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Molecular-level Simulations of Hypersonic Flow past a Cylinder

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Presentation Outline

- Brief overview of molecular level (rarefied) gas dynamics
- Direct Simulation Monte Carlo Method
- Hypersonic Flow- Modelling considerations
- Mach 25 Flow past a cylinder
  - Aerothermodynamics effects
  - Low-density effects
- Summary & Conclusions

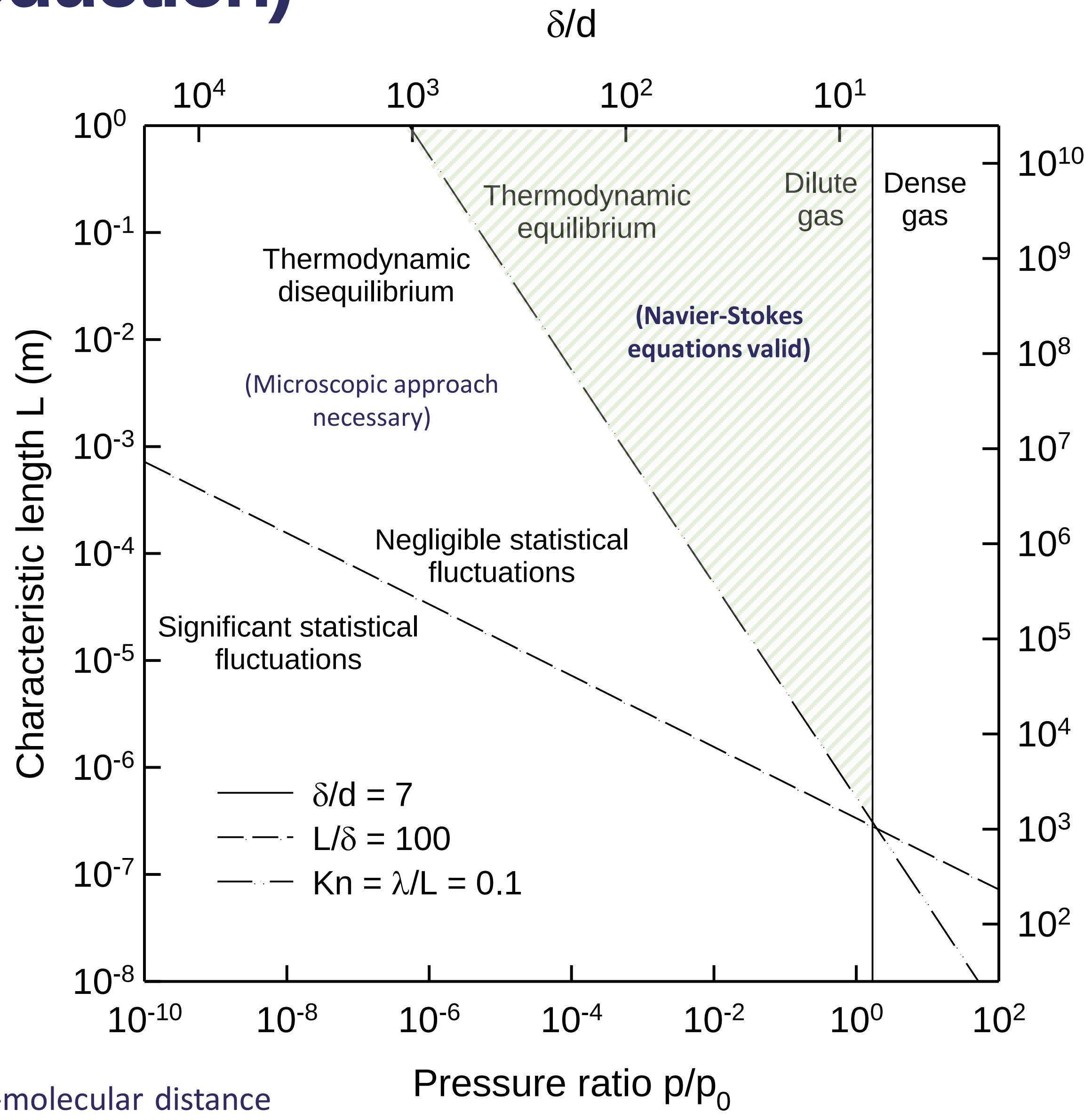
Non-equilibrium Rarefied Gas Dynamics (A brief introduction)

Key Points:

- The shaded region is where Navier-Stokes and Fourier's law can be applied. Below that line thermodynamic equilibrium breaks down, followed by the continuum assumption.

- Traditional CFD based on Navier-Stokes equations not valid, when either the gas density is very low or in devices with extremely small dimensions.

- Alternate modelling approaches needed in these non-equilibrium flow regimes.



d is the molecular diameter and δ is the inter-molecular distance

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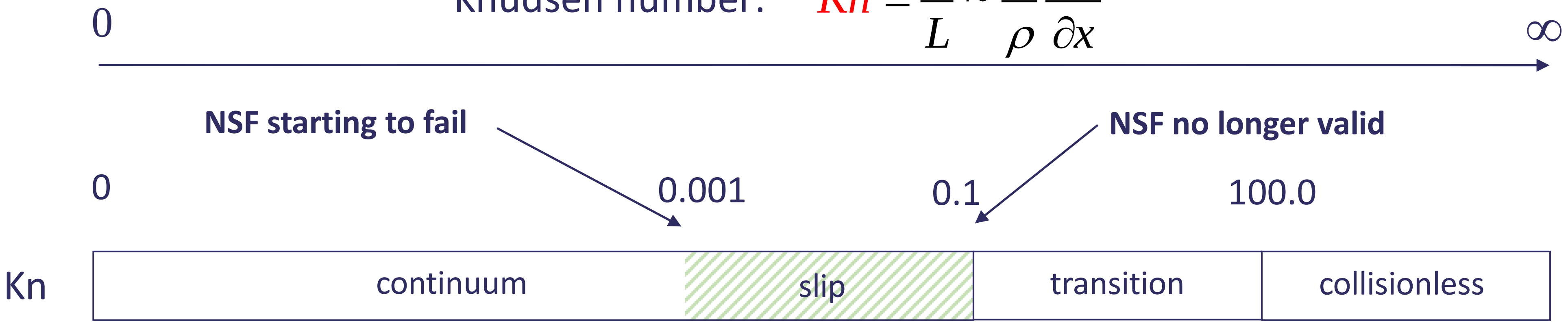
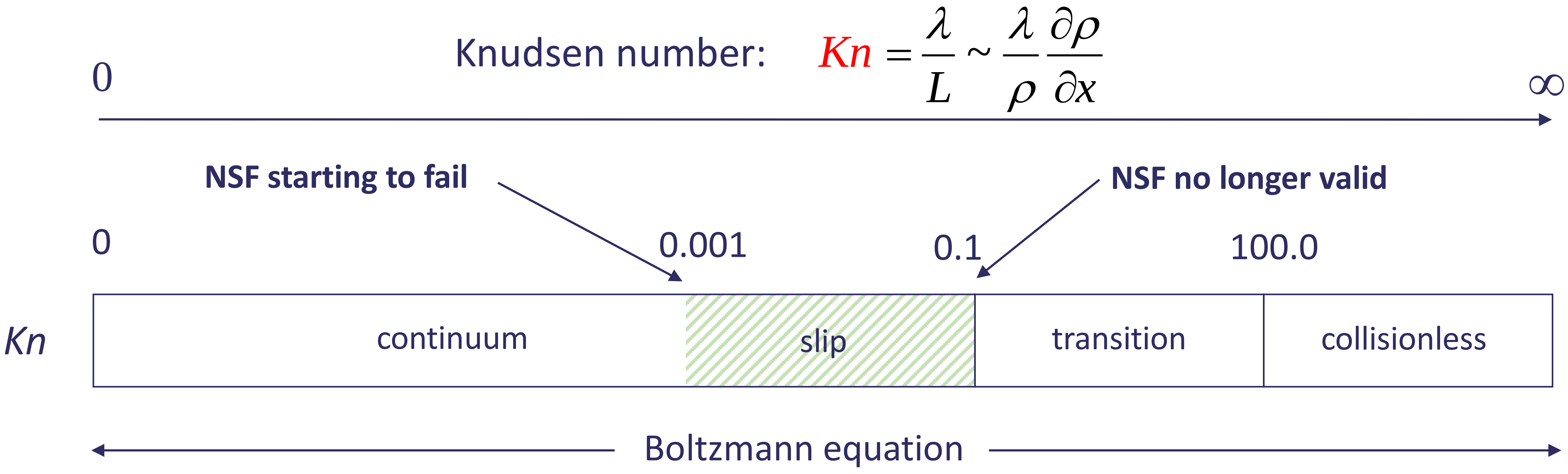
Going beyond the traditional Navier-Stokes equations

Knudsen number: $Kn = \frac{\lambda}{L} \sim \frac{\lambda}{\rho}\frac{\partial \rho}{\partial x}$



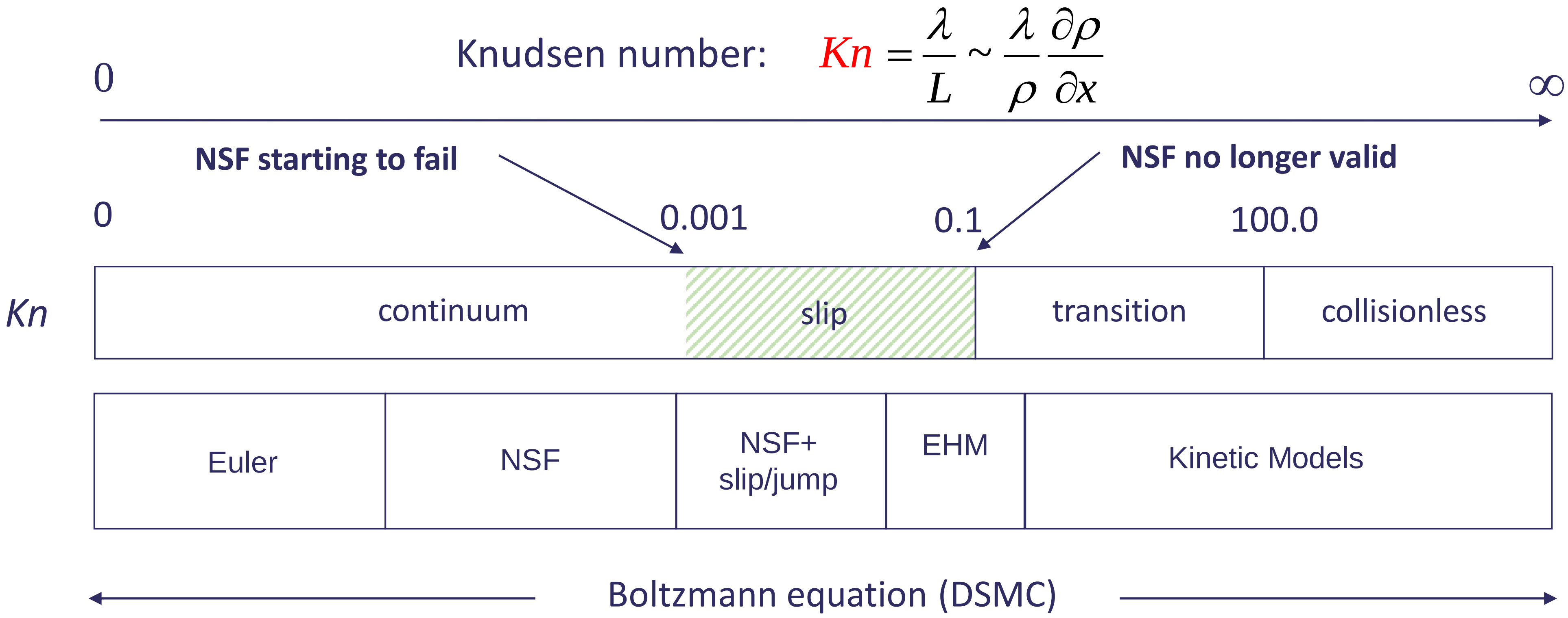
- Mean free path (λ) is the average distance between successive molecular collisions.
- Knudsen number can be high when either λ is large (low-density) or L is very small.
- Insufficient molecular collision frequency at high Knudsen numbers.

Going beyond the traditional Navier-Stokes equations



- The Boltzmann Equation describes discrete nature of gases – molecular representation
- Difficult to solve in its full form ($f(x_i,c_i,t)$ - 7 independent variables)

Modelling considerations for different flow regimes



Key Message: Molecular (Kinetic) level methods like DSMC needed, in situations where traditional CFD is invalid. Example applications: ***high-altitude hypersonics***, ***vacuum gas dynamics*** and ***micro-nanofluidics***.

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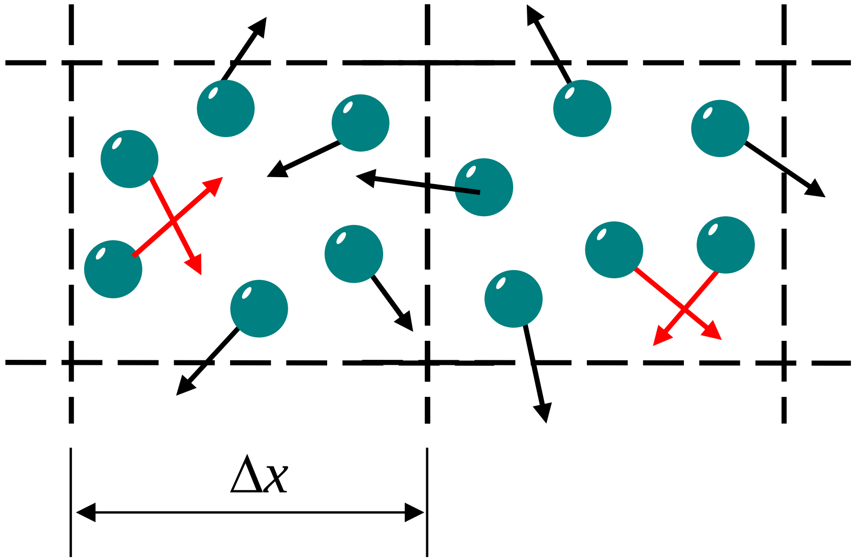
Direct simulation Monte Carlo (DSMC) method

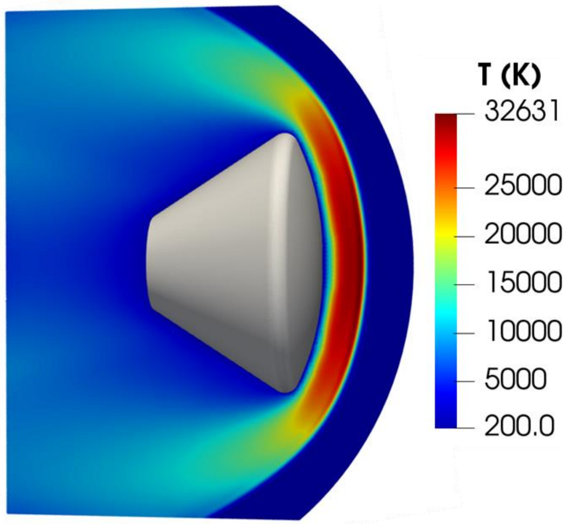
- The defacto standard for rarefied gas flow simulations
- Developed by Graeme Bird in the 1960s
- *Direct Simulation* – direct physical modelling based on kinetic theory for a dilute gas.
- *Monte Carlo* – statistical mechanics
- Each DSMC particle represents a collection of gas molecules
- Valid for all flow regimes but computationally very intensive for near-continuum flows.
- Particle method well-suited for HPC simulations.



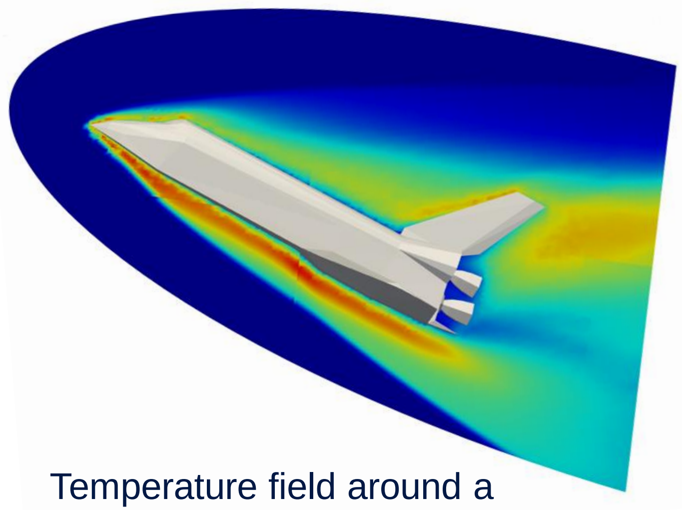
To ensure accuracy, Δx and Δt need to be less than mean free path & mean free time respectively.

Hypersonic flow – Modelling considerations

- Hypersonic flow is a key feature of flight vehicles associated with satellite deployment, space tourism, planetary exploration etc.
- Hypersonic flow implies Mach number ≥ 5, but this could be as high as 30 for re-entry type flows.
- **Aerothermodynamics** - Gas temperature increases with Mach number. Molecular vibration excitation, gas dissociation, chemical reactions and ionization occur successively with increase in Ma.
- **Low density effects** - Gas density decreases with increase in altitude implying an increase in both mean free path and Knudsen number with altitude.



Orion capsule re-entry simulation (Temperature field)



Temperature field around a NASA **Space Shuttle** (Mach 25)

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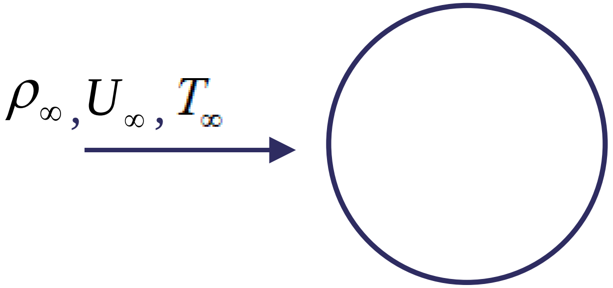
2D Flow past a Cylinder at Ma_∞=25

- Simulations consider a 5 species air mixture (N_2, O_2, N, O and NO) including real-gas effects and chemical reactions.
- **Chemical reactions are based on the Total Collision Energy (TCE) model. 19 dissociation/exchange reactions activated.**
- Knudsen number varied by changing the gas density and keeping the cylinder diameter constant.
- 3 Knudsen numbers considered, i.e., Kn=0.001, Kn=0.01 & Kn=0.1, corresponding to altitudes ~ H=80km, H=100km and H=115km.
- Cylinder wall temperature kept constant at T_w=1000K and considers diffuse wall reflections.



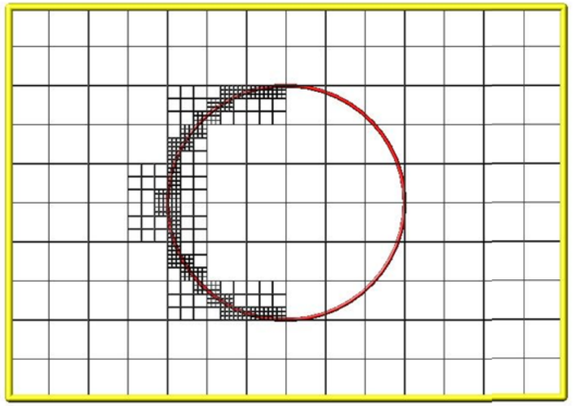
Flow conditions at Kn=0.001

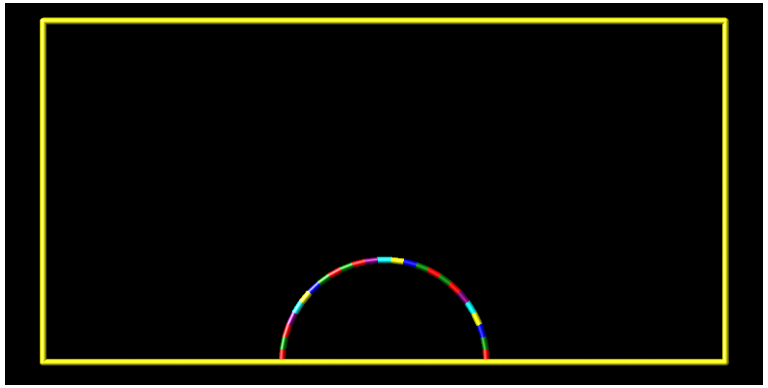
N_2 number density	0.91E21 m^{-3}
O_2 number density	0.24E21 m^{-3}
Free stream temperature	190 K

SPARTA DSMC Code

- **S**tochastic **PA**rallel **R**arefied-gas **T**ime-accurate **A**nalyzer
- Open source DSMC code developed at Sandia National Lab*

  - available from: http://sparta.sandia.gov
- Highly scalable code designed to work efficiently on massively parallel computers
- Parallelized using MPI and domain decomposition
- Extensible code written using object-oriented C++
- Cartesian, hierarchical grids with multiple levels of refinement



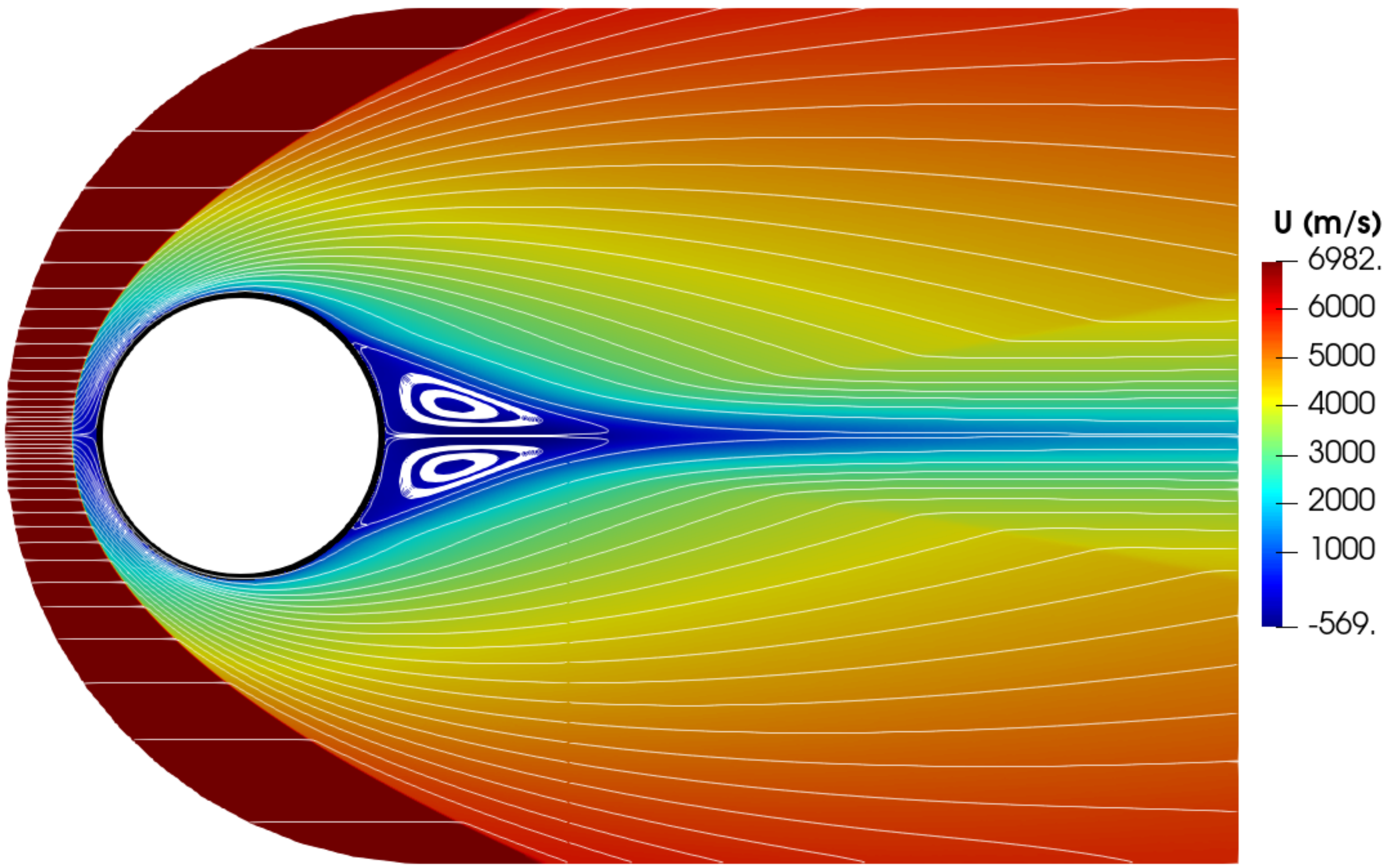


Supersonic flow past a cylinder
(SPARTA DSMC Simulation)

Aerothermodynamics Effects

(Kn=0.001 & Ma=25)

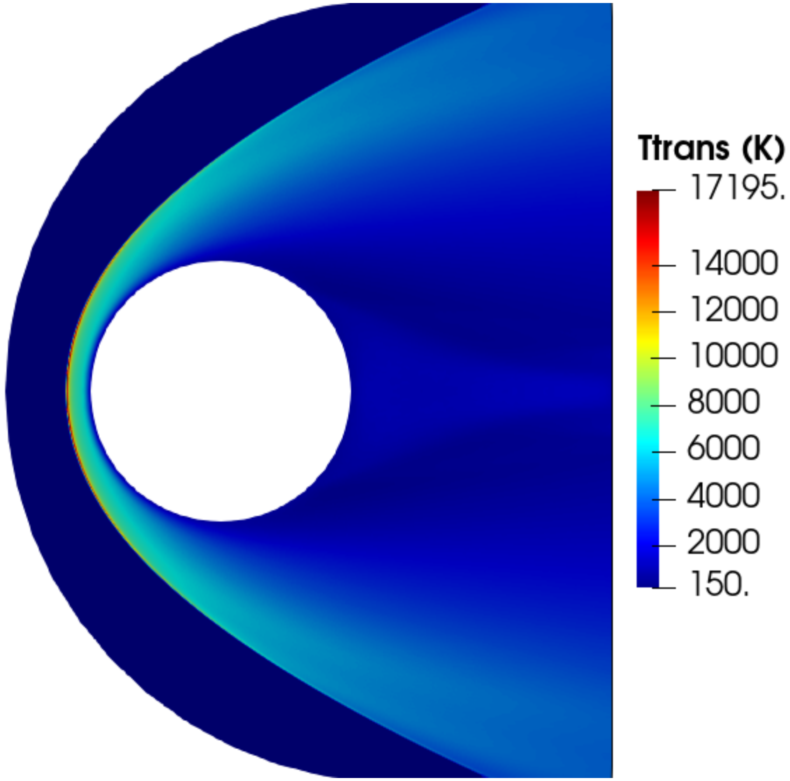
Near-continuum (Kn=0.001) hypersonic flow



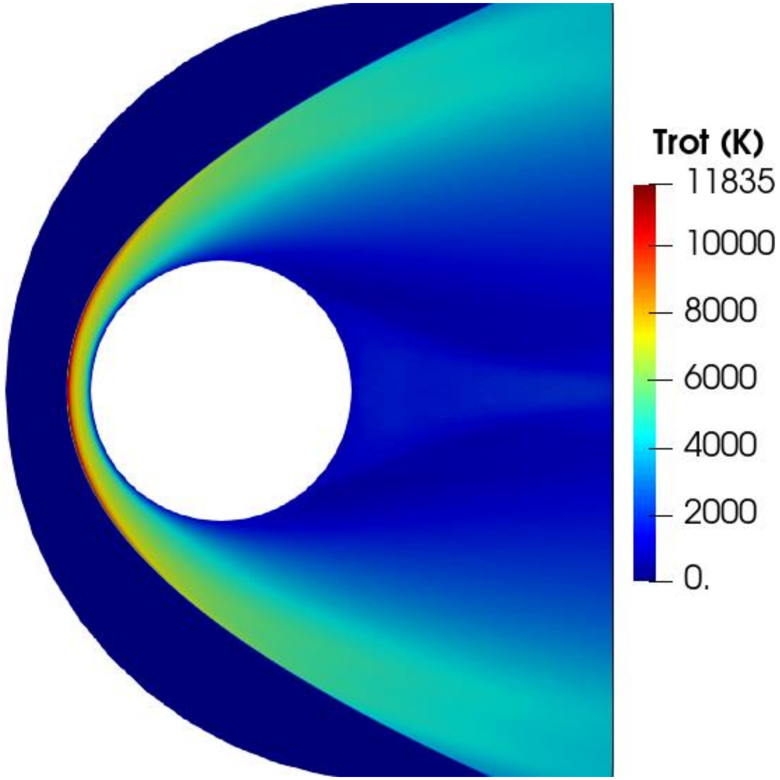
Typical features associated with a high-Ma, continuum flow like a 'thin' shock, wake-recirculation region, downstream re-compression shock etc. captured.

Temperature Component Fields – Reacting Flow

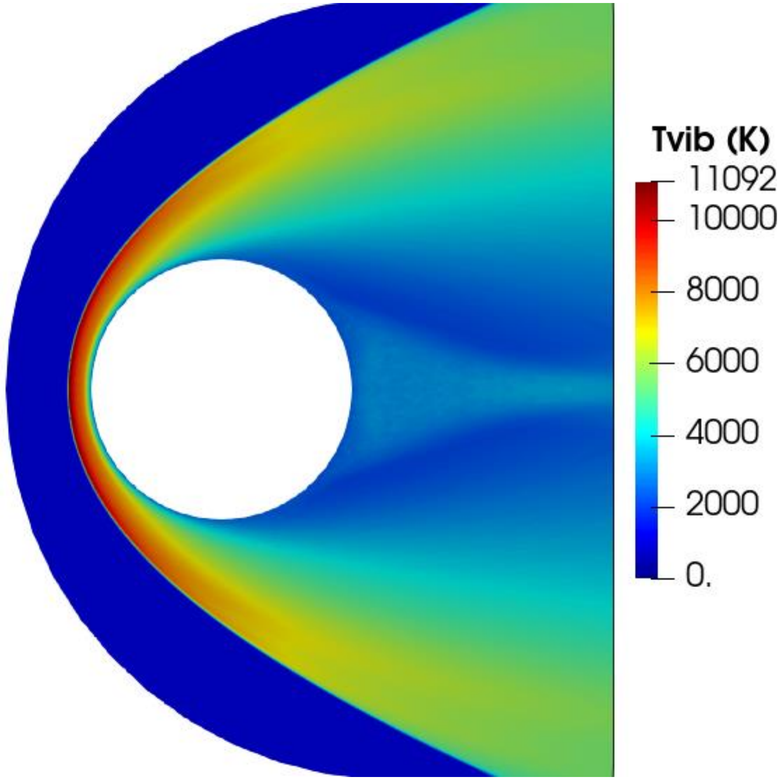
Translational



Rotational

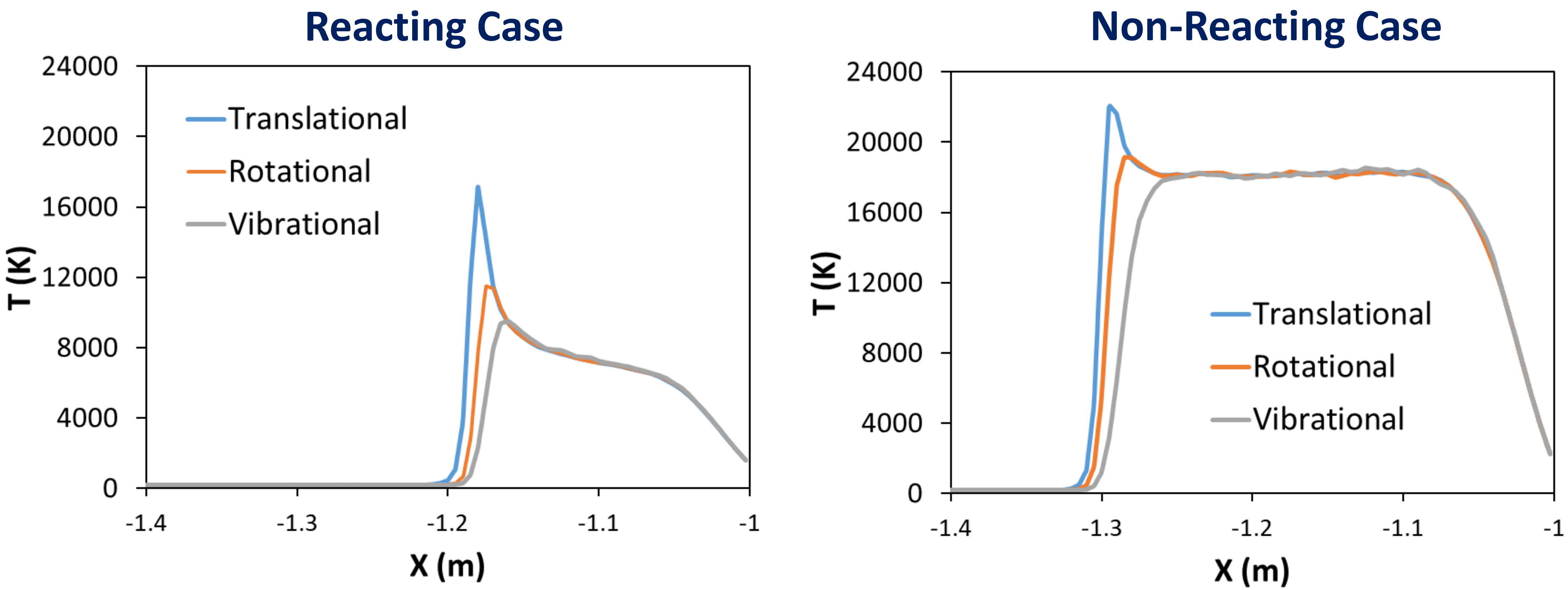


Vibrational



- Rotational mode exists for polyatomic gases; Vibrational excitation at high Mach numbers.

Temperature Components for Kn=0.001, Ma=25
(along the stagnation line upstream of the cylinder)



Shock structure, shock standoff distance and Temperature components significantly different if chemical reactions are ignored.

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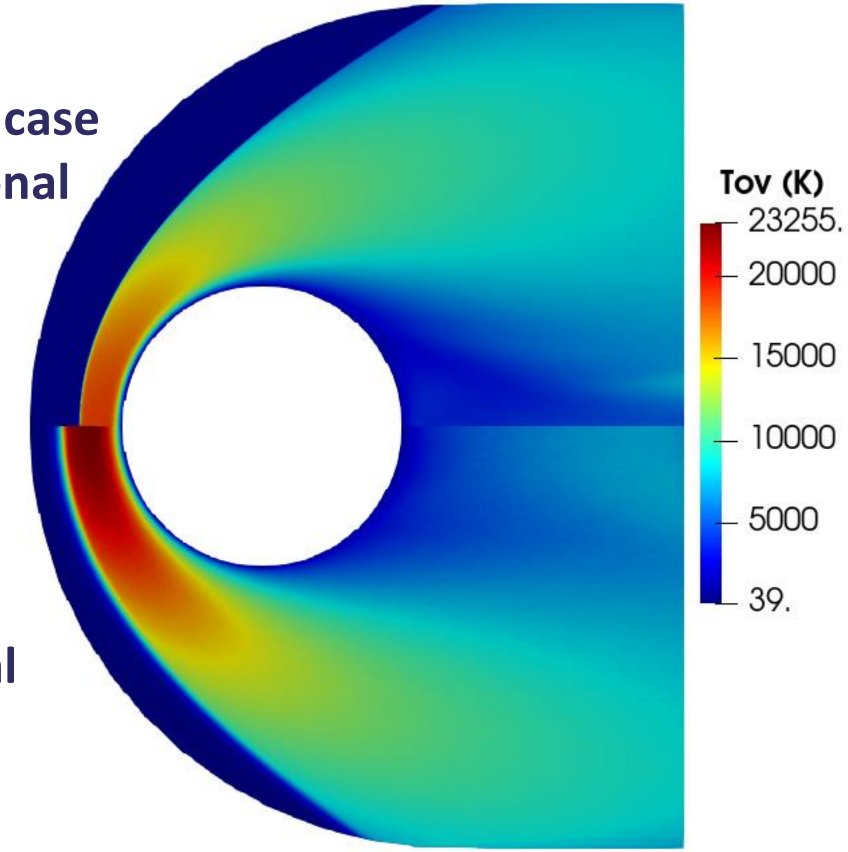
Effects of Vibrational mode & Chemical reactions on the Overall Temperature

Real gas effects very important as some of the kinetic energy is utilised for exciting the vibrational mode first and then for molecular dissociation and chemical reactions.

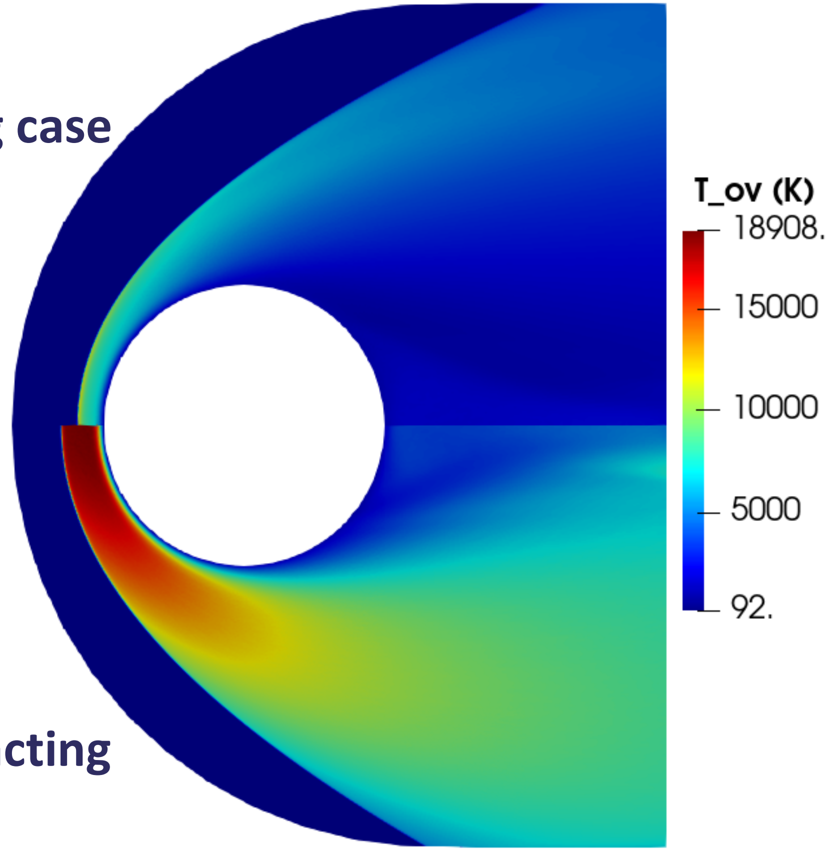
Non Reacting case (with Vibrational mode)

No Vibrational mode



Reacting case

Non Reacting case



(Kn=0.001, Ma=25)

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Low Density (rarefaction) Effects

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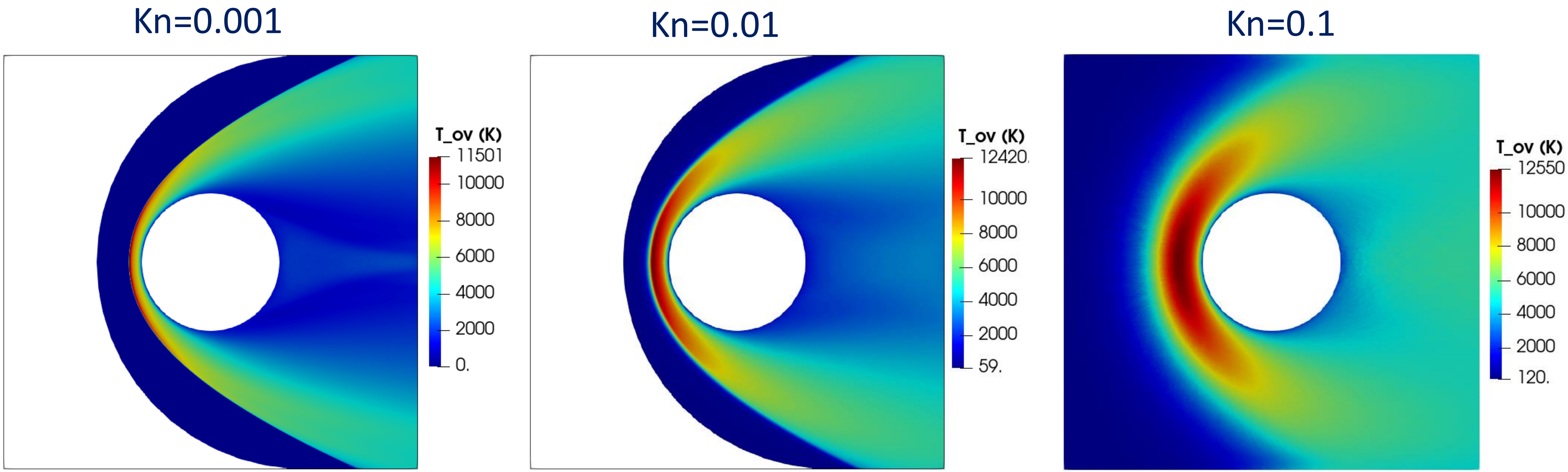
Overall Temperature field at different Kn values



Flow rarefaction significantly affects the shock structure and shock standoff distance.

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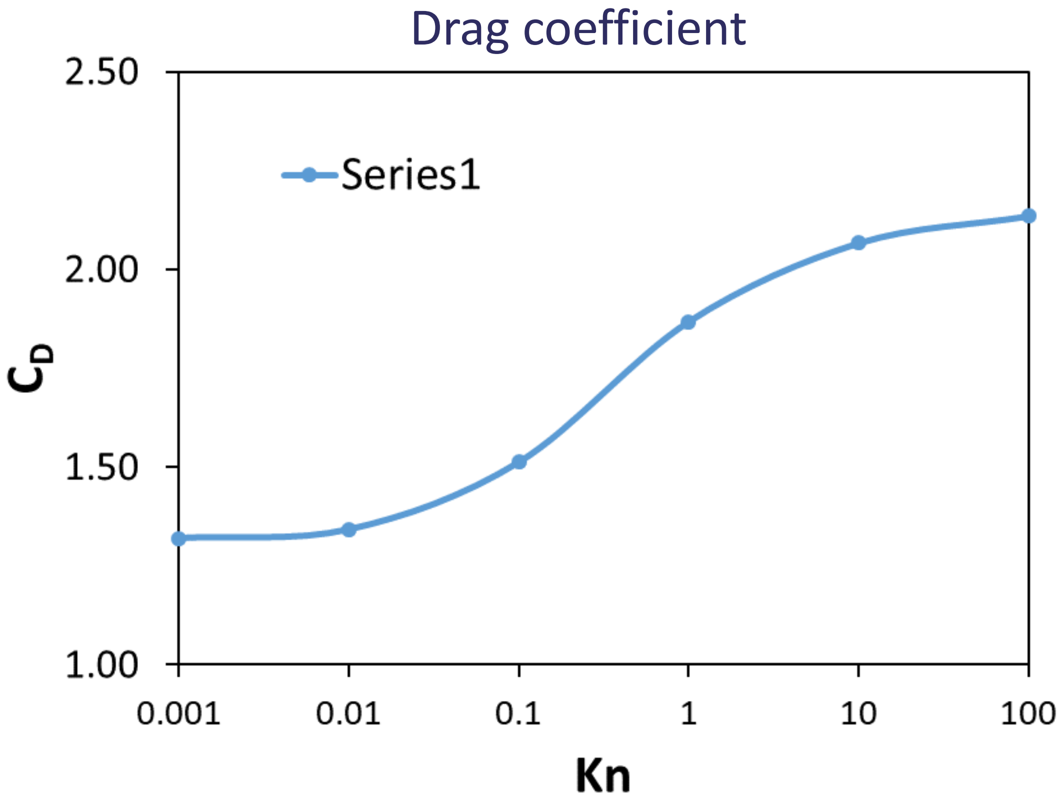
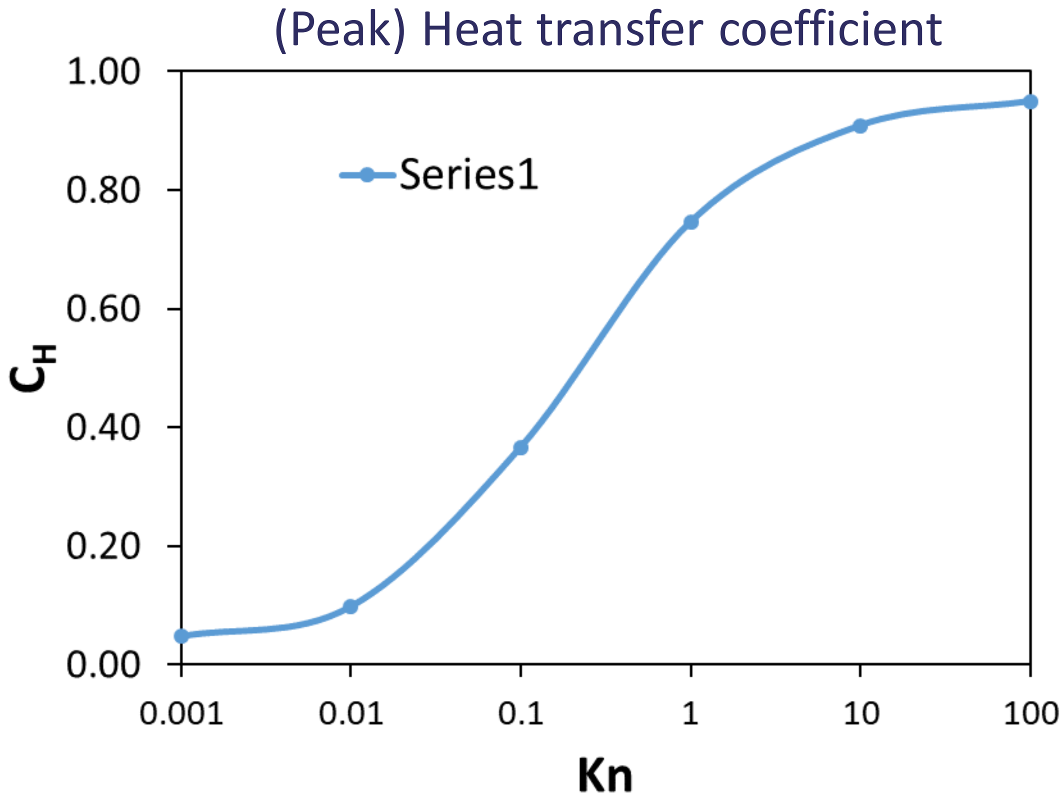
Effect of Rarefaction on Aerothermodynamics Coefficients



$$C_D = F_D / (\tfrac{1}{2} \rho A U_\infty{}^2)$$



$$C_h = q_w / (\tfrac{1}{2} \rho U_\infty{}^3)$$

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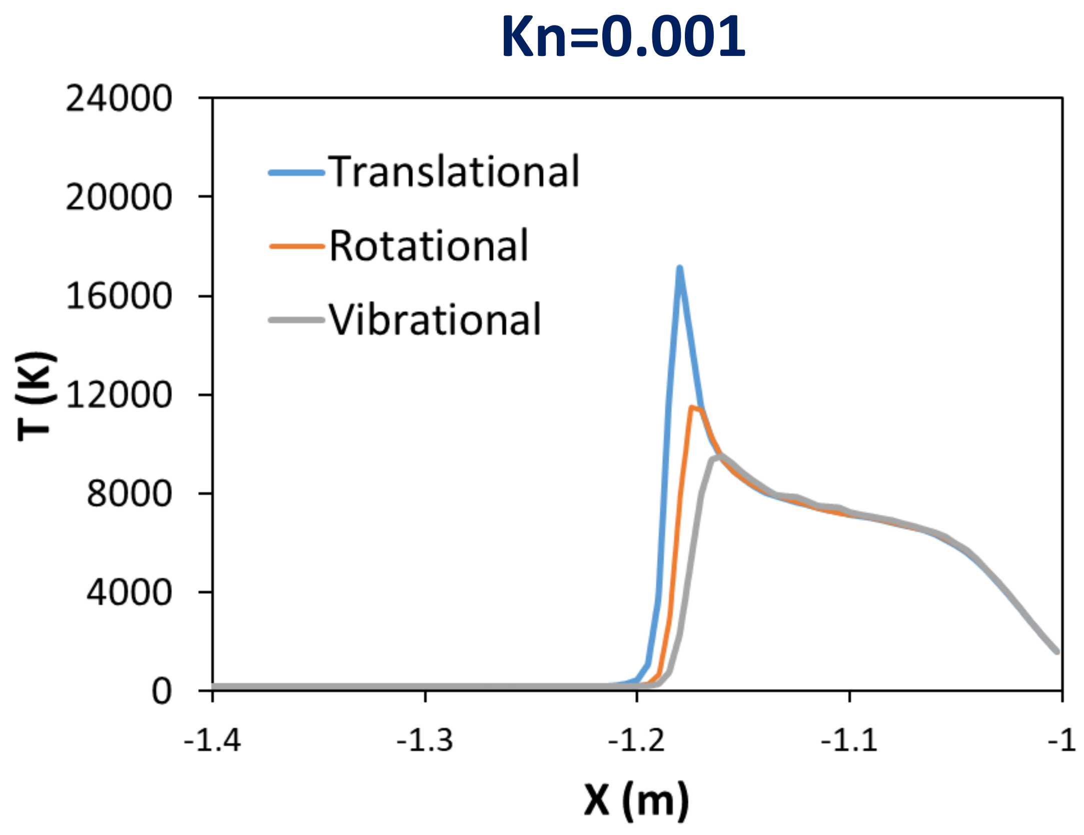
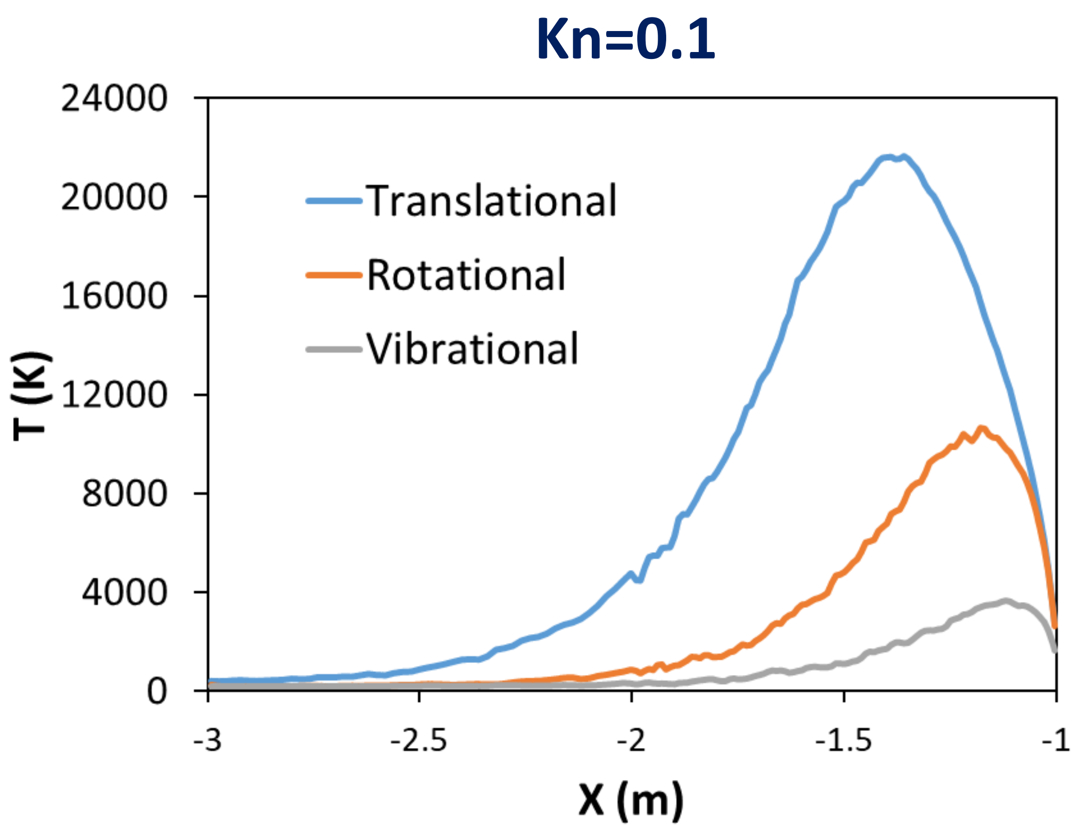
Variation of Temperature Components with Kn

(along the stagnation line upstream of the cylinder)





Significant degree of thermal non-equilibrium for hypersonic flows as the flow transitions from continuum to slip to transition regime.

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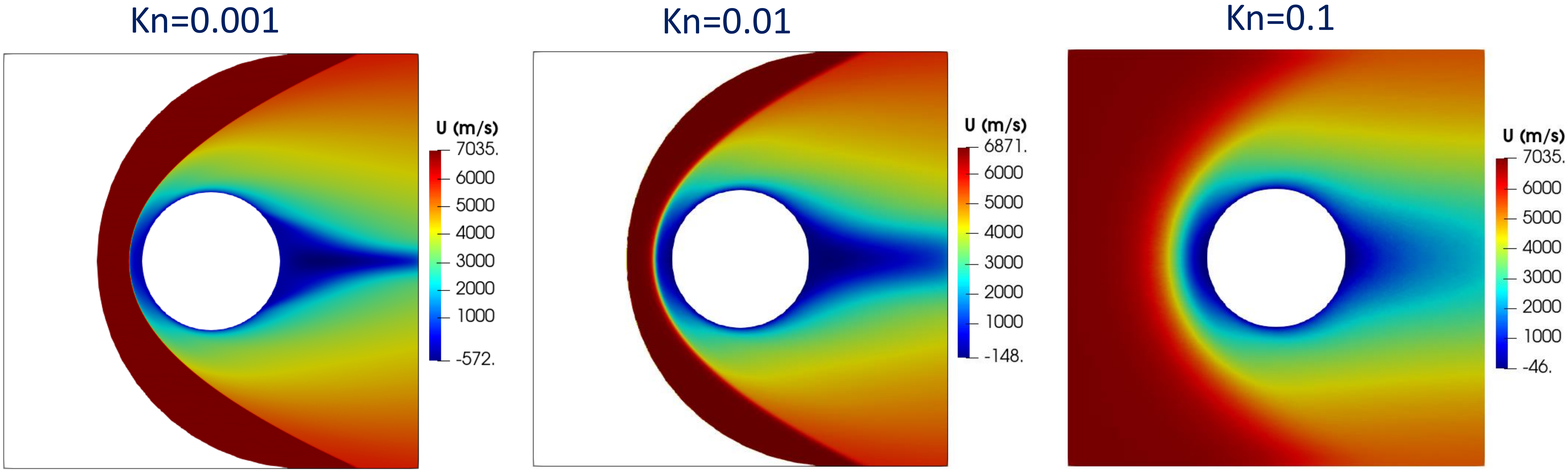
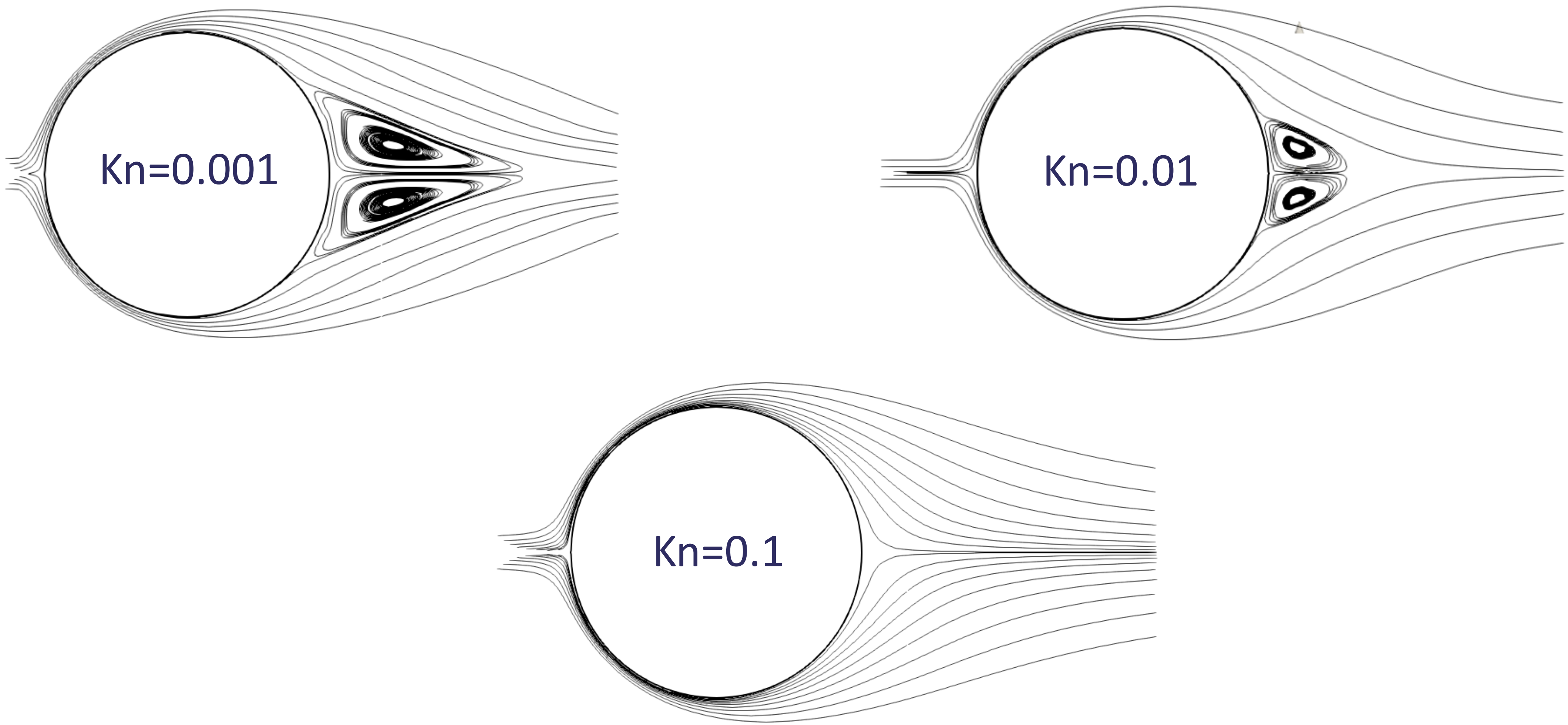
Velocity field at different Kn values



Effect of flow rarefaction on the vortex size
(Velocity streamlines)



Summary & Conclusions

- High-altitude hypersonics is characterized by unique conditions such as extremely high Mach numbers and temperatures & non-equilibrium effects.
- Aerothermodynamics and low-density rarefaction effects significantly affect the flow and thermal aspects.
- Molecular level methods like DSMC enable high-fidelity modelling.
- Advances in HPC imply that DSMC can also complement the development of numerical models in the near-continuum regimes.