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# *Physics of Coupled, Multi-Scale Nonequilibrium Flows*


***D. A. Levin* and V. Patil****

***Sergey G. Gimelshein*****

***Joanna M. Austin******

**Department of Aerospace Engineering*

*The Pennsylvania State University, University Park, PA 16802*

*** University of Southern California, Los Angles, CA 90089*

****University of Illinois, Urbana-Champaign, IL 61801*



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# Research Motivation

- Hypersonic flows are characterized by spatial regions with both sub and supersonic flow in various degrees of thermochemical non-equilibrium and multiple length scales..

- Navier-Stokes (NS) based continuum techniques encounter physical challenges in rarefied regions and are unable to capture the non-equilibrium phenomena.
- An accurate modeling of such flows requires a kinetic consideration.
- Kinetic methods, such as DSMC, are accurate but can be expensive, especially when applied to high density, low Kn flows.
- DSMC is a relatively mature approach to solving the Boltzmann equ. *What's new?*

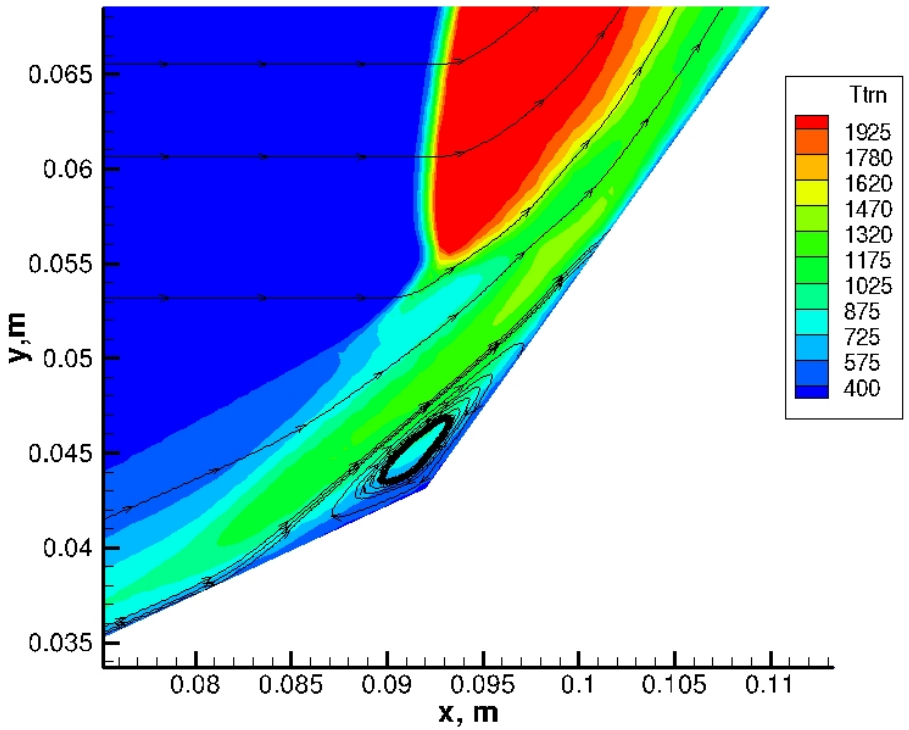
# (1) Double Cone Studies of Moss and Bird*

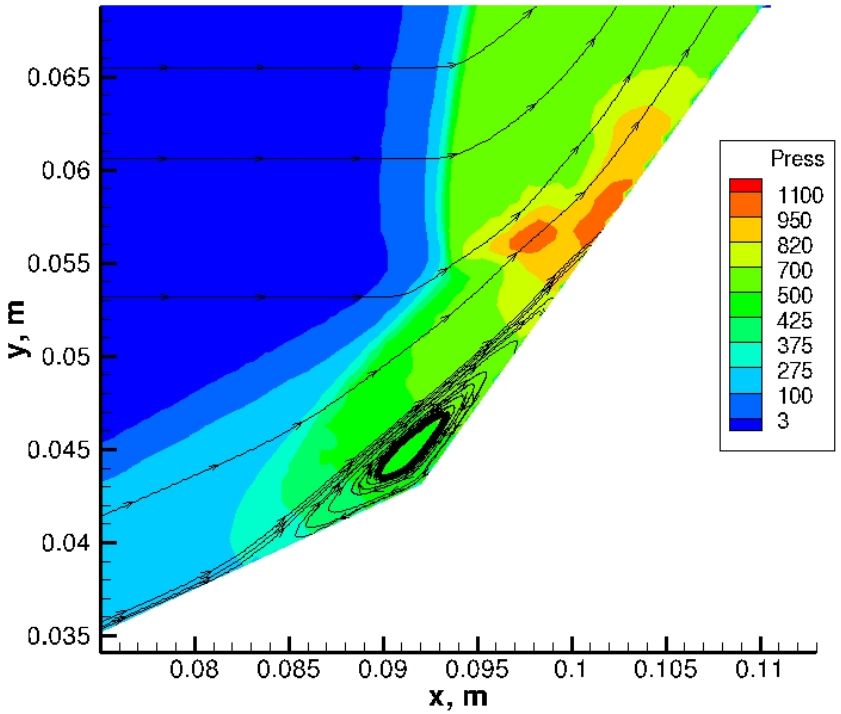
Experimental conditions performed for Mach 15.6 nitrogen flow about a 25-/55-deg bi-conic model

| Freestream Parameters : | |
|---|---|
| Temperature, *K* | 42.6 |
| Number Density, $m^3$ | $3.779 \times 10^{21}$ |
| Speed, m/s | 2073 |
| Density, $kg/m^3$ | $1.757 \times 10^{-4}$ |
| Pressure, Pa | 2.23 |
| Mach number | 15.6 |
| Reynolds number | $1.37467 \times 10^{5}$ |
| Knudsen number | $1.7 \times 10^{-4}$ |

***Moss, J. N. and Bird, G. A., "Direct Simulation Monte Carlo of Hypersonic Flows with Shock Interactions," *AIAA Journal*, Vol. 43, No. 12, 2005, pp. 2565-2573.**

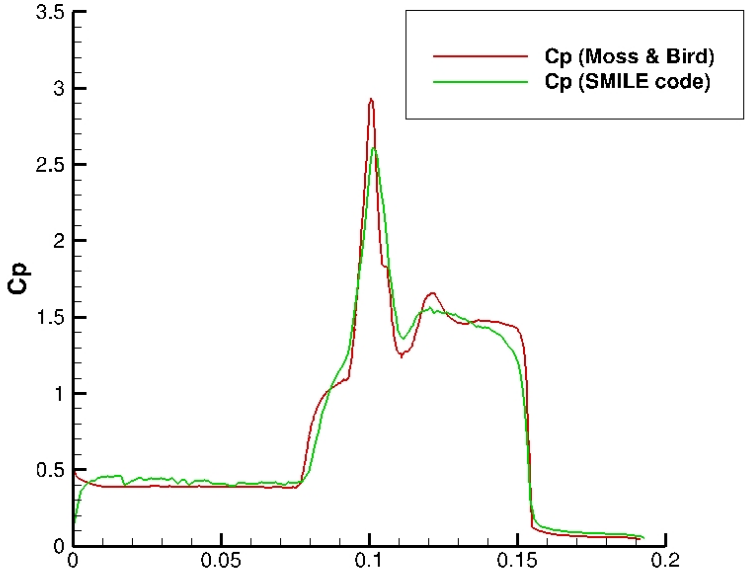
# Double Cone Temperature and Pressure Contours

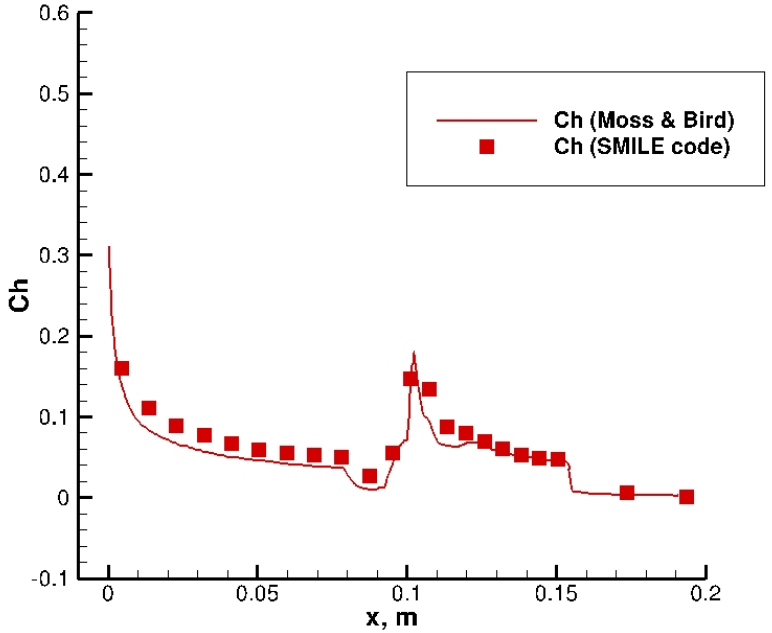


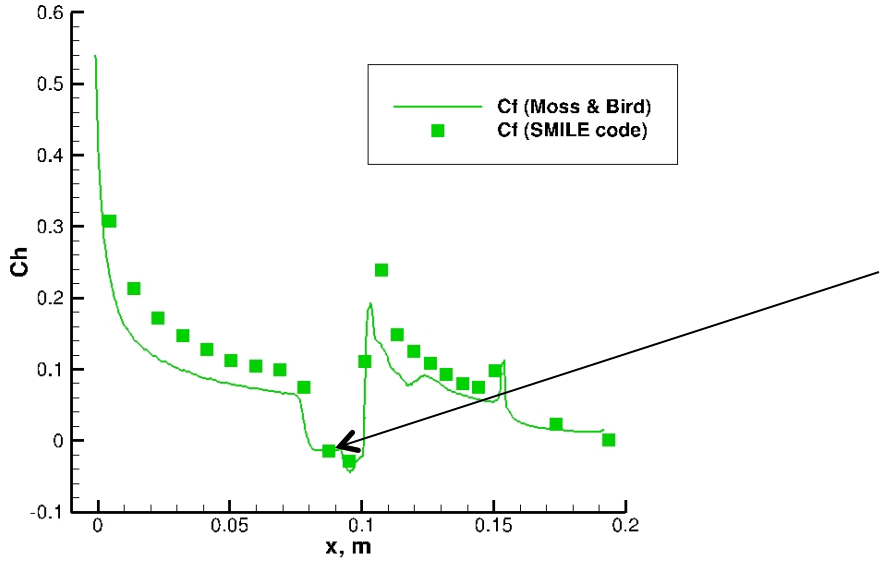




- **Physics is dominated by presence of separation zone and**
- **Sharp leading edge.**

# Comparison of Surface Profiles – Double Cone Configuration




- **Separation zone well modeled.**

# (2) HET Mach 7 Nitrogen Flows

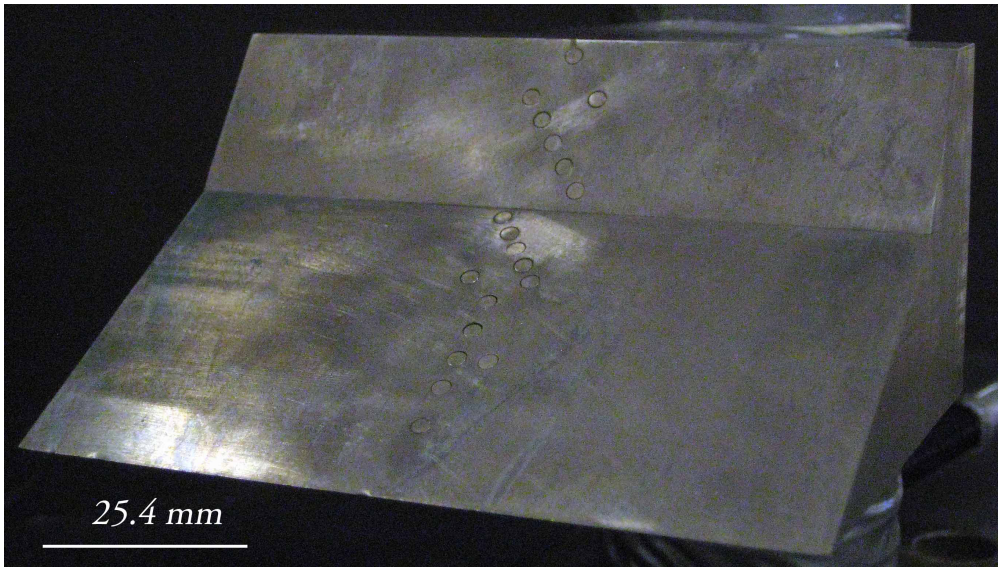



Figure 2. The experimental double wedge model used in the current study. The coaxial thermocouple gauges can be seen along the center of the model. Note: Some gauges are staggered to increase spatial resolution.

- Computational study of the complex shock interactions resulting from the hypersonic flow about a double wedge configuration presented in the paper AIAA 2012-0284 by A.B. Swantek and J. M. Austin.
- Stagnation enthalpies from 2-8 MJ/kg, about a 30-/55-deg double wedge model.

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# Summary of 2 HET Freestream Conditions

| Freestream Parameters | M 7_8 (High Enthalpy) | M 7_2 (Low Enthalpy) |
|---|---|---|
| Mach number | 7.14 | 7.11 |
| Static Temperature, K | 710 | 191 |
| Static Pressure, kPA | 0.78 | 0.39 |
| Velocity, m/s | 3812 | 1972 |
| Density, $kg/m^3$ | 0.0037 | 0.0069 |
| Number Density, $/m^3$ | $7.96 \times 10^{22}$ | $1.48 \times 10^{23}$ |
| Stagnation Enthalpy, MJ/kg | 8.0 | 2.1 |
| Unit Reynolds number, /m | $0.4156 \times 10^{6}$ | $1.0653 \times 10^{6}$ |
| Knudsen number | $4.0256 \times 10^{-4}$ | $1.5742 \times 10^{-4}$ |

# Convergence of Solution*

- **Total number of simulated particles = $9.8 \times 10^7$**

  **Number of particles per cell = > 30**

  **Number of particles per $\lambda^2$ = 3 to 4**

  **Therefore, sufficient number of particles present in domain.**

- **Local Knudsen number (Kn = λ/L) –**

  **Local Kn values > 0.1 everywhere in domain.**

  **Therefore, cell size of sufficient order.**

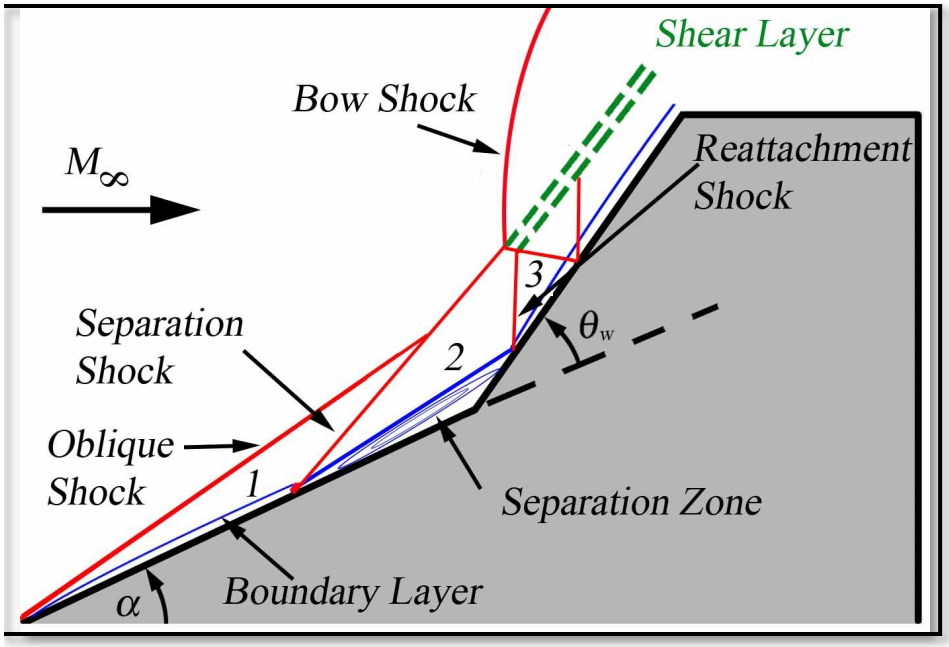
- **Mean time between collisions > Timestep**

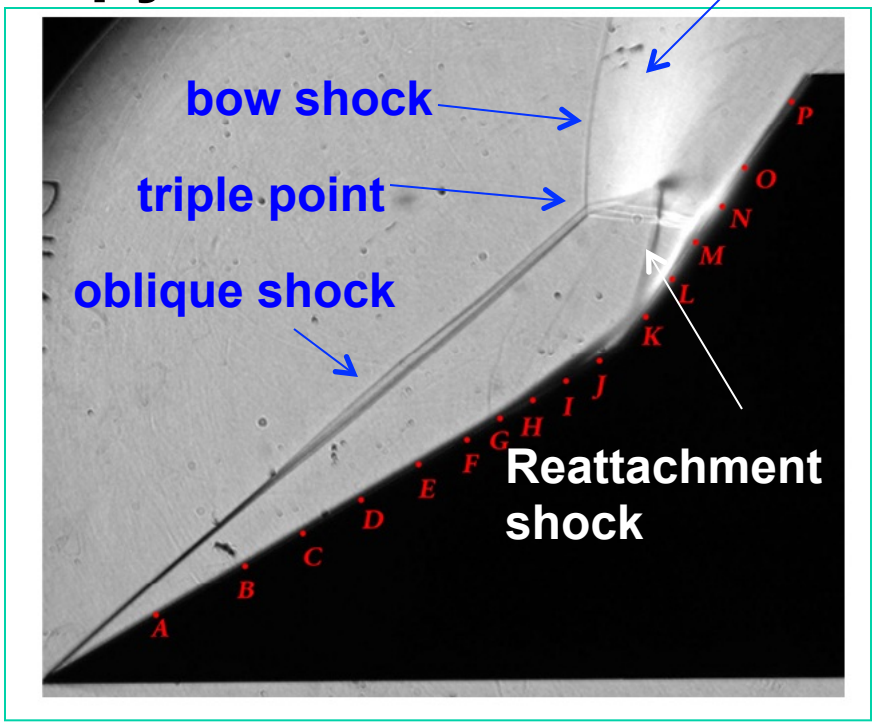
- **So, we can conclude that the solution is converged.**

| Numerical Parameters | M 7_8 (High Enthalpy) |
|---|---|
| Total number of time-steps (NSTEP) | 100,000 |
| Time step (TAU), s | $1.0 \times 10^{-9}$ |
| Number of molecules in one simulated particle (PFnum) | $1.0 \times 10^{13}$ |
| Number of cells | 450 x 400 |
| Cell size, m | $2.0 \times 10^{-4}$ |
| Grid Adaptation (NPG) | 20 |
| Number of processors | 64 |

***Many thanks to Dr. Ryan Gosse for providing assistance with the Air Force HPC Machines.**

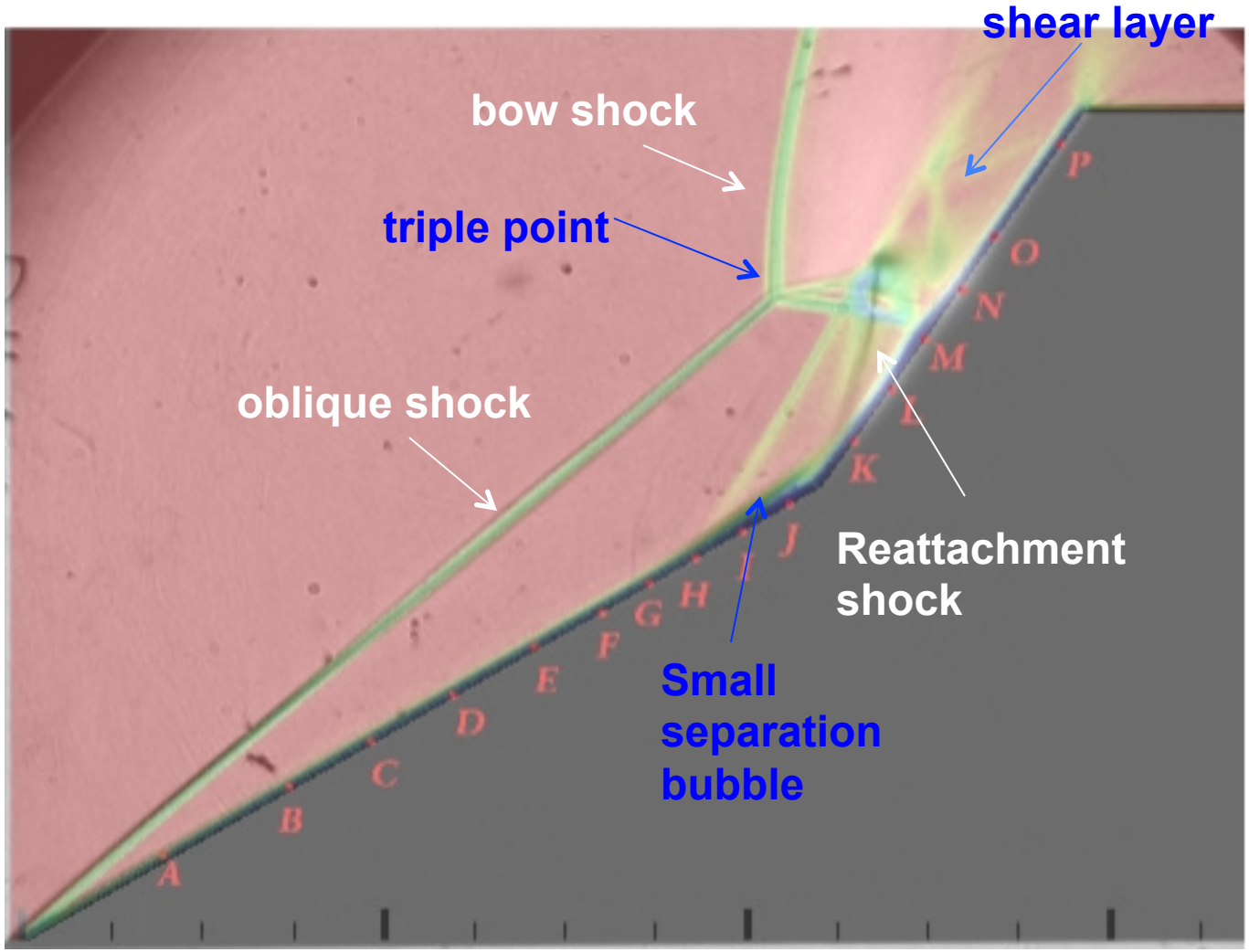
# Strong Shock Interactions – High Enthalpy Case



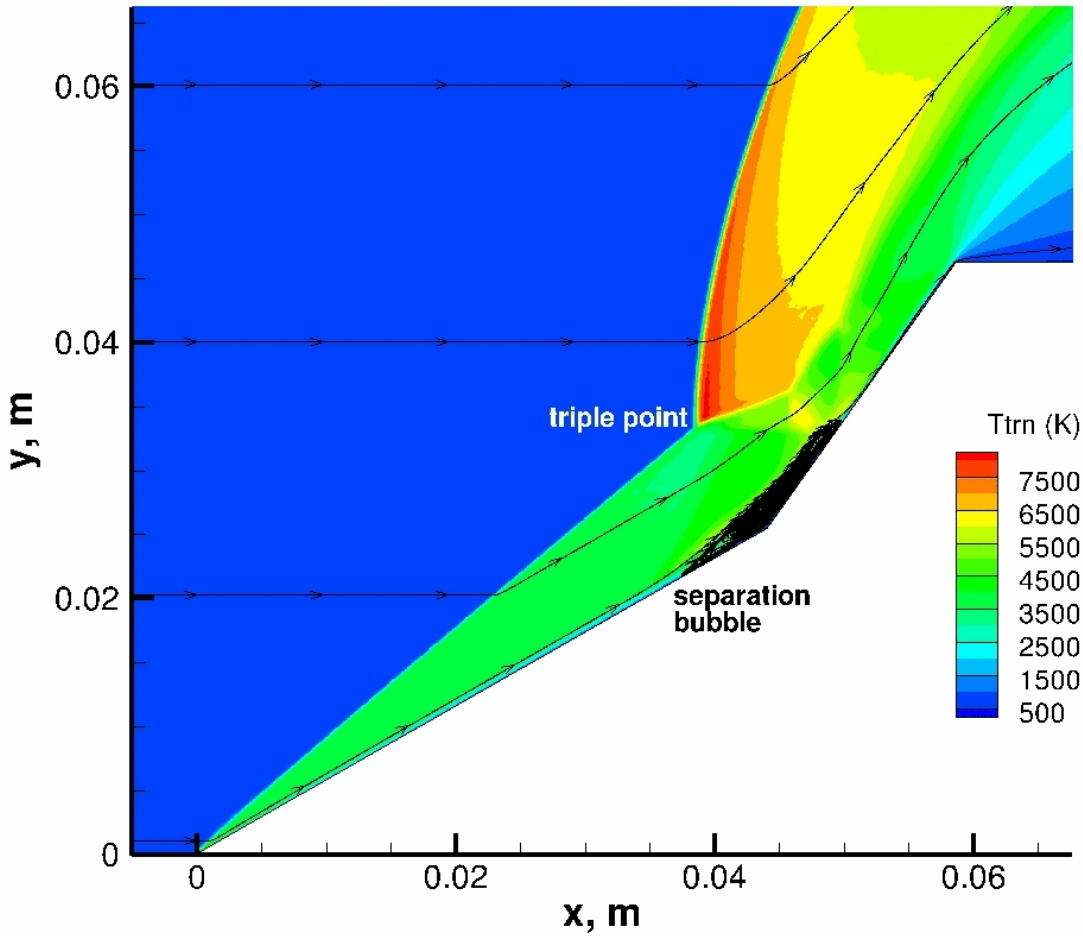

- separation and reattachment shocks
- triple point
- shear layers
- boundary layer interactions
- attached shock from the first cone/wedge interacts with the detached bow shock from the second cone/wedge.

# HE case : Schlieren Comparison




- Overlap of Schlieren plot from DSMC result at 100,000 timesteps (100μs) with Schlieren Image from experimental data (test time is 242μs).
- Best agreement with the shock structure and the size of the separation region between the experimental and computational Schieren images.

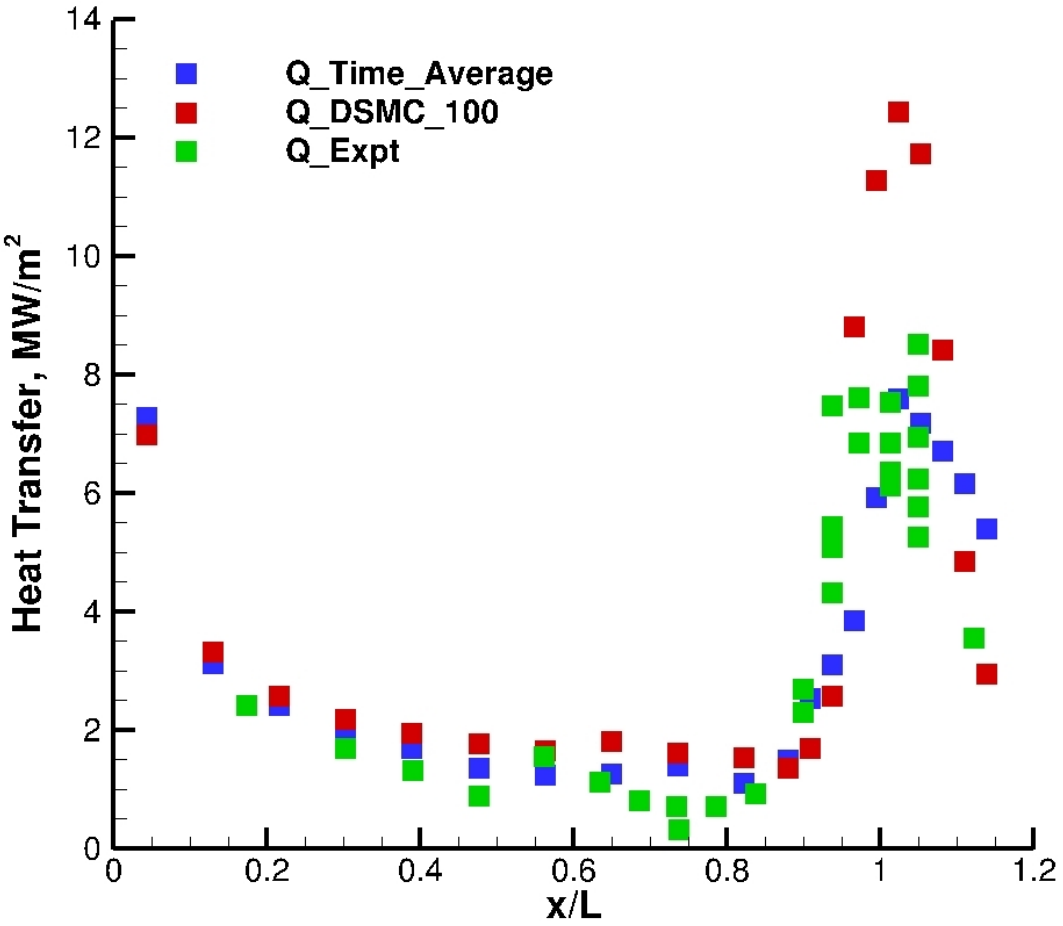
# HE case : Time dependent solution




Translational Temperature Contour Plots
(70μs, 100μs, 160μs, 300μs)

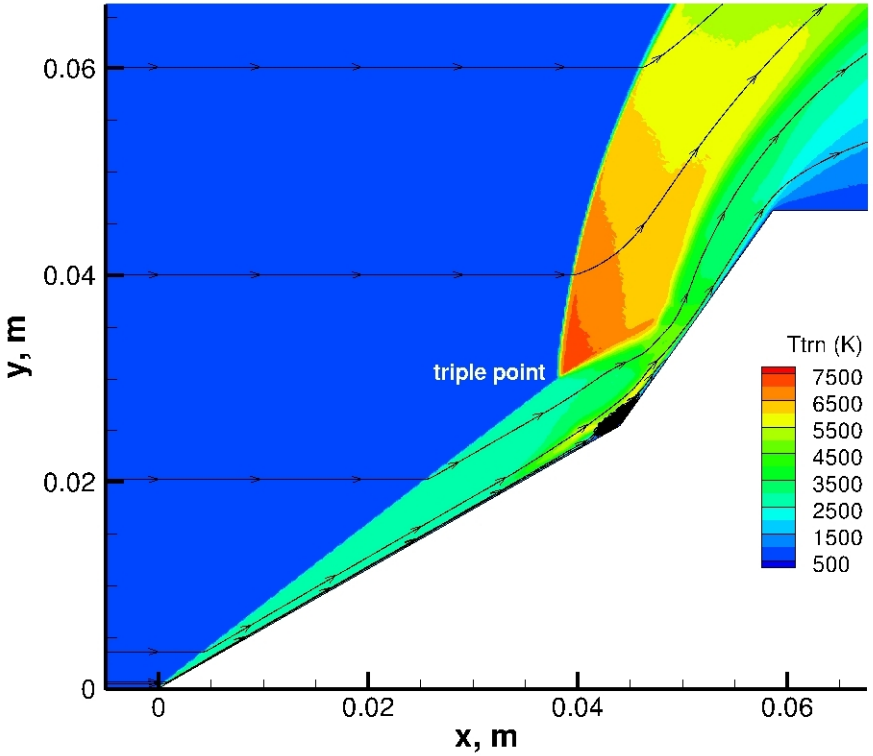
- The size of the separation bubble keeps on increasing.
- The triple point location starts to shift downstream.
- Separation shock moves ahead on the leading edge and interacts earlier with the oblique shock leading to new flow features.
- Flow is unsteady and does not attain a steady state.

# HE case : Heat Transfer

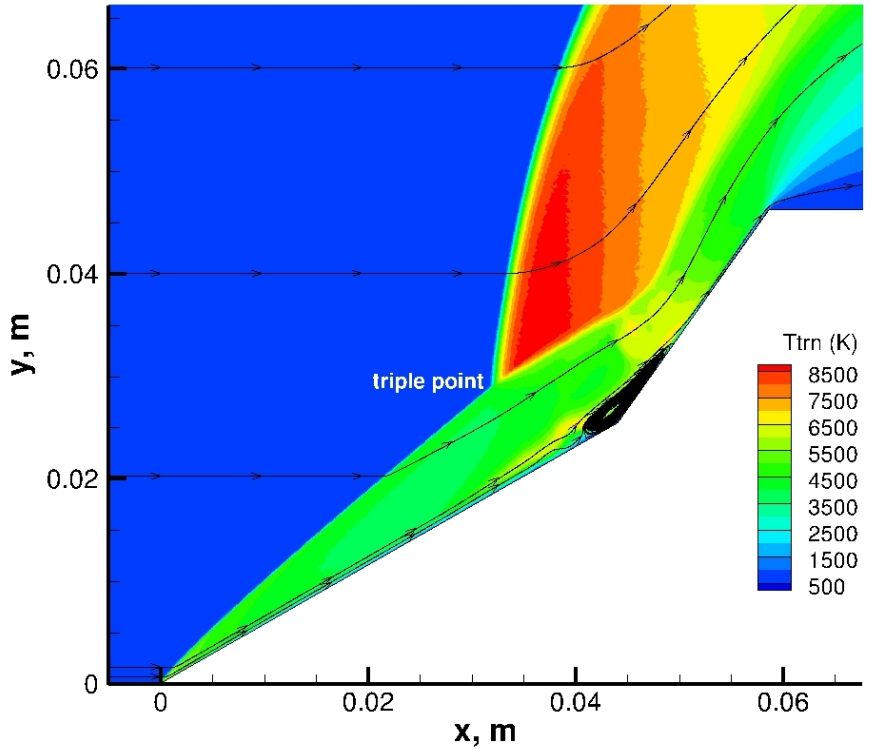



- The computational results show a similar trend to the experimental values and capture the jump at the hinge (x/L = 0.8).
- But the DSMC computations tend to over-predict the heat transfer rates in the area of shock impingement on the aft wedge.
- The weighted time average of heat transfer (from 100μs to 400μs) brings the peak heat transfer into better agreement with the experiment.

# HE case : R-T and V-T relaxation



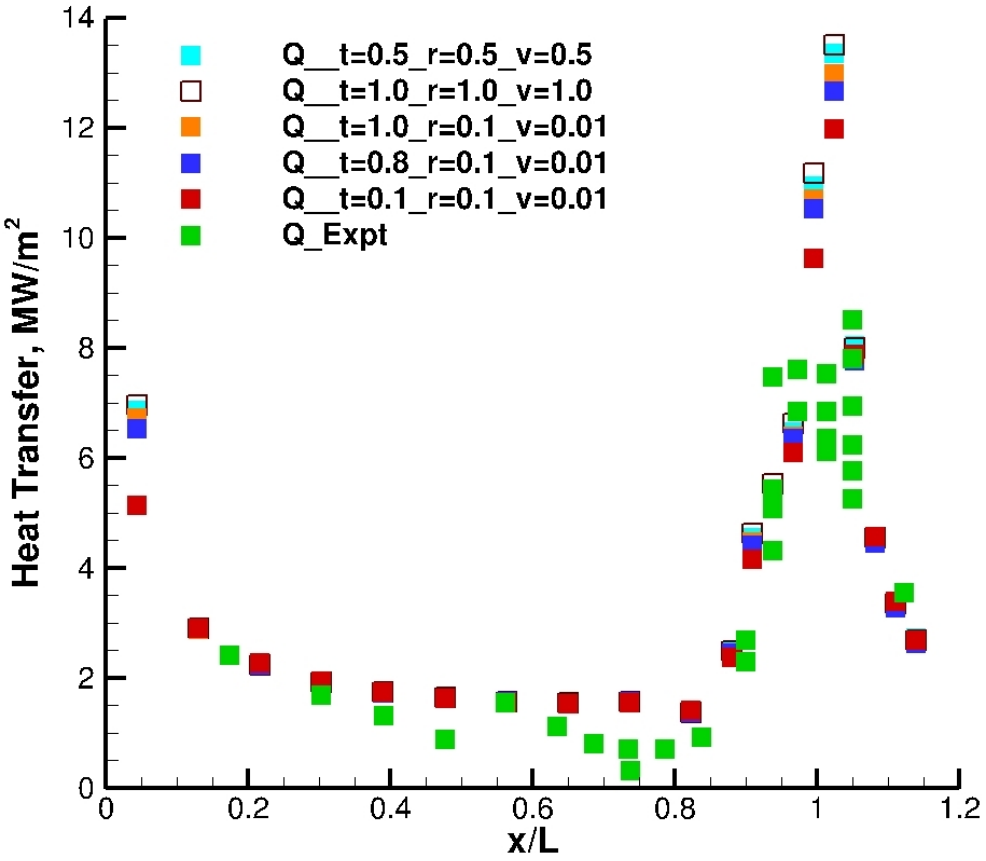

Fast relaxation ($Z_r = Z_v = 2$)




Slow relaxation ($Z_r = Z_v = 1000$)

- **Constant values for relaxation numbers: fast relaxation rate $Z_r = Z_v = 2$ and slow relaxation rate $Z_r = Z_v = 1000$.**
- **Temperature dependent rotational and vibrational relaxation numbers for previous cases were about 8-10 for $Z_r$ and around 1200 for $Z_v$.**

# HE case : Gas Surface Interactions

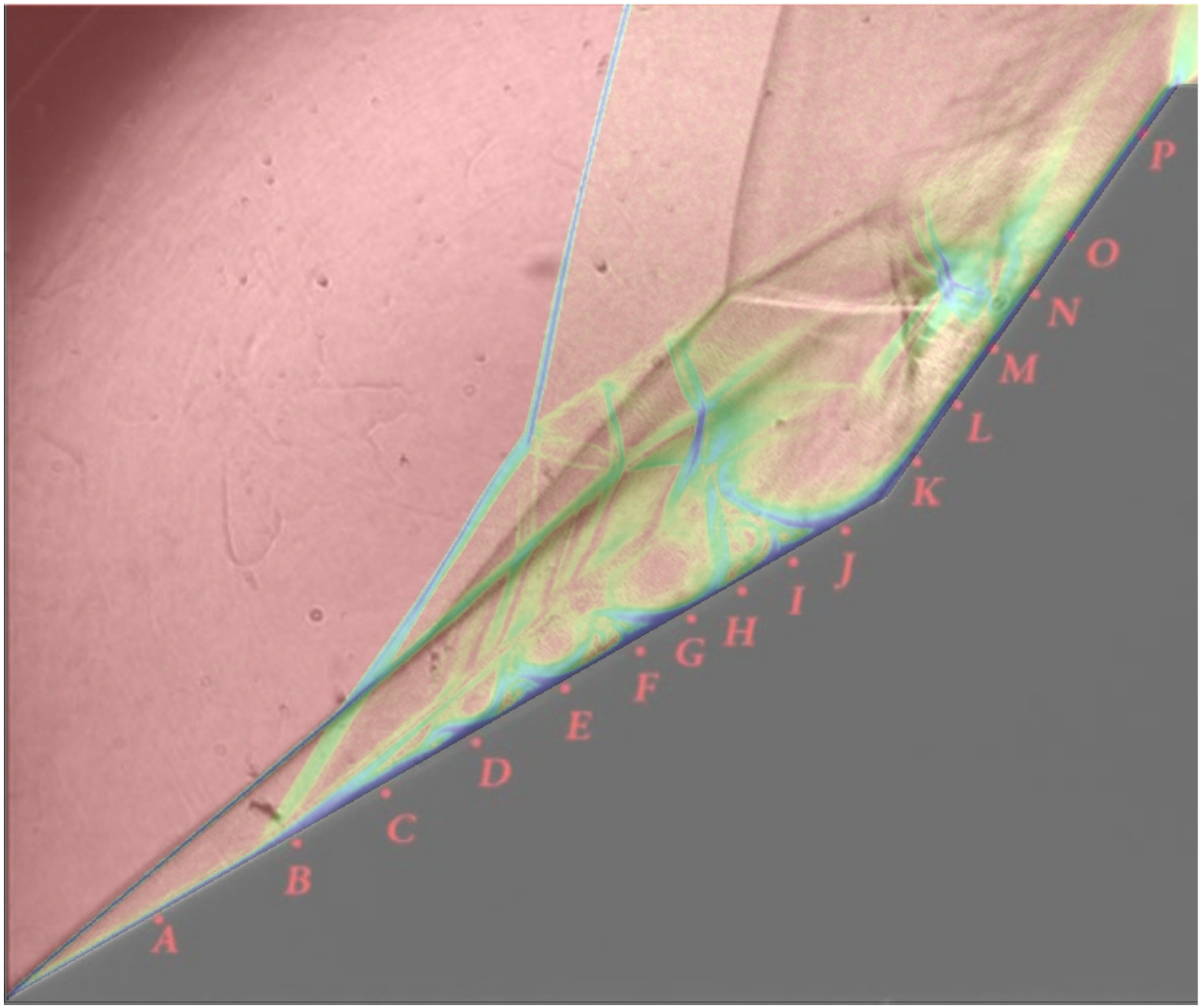



- Heat transfer rates are dependent on the gas - surface interaction model used.
- Thermal energy accommodation coefficients were varied.

| $\alpha_{trans}$ | $\alpha_{rot}$ | $\alpha_{vib}$ |
|---|---|---|
| 0.5 | 0.5 | 0.5 |
| 1.0 | 1.0 | 1.0 |
| 1.0 | 0.1 | 0.01 |
| 0.8 | 0.1 | 0.01 |
| 0.1 | 0.1 | 0.01 |

- It is reasonable to assume the following values for the surface energy accommodation coefficients, $\alpha_{trans}$= 0.8, $\alpha_{rot}$= 0.1, $\alpha_{vib}$= 0.01 based on the material used for the double wedge model experiment.

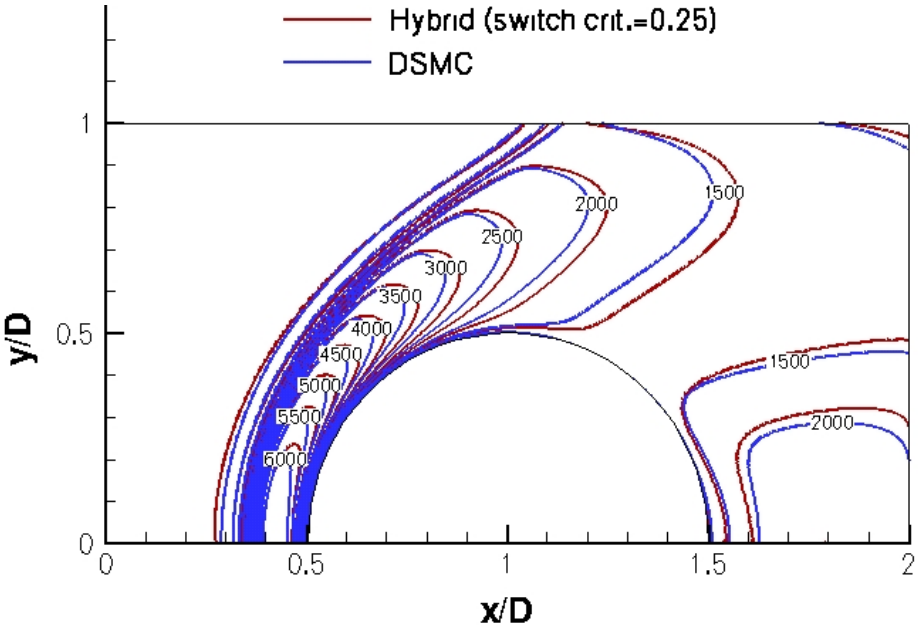
# LE case : Schlieren comparison




- Superimposition of the predicted Schlieren at 320µs with the experimental image.
- Good agreement with the oblique shock and the size of the separation region.
- Different shock structure is observed near the second wedge.
- Triple point in experiment occurs at a higher y location as compared to the DSMC result, due to the difference in the interaction between the separation and oblique shocks.

# Outstanding Scientific Issues

- To develop a basic computational framework based on the ellipsoidal statistical Bhatnagar-Gross-Krook (ES-BGK) model of the Boltzmann equation, capable of solving polyatomic multi-species gas flows.
- The new particle-based (Hybrid?) method should have the following features:
  - Be more efficient than DSMC in modeling high density flows,
  - Provide a transition to NS
  - Be sufficiently general to include internal energy
  - Apply to shock-shock interactions
- Start with flows where chemical reactions are not important.



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# Simplifications of Kinetic Equations

## Boltzmann equation (spatially non-uniform case):

$$\frac{\partial}{\partial t}(nf)+\vec{v}.\frac{\partial}{\partial \vec{r}}(nf)+\vec{F}.\frac{\partial}{\partial \vec{v}}(nf)=\left[\frac{\partial}{\partial t}(nf)\right]_{collisions}$$

$$\left[\frac{\partial}{\partial t}(nf)\right]_{collisions}=\int_{-\infty}^{\infty}\int_{0}^{4\pi} n^2\left(f^*f_1^*-ff_1\right)\, v_r\sigma d\Omega d\vec{v}$$

**Thermal diffusion rate**
**Viscous diffusion rate**
$(Pr = C_p\mu/\kappa)$

## BGK collision model (much simpler):

$$\left[\frac{\partial}{\partial t}(nf)\right]_{collisions}=n\nu\left(f_e-f\right) \qquad \nu = Pr\frac{nkT}{\mu}$$

**Lacks accuracy**
$(Pr = 1.0)$

## ES-BGK collision model (still simple):

$$\left[\frac{\partial}{\partial t}(nf)\right]_{collision}=n\nu\left(f_{ellipsoidal}-f\right)$$

**Corrects the *Pr* unity problem**

A fraction of particles in a cell is randomly selected. New velocities are assigned from a Maxwellian/ES distribution function.

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# Solution of BGK/ES-BGK Equation by Statistical Method

- A fraction of particles in a cell randomly selected. New velocities according to the Maxwellian/ES distribution function assigned.

- The velocities of particles, not selected, remain unchanged.

- Internal modes are relaxed to equilibrium at appropriate rates.

- The relaxation frequency for rotational equilibrium:

$$\nu_R = \frac{F_{coll}}{Z_R}$$

- Rotational collision number:

$$Z_R = \frac{3/5 Z_R^{\infty}}{1 + (\pi^{1/2}/2)(T^*/Teq)^{1/2} + (\pi + \pi^2/4)(T^*/Teq)}$$

- Number of particles selected for relaxation:

$$N_C = N(1 - \exp(-\nu \Delta t))$$

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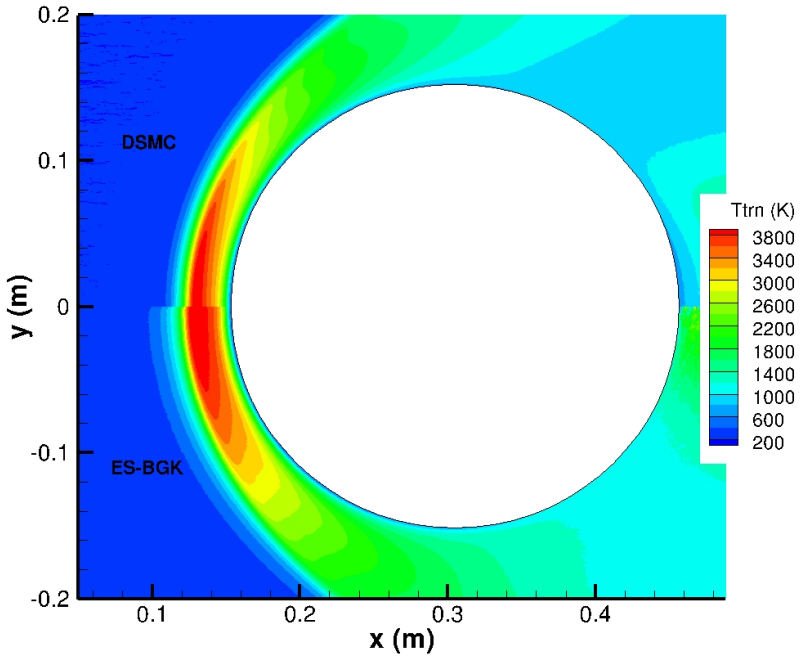
# Two Simple Test Cases DSMC vs BGK

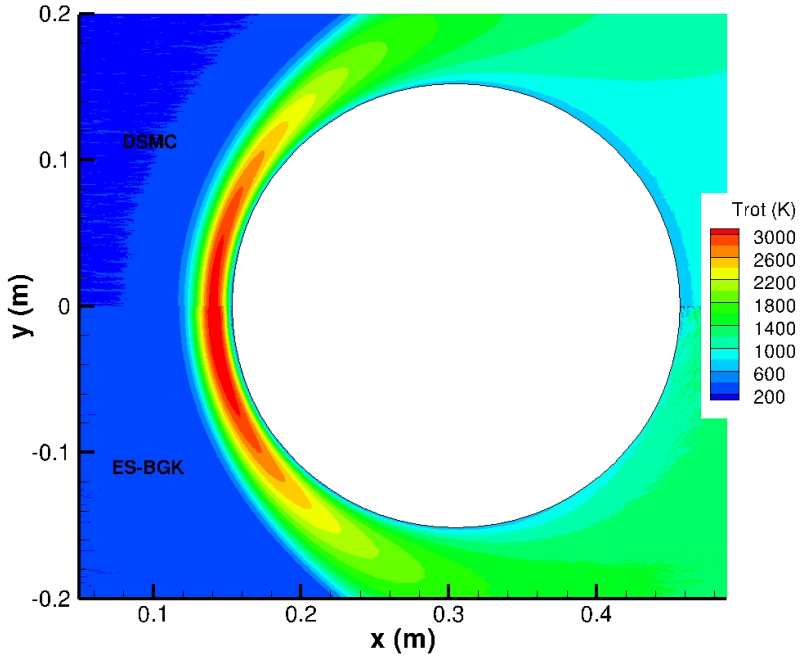
| Freestream Parameters | Case 1: High M | Case2: Low M |
|---|---|---|
| Sphere diameter (m) | 0.05 | 0.3048 |
| Mach number – M | 14.56 | 9.13 |
| Static Temperature (K) | 200 | 200 |
| Static Pressure (kPa) | 2.577 | 1.222 |
| Velocity (m/s) | 4200 | 2634.5 |
| Density (/m^3) | $4.34 \times 10^{-4}$ | $2.06 \times 10^{-5}$ |
| Knudsen number | $1.28 \times 10^{-3}$ | $8.9 \times 10^{-3}$ |

# Case II Mach 9: Comparison of Temperature Contours: *In Progress*

## Translational Temperatures

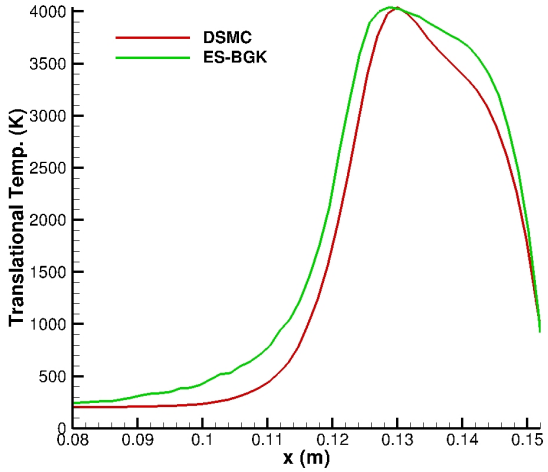



## Rotational Temperatures

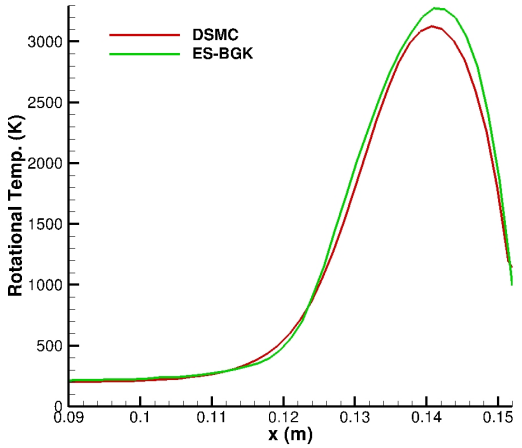



- **Translational temperature profiles are similar, but thickness of the shock is wider in ES vs. DSMC.**
- **The width of the DSMC shock is about 0.015 m while the ES-BGK shock width is around 0.02 m.**
- **Rotational temperatures are in better agreement**

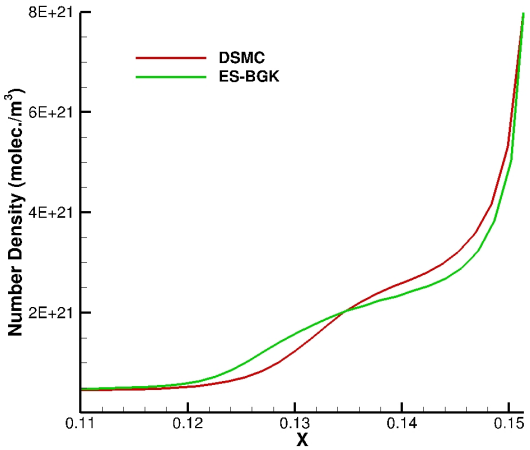
# Case II : Stagnation Line Profiles: *In Progress*



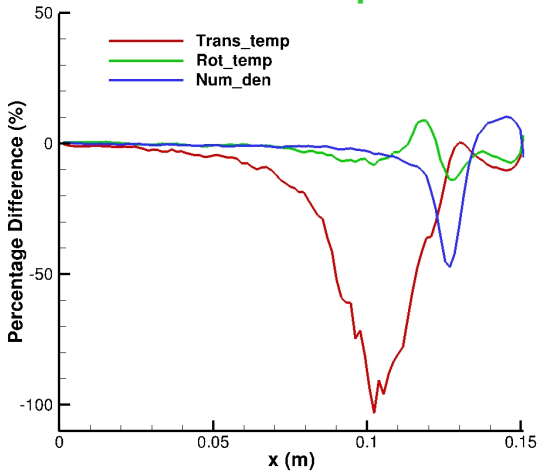

Translational temperature




Rotational temperature




Number density




Percentage difference

- **Difference in DSMC vs ES-BGK number density and rotational temperatures are small.**
- **But the translational temperature shows considerable deviation, due to the difference in the shock width.**

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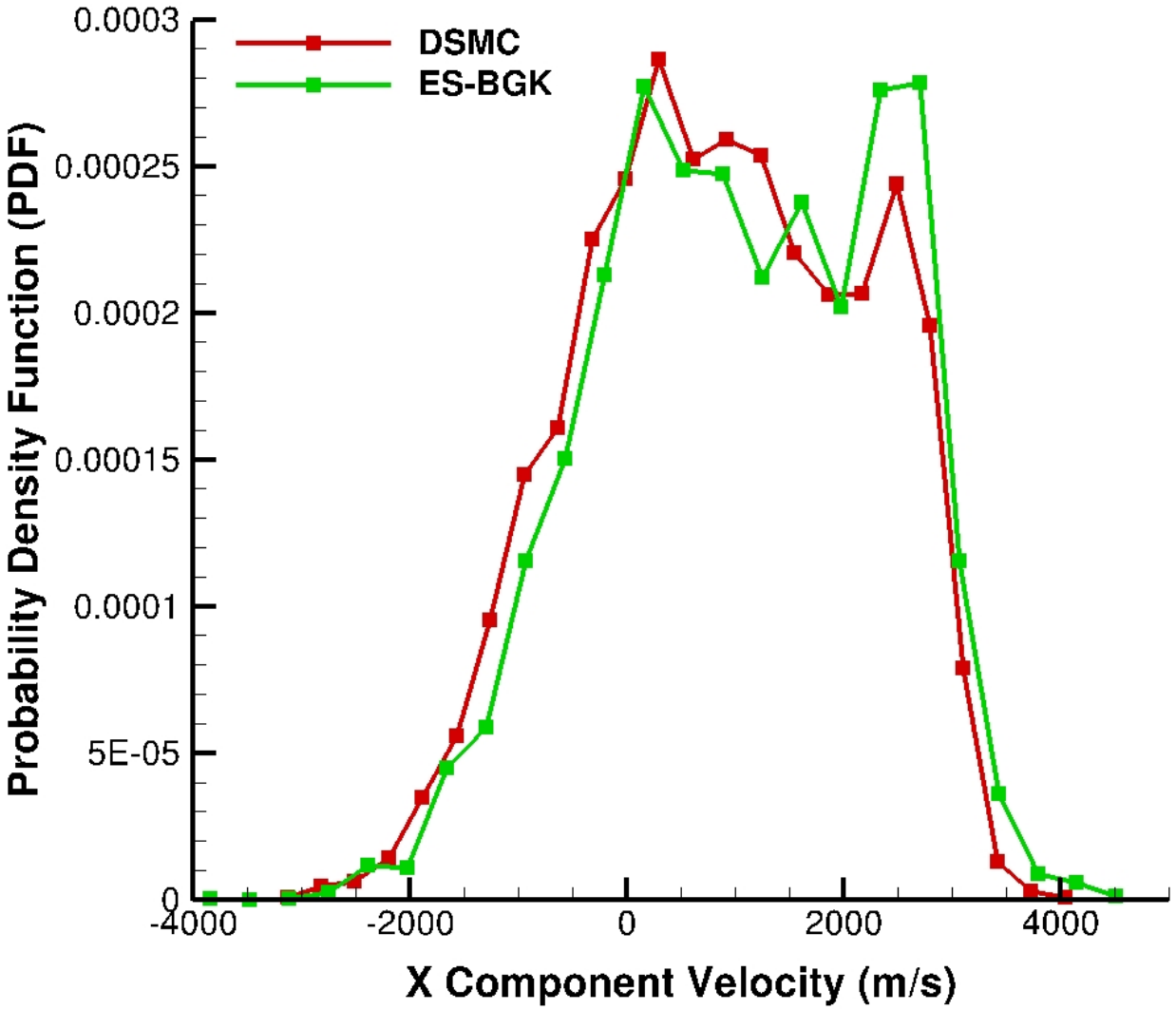
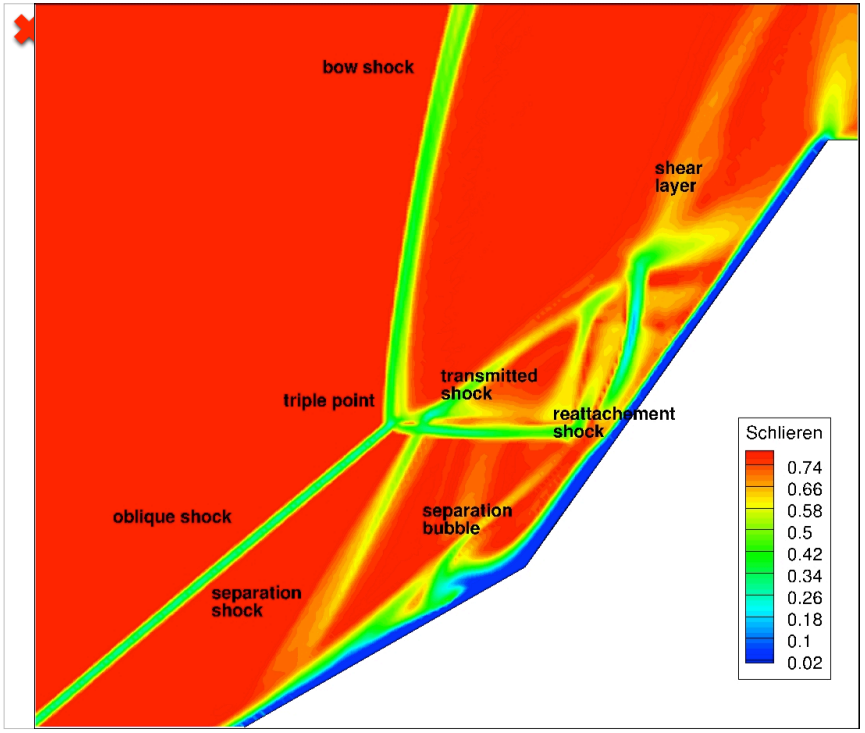
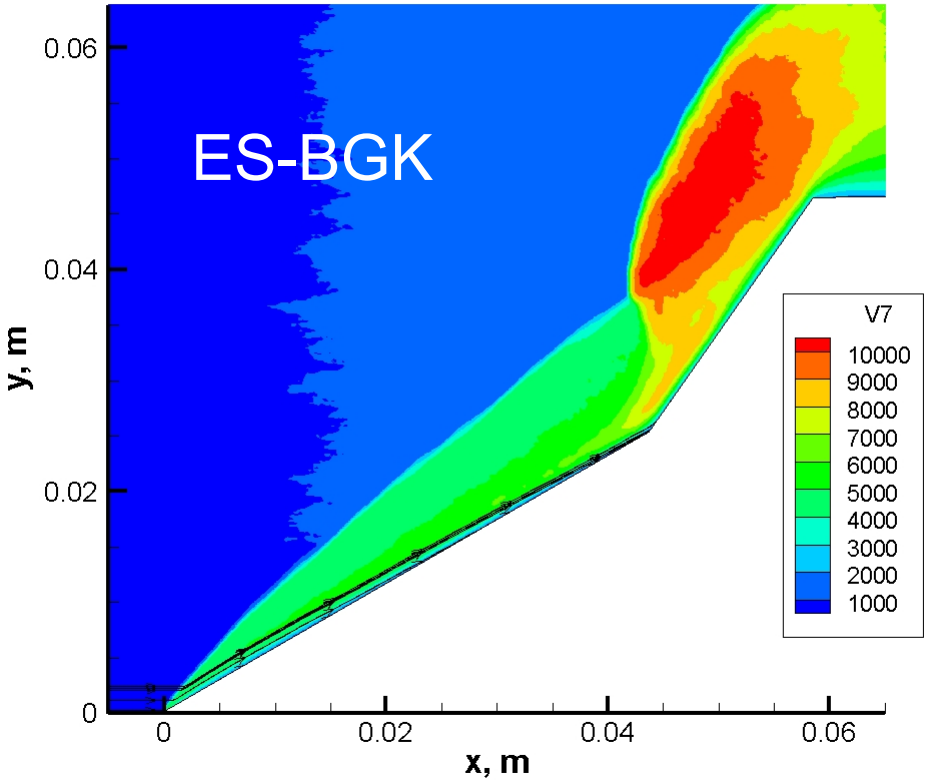
# Case II : Velocity PDF inside Shock




- Departure from Maxwellian distribution is seen at x=0.13 (for DSMC) and x=0.125 (for ES-BGK), in the center of the shock.
- Both ES-BGK and DSMC predict the bi-modal nature of the x-component velocity distribution.

# Comparison of DSMC vs BGK Shock-Shock Interactions




- DSMC resolves experimentally observed complex shock structures,
- In BGK, an oblique shock, bow shock, and triple point can be seen, but, there is no separation region. Why not?

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# *Outstanding Scientific Issues*

- **Our fundamental understanding of laminar shock-shock interactions is far from complete:**
  - **Essentially no chemistry, single species,**
  - **Eliminates many uncertainties in physical models.**
- **Top priorities are the investigation of 3-D vs 2-D affects on the unsteadiness of the DSMC modeled flows.**
- **This data set is part of the AVT-205 so that comparisons with NS/CFD will be interesting.**
- **Development of particle-based algorithm, ES-BGK for compression and shock-shock interactions:**
  - **progression from simple to hard, i.e., flow over a sphere, flow over a flat plate at variable AOA to get separation, and double wedge.**
  - **is there a break down criteria?**
  - **will ES-BGK provide a bridge between DSMC and NS?**
  - **is it computationally worth it compared to promise of new AMR grid techniques?**
- ***Future transitions: modeling of NO formation.***

# *Acknowledgments*

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