State-to-State Transport in Hypersonic Flows

- Master Thesis in Aerospace Engineering
- Ana Catarina Garbacz Gomes
- Nr: 75687

- Instituto Superior Técnico
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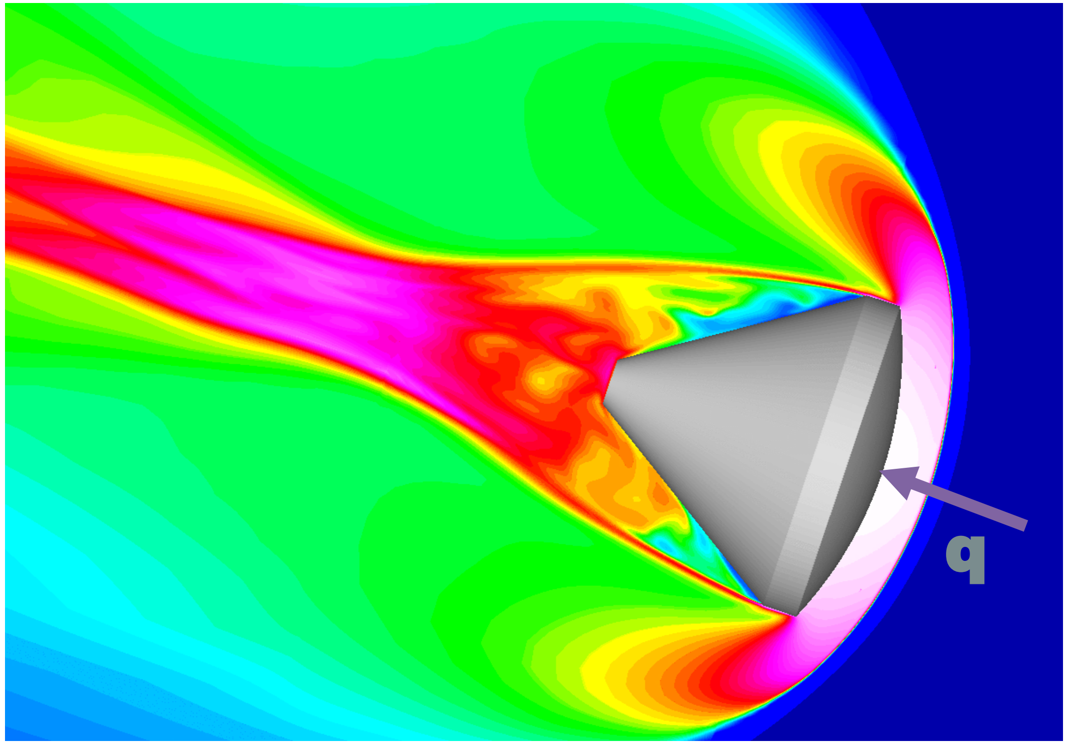
Motivation



- Interplanetary Missions

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- TPS Design

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- Hyperbolic reentry flow analysis

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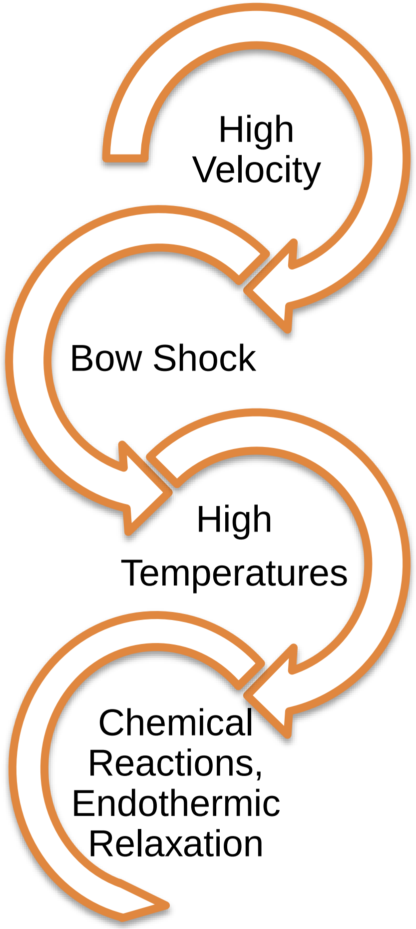
- Uncertainties in heat flux prediction:
  - Up to 50% for convective flux
  - More than 100% for radiative flux

Hypersonic Reentry



High Velocity

Bow Shock

High Temperatures

Chemical Reactions, Endothermic Relaxation

Strong thermal and chemical nonequilibrium

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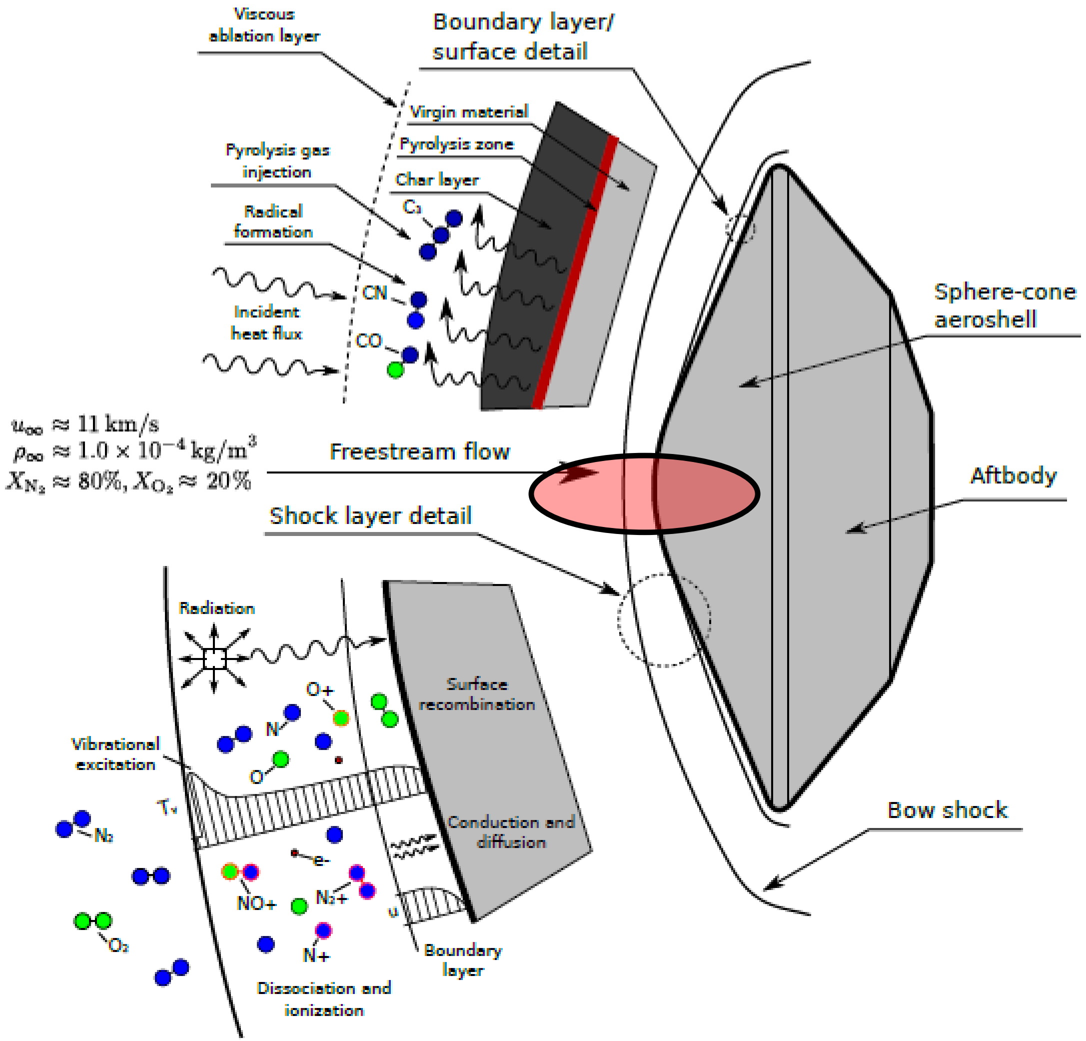
Detailed Microscopic Models



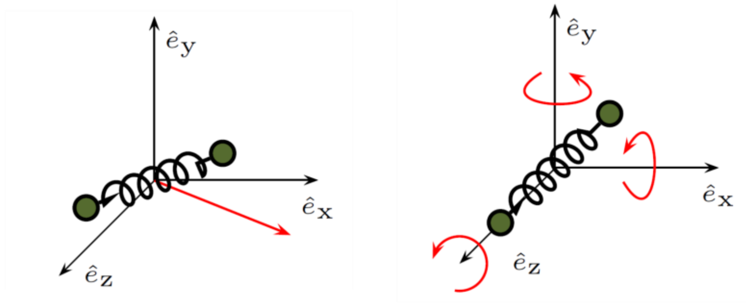
(D. F. Potter. Modelling of radiating shock layers for atmospheric entry at Earth and Mars. PhD thesis, The University of Queensland, Australia, 2011..)

Approach

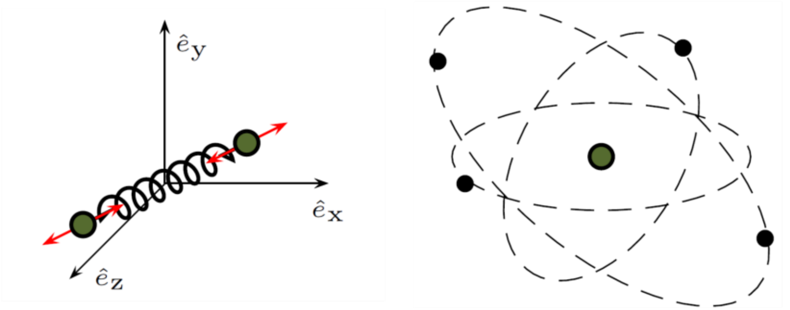
1. Multi-Temperature
2. State-to-State (more detailed)

Macroscopic to Microscopic

- **Multi-Temperature:** Boltzmann distribution
- **State-to-State:** non-Boltzmann distribution

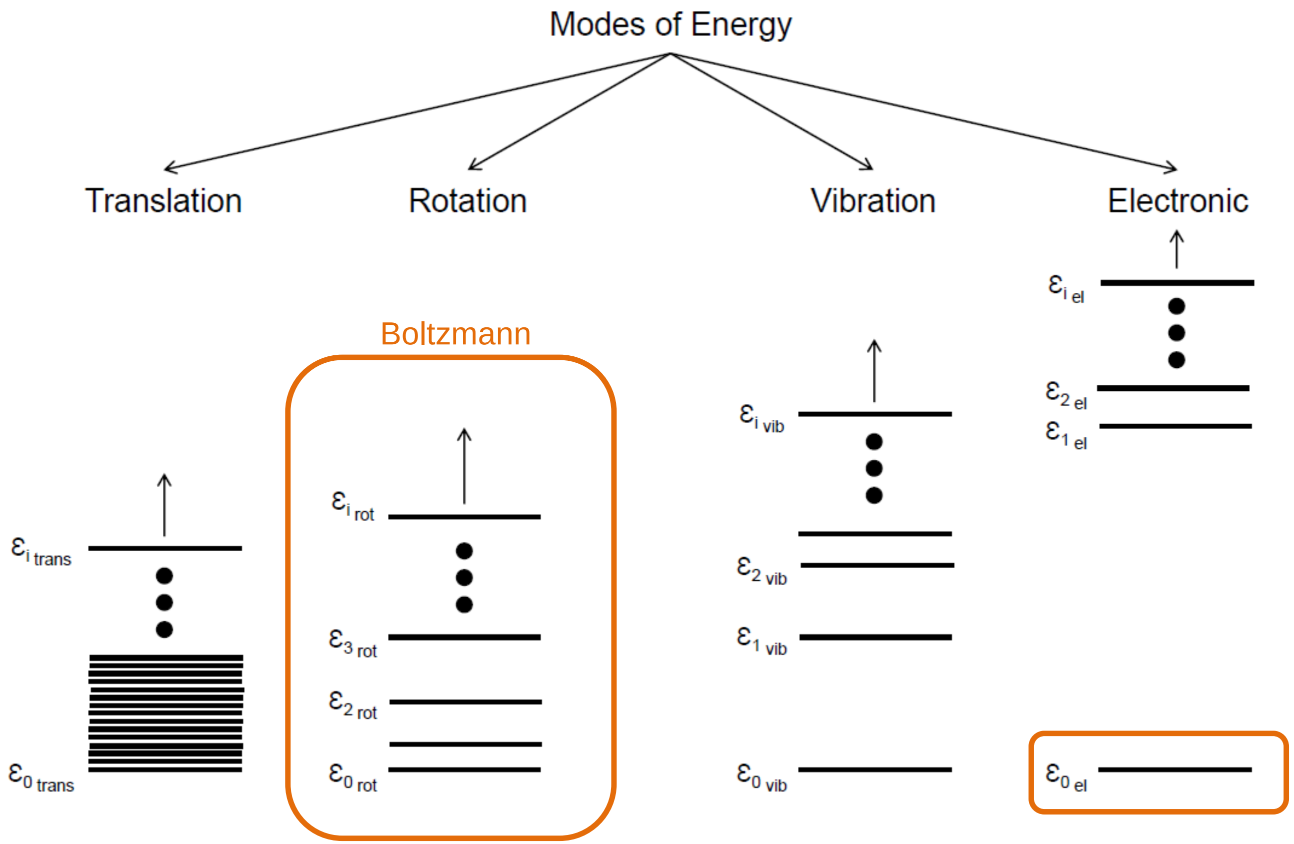


(a) Translational Mode (b) Rotational Mode



(c) Vibrational Mode (d) Electronic Excitation Mode

(adapted from: B. Lopez. Simulation des Écoulements de Plasma Hypersonique Hors Équilibre Thermochimique. PhD thesis, Université D'Orléans, 2010.)



Modes of Energy

Translation

Rotation

Vibration

Electronic

Boltzmann

$\varepsilon_{i\ trans}$ $\varepsilon_{0\ trans}$

$\varepsilon_{i\ rot}$ $\varepsilon_{3\ rot}$ $\varepsilon_{2\ rot}$ $\varepsilon_{0\ rot}$

$\varepsilon_{i\ vib}$ $\varepsilon_{2\ vib}$ $\varepsilon_{1\ vib}$ $\varepsilon_{0\ vib}$

$\varepsilon_{i\ el}$ $\varepsilon_{2\ el}$ $\varepsilon_{1\ el}$ $\varepsilon_{0\ el}$

(adapted from: J. D. Anderson. Hypersonic and High Temperature Gas Dynamics. AIAA, 2nd edition, 1989.)

Physical Models

- Multi-Temperature Approach:
  - Boltzmann distribution
- Kinetic Scheme: Air5-STELLAR-Boltzmann
- Thermal energy source term:

$$\dot{\Omega}_{V-T,s} = \rho_s \frac{\varepsilon^{eq}_{vib,s}(T_{tra}) - \varepsilon_{vib,s}(T_{vib})}{\tau_{VT,s}}$$

- Transport Models: Gupta-Yos/CCS

🟩 Transport Terms 🟥 Source Terms

Conservation equations:

$$\frac{\partial(\rho c_i)}{\partial t} + \vec{\nabla} \cdot (\rho c_i \vec{u}) = \vec{\nabla} \cdot \boxed{\vec{J}_i} + \boxed{\dot{\omega}_i}$$

$$\frac{\partial(\rho \vec{u})}{\partial t} + \vec{\nabla} \cdot (\rho \vec{u} \otimes \vec{u}) = \vec{\nabla} \cdot \boxed{[\tau]} - \vec{\nabla} p$$

$$\frac{\partial(\rho E)}{\partial t} + \vec{\nabla} \cdot (\rho E \vec{u}) = \vec{\nabla} \cdot \left(\sum_k \boxed{\vec{q}_{C_k}} + \sum_i \boxed{\vec{J}_i} h_i + \vec{u} \cdot \boxed{[\tau]} - p\vec{u} \right)$$

$$\frac{\partial}{\partial t}(\rho \varepsilon_k) + \vec{\nabla} \cdot (\rho \vec{u} h_k) = \vec{\nabla} \cdot \left(\boxed{\vec{q}_{C_k}} + \sum_i \boxed{\vec{J}_i} h_{i,k} \right) + \boxed{\dot{\Omega}_k}$$

Physical Models

🟩 Transport Terms 🟥 Source Terms

Conservation equations:

- State-to-State Approach:
  - non-Boltzmann distribution
- Kinetic Scheme: Air5-STELLAR
  - Vibrational state-specific reaction rates – FHO model
- Transport Models: Model 0, Model 1

$$\frac{\partial(\rho c_v)}{\partial t} + \vec{\nabla}.(\rho c_v \vec{u}) = \vec{\nabla}.\boxed{\vec{J}_v} + \boxed{\dot{\omega}_v}$$

$$\frac{\partial(\rho \vec{u})}{\partial t} + \vec{\nabla}.(\rho \vec{u} \otimes \vec{u}) = \vec{\nabla}.\boxed{[\tau]} - \vec{\nabla} p$$

$$\frac{\partial(\rho E)}{\partial t} + \vec{\nabla}.(\rho E \vec{u}) = \vec{\nabla}.\left(\sum_k \boxed{\vec{q}_{c_k}} + \sum_v \boxed{\vec{J}_v} h_v + \vec{u}.\boxed{[\tau]} - p\vec{u} \right)$$

Physical Models – Transport

Multi-Temperature: Boltzmann	State-to-State: non-Boltzmann	
Gupta-Yos/CCS	Model 0	Model 1
$(D_{ij}, \mu, \lambda) = f(x_i, \boxed{\Delta_{ij}}, C_i)$	$(D_{ij_{vw}}, \mu, \lambda) = f(x_v, C_i, \boxed{\Delta_{ij}})$	$(D_{ij_{vw}}, \mu, \lambda) = f(x_v, C_i, \boxed{\Delta_{ij} \times S_v})$

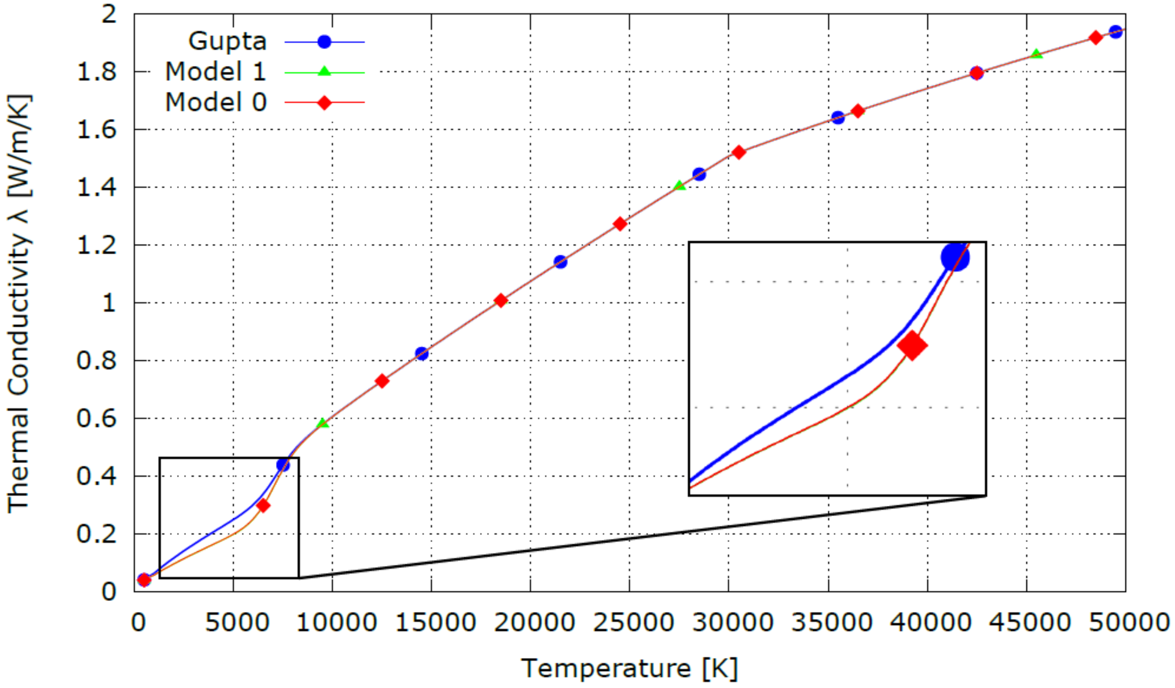
- *D* – mass diffusion, μ – viscosity, λ – thermal conductivity
- x – molar fraction, Δ – collision term, C – coefficient, S – state-specific factor
- i/j – chemical species, v/w – vibrational level

Numerical Setup – Verification & Validation

SPARK

Software Package for Aerodynamics Radiation and Kinetics

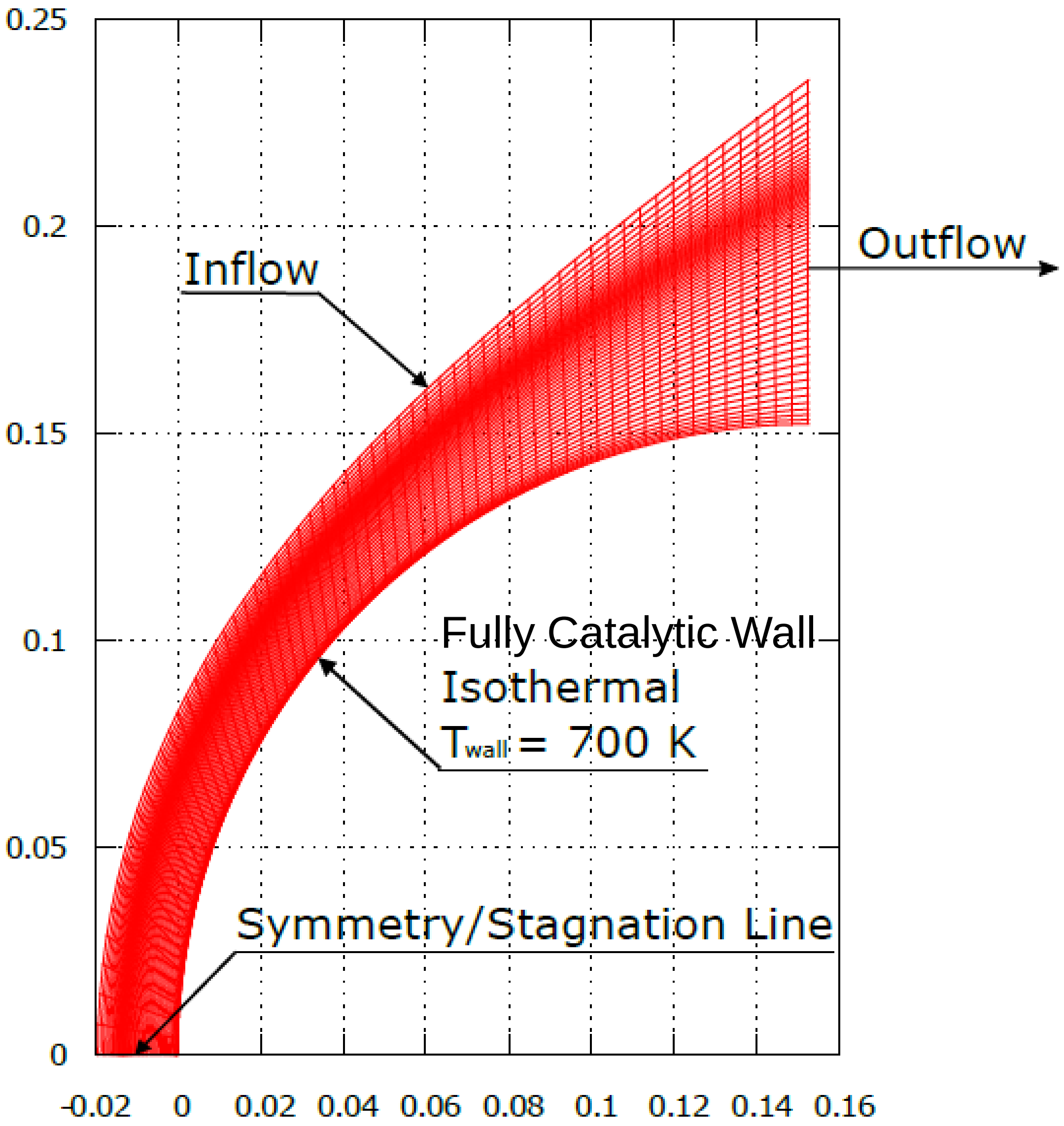
- Equilibrium, Temperature-dependent transport coefficients
  - N_2, N
  - 500 – 50,000 K
  - Ambient pressure
  - Models: Gupta-Yos/CCS, Model 0, Model 1



Numerical Setup – Problem Definition

- Application case study:
  - N_2 Flow over a sphere r = 0.15 m – 2D axissymetric
  - N_2/N mixture
    - 61 vibrational levels $N_2(v)$
    - 1 electronic level N

    } 62 pseudo-species
  - Upstream conditions:
    - V_∞ = 7 km/s
    - p_∞ = 27 Pa
    - T_∞ = 300 K, 700 K



Numerical Setup - Simulations

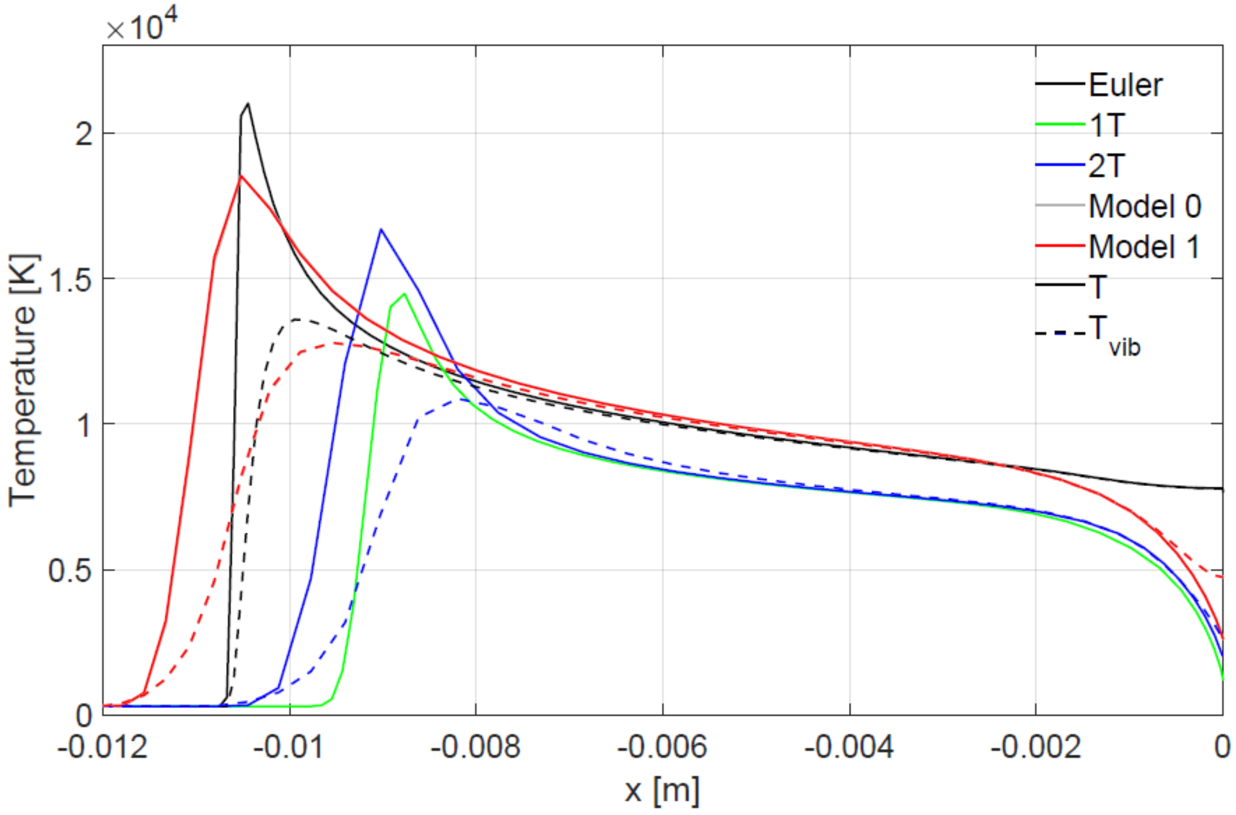
SPARK

Software Package for Aerodynamics Radiation and Kinetics

	Internal Modes Description Model	Transport Model	Kinetic Scheme	T_∞ [K]
Test-case 1	Boltzmann (One-temperature)	Gupta-Yos/CCS	Air5-STELLAR-Boltzmann	300
Test-case 2	Boltzmann (Two-temperature)	Gupta-Yos/CCS	Air5-STELLAR-Boltzmann	300
Test-case 3	Vibrational state-specific	- (Euler)	Air5-STELLAR	300
Test-case 4	Vibrational state-specific	Model 0	Air5-STELLAR	300
Test-case 5	Vibrational state-specific	Model 1	Air5-STELLAR	300
Test-case 6	Vibrational state-specific	Model 0	Air5-STELLAR	700
Test-case 7	Vibrational state-specific	Model 1	Air5-STELLAR	700

Results – Transport Models $T_\infty = 300$ K

Temperature

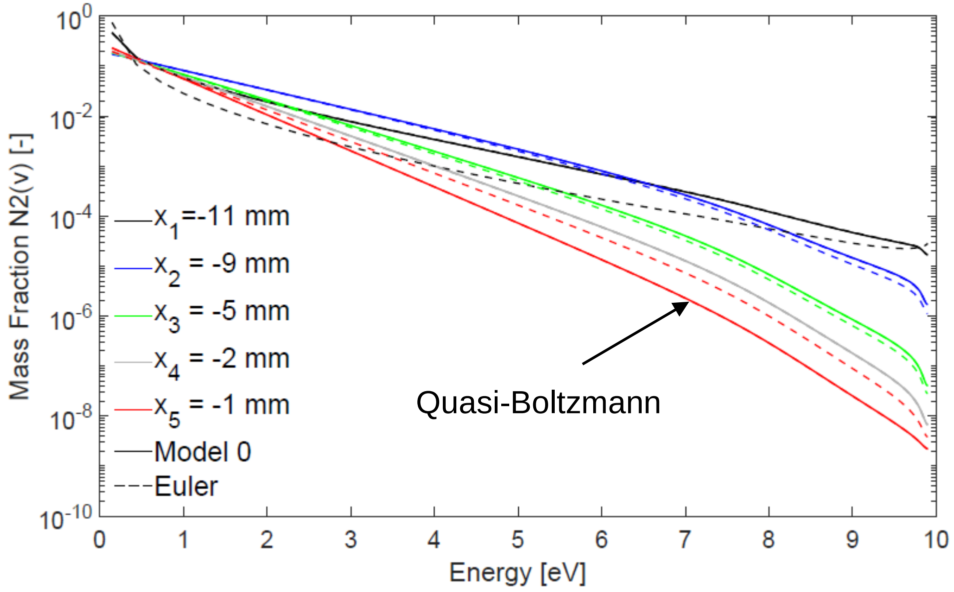


- Impact of Model 1 is negligible – consistent with verification analysis (Model 0 vs. Model 1).
- Transport phenomena leads to a 15% lower peak temperature and larger shock layer thickness (Euler vs. Model 0).
- Larger shock standoff distance and higher peak temperature for more detailed models (respectively, State-to-State, 2T, 1T).
- Equilibrium is not completely achieved near the wall.

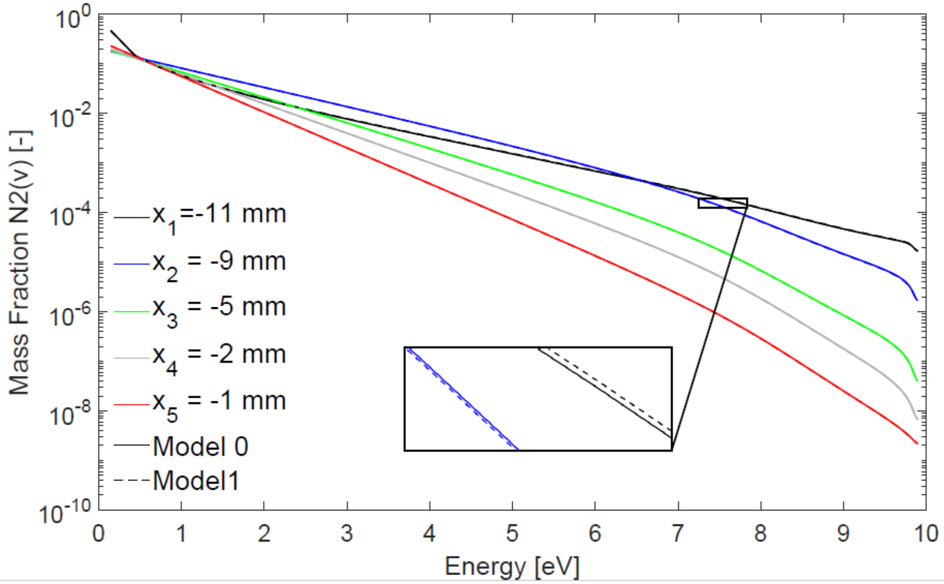
Results – Transport Models
T_{∞} = 300 K

Vibrational Distribution Functions $N_2(v)$ – 300 K

- Lower/higher mass fractions in the shock/boundary layer regions for Euler (Euler vs. Model 0).
- With Model 0, Boltzmann equilibrium is nearly reached in the boundary layer, as opposed to Euler (Euler vs. Model 0).
- Impact of Model 1 is more enhanced in the shock layer, yet negligible (Model 0 vs. Model 1).



Euler vs. Model 0

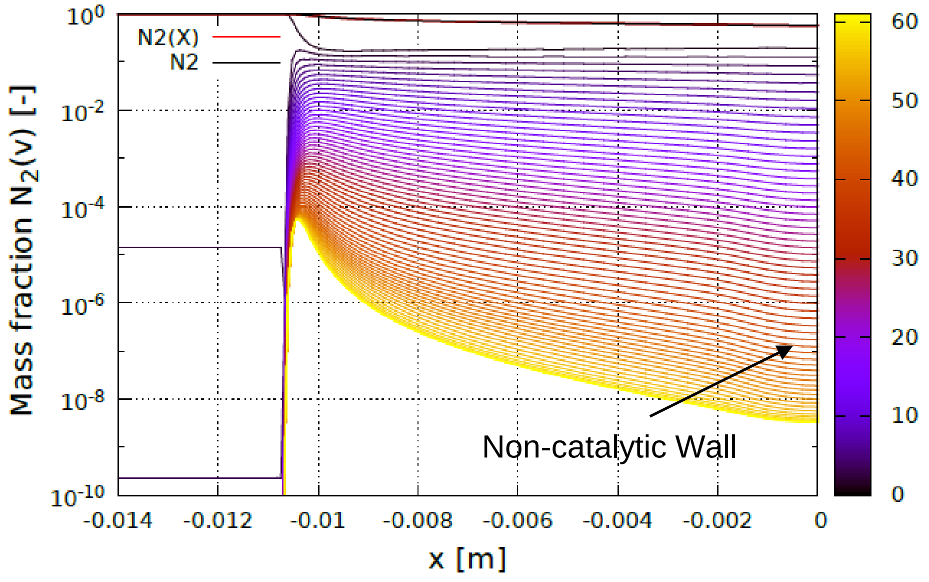


Model 0 vs. Model 1

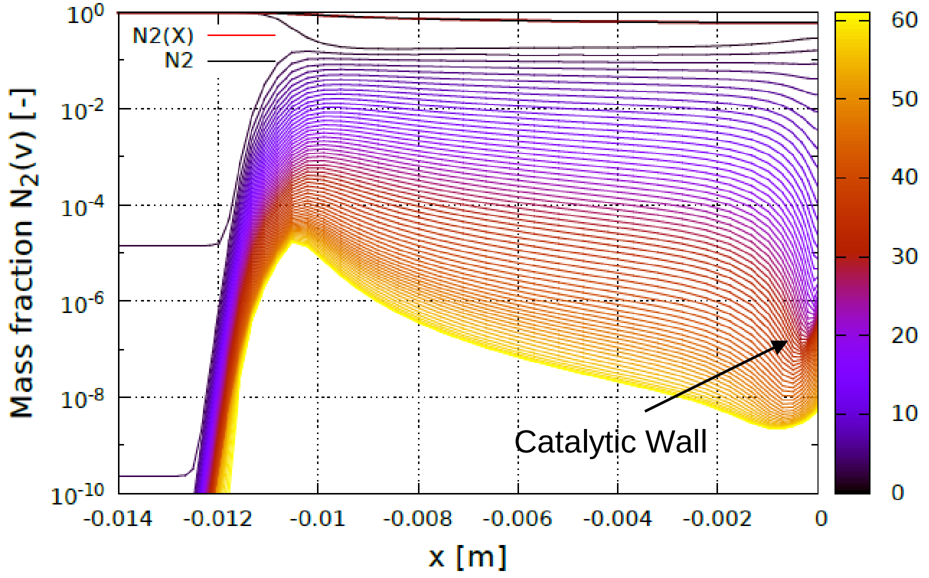
Results – Transport Models
$T_\infty = 300$ K

Mass Fractions – Vibrational Levels $N_2(v)$ – 300 K

- Peak temperature - sudden increase in the population of upper vibrational levels.
- At x = -10.5 mm, dissociation takes over.
- Mass diffusion effects in Model 0 result in smoother curves.
- Recombination effects in the boundary layer, for Model 0.



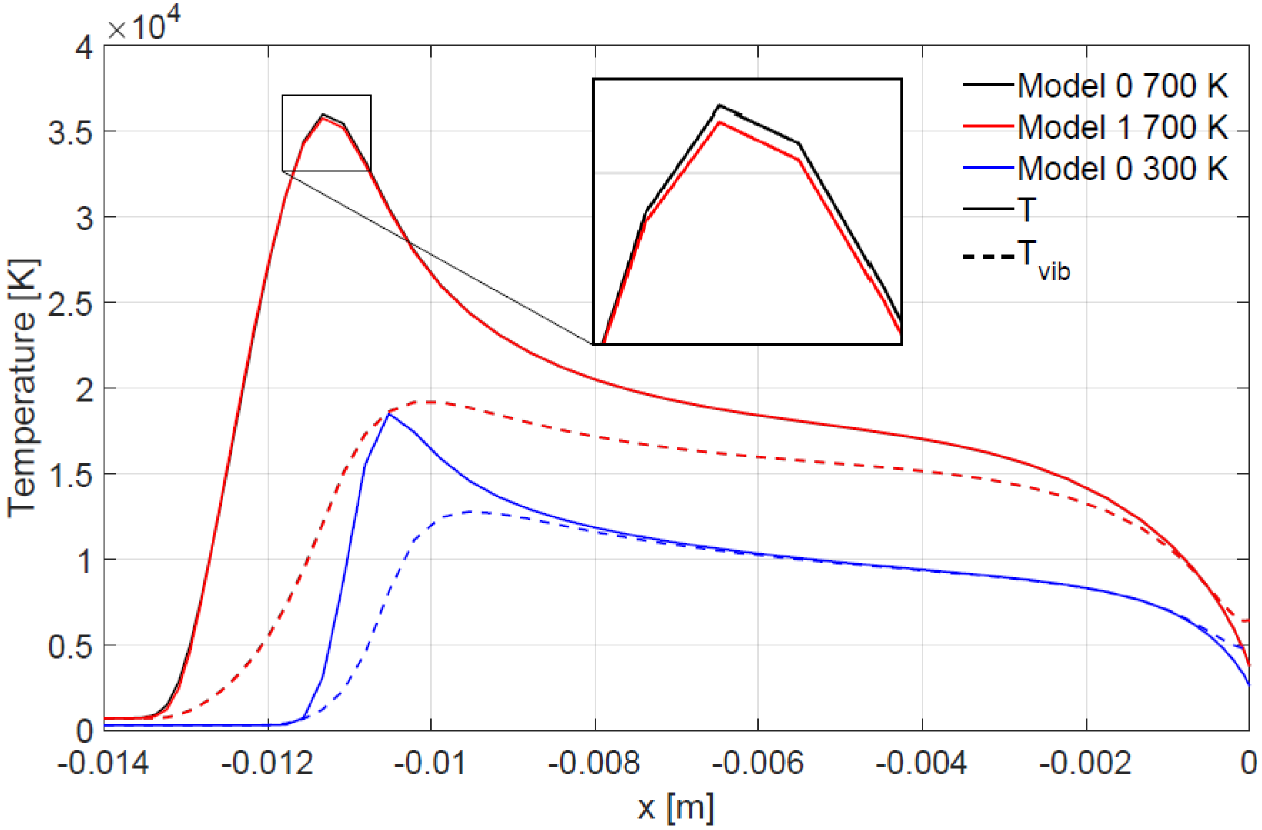
Euler.



Model 0.

Results – Freestream Temperature

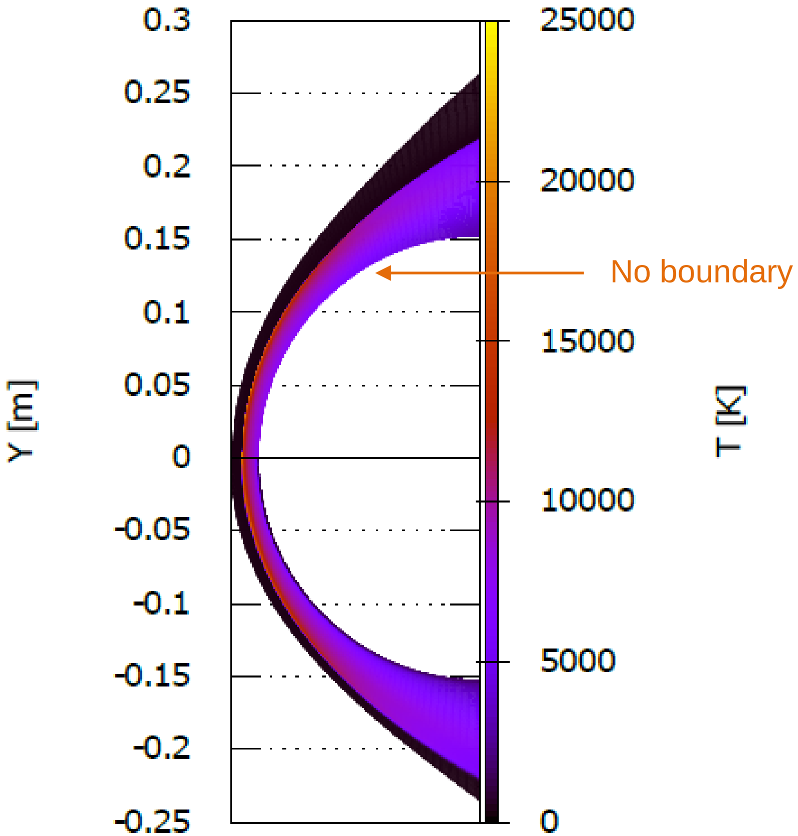
Temperature – T_∞ = 300 K vs. T_∞ = 700 K



- 10% larger shock standoff distance and 50% higher peak temperature for T_∞ = 700 K.
- Model 1 leads to a more diffusive peak temperature.
- Equilibrium is not completely achieved near the wall.

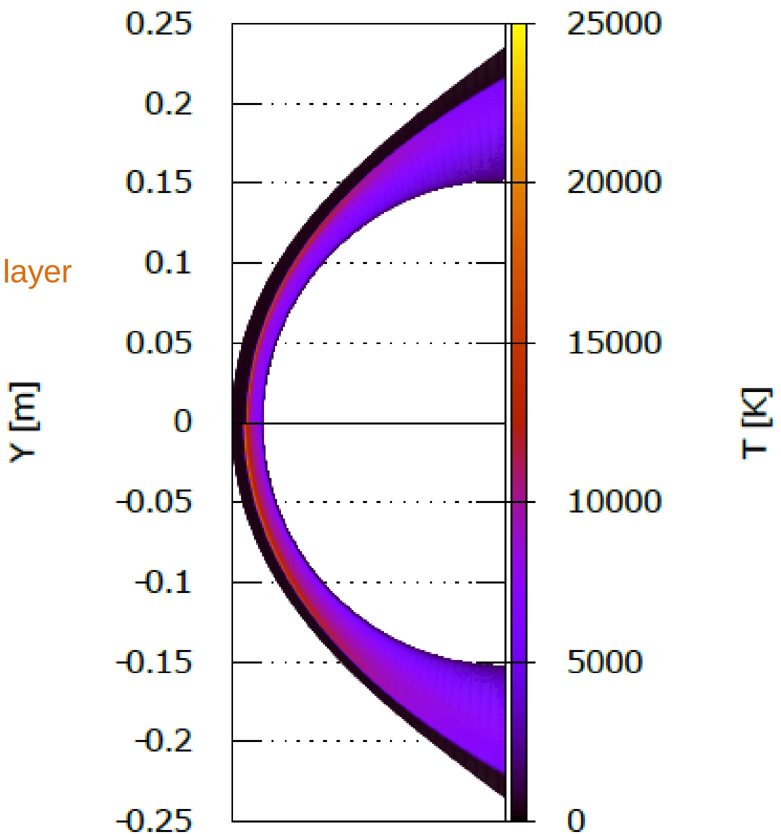
Results – Temperature Fields

2D Temperature field

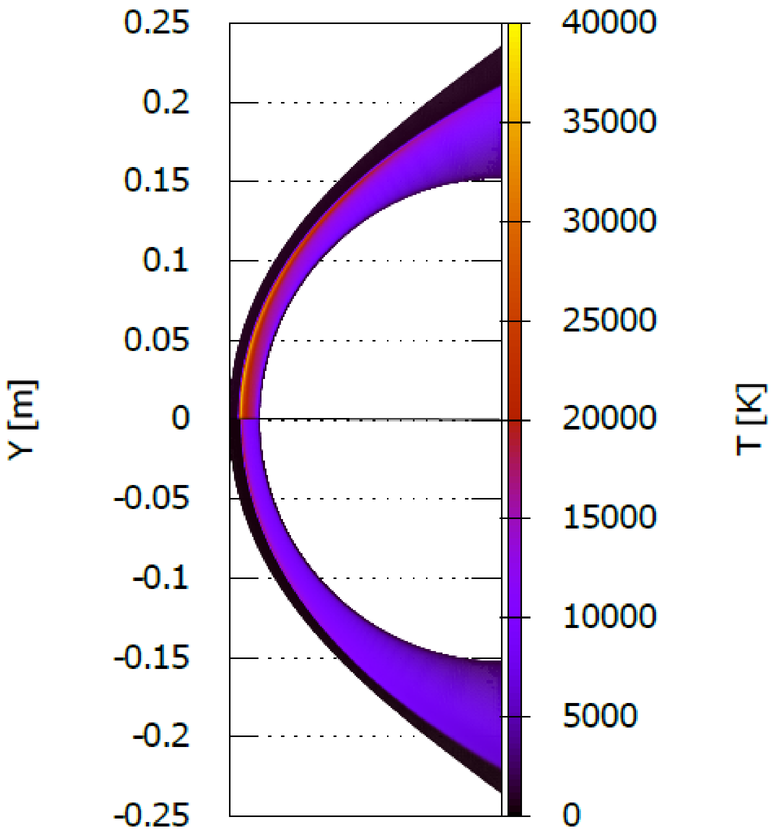


No boundary layer

Euler vs. Model 0, T_∞ = 300 K
(top) (bottom)



2T vs. Model 0, T_∞ = 300 K
(top) (bottom)



Model 0, T_∞ = 300 K vs. T_∞ = 700 K
(top) (bottom)

Conclusions

- State-to-State Navier-Stokes simulations are a significantly stiff problem:
  - Convergence was very slow – CFL around 0.01.
  - Simulations crashed when trying implicit schemes.
- A grid convergence study is required, given the uncertainties in the boundary layer region.
- Model 0 has a significant impact on the prediction of radiative heat fluxes.
- Model 1 does not influence flow properties.

Future Work

- More rigorous mesh refinement in the boundary layer region.
- Inclusion of a detailed state-specific transport model in the governing fluid dynamic equations – Kustova’s model.
- Paper - AIAA Science and Technology Forum and Exposition 2019
  - “Simplified Transport Modelling Strategies for Fully Coupled Navier-Stokes and State-Specific Simulations of Hypersonic Flows”, Ana Garbacz Gomes, Mário Lino Da Silva, Maria Castela, Bruno Lopez.

Thank You

Master Thesis in Aerospace Engineering

Ana Catarina Garbacz Gomes

Nr: 75687

Instituto Superior Técnico

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