Sparta: Validation and Verification

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DSMC15 Short Course

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U.S. DEPARTMENT OF ENERGY

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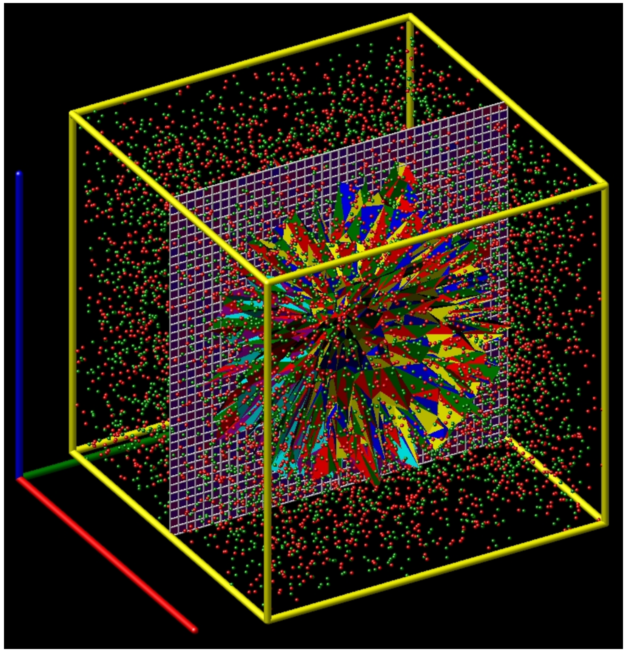
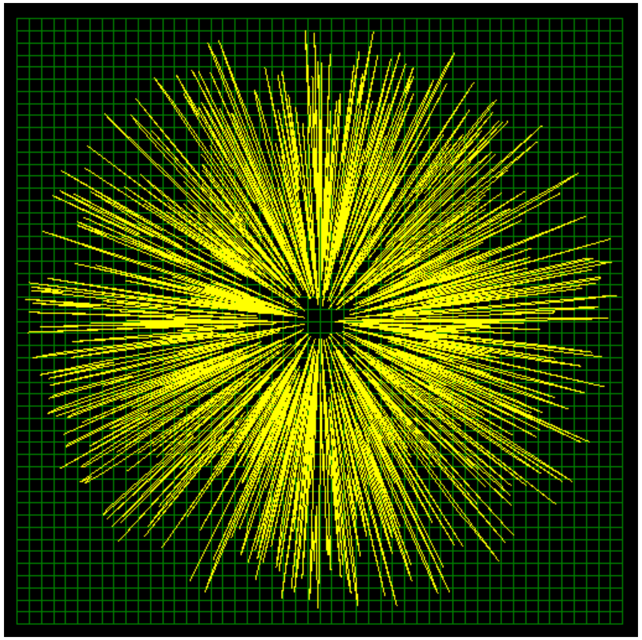
NNSA National Nuclear Security Administration

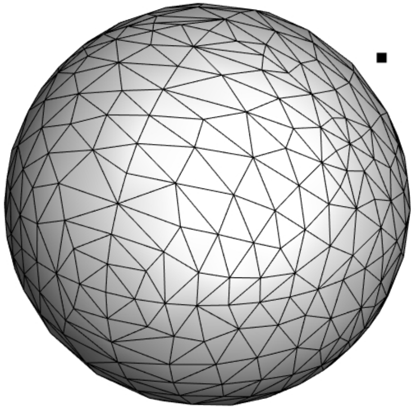
Geometry Description

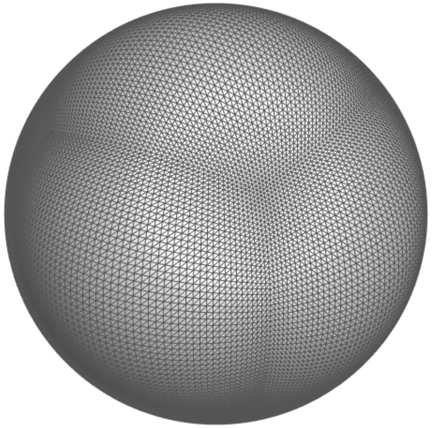
- SPARTA now computes all the cut cell volumes, identifies any split cells, colors all grid cells as inside, outside, or cut/split.
- Each surface in a split cell is tagged by which split volume it belongs to, which will be needed for tracking particles into the split cells.
- Infinitely thin surfaces are detected and correctly dealt with during molecular advection.





Volume calculation



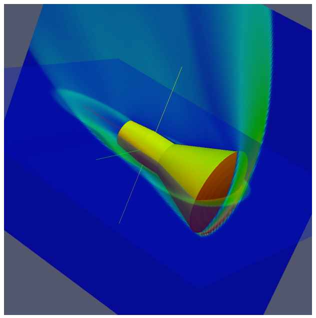


Method/resolution	Flow-field volume (m^3)
1200 elements	59.86171
15000 elements	59.81132
Theory	**59.81121**

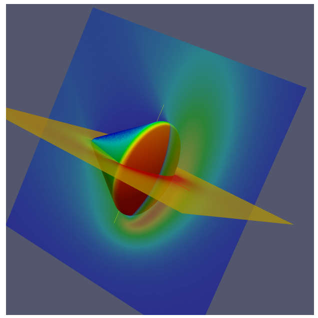
SPARTA uses Cartesian cells to discretize physical space. Cells near surfaces are “cut” by the geometry. For the accurate calculation of the collision frequency,- an accurate calculation of the cut-cell volume is needed.

Simulations of Re-entry Vehicles

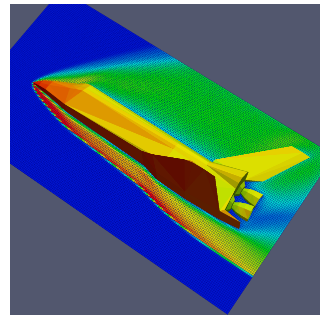
Gemini
1961-1966



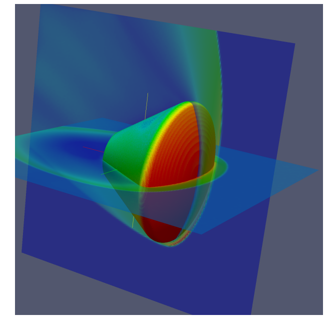
Apollo
1963-1972



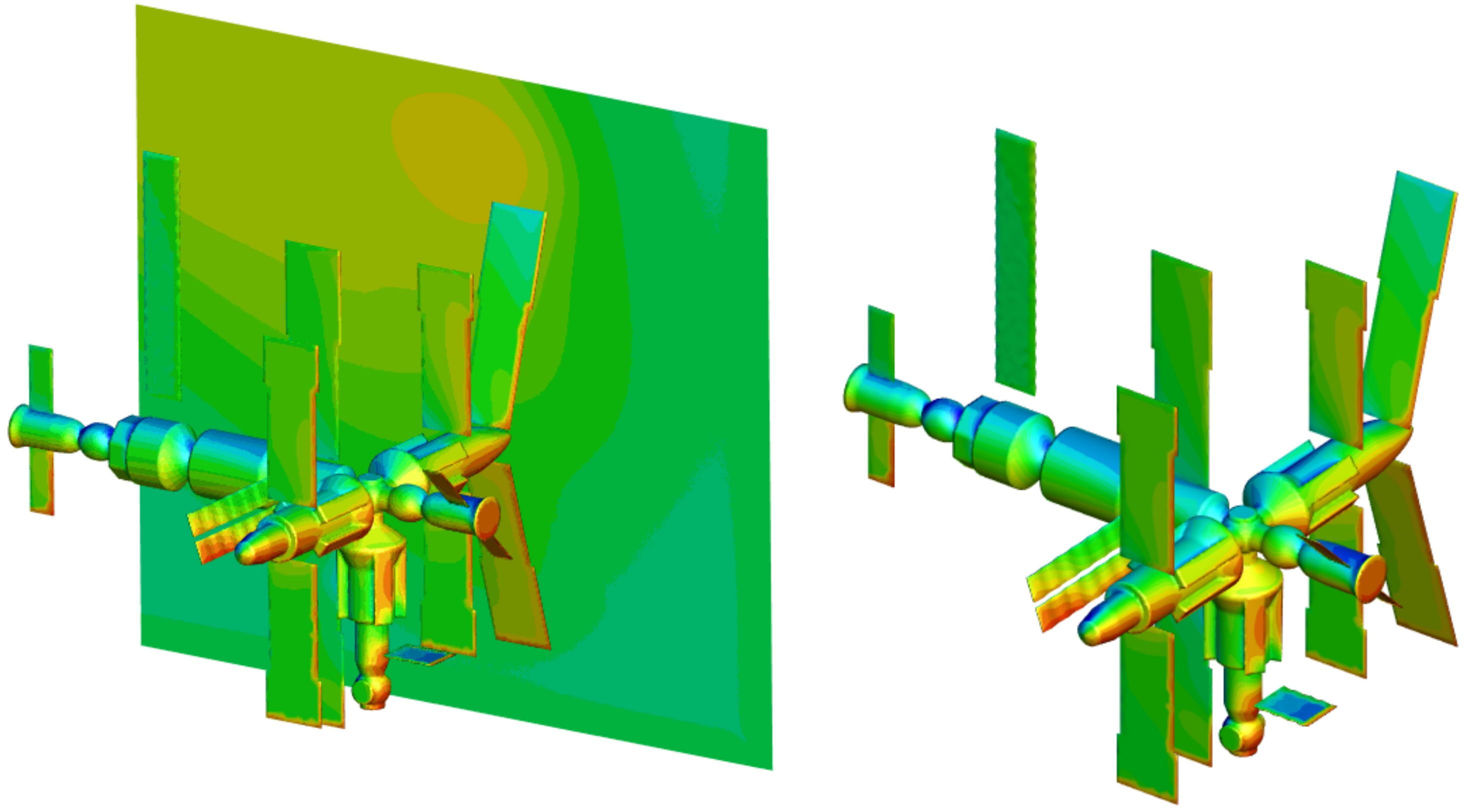
Space Shuttle
1981-2011



Orion
2014-?



Simulation of Mir Space Station



Grid generation (10^7 cells) completed in 0.3 seconds on 16 processors
Geometry comprises multiple “water-tight” bodies

Verification test cases

- **Closed box**
  - Collision frequency
  - Conservation of mass, momentum, energy
  - Inflow boundary conditions
  - Internal energy relaxation
  - Chemical reactions
- **Sonine polynomials**
- **Axisymmetric flow**
- **Flow over a sphere**

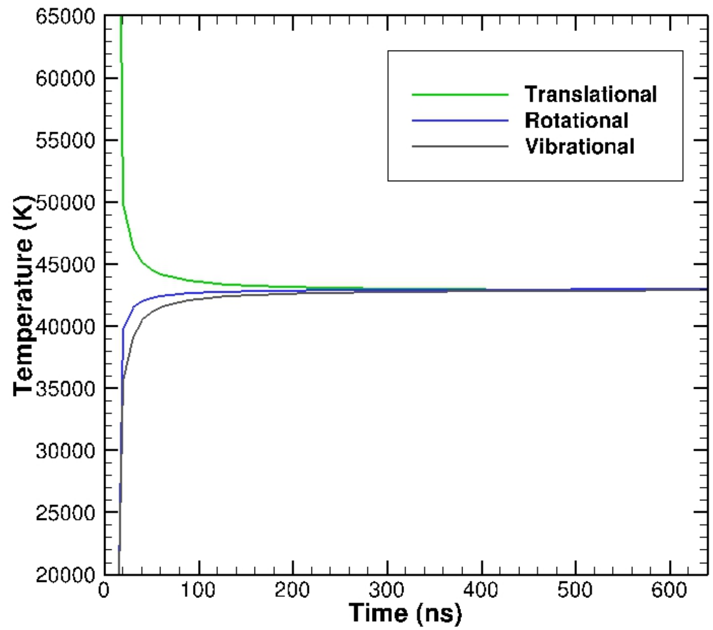
Collision Frequency

- Collision frequency inside a closed isothermal box (argon at 2 torr pressure at 273.15 K)

Step	CPU	Np	Natt	Ncollave	temp
0	0	10000	0	0	274.40561
100	0.048908949	10000	968	700.8	274.40561
200	0.097182035	10000	985	702.64	274.40561
300	0.14856601	10000	1005	704.95333	274.40561
400	0.19848394	10000	998	705.7675	274.40561
500	0.24520898	10000	1022	706.47	274.40561
600	0.29146504	10000	1025	706.61833	274.40561
700	0.33719492	10000	1042	706.68571	274.40561
800	0.38323998	10000	1029	706.80125	274.40561
900	0.430583	10000	1052	706.89778	274.40561
1000	0.47937894	10000	1022	706.741	274.40561

Simulated collision frequency = 7.13949×10^{29} s^{-1}, Theoretical = 7.13103×10^{29} s^{-1} giving a theory to simulation ratio of 1.00014

Internal Energy Relaxation



Molecules of a diatomic gas are allowed to perform energy exchange through successive molecular collisions (specular walls). Initially the molecules are assumed to have all their energy in the translational mode. Eventually, all three energy modes, translational, rotational and vibrational, reach thermal equilibration.

Conservation of mass, momentum, energy

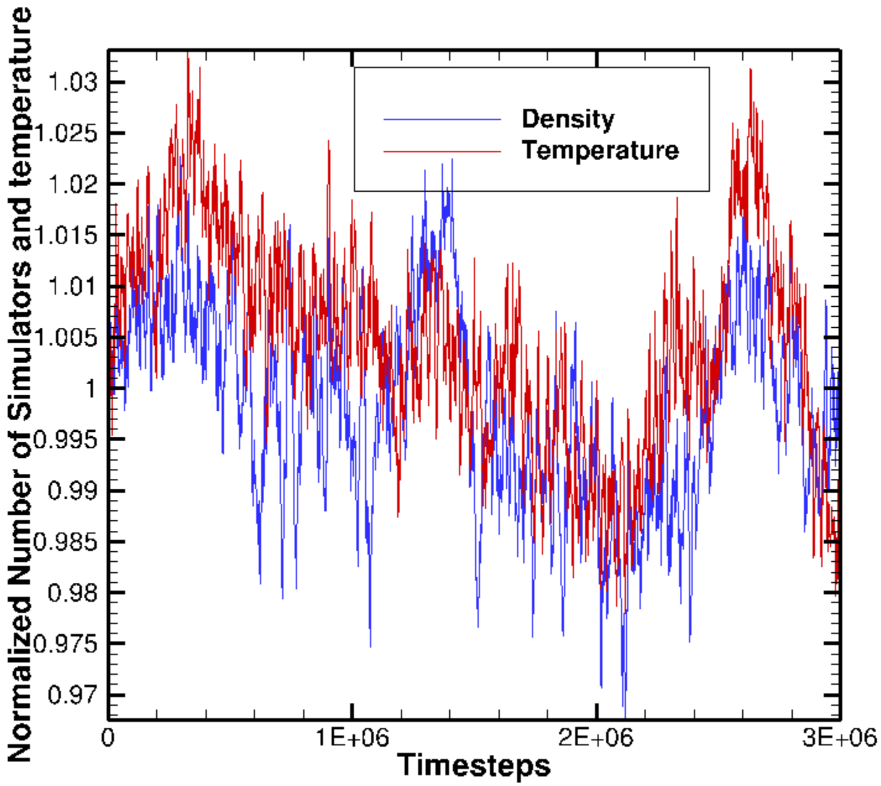
```
variable px particle mass*vx
variable py particle mass*vy
variable pz particle mass*vz
compute px reduce sum v_px
compute py reduce sum v_py
compute pz reduce sum v_pz
compute ke reduce sum ke
compute erot reduce sum erot
compute evib reduce sum evib
variable etot equal c_ke+c_erot+c_evib
stats_style step c_px c_py c_pz v_etot
stats_modify format float %1.15lg
```

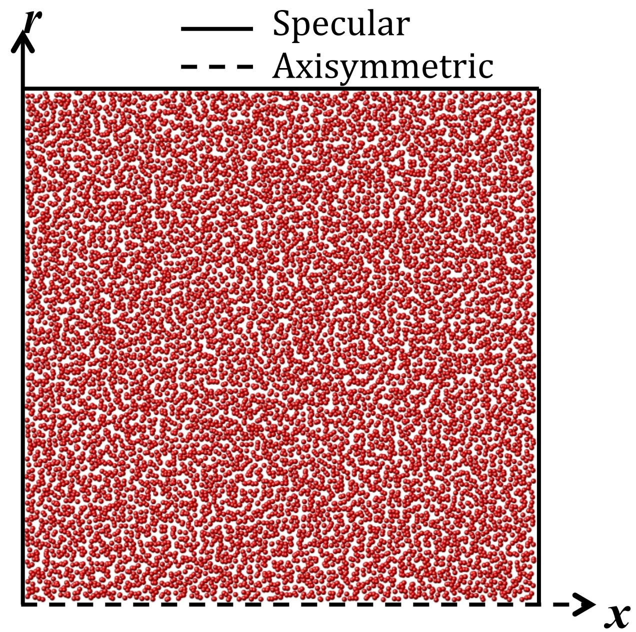
- Mass momentum end energy in the domain must be exactly conserved
- For a diatomic gas the total energy (translational, rotational, vibrational) is conserved
- Fluxes (energy, force) are only conserved to the limit of vanishing discretization

Conservation of mass, momentum, energy

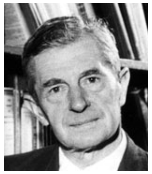
Step	Np	px	py	pz	etot
0	10000	2.83662739288096e-21	1.37629998275074e-22	1.11221277354614e-21	1.31731270155602e-16
1000	10000	2.83662739288095e-21	1.37629998275072e-22	1.11221277354614e-21	1.31731270155601e-16
2000	10000	2.83662739288095e-21	1.37629998275076e-22	1.11221277354614e-21	1.31731270155602e-16
3000	10000	2.83662739288097e-21	1.37629998275068e-22	1.11221277354614e-21	1.31731270155602e-16
4000	10000	2.83662739288096e-21	1.37629998275079e-22	1.11221277354615e-21	1.31731270155602e-16
5000	10000	2.83662739288097e-21	1.37629998275075e-22	1.11221277354615e-21	1.31731270155602e-16
6000	10000	2.83662739288096e-21	1.37629998275074e-22	1.11221277354615e-21	1.31731270155602e-16
7000	10000	2.83662739288097e-21	1.37629998275074e-22	1.11221277354615e-21	1.31731270155602e-16
8000	10000	2.83662739288097e-21	1.37629998275076e-22	1.11221277354615e-21	1.31731270155602e-16
9000	10000	2.83662739288099e-21	1.37629998275078e-22	1.11221277354615e-21	1.31731270155602e-16
10000	10000	2.83662739288098e-21	1.37629998275073e-22	1.11221277354615e-21	1.31731270155602e-16

Axisymmetric Flow

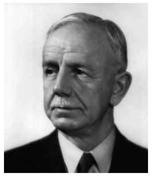




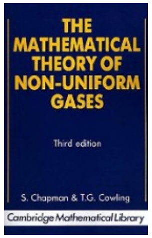
Near-Equilibrium: Chapman-Enskog (CE) Theory



Sydney Chapman



David Enskog



$$f = f^{(0)}(1 + \Phi^{(1)} + \Psi^{(1)}) \qquad f^{(0)} = (n/\pi^{3/2} c_m^3)\exp[-\tilde{c}^2]$$

$$c_m = \sqrt{2k_B T/m} \qquad \tilde{\mathbf{c}} = \mathbf{c}/c_m \qquad \mathbf{c} = \mathbf{v} - \mathbf{u}$$

$$\Phi^{(1)} = -(8/5)\tilde{A}[\tilde{c}]\tilde{\mathbf{c}} \cdot \tilde{\mathbf{q}} \qquad \Psi^{(1)} = -2\tilde{B}[\tilde{c}](\tilde{\mathbf{c}} \circ \tilde{\mathbf{c}} : \tilde{\tau})$$

$$\tilde{A}[\tilde{c}] = \sum_{k=1}^{\infty} (a_k/a_1) S_{3/2}^{(k)}[\tilde{c}^2] \qquad \tilde{B}[\tilde{c}] = \sum_{k=1}^{\infty} (b_k/b_1) S_{5/2}^{(k-1)}[\tilde{c}^2]$$

$$C_p = (5/2)(k_B/m) \qquad \mathrm{Pr} = (2/3)(\mu_\infty/\mu_1)(K_1/K_\infty)$$

- Chapman and Enskog analyzed Boltzmann collision term
  - Perturbation expansion using Sonine polynomials
  - Near equilibrium, appropriate in continuum limit
- Determined velocity distribution
  - Distribution "shape": Sonine polynomial coeffs. a_k/a_1, b_k/b_1
  - Values for all Inverse-Power-Law (IPL) interactions
    - Maxwell and hard-sphere are special cases

Gallis M. A., Torczynski J. R., Rader D. J., "Molecular Gas Dynamics Observations of Chapman-Enskog Behavior and Departures Therefrom in Nonequilibrium Gases", *Physical Review E*, 69, 042201, 2004.

Extracting CE Parameters from DSMC

$$\frac{a_k}{a_1} = \sum_{i=1}^{k} \left(\frac{(-1)^{i-1} k!(5/2)!}{(k-i)!i!(i+(3/2))!} \right) \left(\frac{\langle \tilde{c}^{2i} \tilde{c}_x \rangle}{\langle \tilde{c}^2 \tilde{c}_x \rangle} \right) \qquad \tilde{\mathbf{c}} = \frac{\mathbf{v} - \mathbf{V}}{c_m}$$

$$\frac{b_k}{b_1} = \sum_{i=1}^{k} \left(\frac{(-1)^{i-1} (k-1)!(5/2)!}{(k-i)!(i-1)!(i+(3/2))!} \right) \left(\frac{\langle \tilde{c}^{2(i-1)} \tilde{c}_x \tilde{c}_y \rangle}{\langle \tilde{c}_x \tilde{c}_y \rangle} \right) \qquad c_m = \sqrt{\frac{2k_B T}{m}}$$

DSMC moments of velocity distribution function

- Temperature T, velocity V
- Higher-order moments

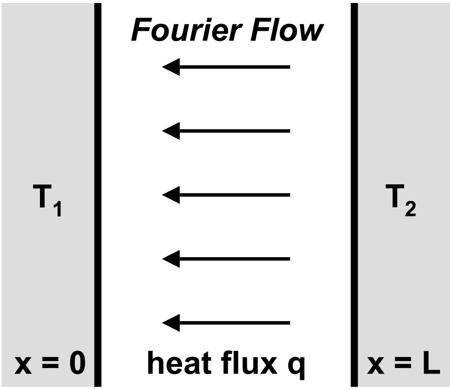
DSMC values for VSS molecules (variable-soft-sphere)

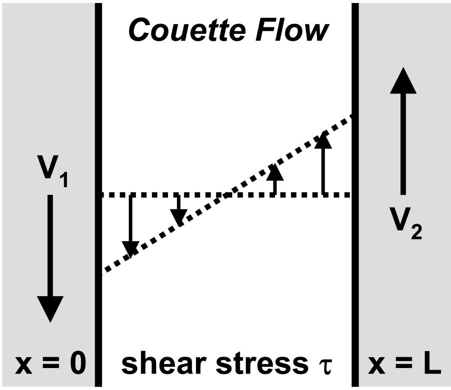
- Sonine-polynomial coefficients: a_k/a_1 and b_k/b_1
- Applicable for arbitrary Kn_L, Kn_q, Kn_τ

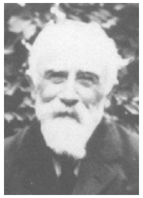
Quantifying Non-Equilibrium
Fourier and Couette Flow

Joseph Fourier

$$q = -K \frac{\partial T}{\partial x}$$







Maurice Couette

$$\tau = \mu \frac{\partial v}{\partial x}$$

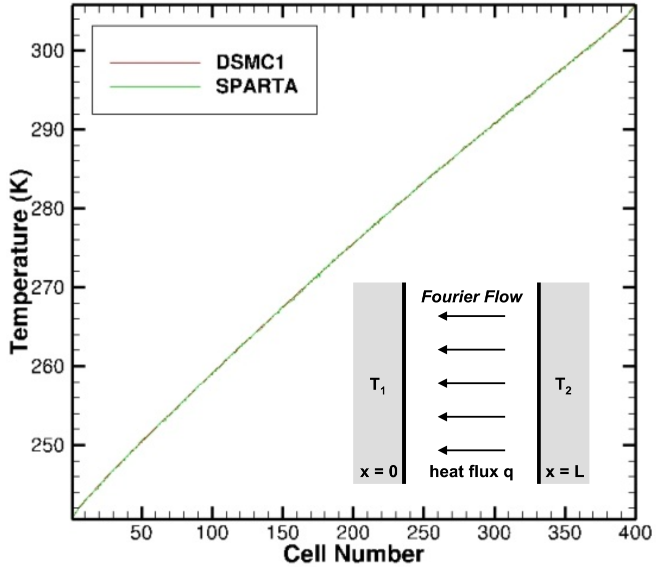
Investigate transport in gas between parallel plates
- Fourier flow: heat conduction in stationary gas
- Couette flow: momentum transport in isothermal shear flow

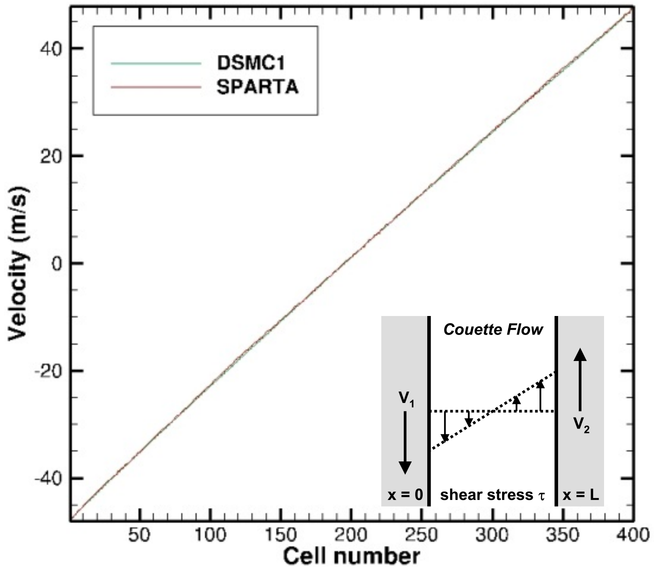
Apply DSMC to Fourier flow and Couette flow
- Heat flux, shear stress: one-dimensional, steady

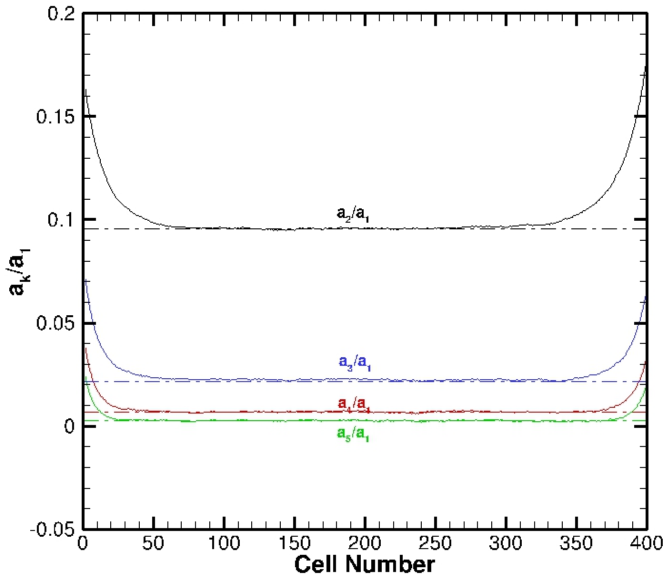
Compare DSMC to analytical "normal solutions"
- Normal: outside Knudsen layers
- Solutions: Chapman-Enskog (CE), Moment-Hierarchy (MH)

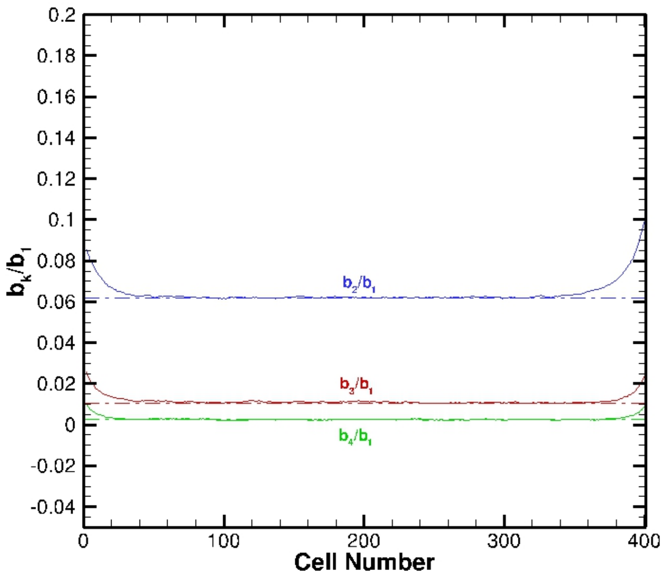
Verify DSMC accuracy at arbitrary heat flux, shear stress
- Thermal conductivity, viscosity; velocity distribution

Sonine Polynomial Coefficients



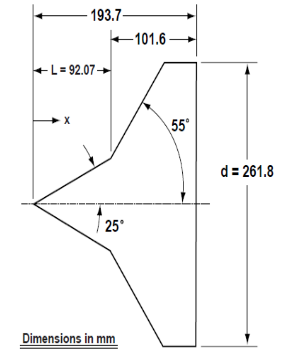


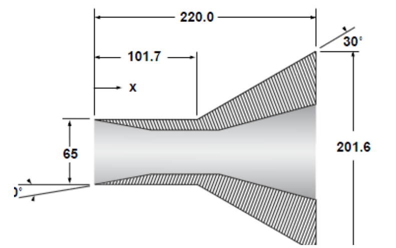


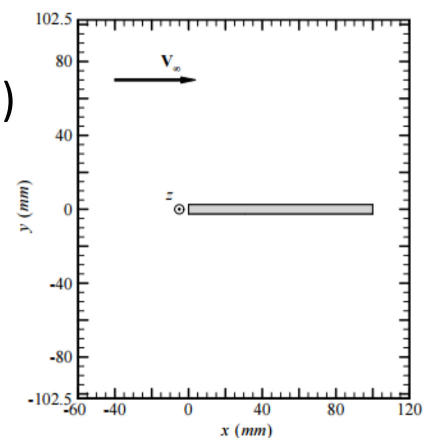


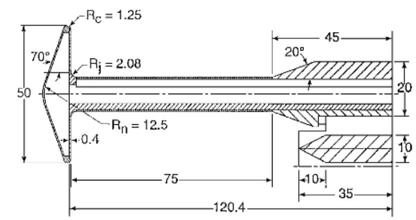
Validation test cases

- Comparisons with experimental data from:
  - CUBRIC Lens
    - 25/55 deg biconic (2D-axisymmetric)
    - Hollow cylinder flare (2D-axisymmetric)
  - SR3
    - 70 deg Cone (2D-axisymmetric)
    - Flat plate (2D)









Simulations performed by A. Klothakis and I. Nikolos, *Modeling Of Rarefied Hypersonic Flows Using The Massively Parallel DSMC Kernel "Sparta"*, 8th GRACM International Congress on Computational Mechanics, Volos, Greece, July 12– 15, 2015

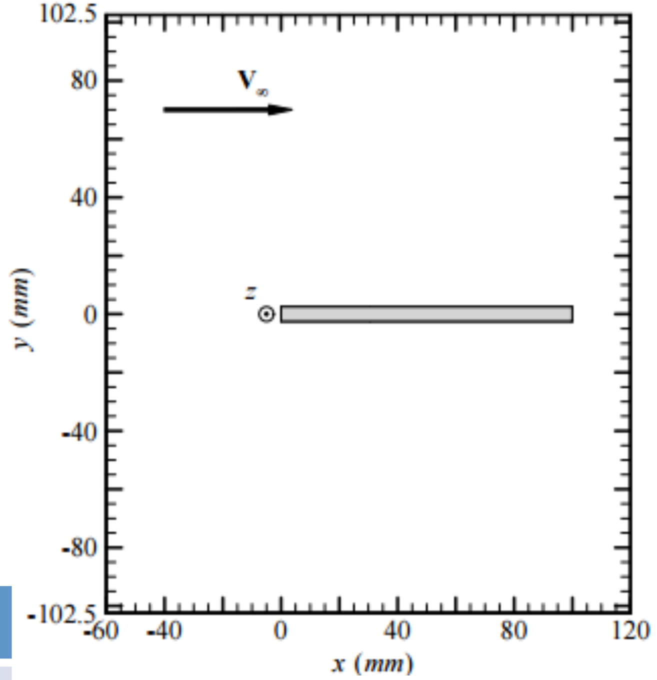
Hypersonic flow around a flat plate

- Geometry: Flat plate

Length : 100mm

Height : 50mm

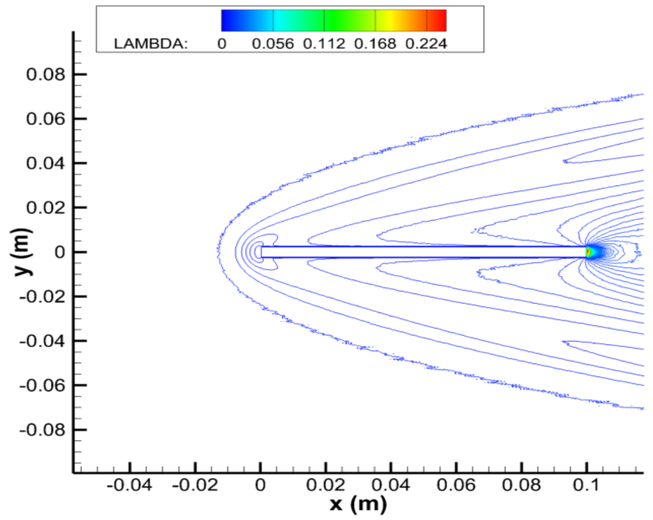
- Flowfield Dimensions : 180mm x 205mm
- Grid size: 360 x 410 cells
- Cell size: 0.5mm x 0.5mm
- λ=1.6mm

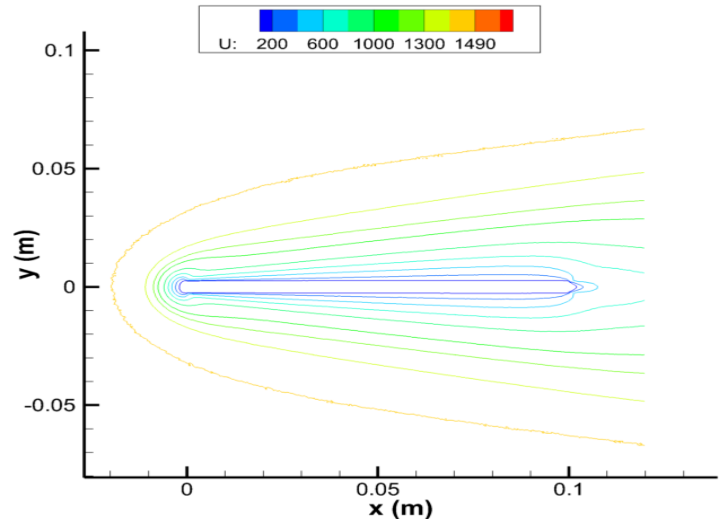


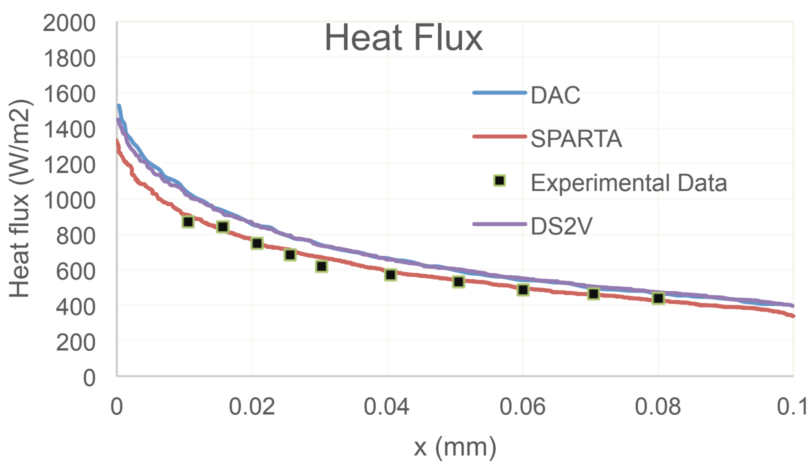
Flow conditions			
V_∞	T_∞	T_w	Density
1504	13.32	290	3,71610[20]

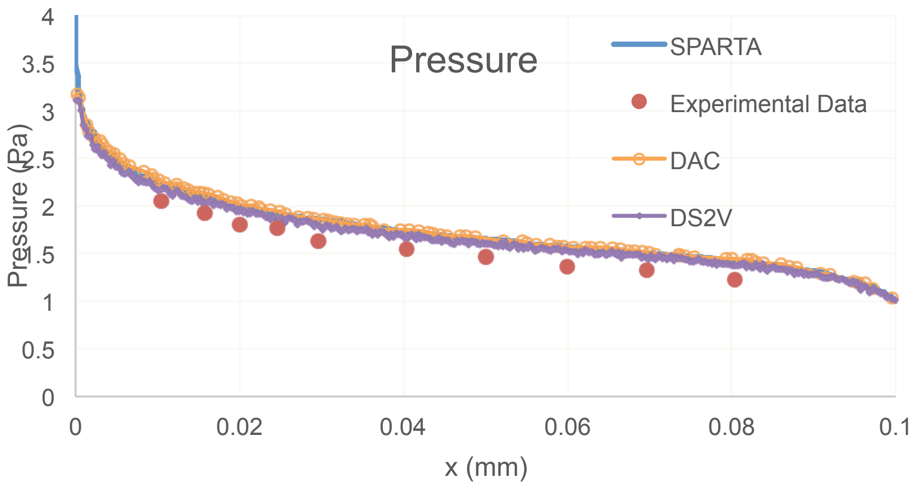
Allègre, J., Raffin, M., Chpoun, A., Gottesdiener, L. (1992), "Rarefied Hypersonic Flow over a Flat Plate with Tuncated Leading Edge", *Progress in Astronautics and Aeronautics,* pp. 285-295

Hypersonic flow around a flat plate



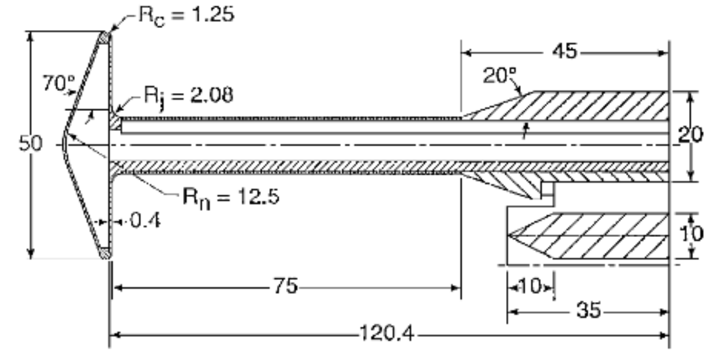






Hypersonic flow around a 70-degree blunt cone

- Geometry: AGARD Group Mars Pathfinder
- Flowfield dimensions: 10cm x 15cm
- Grid: 600x600 cells, 2-level 10x10 cells around the cone area

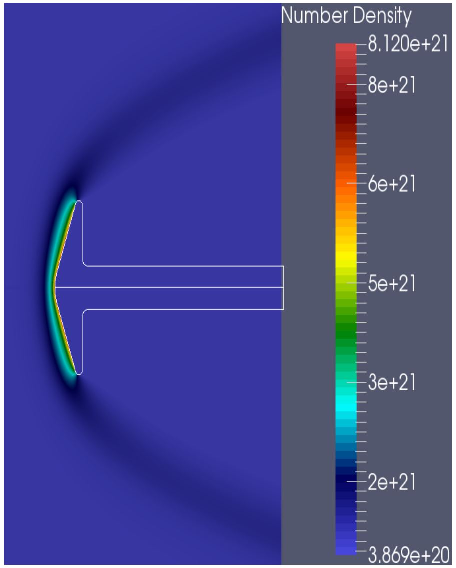


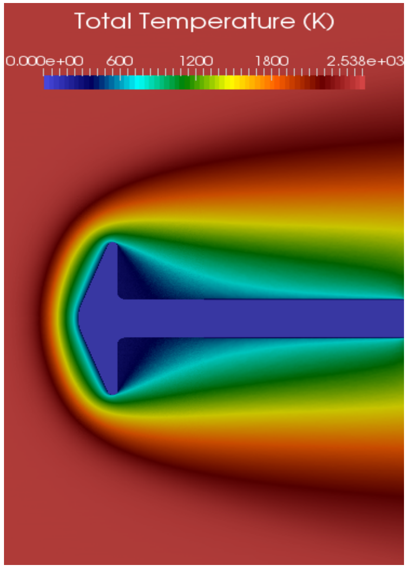
Blunt cone geometry
(Dimensions in mm)

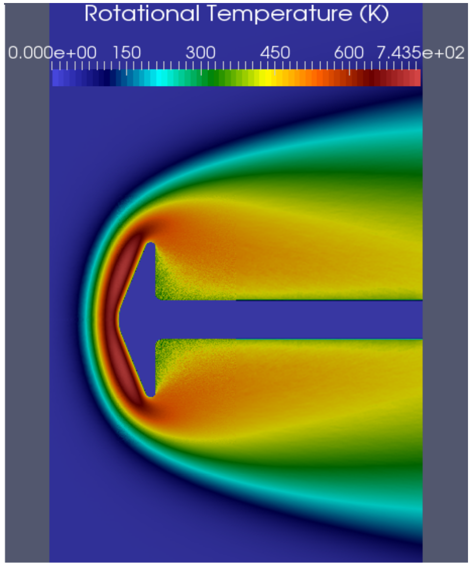
Flow conditions	Gas	Ma	T_0	P_0	Re
1	N_2	20.2	1100	3.5	1420
2	N_2	20	1100	10	4175

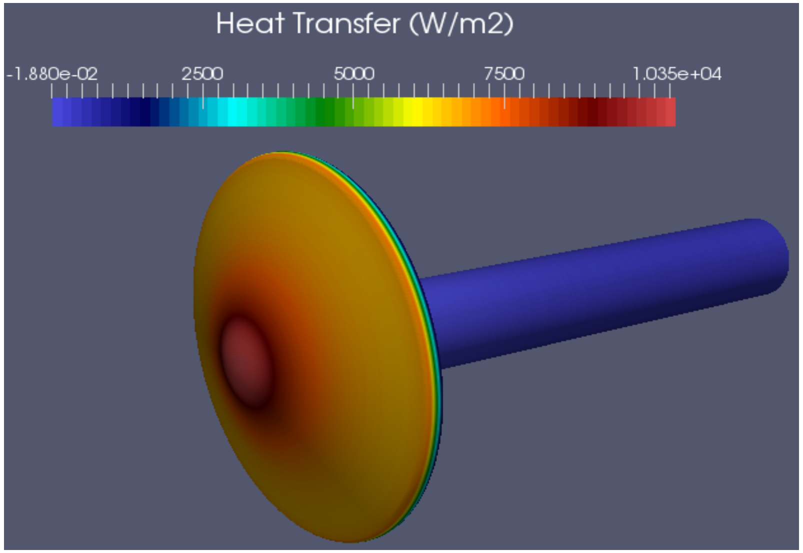
Allègre, J., Bisch, D., Lengrand, J. C. (1997), "Experimental Rarefied Heat Transfer at Hypersonic Conditions over a 70-Degree Blunted Cone", Journal of Spacecraft and Rockets, Vol. 34, No. 6, pp. 724-728.

Hypersonic flow around a 70-degree blunt cone

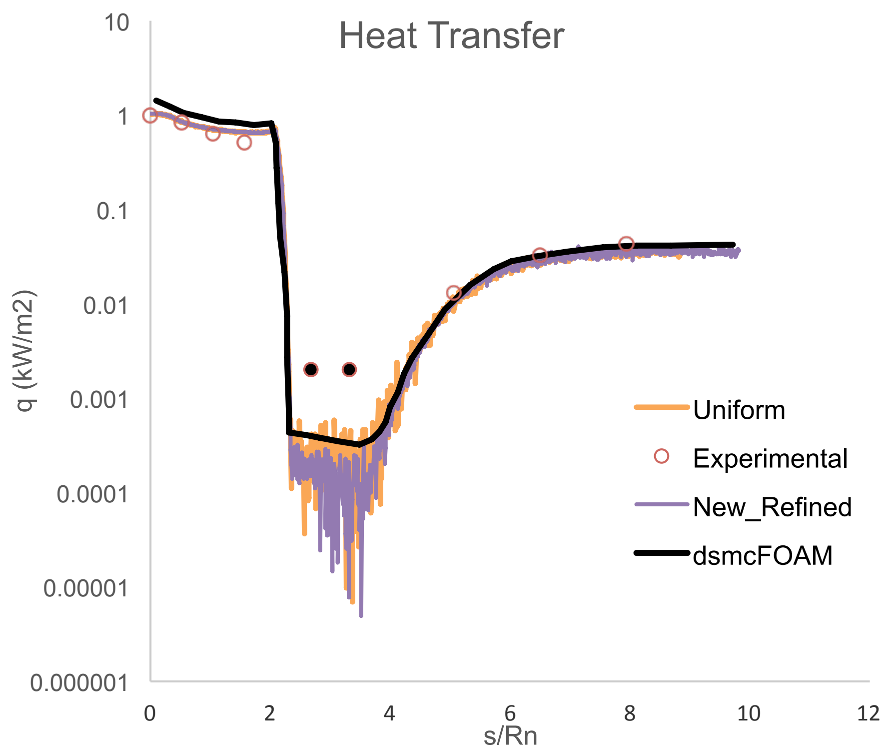


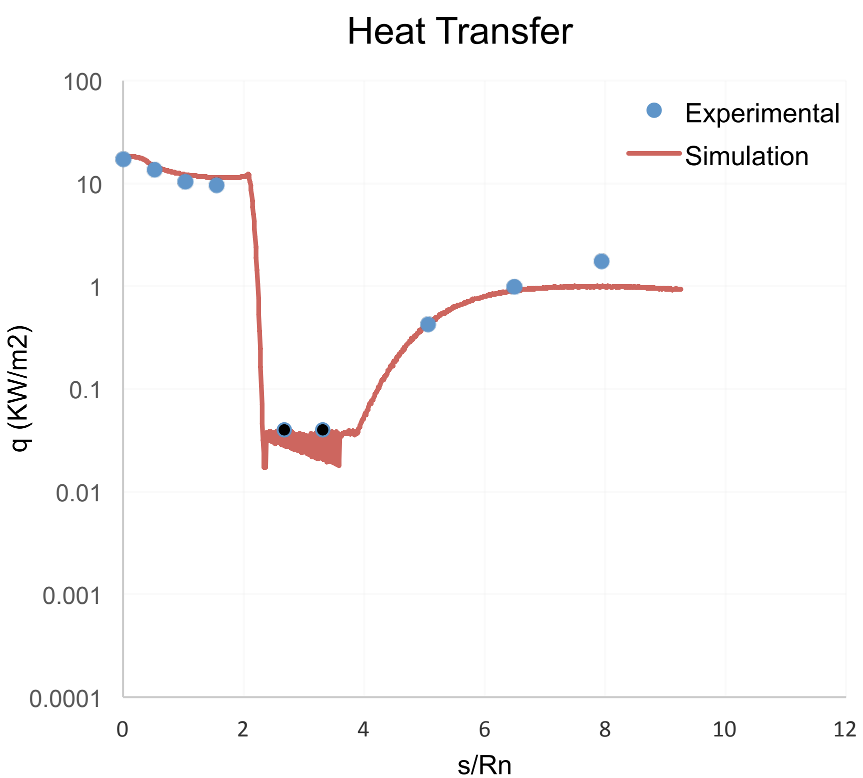






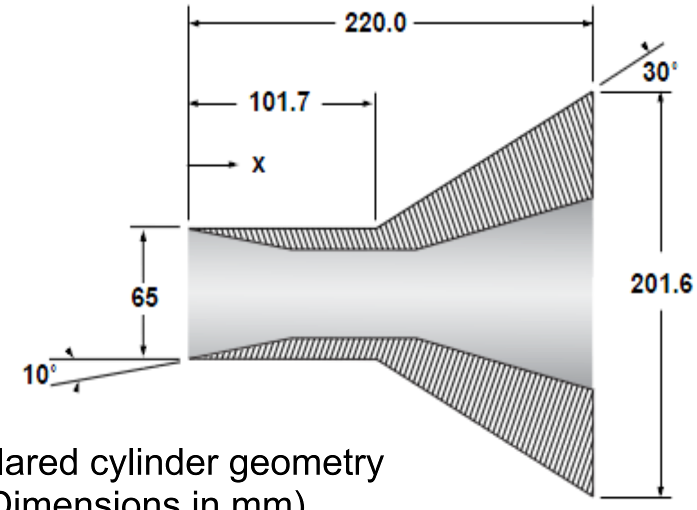
Hypersonic flow around a 70-degree blunt cone





Hypersonic flow around a flared cylinder

- Flowfield dimensions: 22cm x 12cm
- Grids : Uniform 1000x1800 cells, 2-Level 957x440 cells second level 10x10 cells

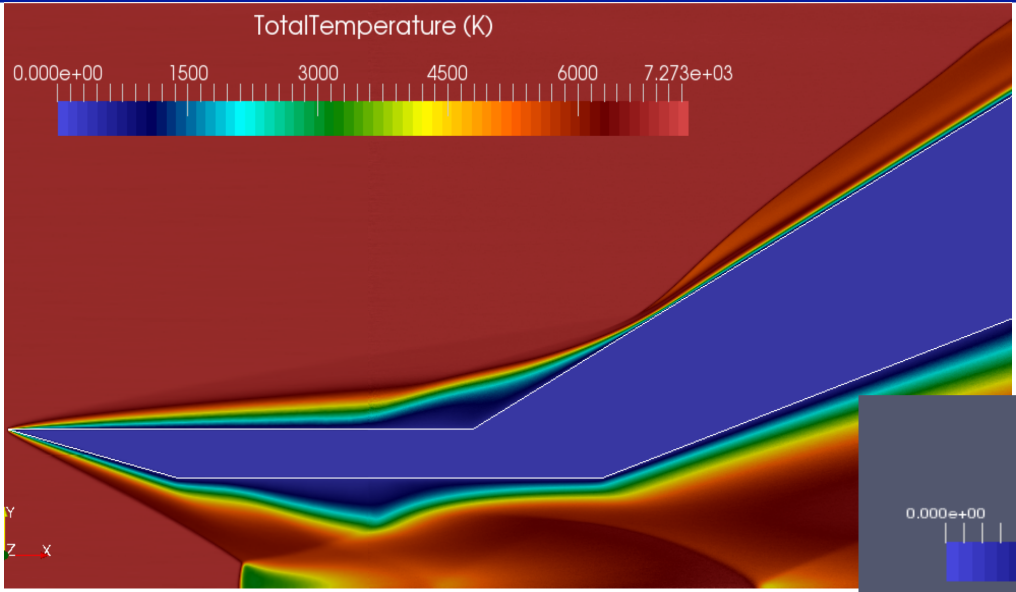


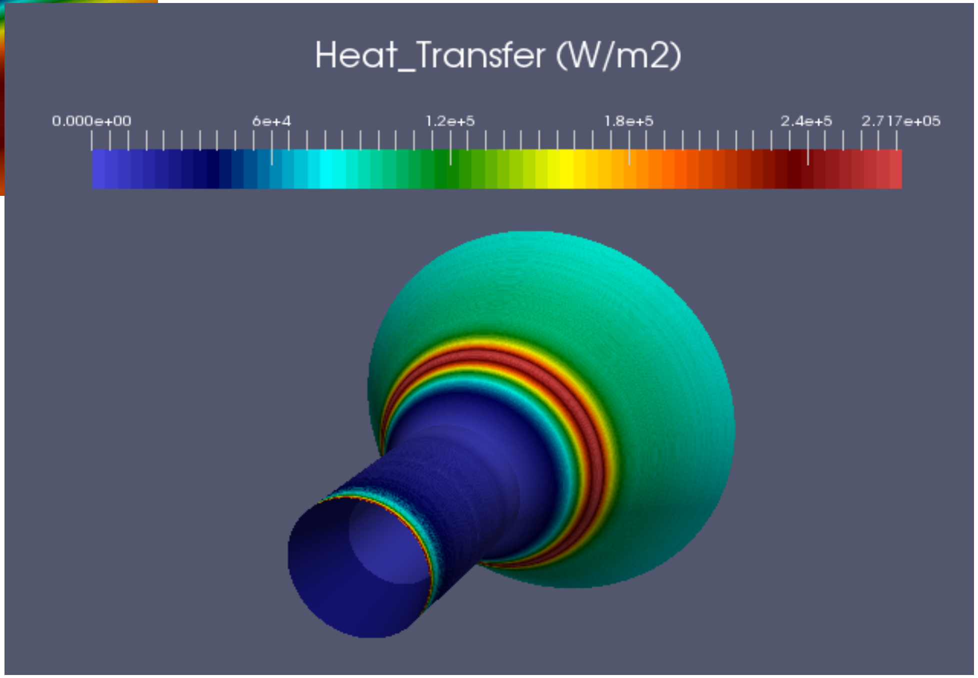
Flared cylinder geometry
(Dimensions in mm)

Conditions	Flow Velocity (m/s)	Number Density, m^{-3}	Flow temperature (K)	Gas	Surface Temperature (K)
LENS Run 11	2484	3.78×10^{21}	95.6	N_2	297.2

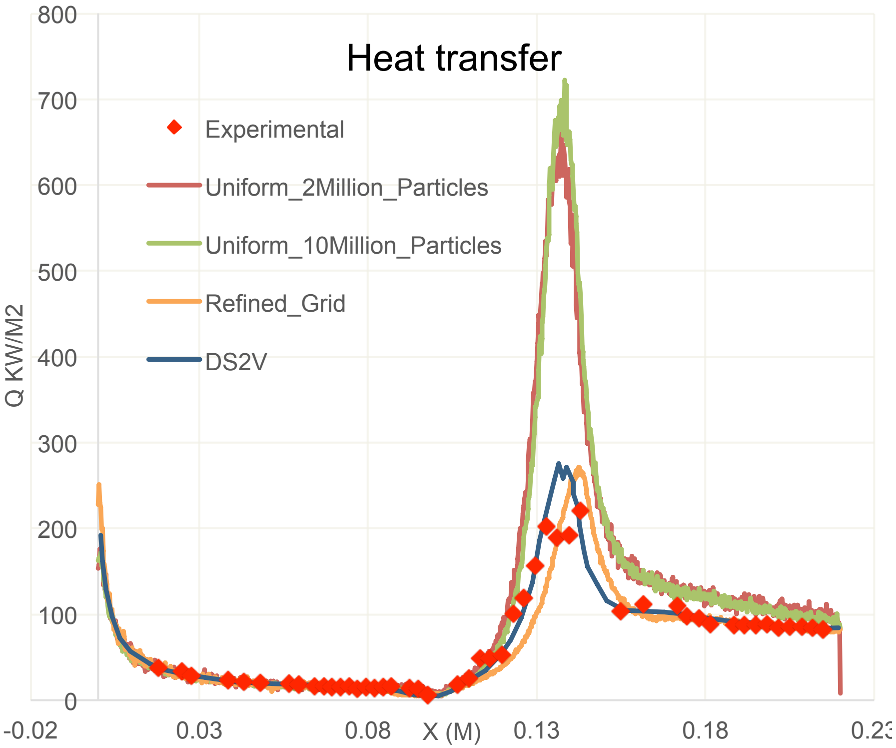
Holden, M., Harvey, J., Wadhams, T., and MacLean, M., "A Review of Experimental Studies with the Double Cone Configuration in the LENS Hypervelocity Tunnels and Comparisons with Navier-Stokes and DSMC Computations," AIAA 2010-1281, 48th AIAA Aerospace Sciences Meeting, Orlando, FL, January 4-7, 2010.

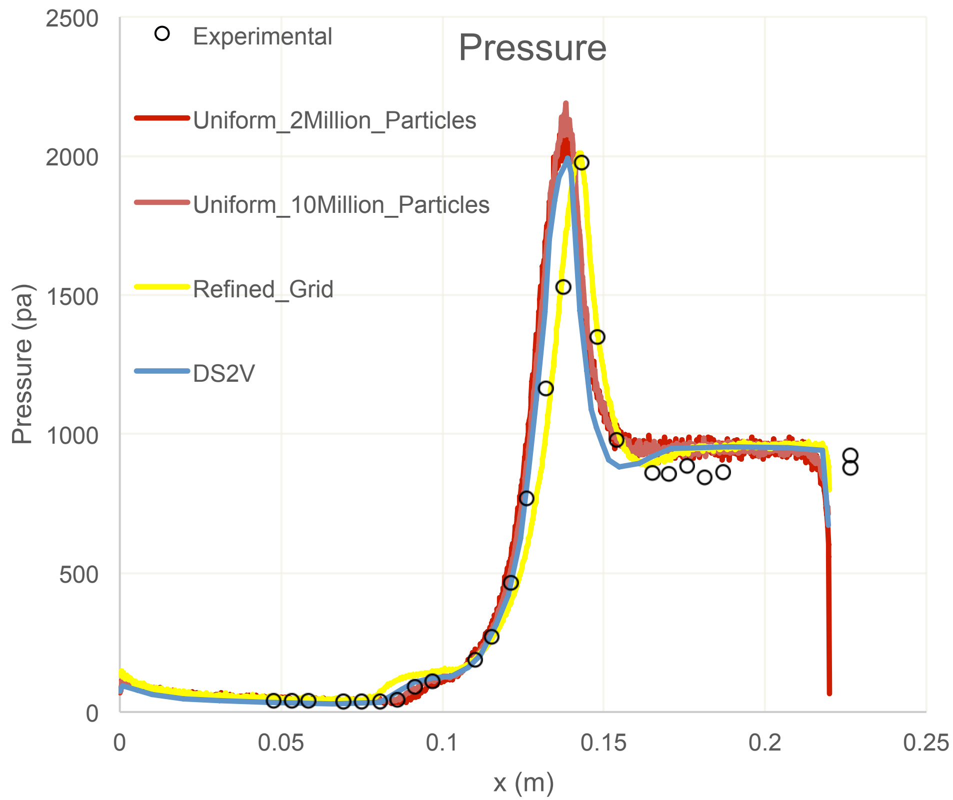
Hypersonic flow around a flared cylinder





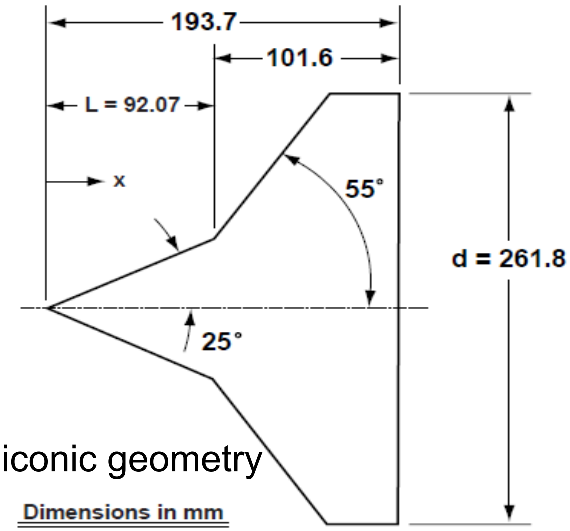
Hypersonic flow around a flared cylinder





Hypersonic flow around a 25/55 degree biconic

- Flowfield dimensions: 22cm x 50cm
- Grid : 2 level grid, first level 870x870 cells, second level 10x10 cells refinement o the first level, second level starts from 5cm after the biconic's leading edge and ends at the end of the biconic's surface.

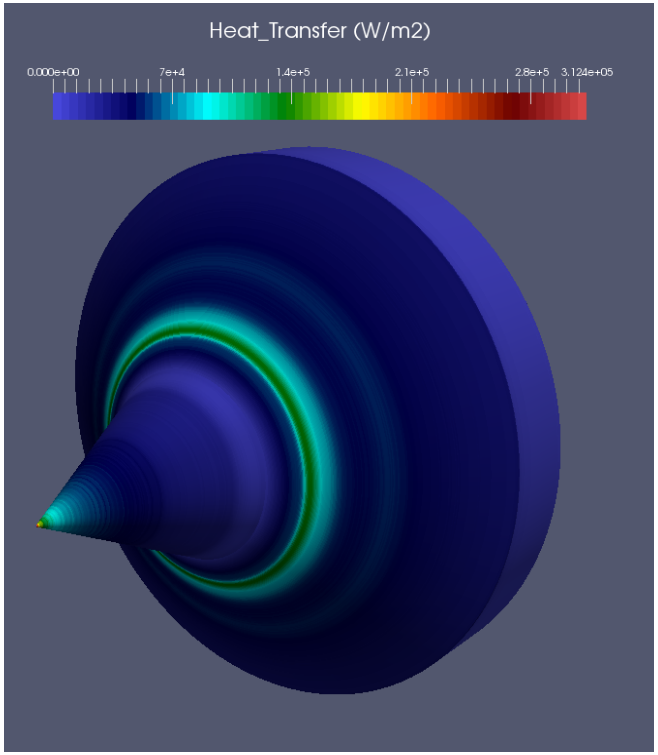


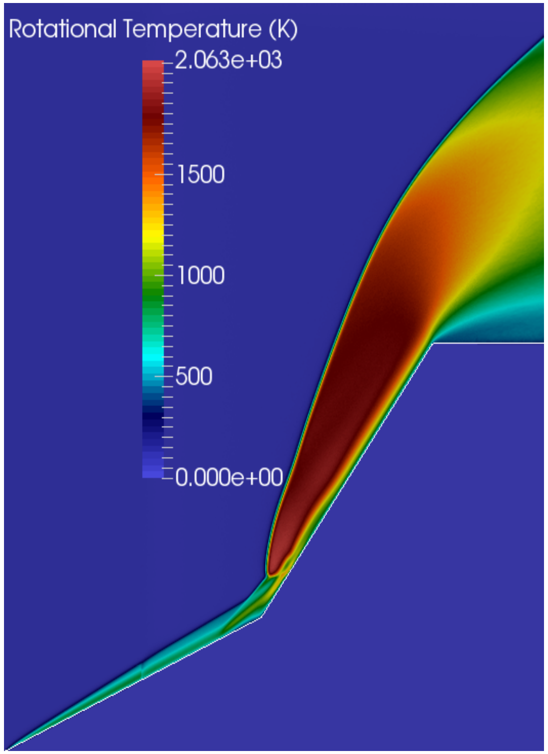
Biconic geometry

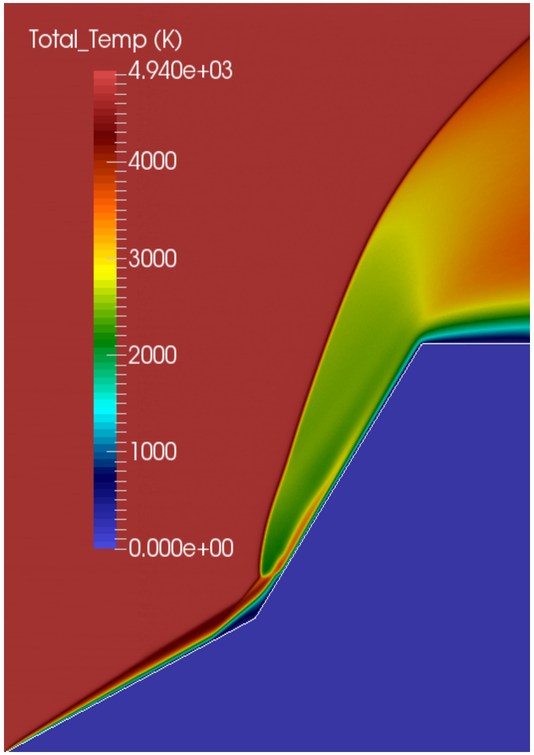
Conditions	Flow Velocity (m/s)	Number Density, m^{-3}	Flow temperature (K)	Gas	Surface Temperature (K)
CUBRC Run 7	2072.6	3.0×10^{18}	42.61	N_2	297.2

Holden, M., Harvey, J., Wadhams, T., and MacLean, M., "A Review of Experimental Studies with the Double Cone Configuration in the LENS Hypervelocity Tunnels and Comparisons with Navier-Stokes and DSMC Computations," AIAA 2010-1281, 48th AIAA Aerospace Sciences Meeting, Orlando, FL, January 4-7, 2010.

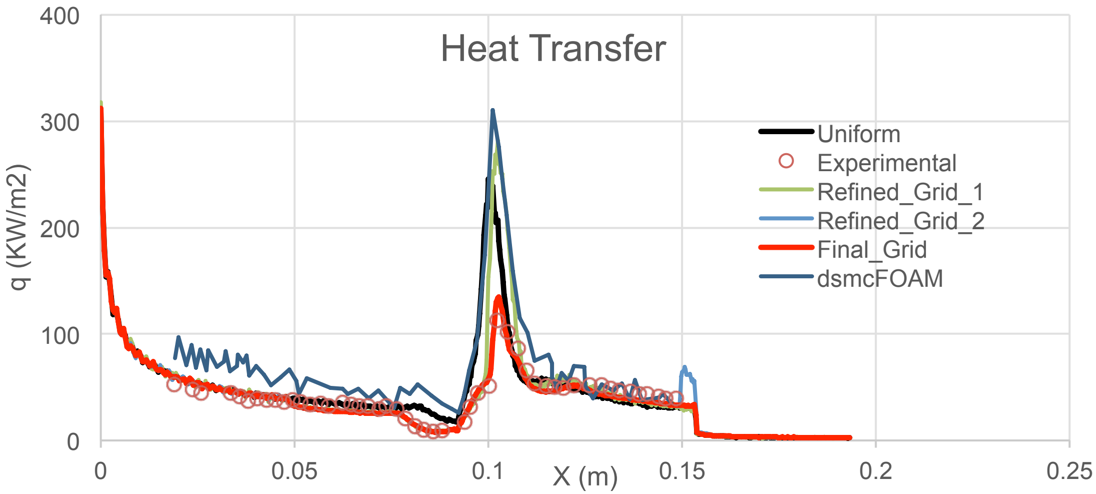
Hypersonic flow around a 25/55 degree biconic

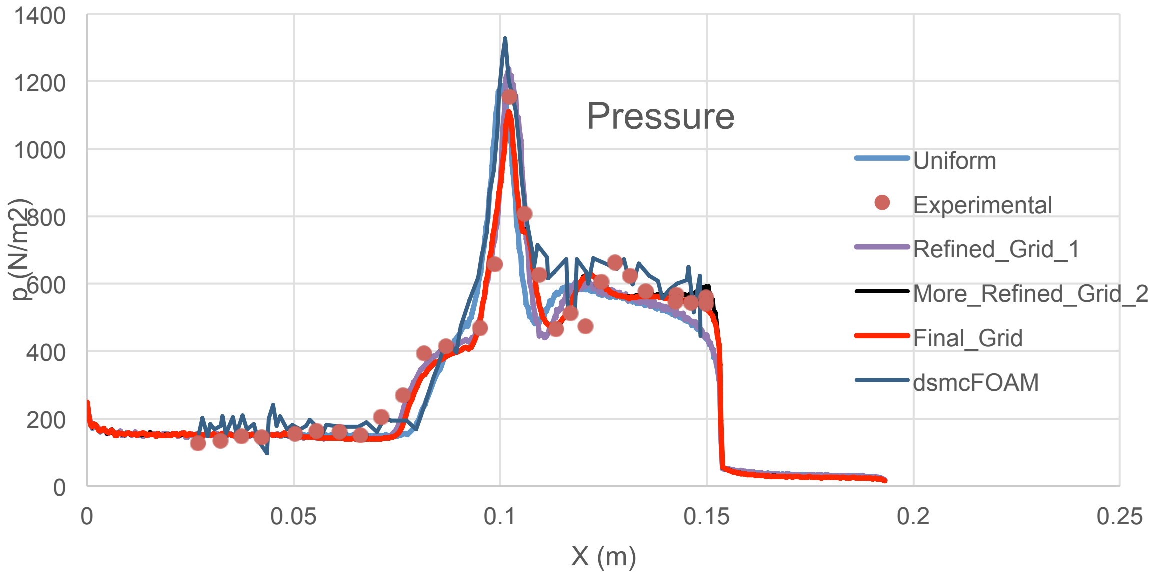




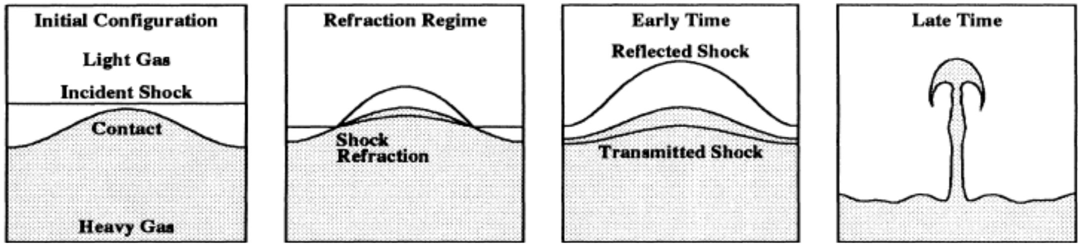


Hypersonic flow around a 25/55 degree biconic

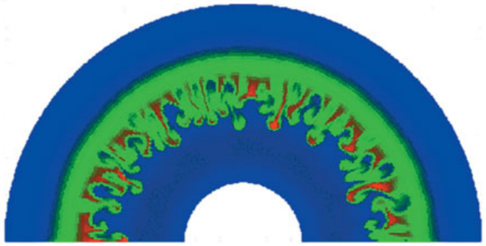




Hydrodynamic Instabilities: Richtmyer-Meshkov Instability (RMI)



Grove et al., Phys. Rev. Lett., 71(21), 3473 (1993).

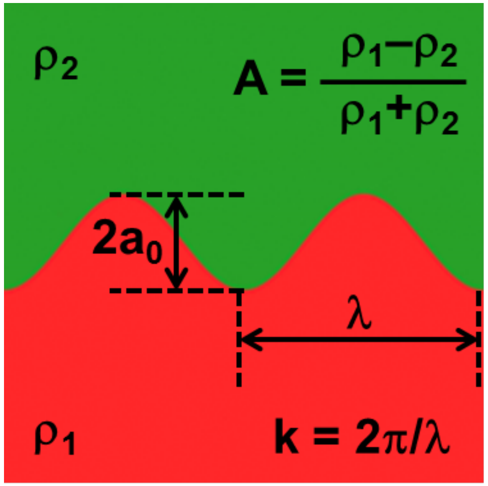


ICF target compression

RMI applications include stellar evolution, inertial confinement fusion, shock-flame interaction

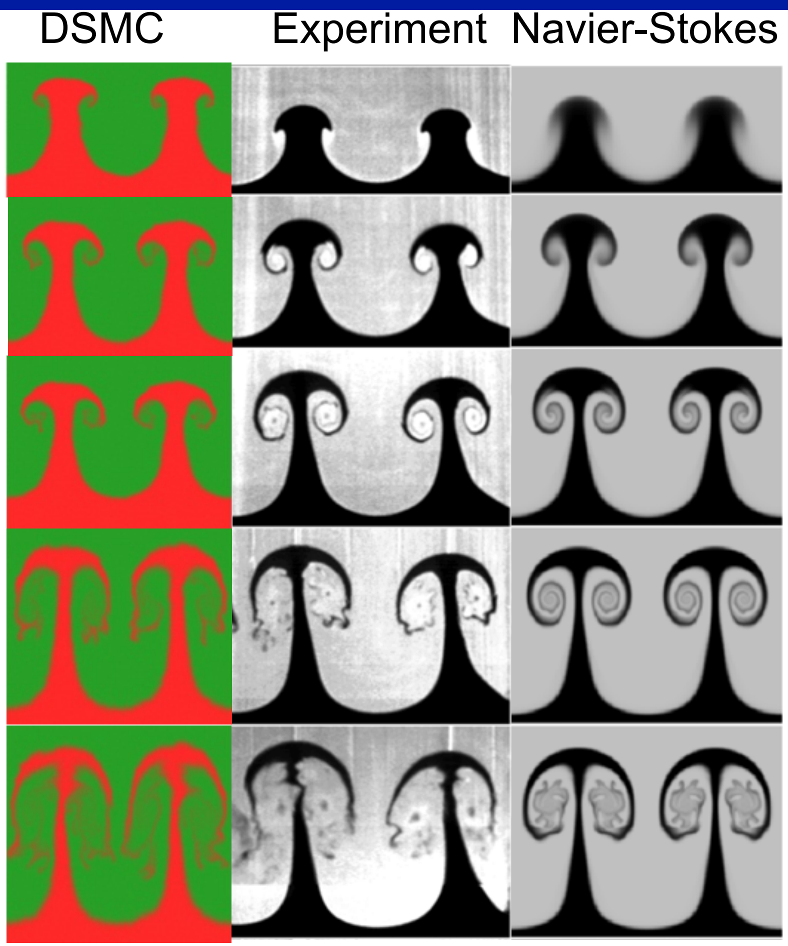
RMI combines multiple fluid-flow phenomena

- Shock transmission and reflection
- Hydrodynamic instabilities
- Linear and nonlinear growth
- Diffusion and turbulent mixing
- Compressibility effects
- Chemical reactions



RMI basic geometry

RMI in Air-SF_6 Mixture: Mach = 1.4 Shock



Morgan *et al.* JFM 2012