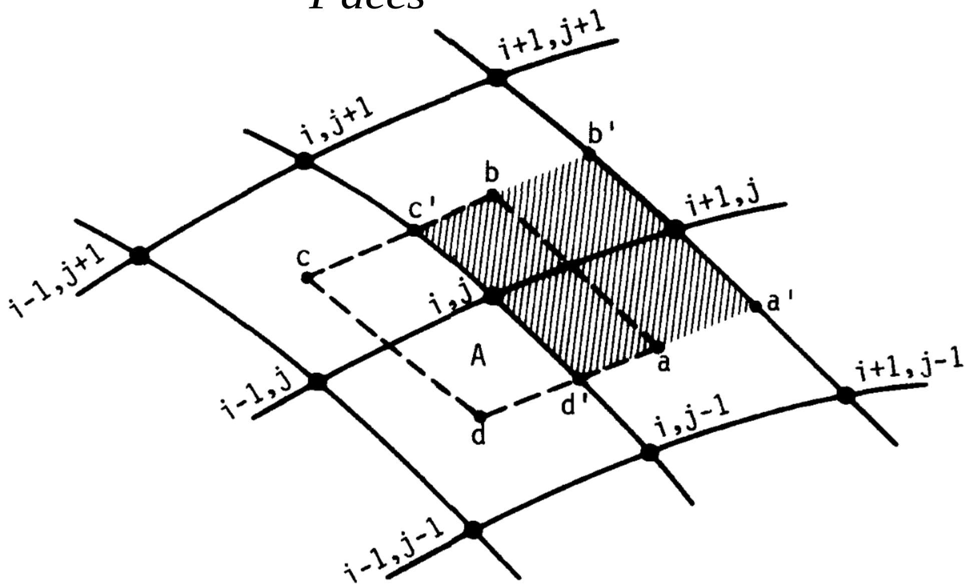


Hypersonic cruise missiles (source: defence Advanced Research Agency illustration)

Orion capsule (source: NASA)

Numerical method

$$V_{i,j}\frac{d\mathbf{U}_{i,j}}{dt}+\sum_{Faces}\mathbf{F}_{num}\cdot\mathbf{n}\Delta S=V_{i,j}\mathbf{W}_{i,j}$$



Cell-centered Finite Volume Space discretization on a Multi-block structured mesh

$$\mathbf{F}_{num}=\mathbf{F}_{E,num}-\mathbf{F}_{V,num}$$

Reactive Navier-Stokes equations:

- **Advection and pressure term** (hyperbolic)
- **Shear-stress, heat flux terms** (diffusive)
- **Chemical source terms** (stiffness)

Solution strategy:

➢ **Operator splitting approach: Frozen step + Chemical step**

✓ **<u>Frozen step:</u> Method of Lines:**

- **Space discretization + Time integration**
  - **Space dicretization: Inviscid & Viscous terms scheme**
  - **Time integration: Runge-Kutta scheme**

✓ **<u>Chemical step:</u> implicit scheme for stiff terms**

John C. Tannehill, Dale Anderson, Richard H. Pletcher, Computational Fluid Mechanics and Heat Transfer, Taylor & Francis 1997

Numerical method

Operator splitting approach

$$V_{i,j}\frac{d\mathbf{U}_{i,j}}{dt}+\sum_{Faces}\mathbf{F}_{num}\cdot\mathbf{n}\Delta S=0$$

Frozen step: AUSM or Flux Vector Splitting of Steger and Warming with MUSCL approach for higher order accuracy; Gauss divergence approach for viscous terms; Runge-Kutta scheme up to third order for time integration

$$\frac{\partial}{\partial t}\int_{V_0}\mathbf{U}dV=\int_{V_0}\mathbf{W}dV$$

Chemical step

$$\Delta t_c^{(v)}=\Delta t_f/n$$

Sub-time step

$$\frac{\partial\mathbf{y}}{\partial t}=\mathbf{P}-\mathbf{L}\mathbf{y}\qquad \mathbf{y}=\{\rho_i\}_{0\le i\le N}$$

P is a vector and L a diagonal matrix.
P_i and $L_i y_i$ are non-negative and represent, respectively, production and loss terms for component y_i

$$y_i^k(t+\Delta t_c^{(v)})=\frac{\Delta t_c^{(v)}P_i(\mathbf{y}^{k-1})+y_i(t)}{1+\Delta t_c^{(v)}L(\mathbf{y}^{k-1})}$$

Gauss-Seidel iterative scheme

Thermochemical non-equilibrium models for air

MULTI-TEMPERATURE 5 SPECIES PARK MODEL[1]

- 17 reactions + 3 transport equations for the vibrational energies
- Arrhenius type rate coefficients function of an effective temperature calculated as a geometrical mean of translational and vibrational temperatures
- Vibrational levels follow a Boltzmann distribution at temperature Tv
- Tuned on experimental measures
- Not computationally demanding
- It may fail when the conditions are far from those for which it was tuned

5 SPECIES State-to-State (StS) MODEL[2]

- Detailed vibrational kinetics of molecules.
- 68 and 47 vibrational levels for N_2 and O_2 respectively
- Thousands of elementary processes → High accuracy but huge computational cost

[1] C. Park, Nonequilibrium Hypersonic Aerothermodynamics, Wiley, New York, 1990

[2] M. Capitelli et al., Fundamentals Aspects of Plasma Chemical Physics: Kinetics, Springer Science & Business Media, 2015

Combined GPU and MPI Computing

GPUs are very powerful and efficient

MPI allow to efficiently scale the computations across a multiple-nodes GPU cluster

Our implementation has shown speed-ups (single GPU vs single-core CPU) up to 150

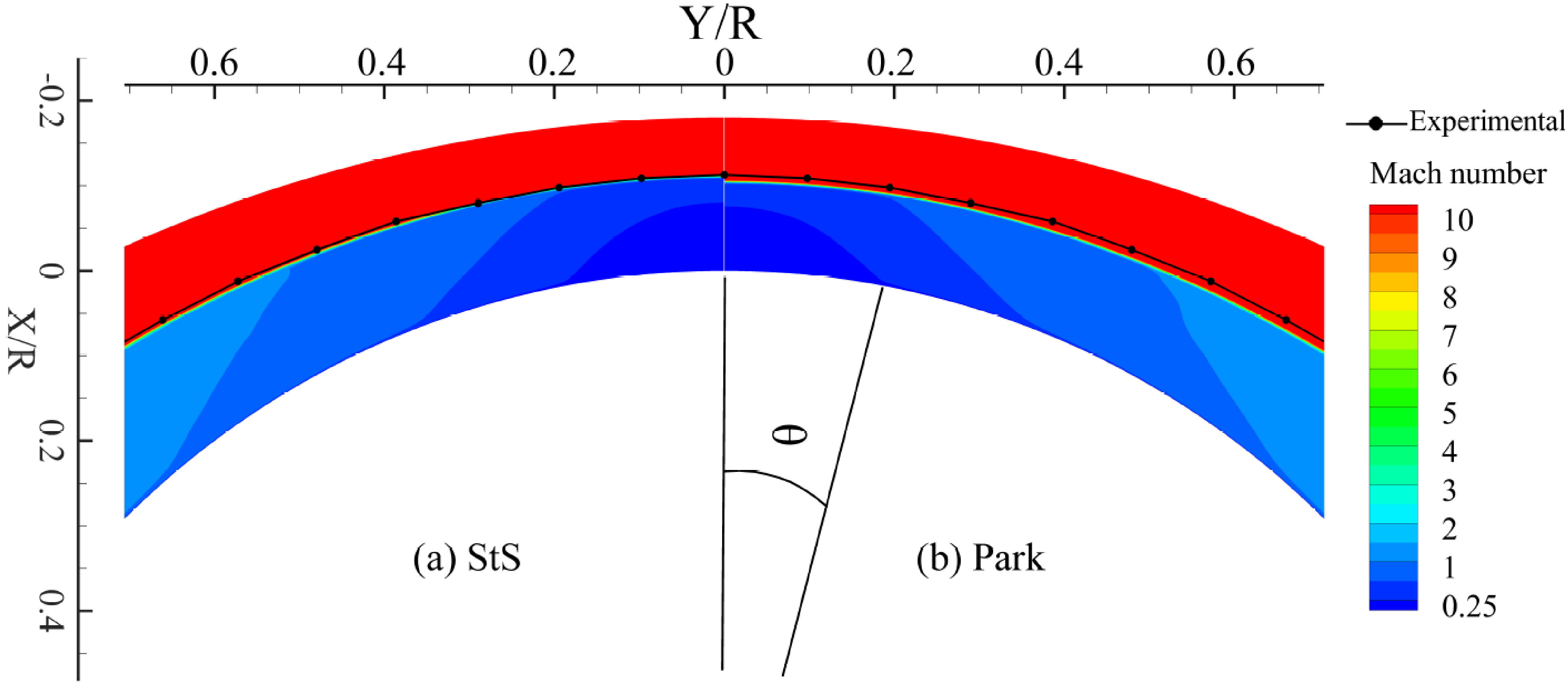
MPI-CUDA: GPU vs CPU computational performance

NVIDIA Tesla K40 (235 W) VS Intel Xeon CPU E5-2630 (6 cores) v2 2.60 GHz (80 W)

	Fluid cells	12 GPUs --Time per iteration (s) (Energy (J))	12 CPUs -- Time per iteration (s) (Energy(J))	Speed up (1 GPU vs 1 core)
StS				
	64x32	6.33 ($1.8*10^4$)	8.17 ($7.8*10^3$)	1.29 (7.7)
	128x64	6.36 ($1.8*10^4$)	26.71 ($2.56*10^4$)	4.2 (25.2)
	256x128	6.90 ($1.9*10^4$)	105.9 ($10.2*10^4$)	15.3 (91.8)
	512x256	15.91 ($4.5*10^4$)	419.5 ($40.3*10^4$)	26.4 (158.4)
	1024x512	68.72 ($19.4*10^4$)	1702.1 ($163.4*10^4$)	24.8 (148.8)
Park				
	64x32	$7.50*10^{-3}$ (21)	$1.59*10^{-3}$ (1.5)	0.21 (1.3)
	128x64	$7.77*10^{-3}$ (22)	$4.55*10^{-3}$ (4.3)	0.59 (3.5)
	256x128	$7.24*10^{-3}$ (20)	$1.68*10^{-2}$ (16)	2.32 (13.9)
	512x256	$1.36*10^{-2}$ (38)	$6.53*10^{-2}$ (63)	4.8 (28.8)
	1024x512	$3.48*10^{-2}$ (98)	$2.46*10^{-1}$ (236)	7.1 (42.6)

Flow past a sphere: Nonaka[4] test case

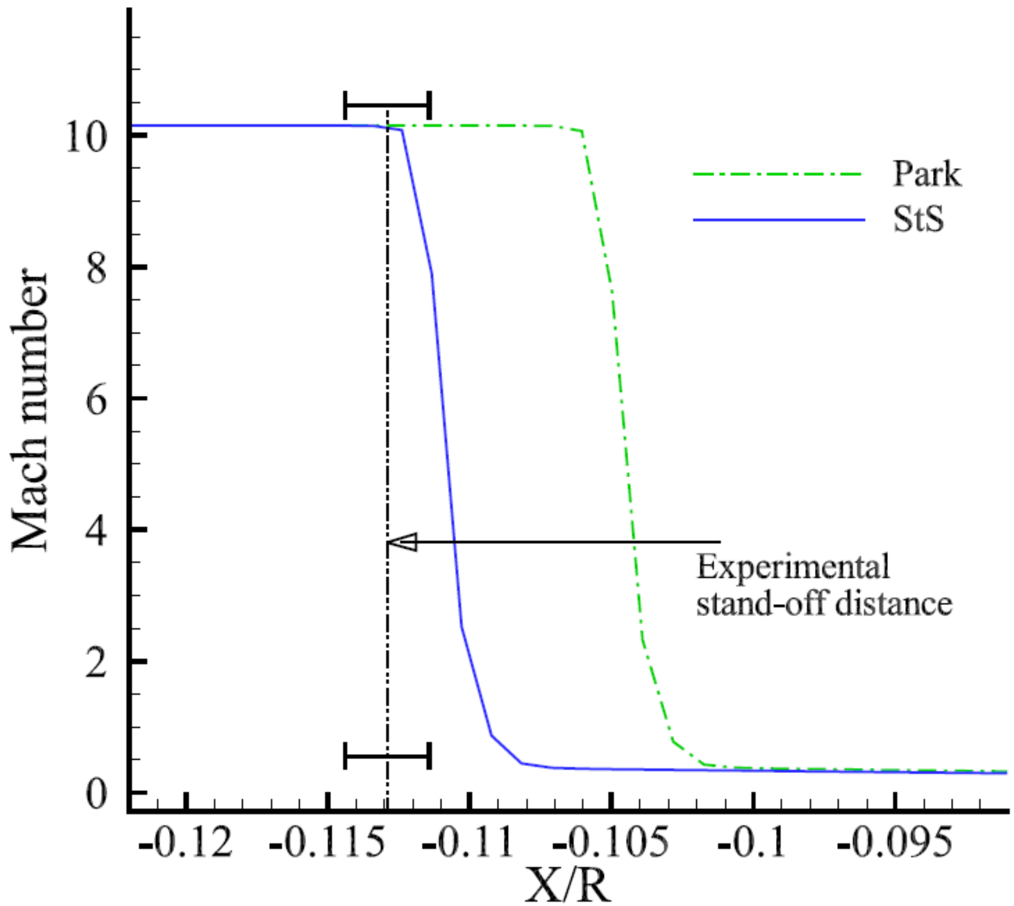
[4]R= 7mm; u_∞=3490 m/s; T_∞=293 K; P_∞= 4825 Pa; Y_{N2}=0.767; Y_{O2}=0.233



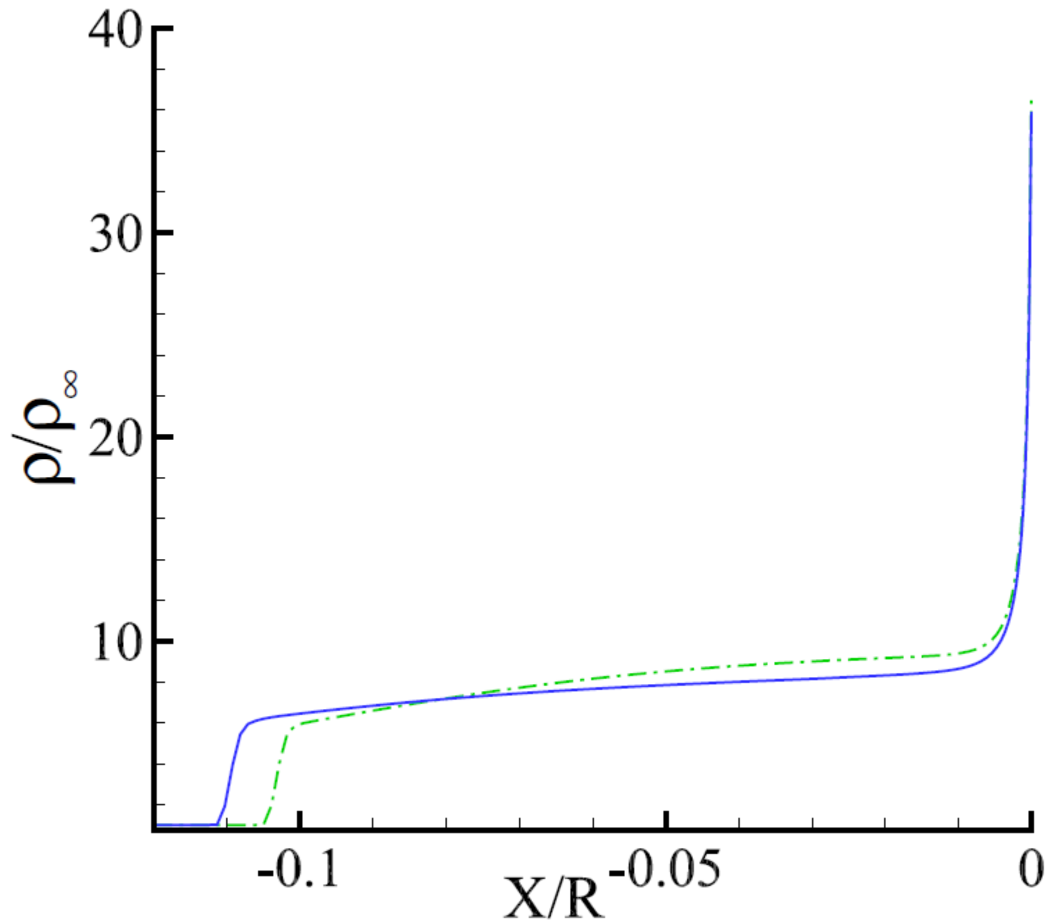
Numerical and experimental shock shape: (a) StS model; (b) Park model

[4]S. Nonaka et al. ,JTHT 14 (2), 2000

Nonaka[4] test case: stagnation line profiles



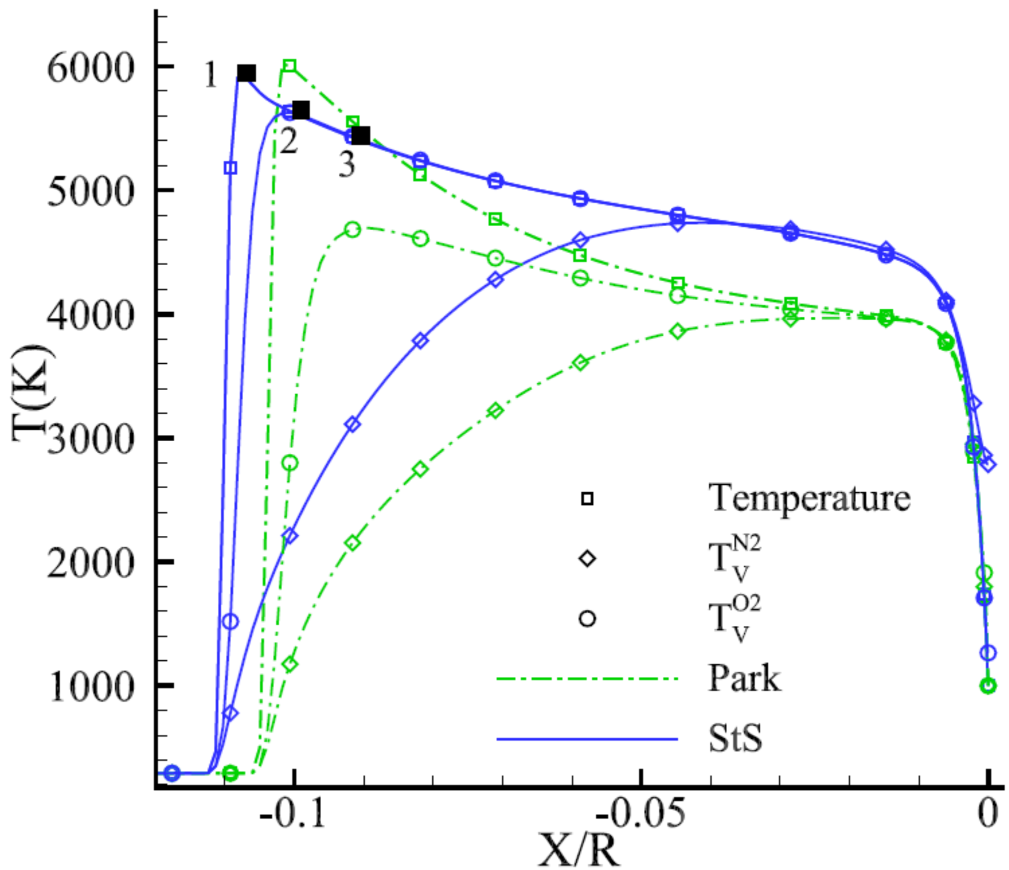
Mach Number



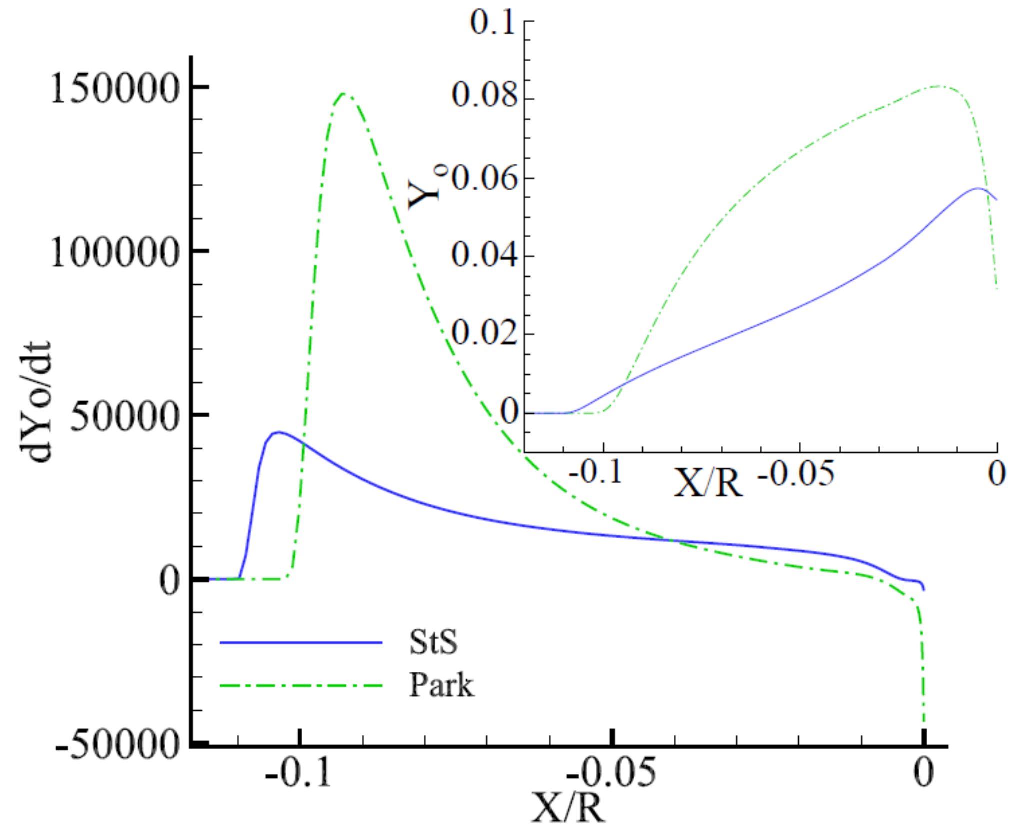
Normalized density

G. Colonna, F. Bonelli and G. Pascazio, "Impact of a fundamental molecular kinetics on macroscopic properties of high-enthalpy flows: the case of hypersonic atmospheric entry." Physical Review Fluids, 4 (3), 033404 (2019).

Nonaka[4] test case: stagnation line profiles



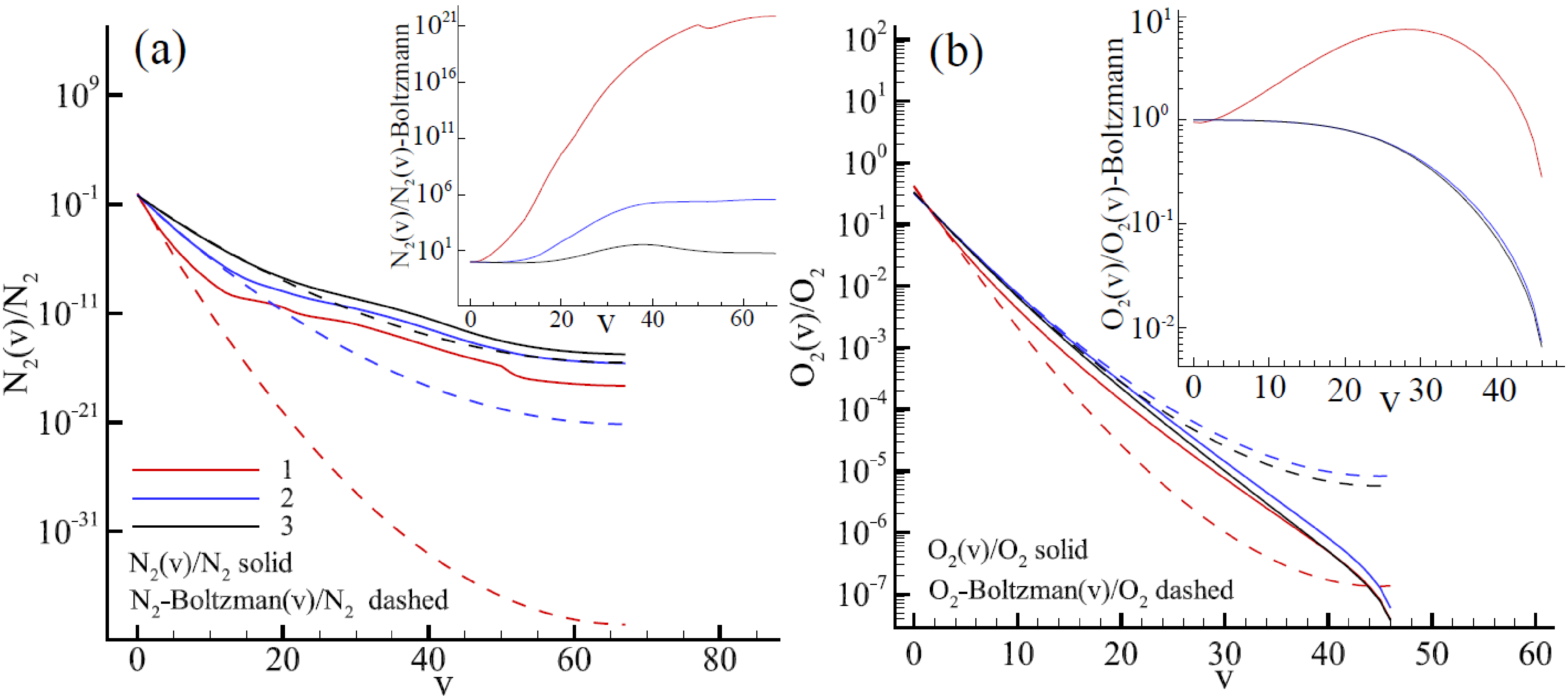
Temperatures



Oxygen atom reaction rate and mass fraction

G. Colonna, F. Bonelli and G. Pascazio, "Impact of a fundamental molecular kinetics on macroscopic properties of high-enthalpy flows: the case of hypersonic atmospheric entry." Physical Review Fluids, 4 (3), 033404 (2019).

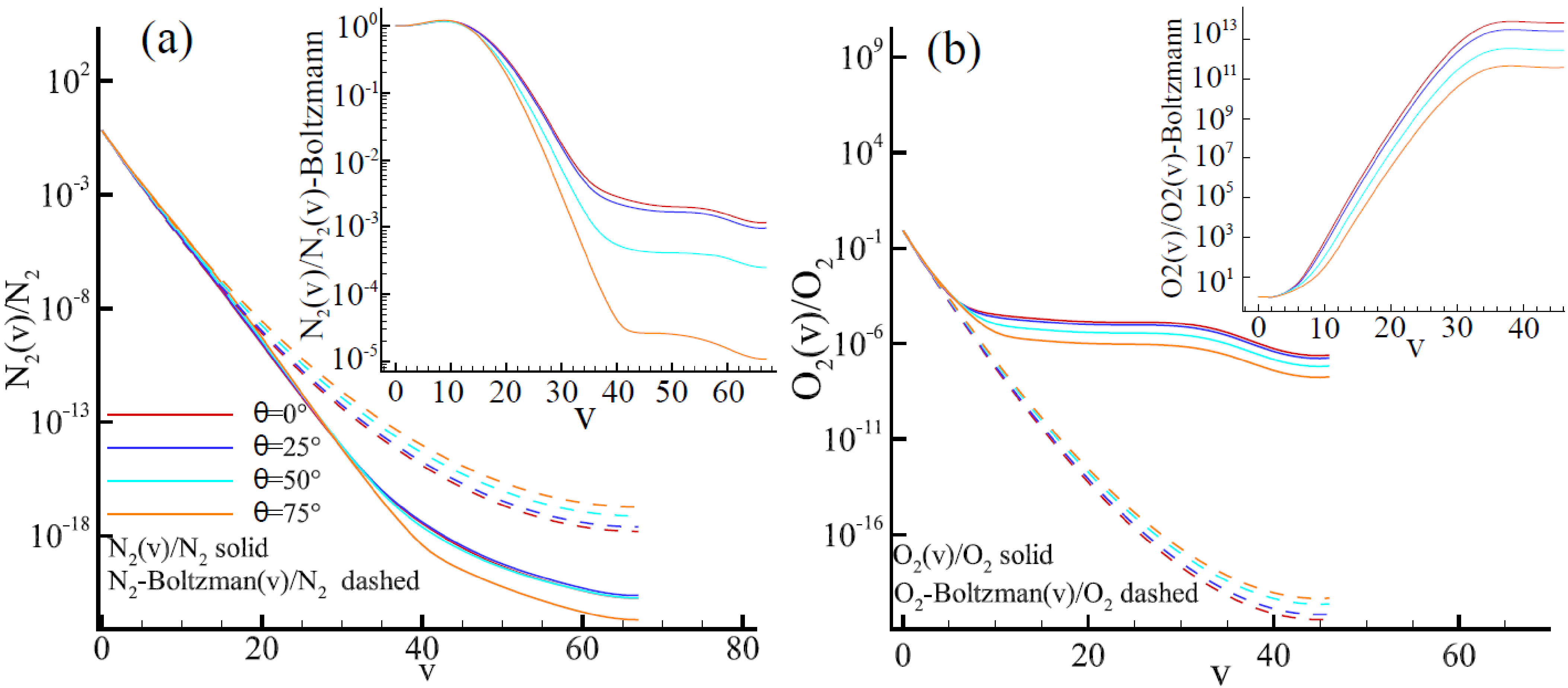
Nonaka[4] test case: vibrational distributions along stagnation line



Stagnation line population with actual to Boltzmann ratio in the inset: (a) N2; (b) O2

G. Colonna, F. Bonelli and G. Pascazio, "Impact of a fundamental molecular kinetics on macroscopic properties of high-enthalpy flows: the case of hypersonic atmospheric entry." Physical Review Fluids, 4 (3), 033404 (2019).

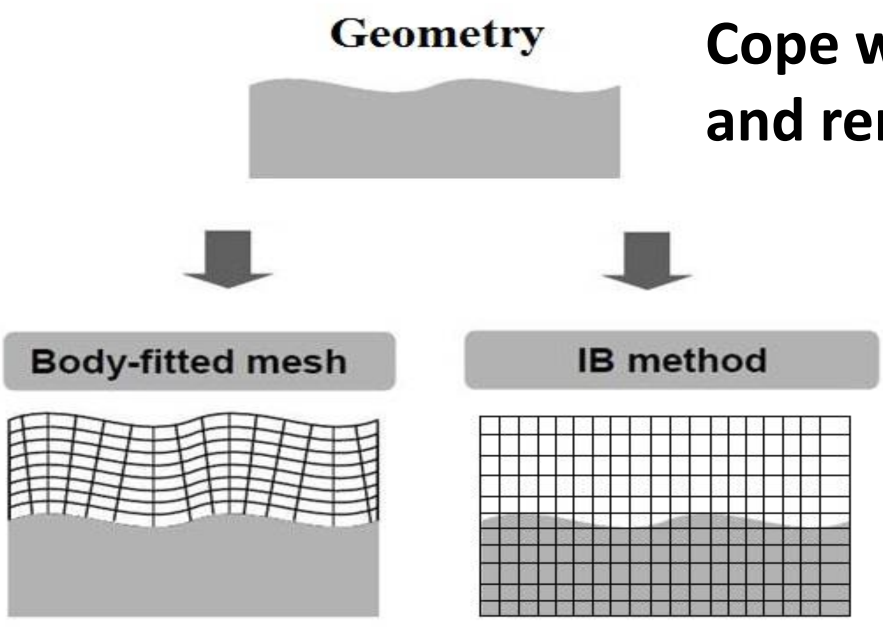
Nonaka[4] test case: vibrational distributions wall profiles



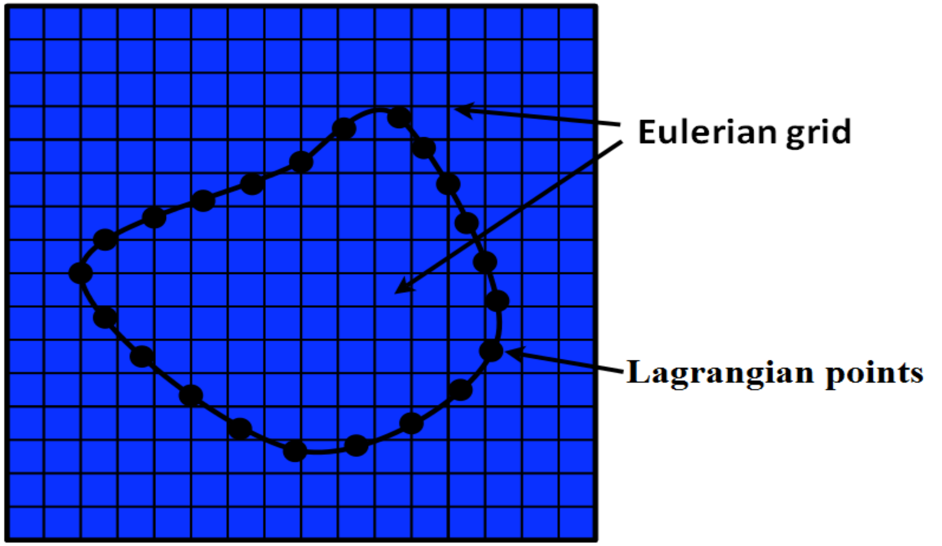
Wall surface populations with actual to Boltzmann ration in the inset: (a) N2; (b) O2

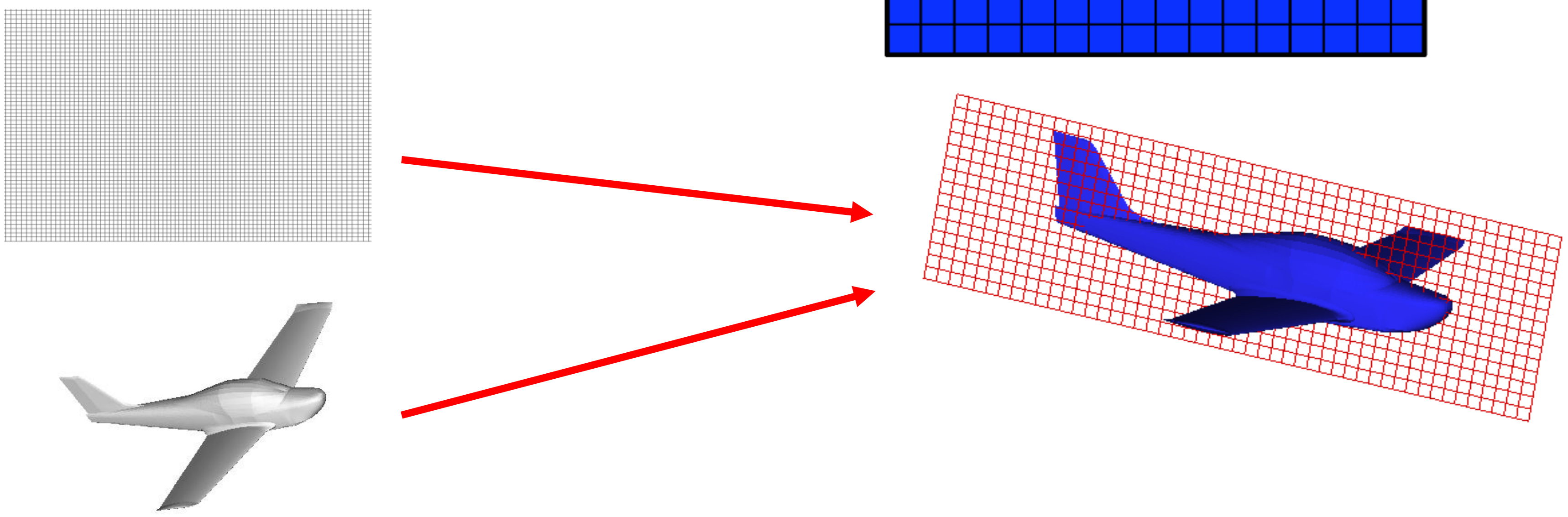
G. Colonna, F. Bonelli and G. Pascazio, "Impact of a fundamental molecular kinetics on macroscopic properties of high-enthalpy flows: the case of hypersonic atmospheric entry." Physical Review Fluids, 4 (3), 033404 (2019).

Immersed-Boundary Method

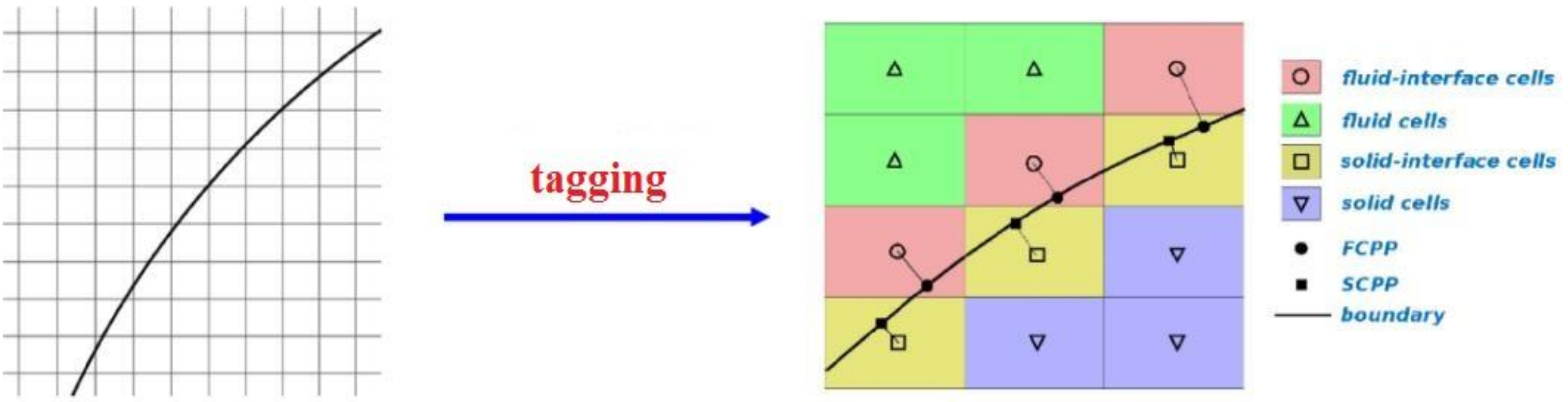


Cope with the time consuming grid generation and remeshing processes





Immersed-Boundary solver for Cartesian grid

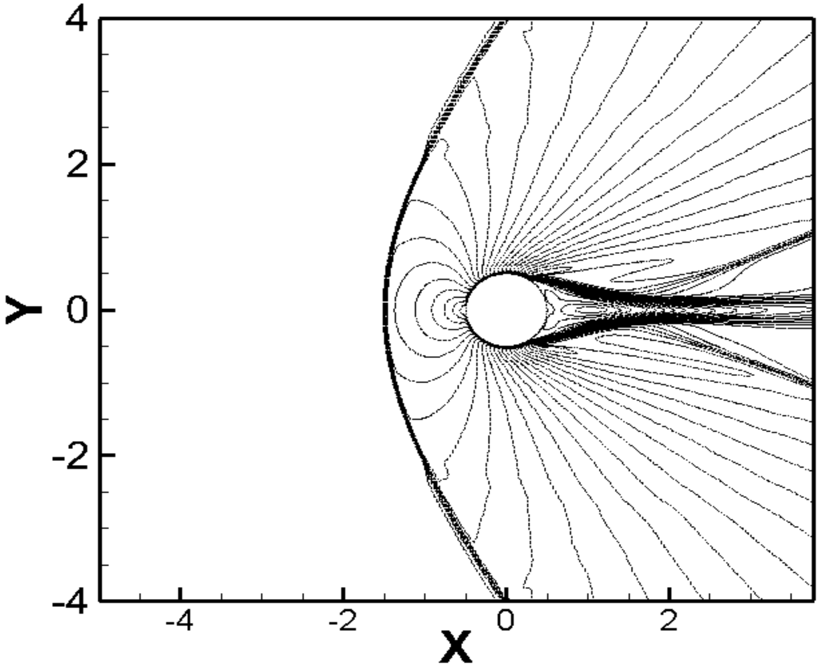


- the centers of the *fluid-interface* and *solid-interface* cells are projected onto the body surface along its normal direction, so as to obtain *fluid-cell projection points* (*FCPP*) and *solid-cell projection points* (*SCPP*);
- the flow variables at the centers of the *fluid* cells and the temperature at the *solid* cells are the unknowns to be computed using a finite-volume dual time stepping solver;
- the *solid* cells do not influence the flow field at all and vice versa;
- the boundary conditions are imposed at the *fluid-interface* and *solid-interface* cells by a local IB reconstruction scheme.

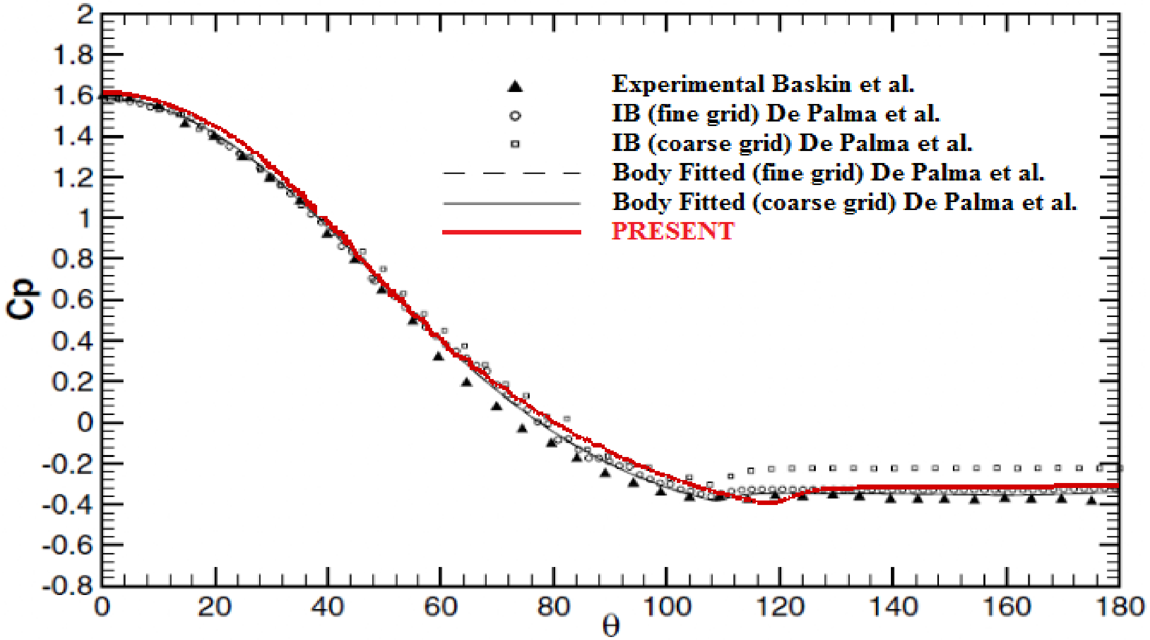
Supersonic flow past a circular cylinder

The new LS reconstruction has been validated and compared with the 1D reconstruction in the case of supersonic turbulent flow past a circular cylinder.

Re = 2000000, Ma = 1.7. **Grid: 139777 cells**



Mach number contours on the finest grid, ΔMa = 0.03.



Pressure coefficient distributions along the external surface of the cylinder.

[1] De Palma et al., Computers & Fluids, 2006

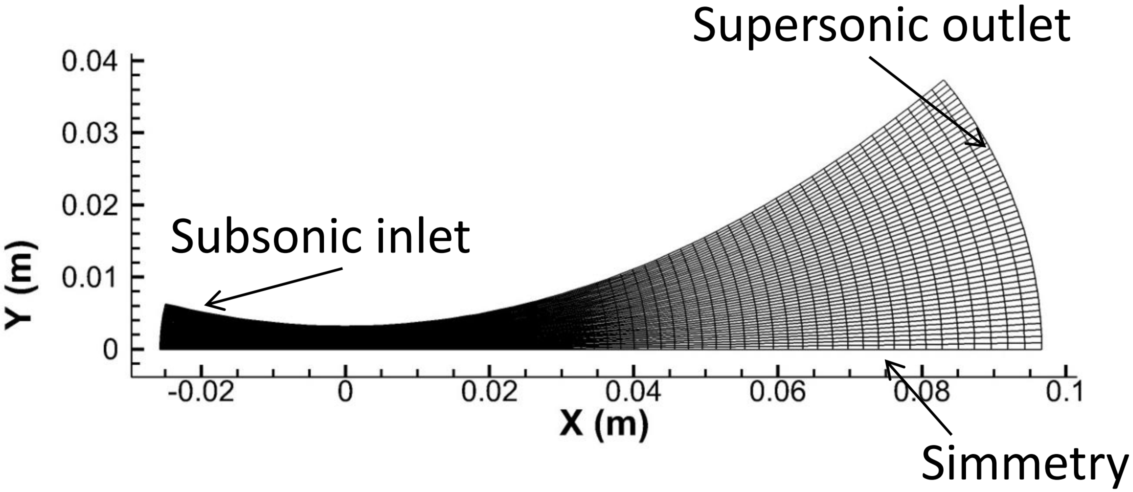
[2] Bashkin et al., Fluid Dynamics, 2002

Sharma nozzle test case

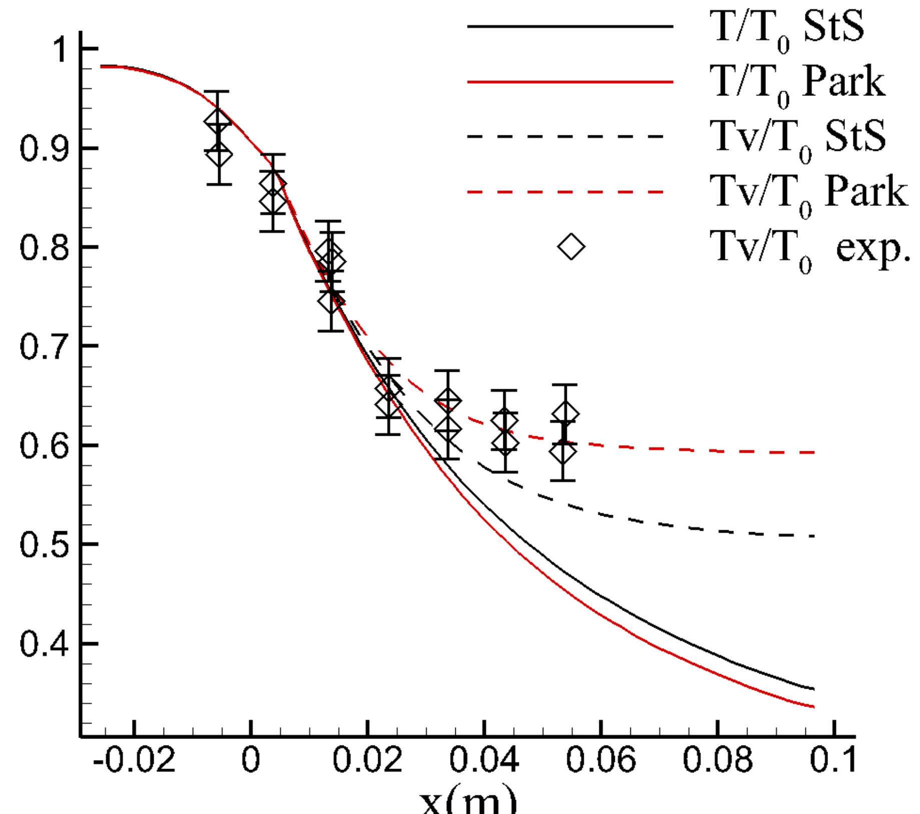
	Before throat	After throat
P	$P_0 = 100$ atm	0.197 atm
T	$T_0 = 5600$ K	300 K
(u, v)	$(0, 0)$	$(0, 0)$
N_2 molar fraction[a]	0.9828	1
$N_2(v)$ distribution	Boltzmann at T_0	Boltzmann at 300 K
N molar fraction[a]	0.0172	1.12923e-79

[a]Equilibrium calculation.

Initial conditions

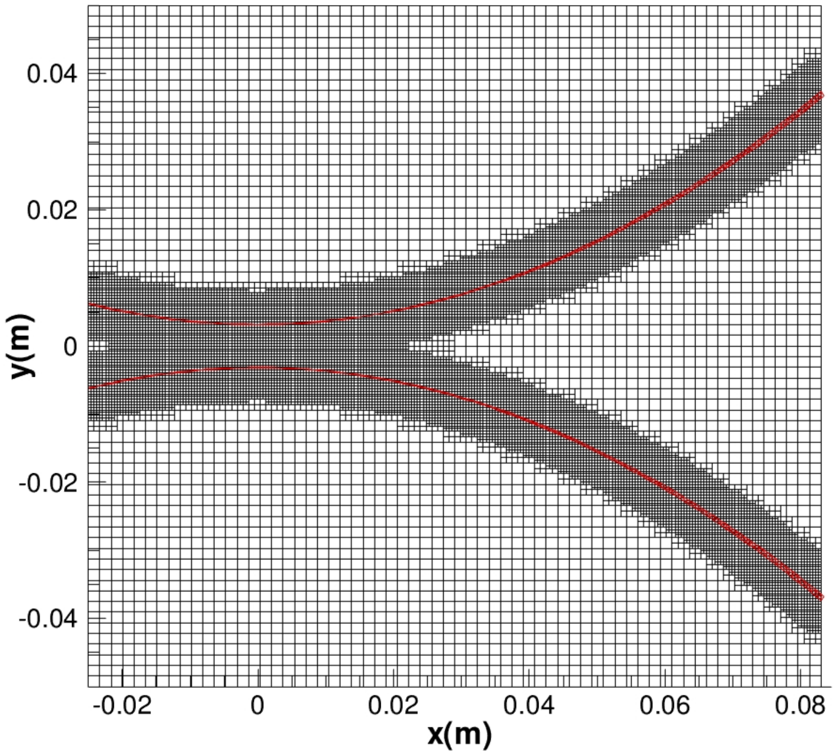


Grid scheme: 65x47 fluid cells



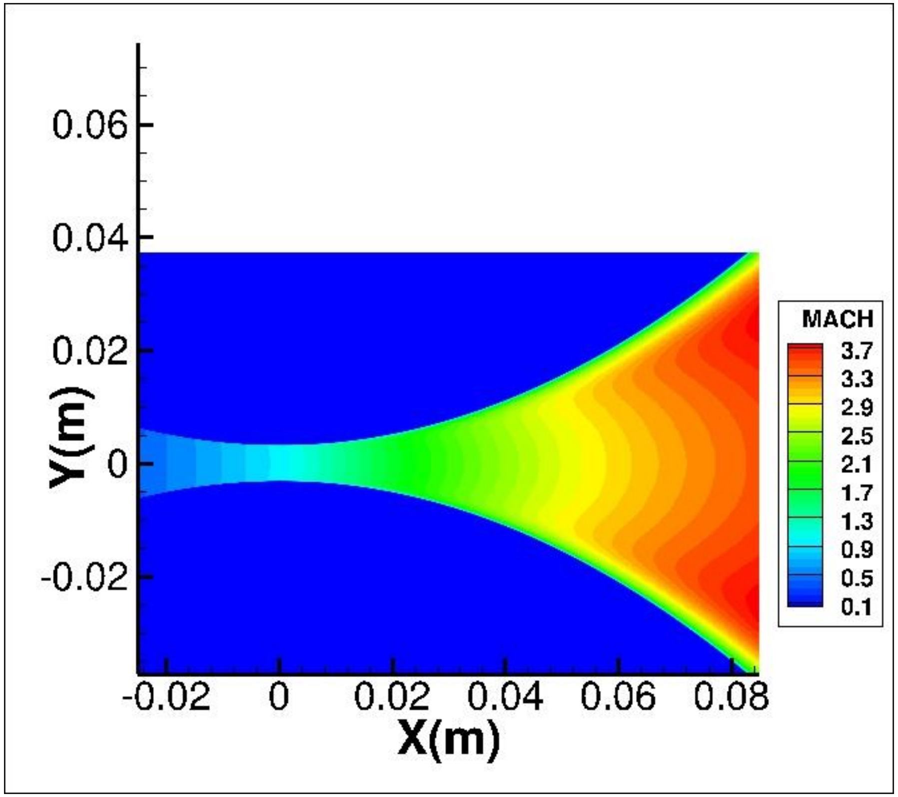
Normalized temperature profiles

Immersed-Boundary Method: Sharma nozzle test case

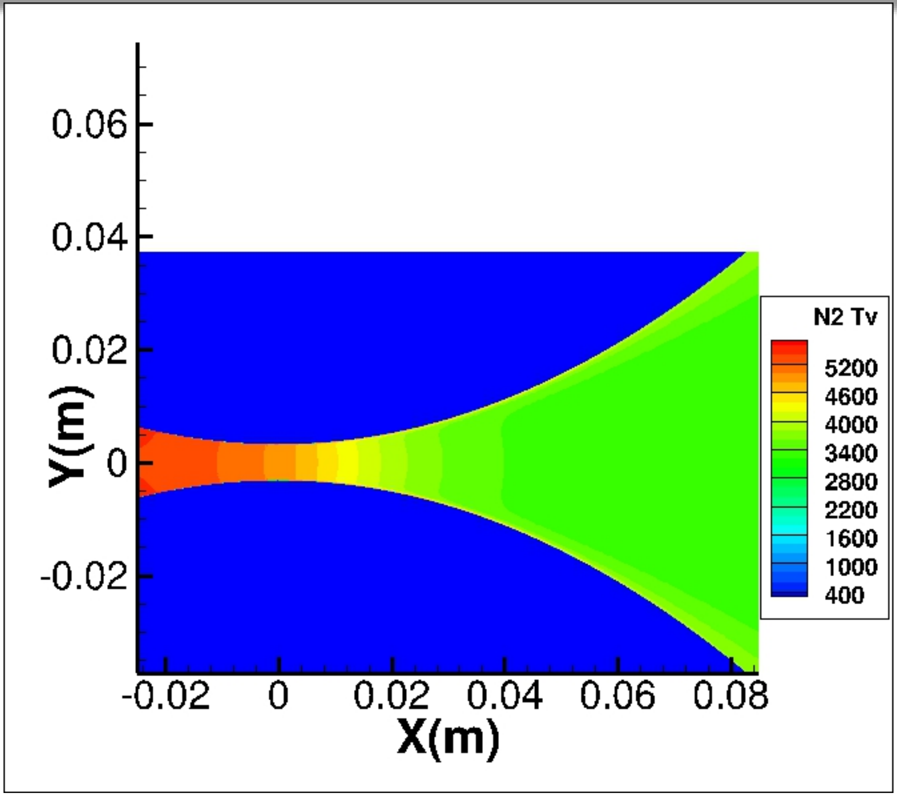


Cartesian mesh

Mach number contours

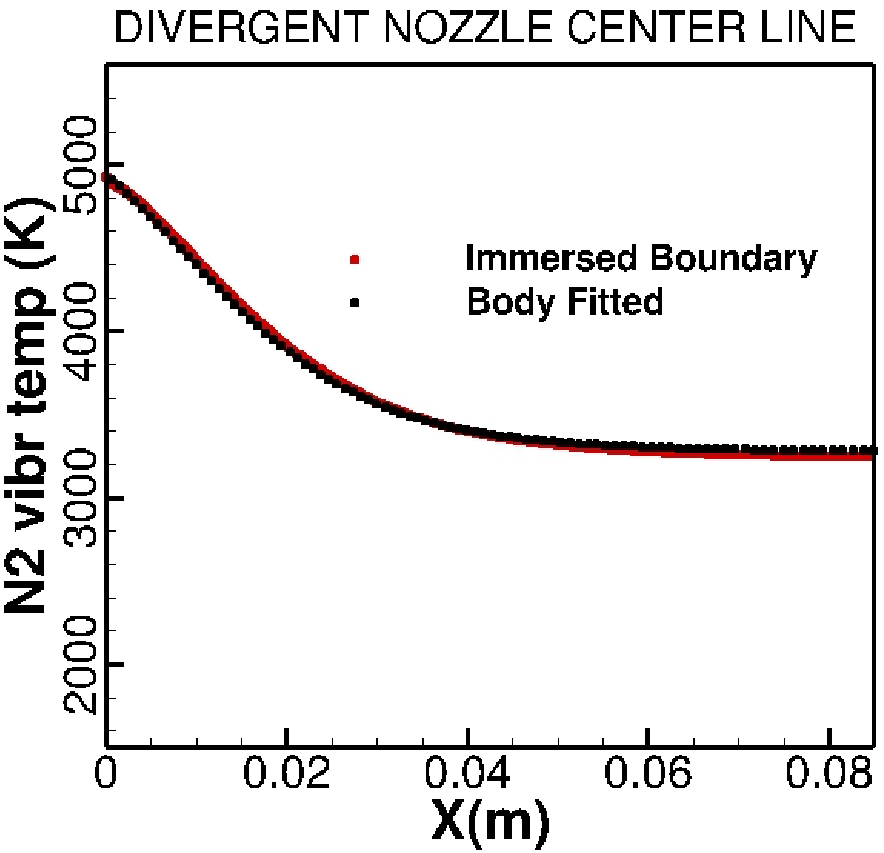


Immersed-Boundary Method: Sharma nozzle test case

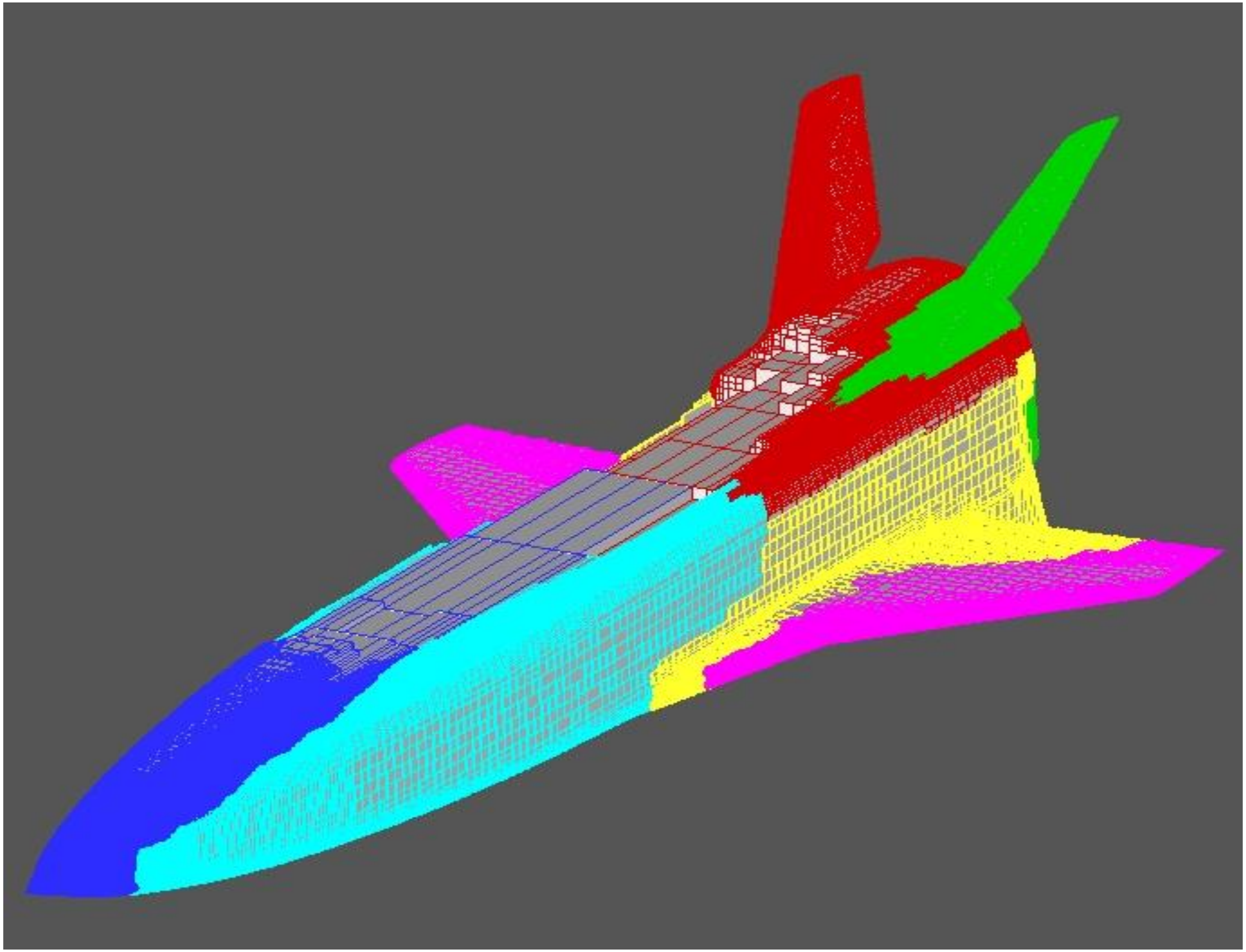


N2 Tv contours

IB vs Body fitted

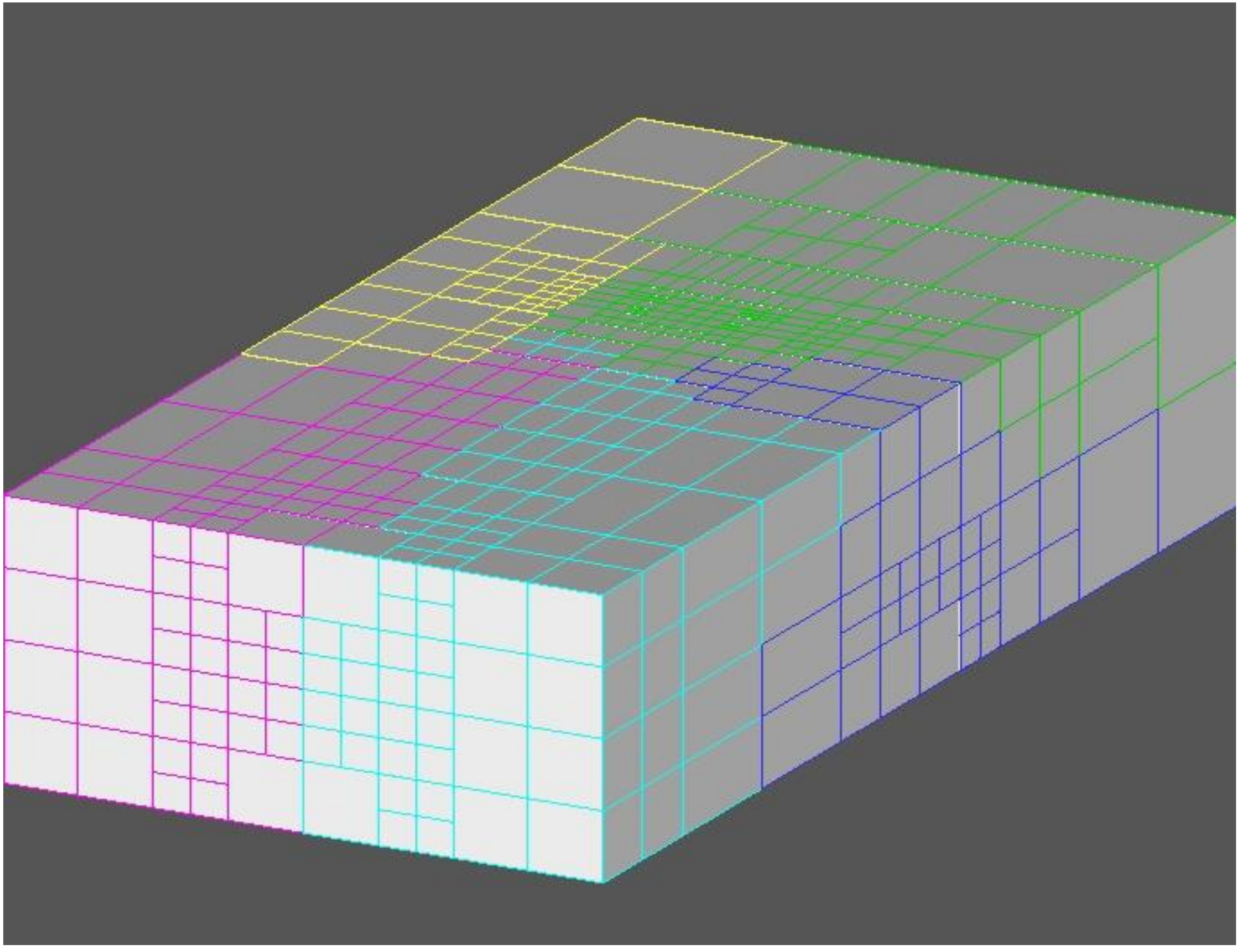


Computational mesh: internal points (solid)



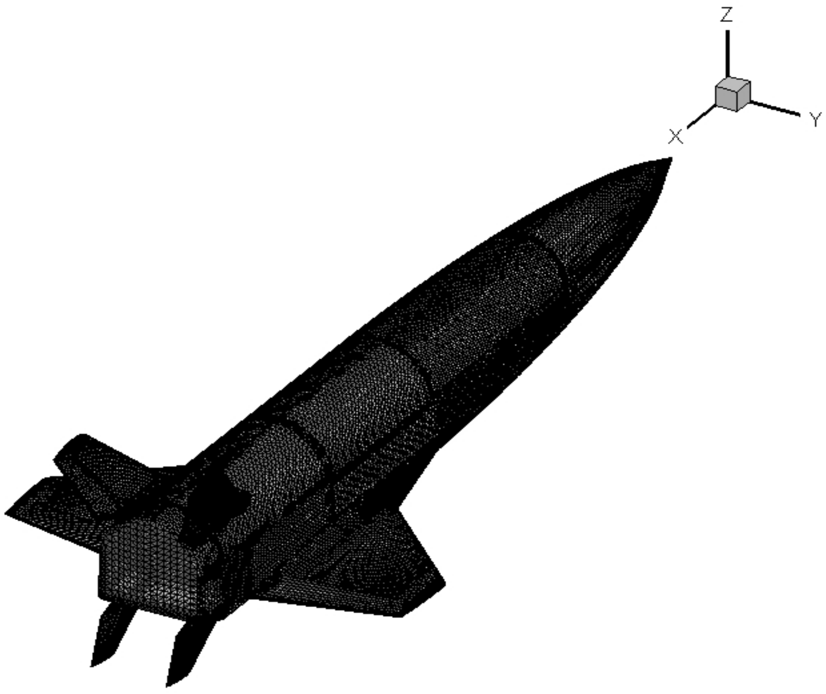
USV – Unmanned Space Veichle

Computational mesh: external points (fluid)

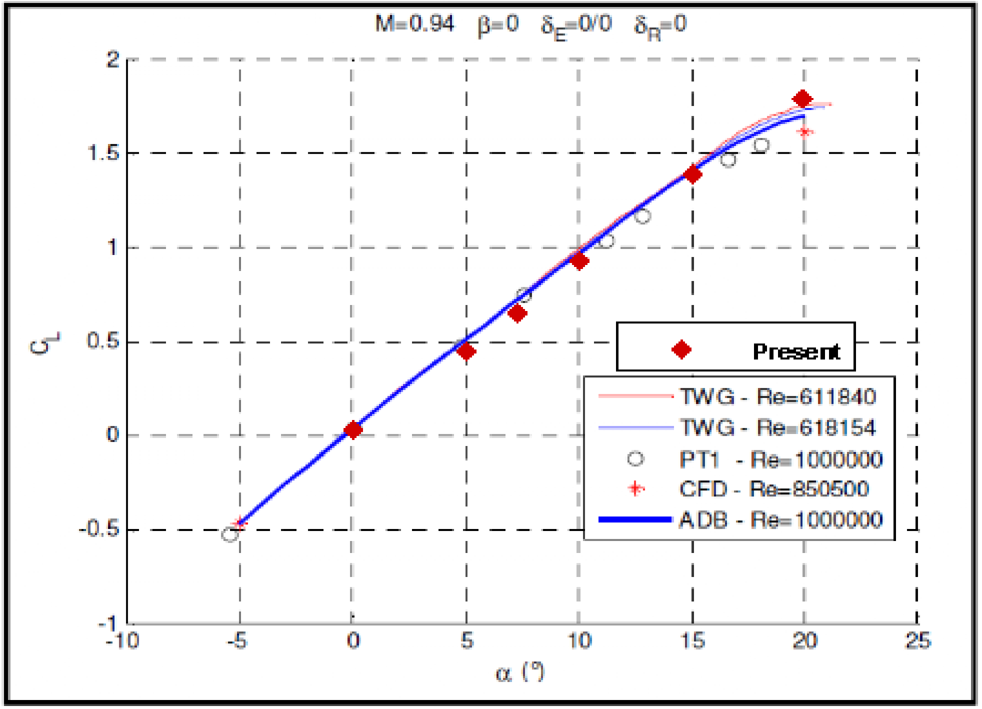


USV – Unmanned Space Veichle

Transonic flow past an Unmanned Space Vehicle



Triangular mesh of the Unmanned Space Vehicle



C_L vs α at $\mathrm{M} = 0.94$

α is the angle of attack

β is the side-slip angle

δ_E is the elevon deflection angle

δ_R is the rudder deflection angle

Conclusions

- We developed an efficient multi-GPU code for two-dimensional fluid dynamics
- We demonstrated the accuracy and the feasibility of fluid dynamic computations of thermochemical non-equilibrium flows by means of detailed state-to-state (StS) vibrationally resolved air kinetics
- The MPI-CUDA approach allowed us to efficiently scale the code across a multiple-nodes GPU cluster with good scalability performance: comparing the single GPU against the single core CPU performance speed-up values up to 150 were found.

Current and future work

- Flow-wall boundary treatment: models for catalysis and ablation
- Extension to 3D with a high-resolution hybrid WENO/central difference scheme
- Introduction of ionized species

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