GPU aided 2D high-enthalpy flow solver with state-to-state kinetics

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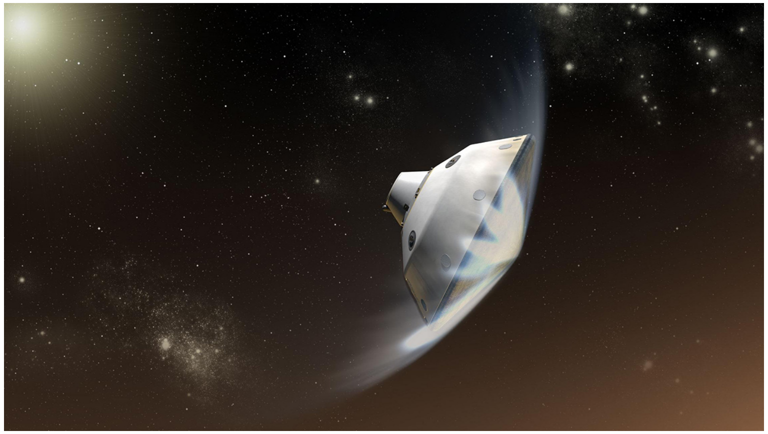
Motivations



In front of bodies moving at hypersonic speed forms a shock wave where temperature can jump from hundreds to many thousands K, inducing vibrational excitation, dissociation and ionization.

It is well known that the system presents regions with strong non-equilibrium, affecting the macroscopic properties of the flow, such as the heat flux to the vehicle surface.

Approaches to treat air in non-equilibrium

Multi-Temperature	State-to-State
5 species	~10^2 species
17 reactions	~10^4 reactions
3 vibrational temperatures	0 vibrational temperatures

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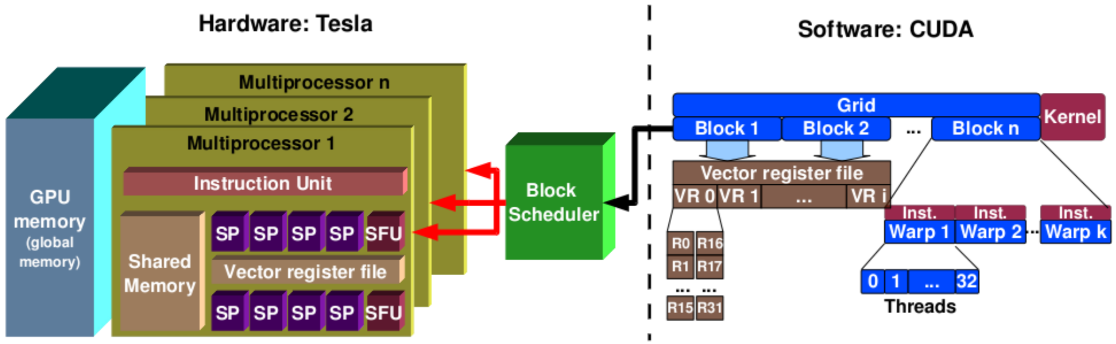
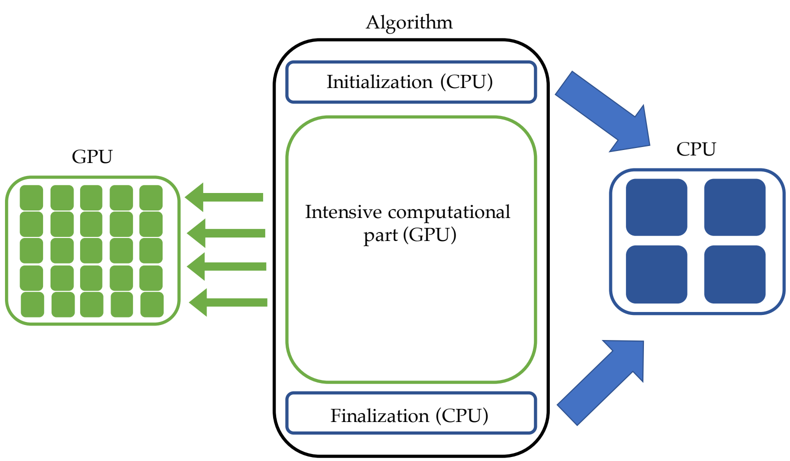
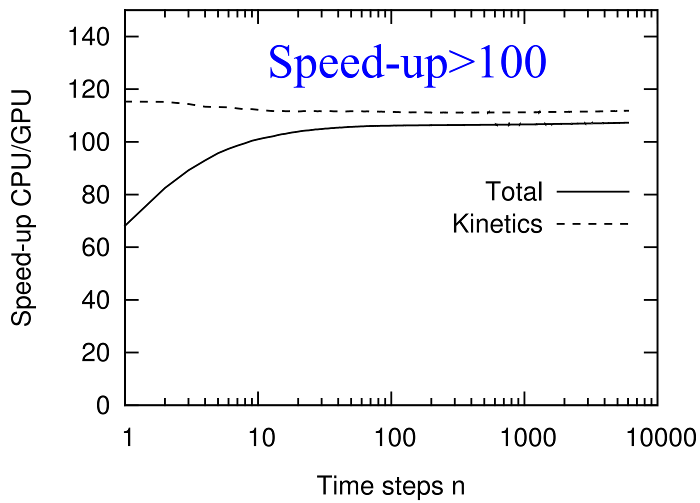
CUDA for GP-GPU

The use of new technology can give relevant improvement in StS kinetics in CFD. Graphical processing units allow considerably speed-ups.



CPU power does not increase fast.
Close to the limits of Moore law
GPU power is growing fast.
As well as the COST.





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5 species State-to-State (StS) model

The State-to-State approach write a relaxation equation for each vibrational level so that it is possible to calculate the distribution of internal states when it departs from the Boltzmann one.

Pure N_2

$$N_2(v)+N_2 \leftrightarrow N_2(v-1)+N_2$$
$$N_2(v)+N \leftrightarrow N_2(v-\Delta v)+N$$
$$N_2(v)+N_2(w-1) \leftrightarrow N_2(v-1)+N_2(w)$$
$$N_2(v)+N_2 \leftrightarrow 2N+N_2$$
$$N_2(v)+N \leftrightarrow 2N+N$$

Pure O_2

$$O_2(v)+O_2 \leftrightarrow O_2(v-1)+O_2$$
$$O_2(v)+O \leftrightarrow O_2(v-\Delta v)+O$$
$$O_2(v)+O_2(w-1) \leftrightarrow O_2(v-1)+O_2(w)$$
$$O_2(v)+O_2 \leftrightarrow 2O+O_2$$
$$O_2(v)+O \leftrightarrow 2O+O$$

Mixed N_2

$$N_2(v)+O_2 \leftrightarrow N_2(v-1)+O_2$$
$$N_2(v_{\max})+O_2 \leftrightarrow 2N+O_2$$
$$N_2(v)+O \leftrightarrow N_2(v-1)+O$$
$$N_2(v_{\max})+O_2 \leftrightarrow 2N+O_2$$

Mixed O_2

$$O_2(v)+N_2 \leftrightarrow O_2(v-1)+N_2$$
$$O_2(v_{\max})+N_2 \leftrightarrow 2O+N_2$$
$$O_2(v)+N \leftrightarrow O_2(v-1)+N$$
$$O_2(v_{\max})+N \leftrightarrow 2O+N$$

$$O_2(v)+N_2(w-1) \rightleftharpoons O_2(v-2)+N_2(w)$$

Zeldovich exchange reactions

$$O_2(v)+N \leftrightarrow NO+O$$
$$N_2(v)+O \leftrightarrow NO+N$$

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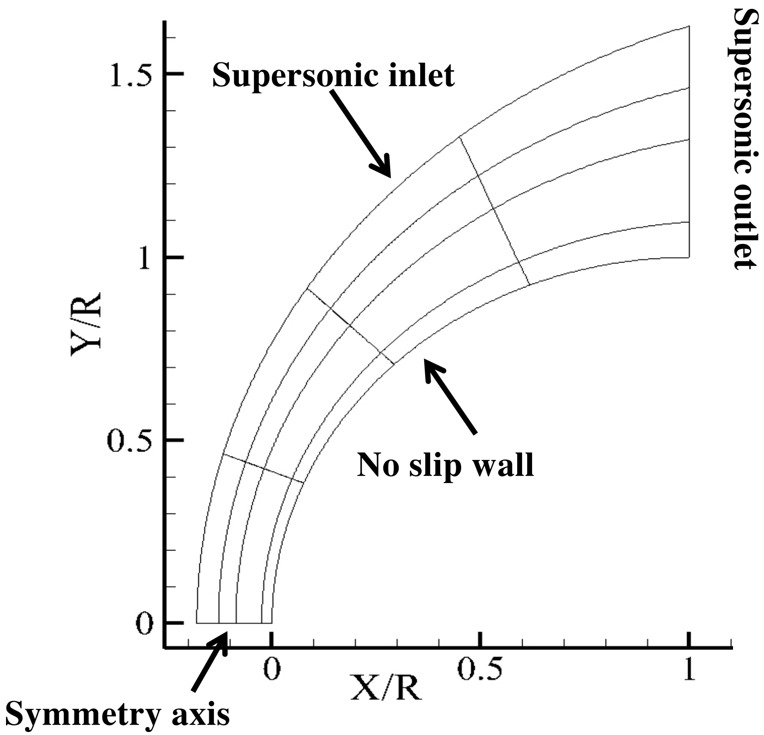
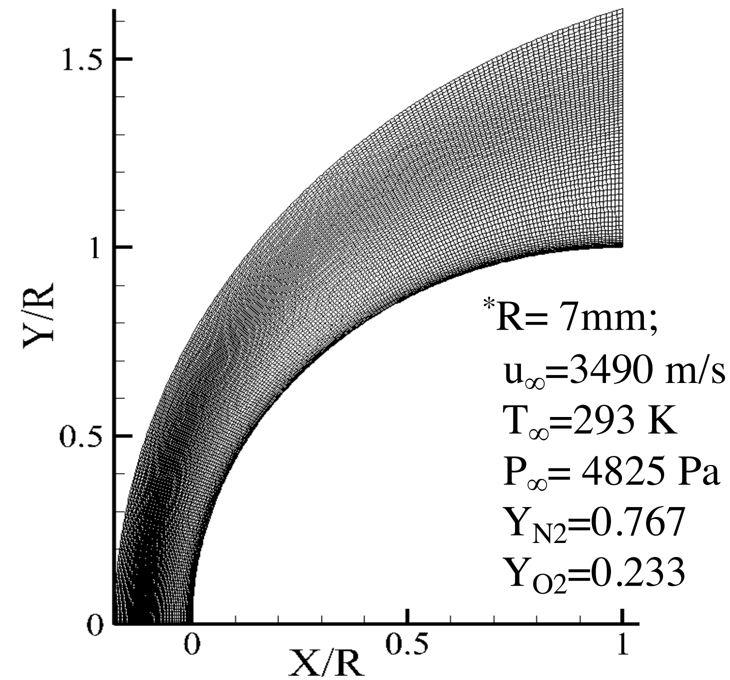
Flow past a sphere: Nonaka* test case

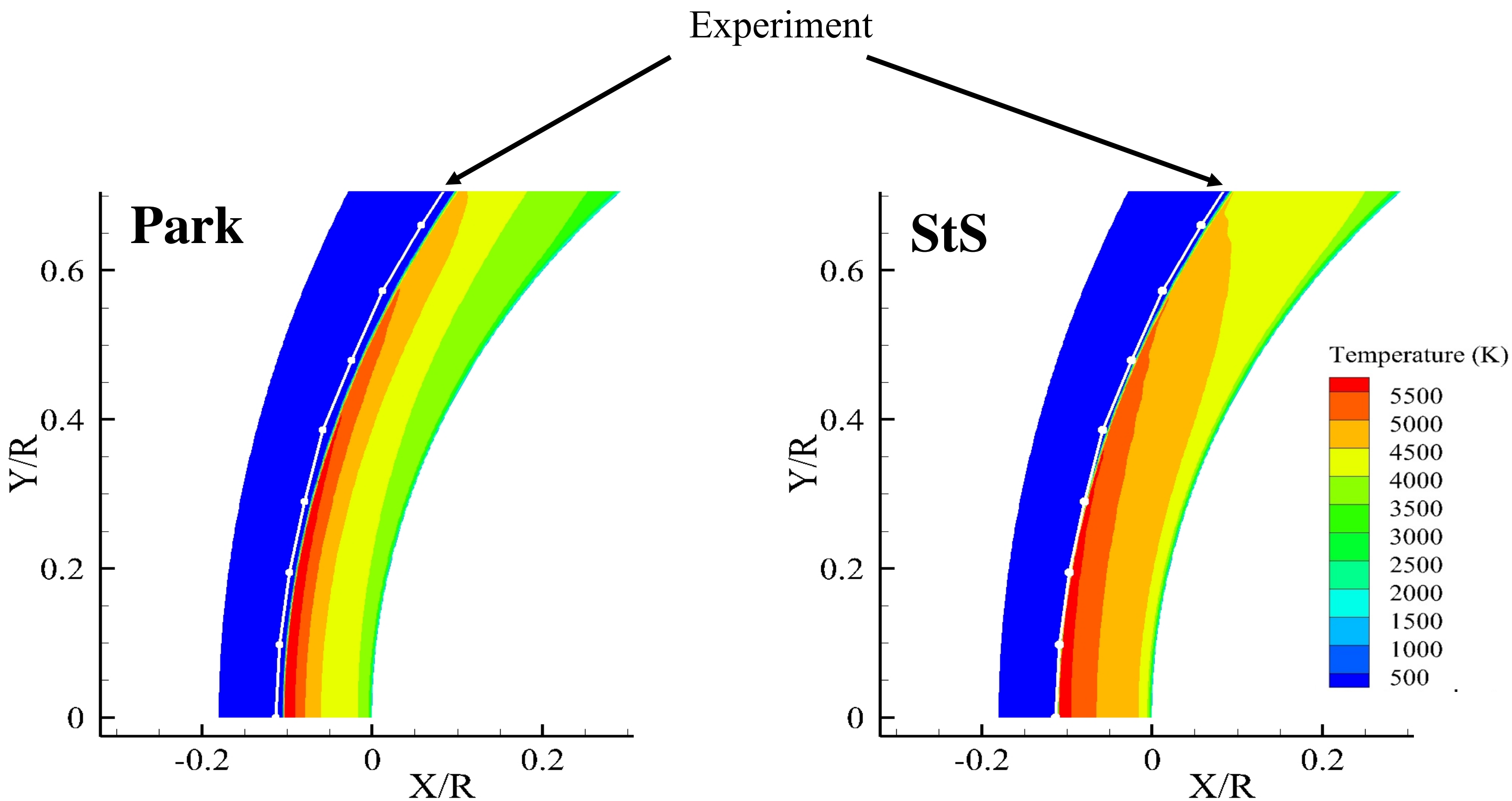
*S. Nonaka et al. ,JTHT 14 (2), 2000





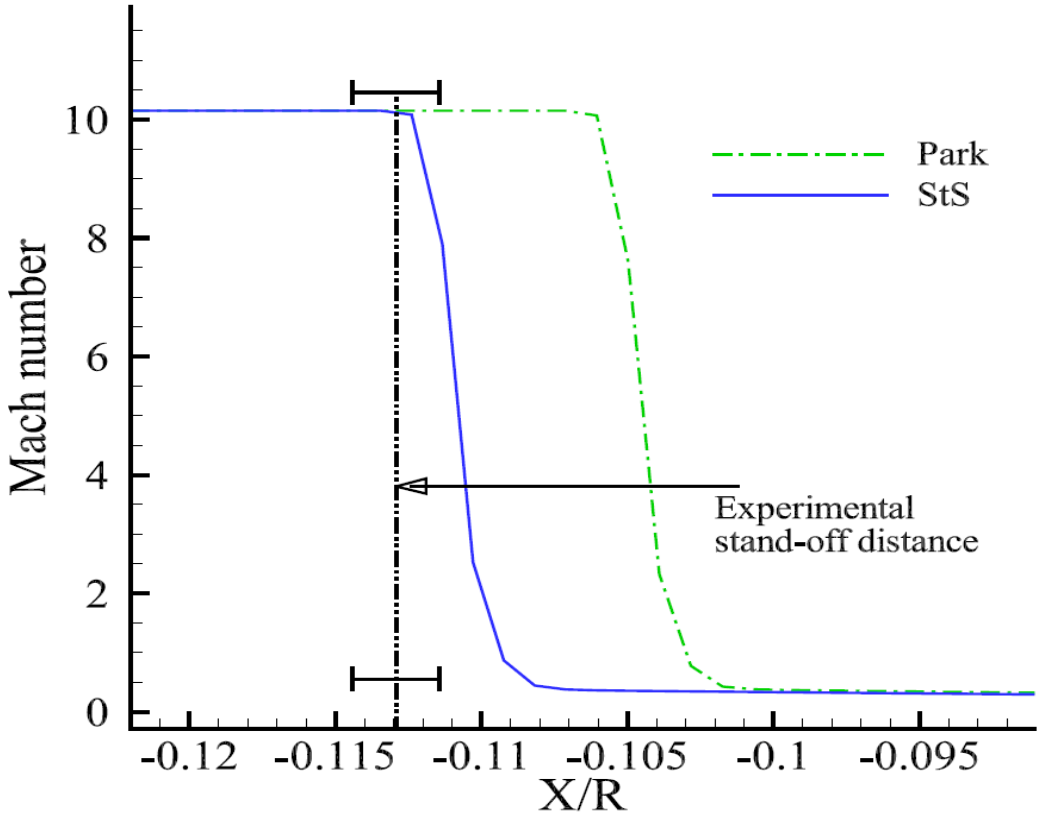
Computational domain,
with an example of 4 x4 MPI partitioning, along with boundary conditions (left).
152x392 computational grid shown every 2 grid points (right).

Nonaka test case



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

Nonaka test case: comparison along stagnation line



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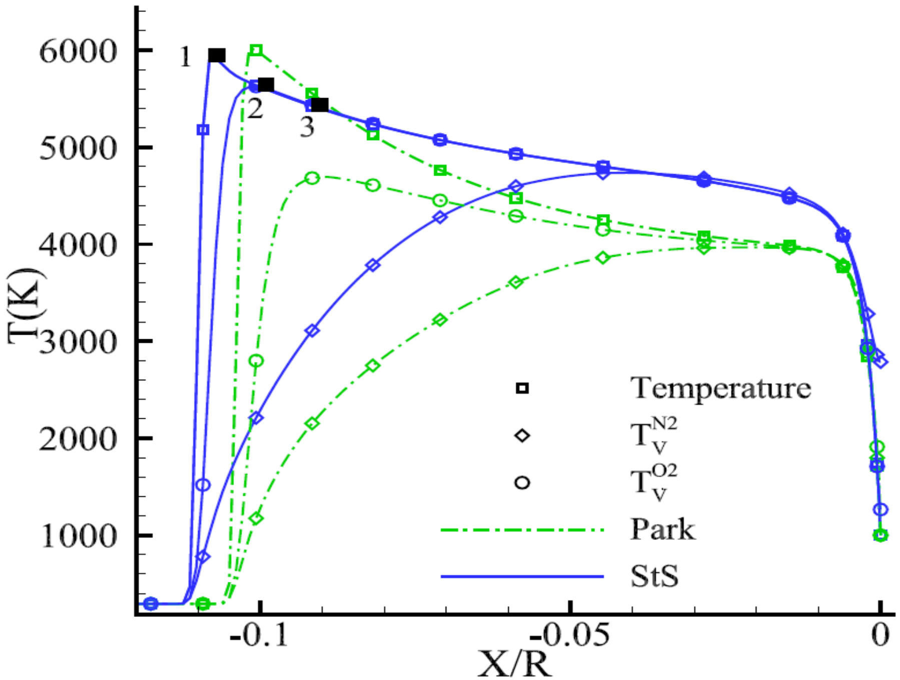
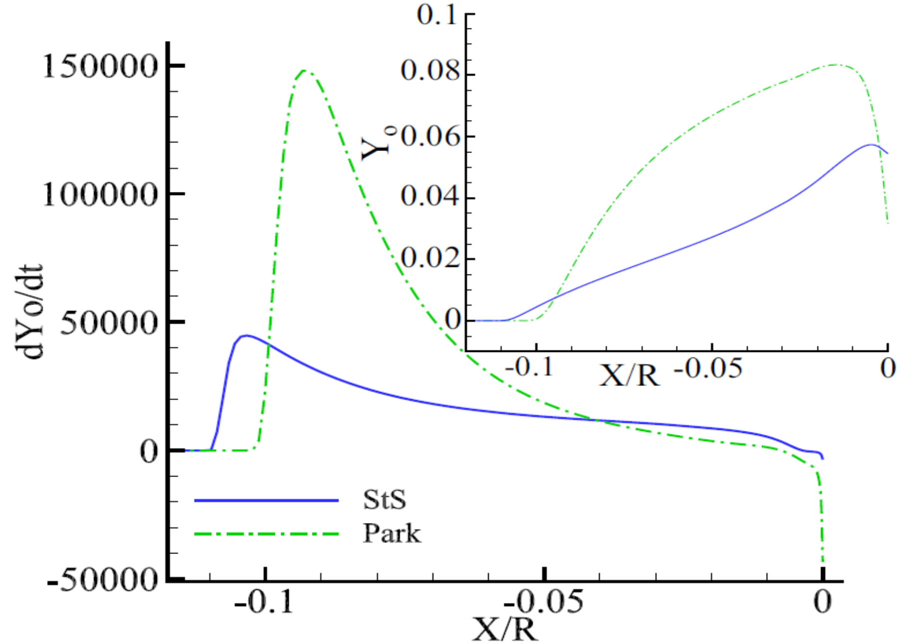


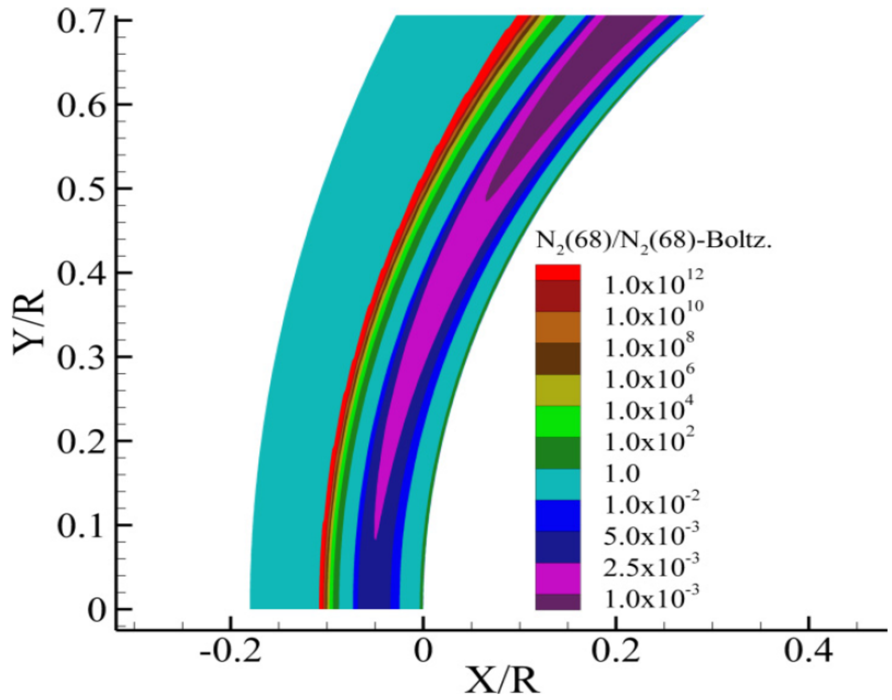
Temperatures

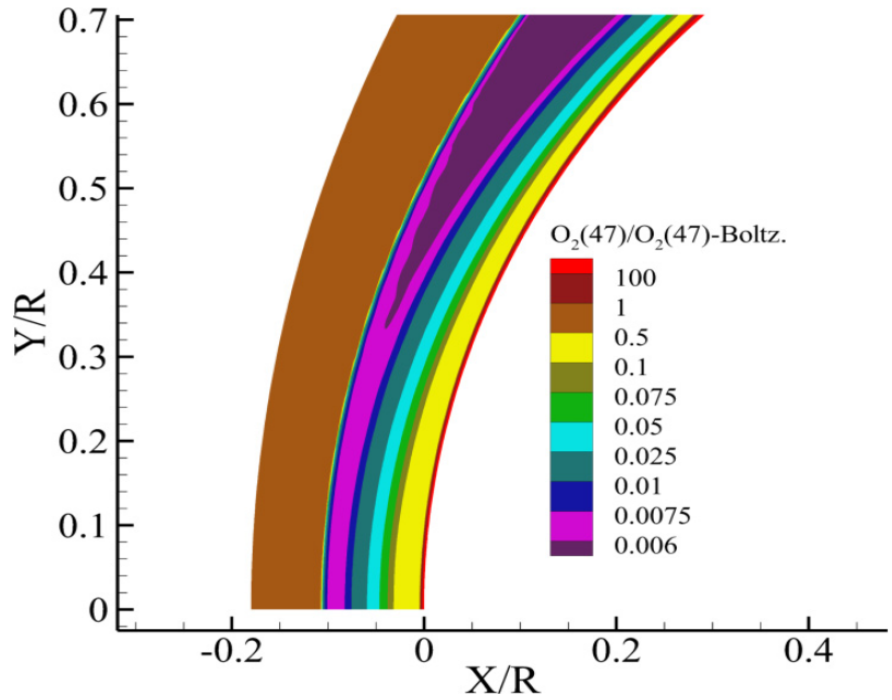


Oxygen atom reaction rate

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

Nonaka test case: highest vibrational level contour plot





Finite rate catalysis model

I. Armenise et al. JTHT 20, 465–476 (2006)
M. Barbato et al. JTHT 14, 412–420 (2000)

atom chemisorption (ch)

$$\mathrm{N} +^{*} \rightarrow \mathrm{N}^{*}$$
$$\mathrm{O} +^{*} \rightarrow \mathrm{O}^{*}$$

molecule chemisorption (chdm)

$$\mathrm{N}_2 + 2^{*} \rightarrow \mathrm{N}^{*} + \mathrm{N}^{*}$$
$$\mathrm{O}_2 + 2^{*} \rightarrow \mathrm{O}^{*} + \mathrm{O}^{*}$$
$$\mathrm{NO} + 2^{*} \rightarrow \mathrm{N}^{*} + \mathrm{O}^{*}$$

Eley–Rideal (ER)

$$\mathrm{N} + \mathrm{N}^{*} \rightarrow \mathrm{N}_2 +^{*}$$
$$\mathrm{O} + \mathrm{O}^{*} \rightarrow \mathrm{O}_2 +^{*}$$
$$\mathrm{N} + \mathrm{O}^{*} \rightarrow \mathrm{NO} +^{*}$$
$$\mathrm{O} + \mathrm{N}^{*} \rightarrow \mathrm{NO} +^{*}$$

Langmuir–Hinshelwood (LH)

$$\mathrm{N}^{*} + \mathrm{N}^{*} \rightarrow \mathrm{N}_2 + 2^{*}$$
$$\mathrm{O}^{*} + \mathrm{O}^{*} \rightarrow \mathrm{O}_2 + 2^{*}$$
$$\mathrm{N}^{*} + \mathrm{O}^{*} \rightarrow \mathrm{NO} + 2^{*}$$

thermal desorption (td)

$$\mathrm{O}^{*} \rightarrow \mathrm{O} +^{*}$$
$$\mathrm{N}^{*} \rightarrow \mathrm{N} +^{*}$$

$$\gamma_{AB} = \frac{\text{Flux of atoms recombining at the surface}}{\text{Flux of atoms impinging on the surface}}$$

$$\gamma_{NN} = \frac{2(-[N_2][S]^2 k_{chdm}^{N_2} + [N][N^*]k_{ER}^{NN} + [N^*]^2 k_{LH}^{NN})}{Z_N}$$

$$\gamma_{OO} = \frac{2(-[O_2][S]^2 k_{chdm}^{O_2} + [O][O^*]k_{ER}^{OO} + [O^*]^2 k_{LH}^{OO})}{Z_O}$$

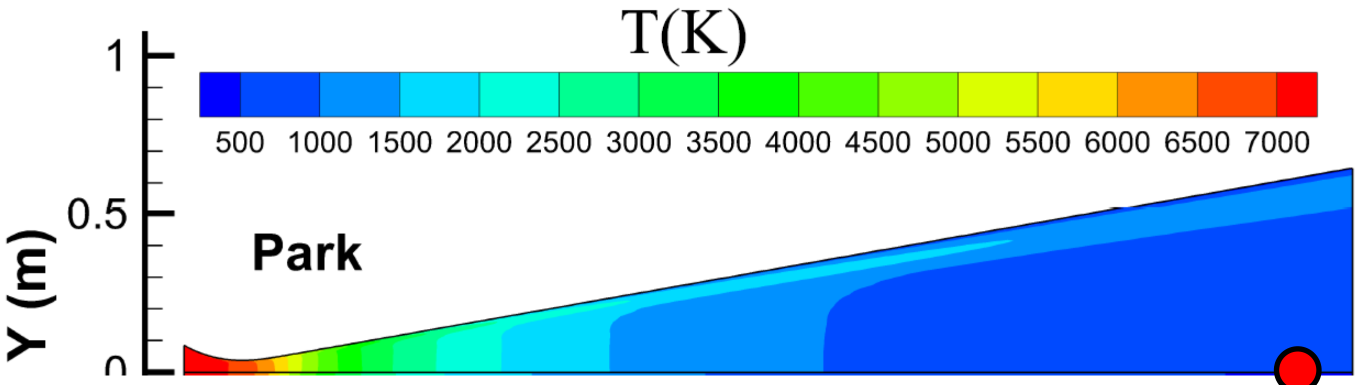
$$\gamma_{NO} = \frac{(-[NO][S]^2 k_{chdm}^{NO} + [N][O^*]k_{ER}^{NO} + [O][N^*]k_{ER}^{ON} + [N^*][O^*]k_{LH}^{NO})}{Z_N}$$

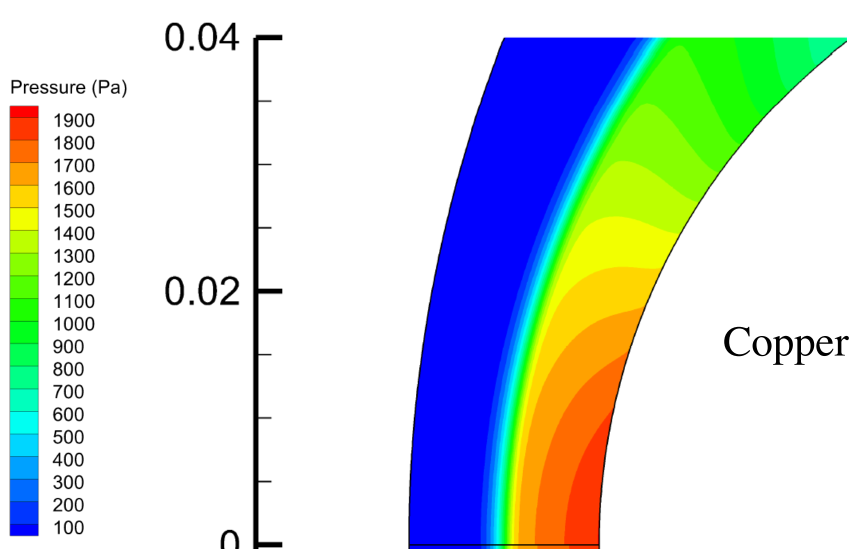
$$\gamma_{ON} = \frac{(-[NO][S]^2 k_{chdm}^{NO} + [N][O^*]k_{ER}^{NO} + [O][N^*]k_{ER}^{ON} + [N^*][O^*]k_{LH}^{NO})}{Z_O}$$

$$Z_A = [A]\sqrt{kT/(2\pi m_A)}$$

CIRA: SCIROCCO Plasma Wind Tunnel test case

F. Bonelli et al., Effect of finite-rate catalysis on wall heat flux prediction in hypersonic flow, Phys. Rev. Fluids 6, 033201





Copper sphere D=10cm, Tw=300 K

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SCIROCCO Plasma Wind Tunnel test cases

StS-1: recombing molecules have the same distribution of incoming ones

StS-2: recombing molecules have uniform distributions

StS-3: recombing molecules populate the highest vibrational level

	Exp.	Park (err. %)	StS-1 (err. %)	StS-2 (err. %)	StS-3 (err. %)	Park FC (err. %)
q_{probe} [kW/m^2]	1543	1708 (10.8%)	1873 (21.38%)	1816 (17.69%)	1774 (14.97%)	2160 (39.99%)

Total heat flux at the stagnation point

[kW/m^2]	Park	StS-1	StS-2	StS-3	Park FC
roto-translational (% contribution)	1082 (63.34%)	1213.3 (64.78%)	1516.0 (83.48%)	1763.8 (99.41%)	1146.6 (53.07%)
diffusive (% contribution)	606.10 (35.48%)	660.17 (35.25%)	300.0 (16.52%)	10.38 (0.59%)	1000.5 (46.31%)
vibrational (% contribution)	20.18 (1.18%)				13.3 (0.62%)

Decomposition of the total heat flux at the stagnation point

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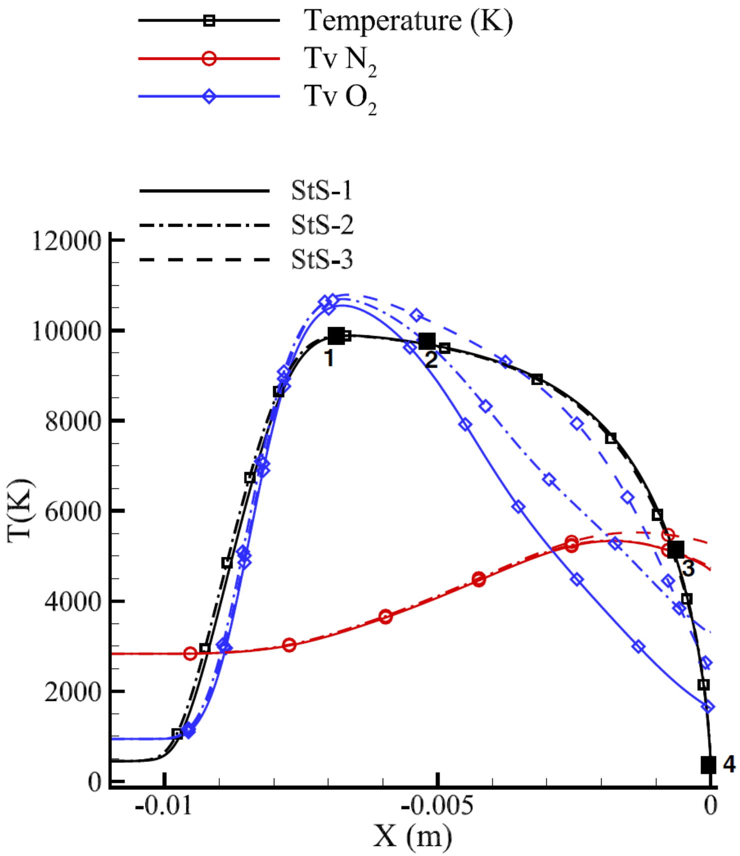
CIRA: SCIROCCO Plasma Wind Tunnel test case stagnation line profiles

F. Bonelli et al., Effect of finite-rate catalysis on wall heat flux prediction in hypersonic flow, Phys. Rev. Fluids 6, 033201



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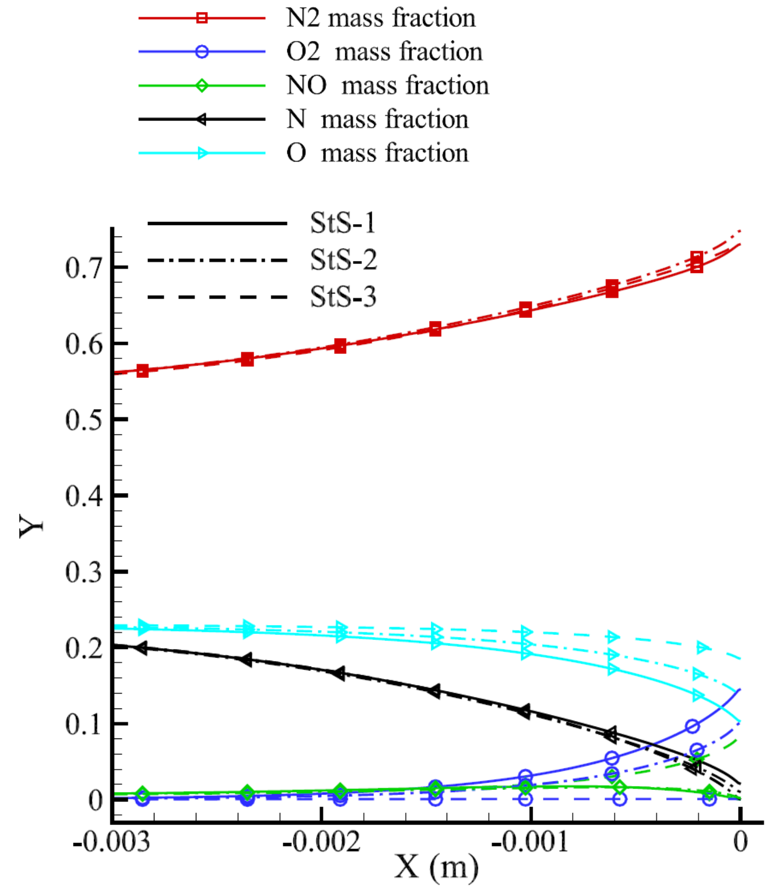

Mass fractions

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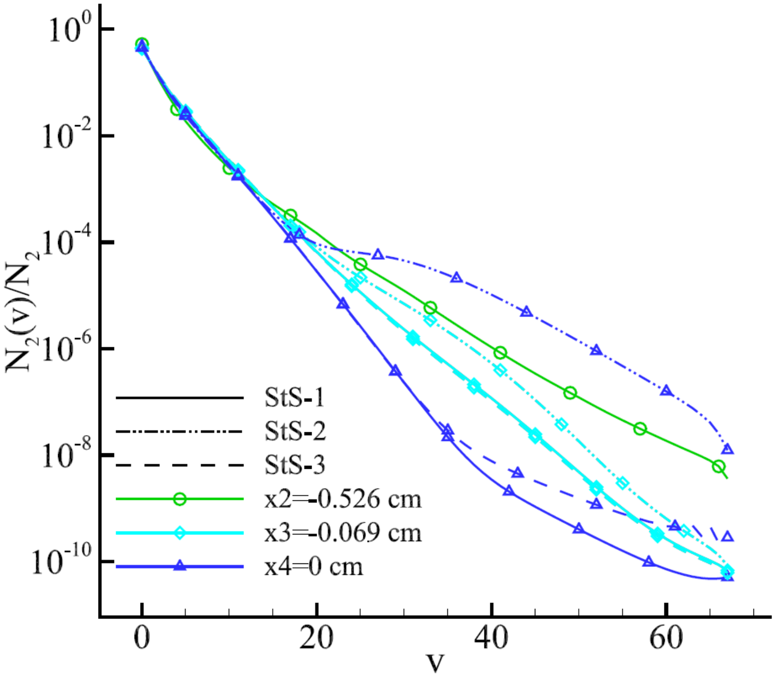
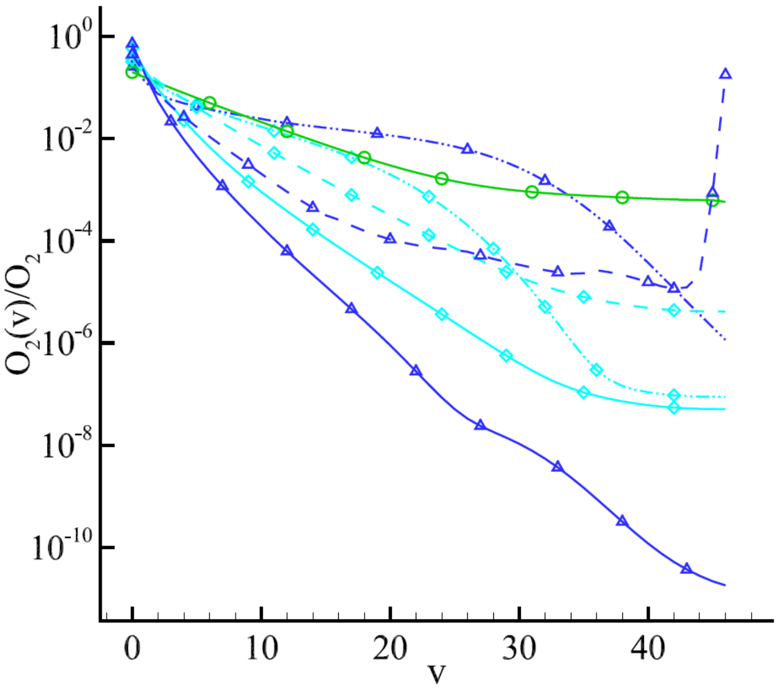
CIRA: SCIROCCO Plasma Wind Tunnel test case – vibrational distributions





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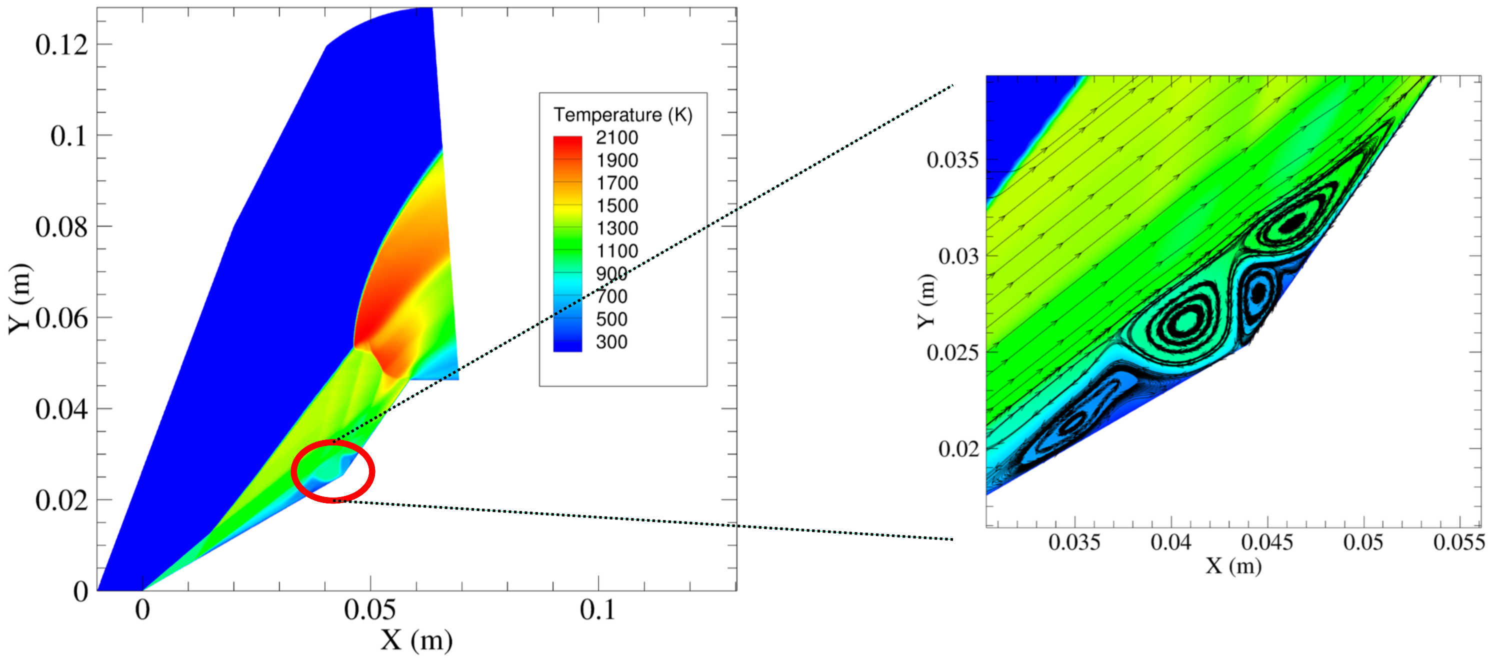
DOUBLE WEDGE TEST CASES

D. Ninni et. Acta astronautica 191 (2022) 178



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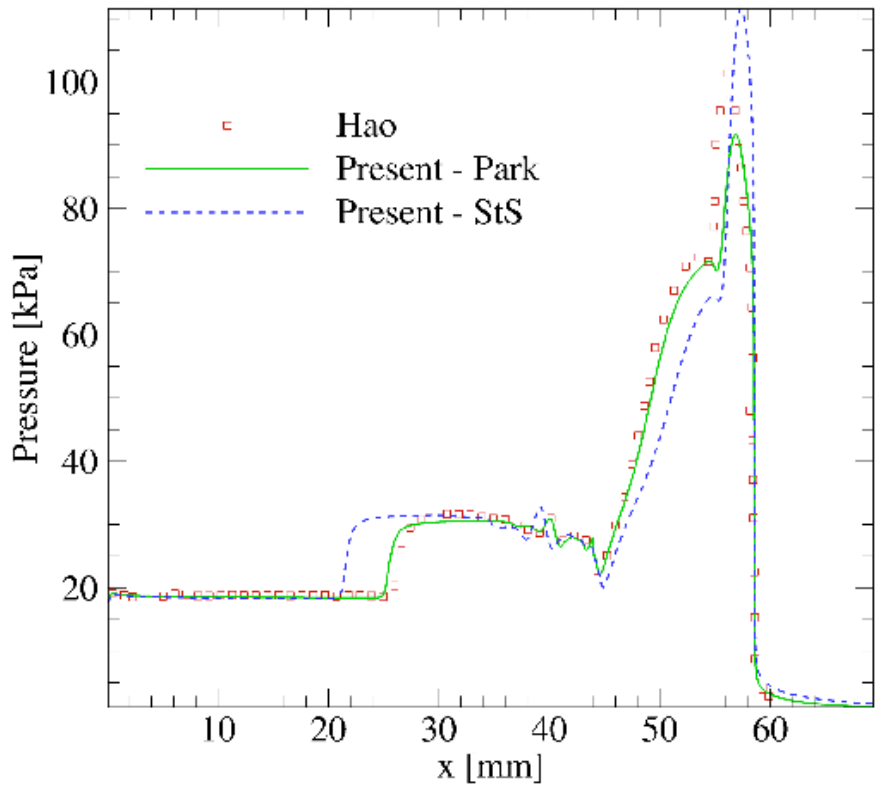
DOUBLE WEDGE TEST CASES: StS vs, Park

D. Ninni et. Acta astronautica 191 (2022) 178



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Conclusions

- The StS model has been implemented in 2D fluid dynamic code accelerated by GPU (speedup ~ 100)
- The code has been applied to blunt body including also state-resolved surface processes and kinetic equation for active surface site occupation.
- Application to unsteady flows as double wedge.
- Comparison with Park multi-temperature models shows differences in all the test cases
- 3D version of the code is under construction,