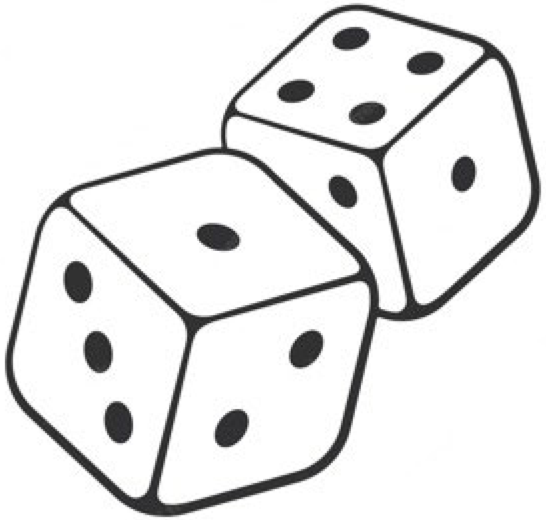
Analysis 101: Intro to DSMC

EDL Summer Seminar Series

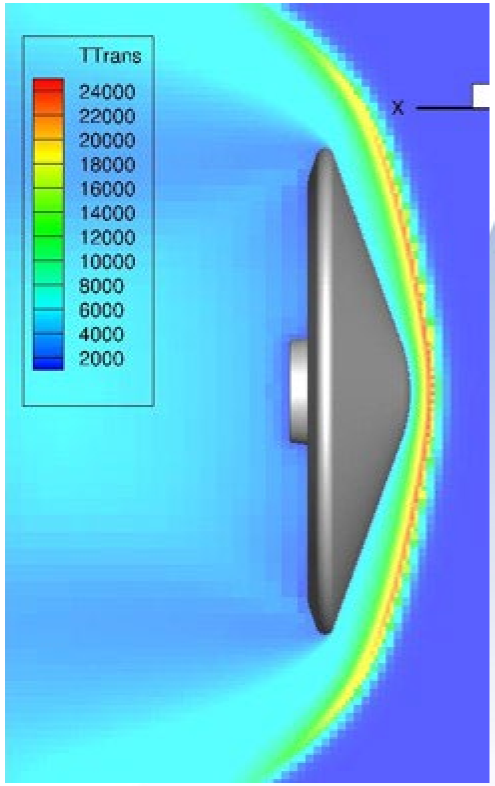


Dr. Arnaud Borner

AMA / NASA ARC

Dr. Derek Liechty

NASA LaRC



Welcome

Dr. Arnaud Borner

- 8 years at NASA ARC as contractor, first in Computational Physics branch, then TPS materials branch. Started as a postdoc.
- PhD from Penn State in 2014, dissertation on particle methods (DSMC, MD) for modeling space propulsion.
- 13 years working DSMC algorithms and codes.
- Other interests: TPS material modeling (micro- and macroscale), hypersonic aerothermodynamics, Venus.

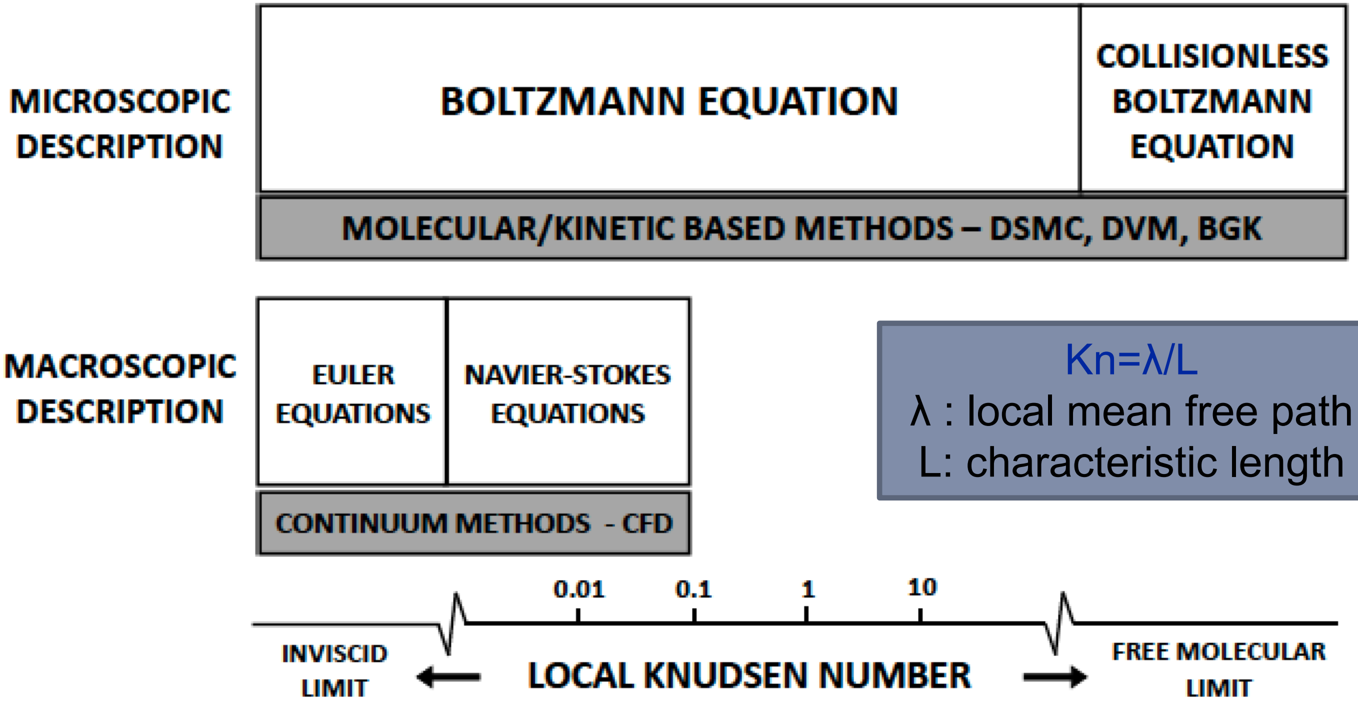
Dr. Derek Liechty

- 26 years at NASA LaRC, in Aerothermodynamics branch. Started as a Co-op.
- PhD from U. Maryland in 2013, dissertation on electronic energy modeling and chemical reactions in DSMC.
- 20 years working DSMC algorithms and codes.

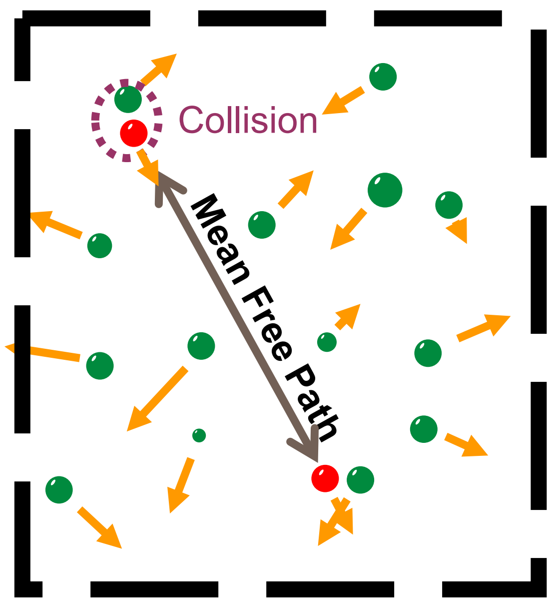
Outline

1. What is DSMC? Theory + Models
2. Codes
3. V&V
4. Applications

Computational Method/Flow Regime



Kn=λ/L
λ : local mean free path
L: characteristic length



- **Both CFD and DSMC approximate the Boltzmann equation**
  - Assumptions are made for CFD
  - DSMC is a solution in the limit of small timesteps and cells

What is DSMC?

Direct Simulation Monte Carlo

- Developed by Dr. Graeme Bird in the ‘60s
- Stochastic model of individual particles and their physics
  - Each DSMC ‘particle’ represents many real particles
- Probabilistic approach
  - Simplified models use cross sections determined from experiments or analytic results.

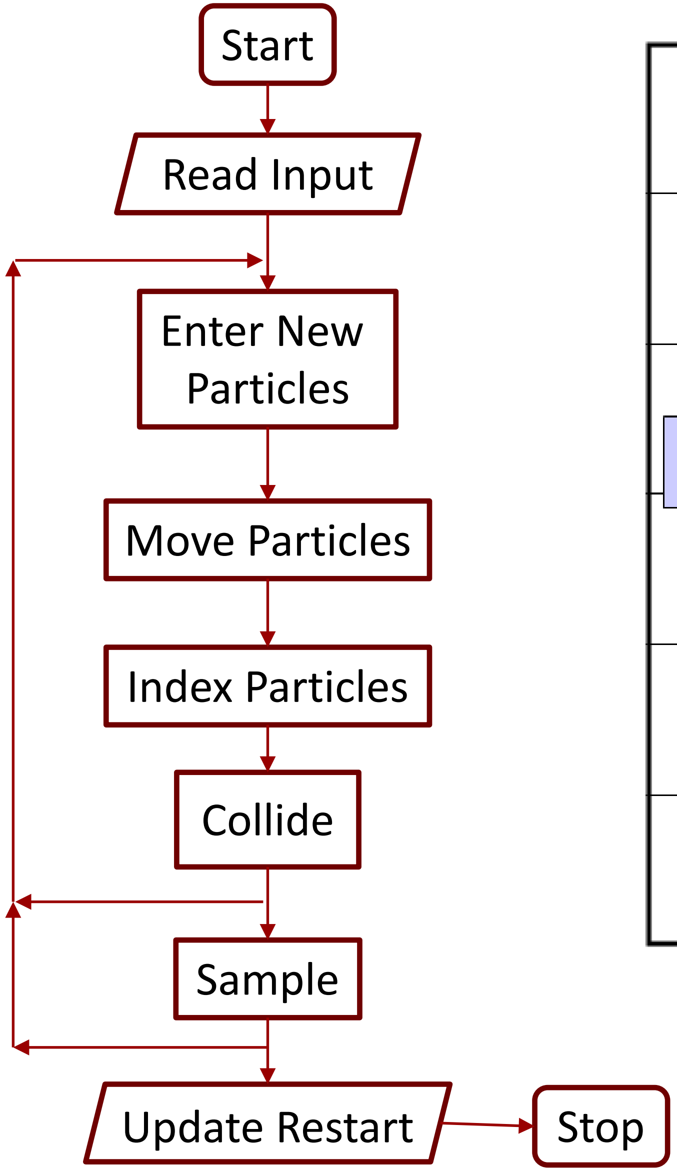

Graeme Bird
(1963, 1994)

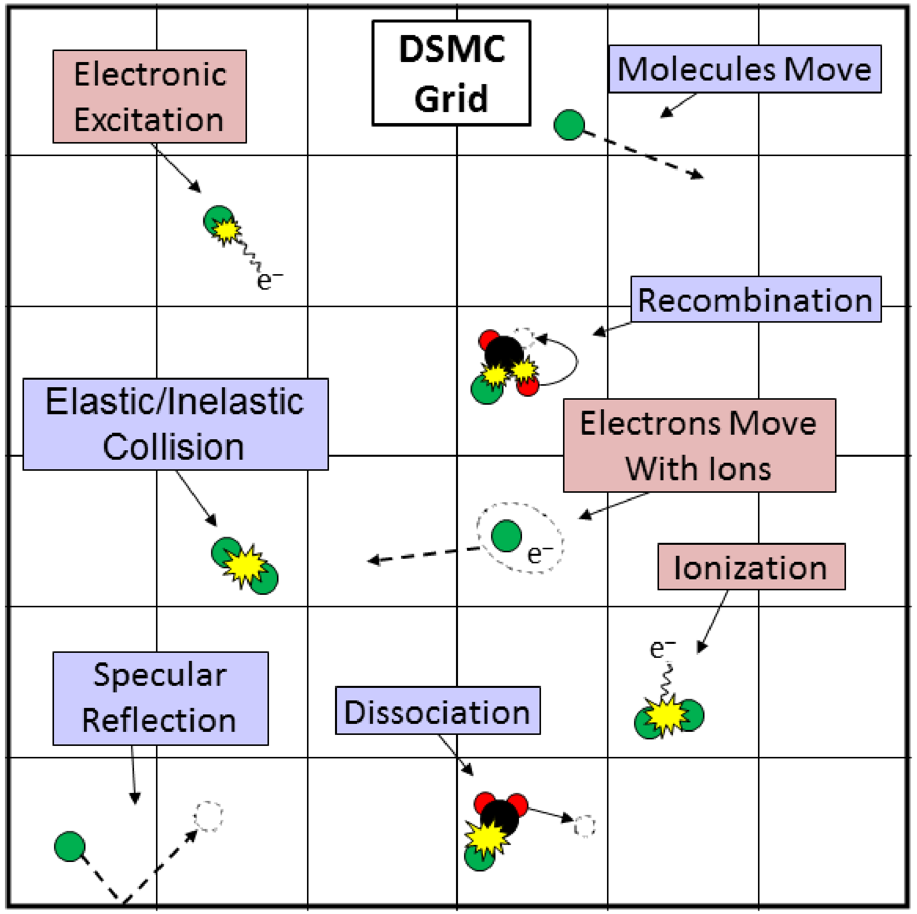
$$\frac{\partial f_A}{\partial t} + v_j \frac{\partial f_A}{\partial x_j} + \frac{1}{m_A}\frac{\partial}{\partial v_j}\left(\vec{F}_j f_A\right) = \iint \left[f_A(\vec{v}\,') f(\vec{w}\,') - f_A(\vec{v}) f(\vec{w}) \right] g \sigma^{AB} \, d\Omega \, d\vec{w}$$

Move

Collide

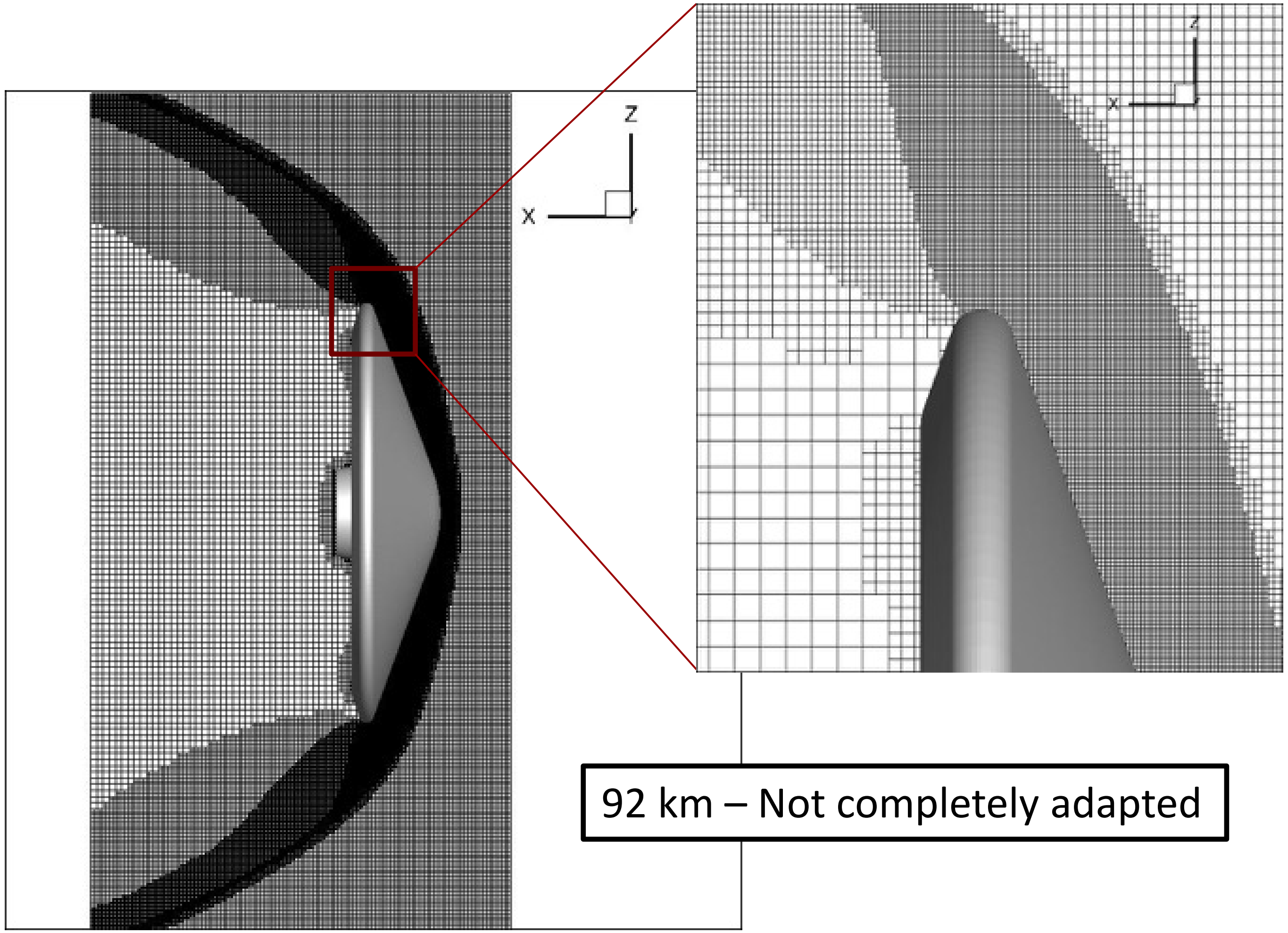
DSMC


Start
Read Input
Enter New Particles
Move Particles
Index Particles
Collide
Sample
Update Restart
Stop

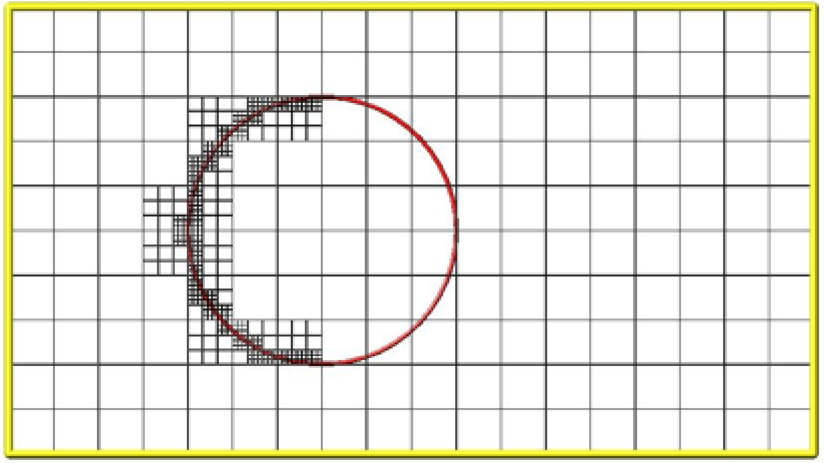

Electronic Excitation
DSMC Grid
Molecules Move
e⁻
Recombination
Elastic/Inelastic Collision
Electrons Move With Ions
e⁻
Ionization
e⁻
Specular Reflection
Dissociation

Grid

- Can use any type of grid, but Cartesian is popular
- Use a cut-cell algorithm to embed the surface grid



92 km – Not completely adapted



Particle Motion

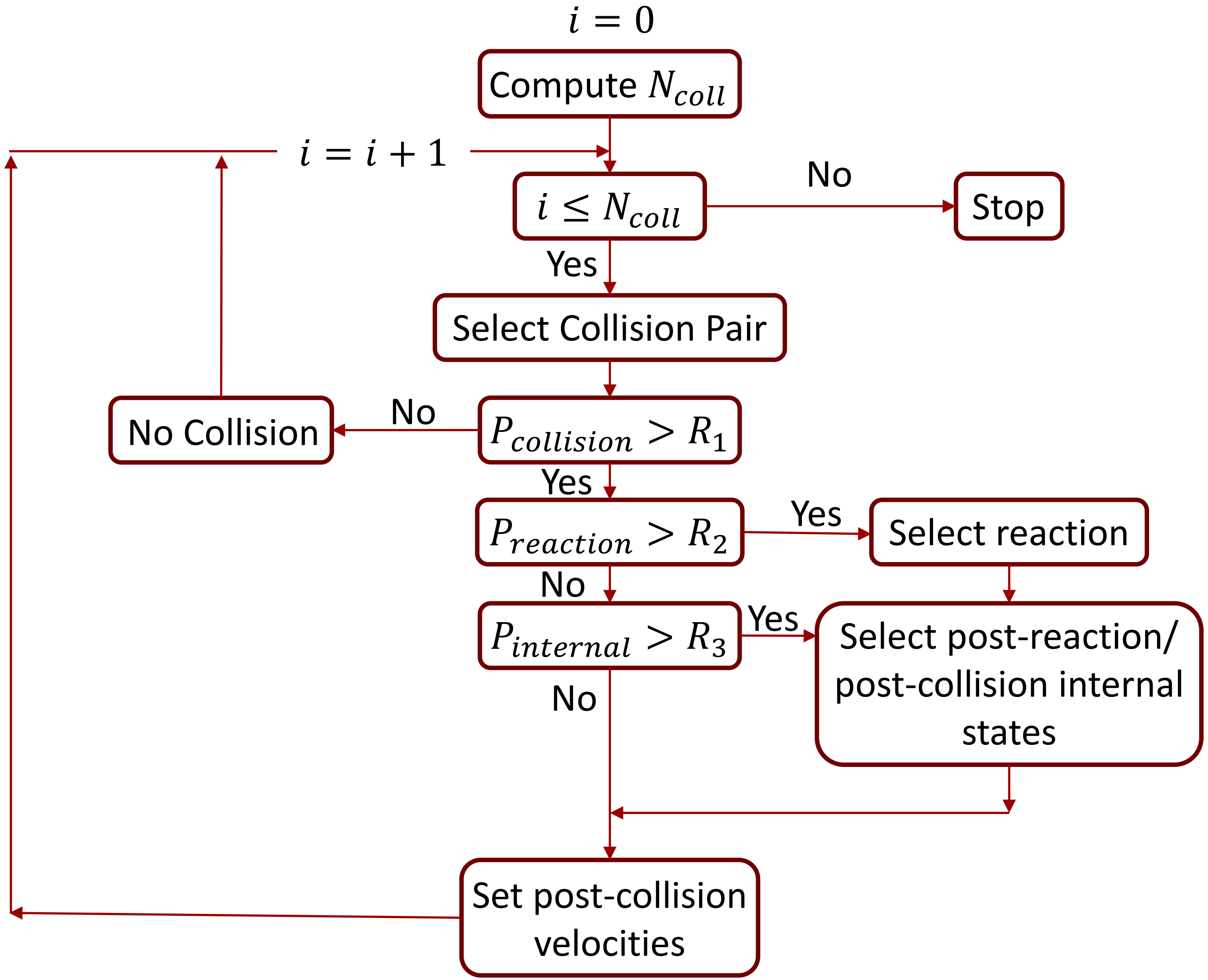
Entering particles

- At each time step, a number of particles are introduced at the boundaries to maintain the number flux of particles based on free stream or surface flux conditions
- For each particle
  - Random location along cell face
  - Velocity is sampled from the velocity distribution function
  - Internal energies are sampled from respective distribution functions
  - Particle time step is set to a random fraction of local simulation time step

Moving particles

- Track motion through cells
- Surface interactions
  - Specular, diffuse, other more complex interactions
  - Chemistry?

Particle Collisions



Particle Collisions

- **Particles are chosen in each cell to collide to reproduce the required macroscopic collision rate**
  - No-Time-Counter (NTC) scheme
    - Number potential collisions: $N_{coll} = \frac{\frac{1}{2}N(N-1)F_{NUM}(\sigma_T c_r)_{max}\Delta t}{V}$
    - Collision is accepted if: $R \leq \frac{(\sigma_T c_r)_{pair}}{(\sigma_T c_r)_{max}} = P_{collision}$
    - If accepted, proceed with collision routine
    - Repeat until N_{coll} pairs are considered
  - Majorant Collision Frequency (MCF) scheme
    - Majorant frequency: $\nu_{max} = \frac{\frac{1}{2}N(N-1)F_{NUM}(\sigma_T c_r)_{max}}{V} > \nu$
    - Time increment sampled from exponential distribution: $\delta t = -\frac{lnR}{\nu_{max}}$
    - Choose a pair and accept if: $R \leq \frac{(\sigma_T c_r)_{pair}}{(\sigma_T c_r)_{max}} = P_{collision}$
    - If accepted, proceed with collision routine
    - Repeat until $\sum \delta t > \Delta t$

Elastic Collision Models (Phenomenological)

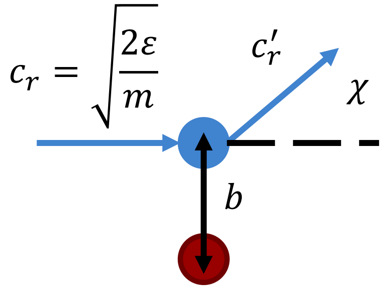
- 1963 (Bird): Hard sphere (HS) model reproduces relaxation to equilibrium with one molecular model parameter - d_{ref}
- 1981 (Bird): Variable hard sphere (VHS) model reproduces viscosity variation based in the inverse power law potential with two molecular model parameters - d_{ref}, ω
- 1991 (Koura & Matsumoto): Variable soft sphere (VSS) model reproduces viscosity and diffusion coefficients based on inverse power law or Lennard Jones potentials with three molecular model parameters - d_{ref}, ω, α
- 1993 (Hassan & Hash): Generalized hard sphere (GHS) reproduces viscosity on diffusion coefficients using least squares fit of experiments or a known intermolecular potential using a minimum of six molecular model parameters
- +Others….

Elastic Collision Models

VHS model

- Hard sphere scattering and power-law of viscosity

$$d_{VHS} = d_{ref}\left(c_{r,ref}/c_r\right)^{\omega-0.5} \quad \chi = \cos^{-1}(b/d_{VHS})$$



- Simple closed form expression for scattering angle makes it the most widely used

VSS model

- A modification introduced of VHS to have both viscosity and diffusion consistent with those of IPL or LJ potential

$$d_{VSS} = d_{ref}\left(c_{r,ref}/c_r\right)^{\omega-0.5} \quad \chi = \cos^{-1}\left(\frac{b}{d_{VHS}}\right)^{1/\alpha}$$

- Only slightly more complex algorithm – should always be used if possible

Internal Energy Modes

- **Atoms/molecules can store energy in their internal modes**
- **Different temperatures can be defined:** $\boldsymbol{T_{trans}, T_{rot}, T_{vib}, T_{ele}}$
- **Under equilibrium, the total thermal energy is equipartitioned**

$$E_i = \frac{1}{2}\varsigma_i k_B T_i$$

- **Degrees of freedom**
  - Translational
    - since all particles move in 3D space, $\varsigma_{trans} = 3$
  - Rotational (can assume continuous or discrete)
    - Diatomic are assumed fully excited with $\varsigma_{rot} = 2$
    - Nonlinear molecules fully excited with $\varsigma_{rot} = 3$
  - Vibrational
    - Normally simple harmonic oscillators

$$\zeta_{vib} = \frac{2\,\Theta_{vib}/T}{exp(\Theta_{vib}/T) - 1}$$

    - Can account for anharmonic oscillators

Internal Energy Modes (cont.)

Degrees of freedom (cont.)

- Electronic
  - Most DSMC simulations DO NOT account for electronic energy!!!
  - Incorrect for high energy flows – CFD accounts for this in the collision integrals and DSMC will NEVER match CFD if it does not account for electronic energy

$$e_{el} = \frac{1}{2}\zeta_{el} R T_{el} = R T^2 \frac{\partial}{\partial T} ln Q_{el}$$

$$Q_{el} = \sum_i g_i e^{-\Theta_i/T}$$

$$\zeta_{el} = \frac{2\sum_i g_i \Theta_i e^{-\Theta_i/T}}{T_{el}\sum_i g_i e^{-\Theta_i/T}}$$

Internal Energy Redistribution

Larsen-Borgnakke (LB) model

- Standard phenomenological approach describing energy exchange between translational and internal modes
- Post-collision internal and translational energies are sampled from the collision equilibrium distribution to satisfy detailed balance
- For any internal mode

$$E_c = E_{t,1+2} + E_{int,1}$$

- The probability of a post-collision energy $E'_{int,1}$ is the ratio of the joint distribution function to the maximum value of the function

$$P_{LB} = \frac{f}{f_{max}} = \left(1 - \frac{E'_{int,1}}{E_c}\right)^{1.5-\omega_{12}}$$

Internal Energy Relaxation

- **The probability of undergoing an energy exchange during a collision, P_{int}, to reproduce a relaxation rate τ_{int} is based on the definition of relaxation numbers**

$$Z_{int}^{C} = \frac{\tau_{int}}{\tau_c} = \begin{array}{c}\text{Average number of} \\ \text{collisions within } \Delta t = \tau_{int}\end{array} \longrightarrow P_{internal} = \frac{C}{Z_{int}^{C}} = \frac{1}{Z_{int}^{DSMC}}$$

- **Constant C is found by linking the rate of energy exchange predicted by theory (macroscopic) to the collision-based DSMC-LB procedures (microscopic)**

$$Z_R^{DSMC} = Z_R^C \frac{\varsigma_t}{\varsigma_t + \varsigma_r} \qquad Z_V^{DSMC} = Z_V^C \frac{\varsigma_t}{\varsigma_t + A(T_t)}$$

Internal Energy Relaxation

- **The most popular RT and VT relaxation rates used in DSMC are given by**
  - Parker:

$$Z_r^C(T_t) = \frac{Z_r^\infty}{1 + (\pi^{3/2}/2)(T^*/T_t)^{1/2} + (\pi^2/4 + \pi)(T^*/T_t)}$$

  - Millikan & White

$$Z_v^C(T_t) = \frac{exp\left[A\left(T_t^{-1/3} - B\right) - 18.42\right]}{p^{atm}\tau_c}$$

- **There are also formulations based on the collision energy, so a temperature doesn't have to be defined**

Chemistry Modeling

- **In general, there are two main steps in the modeling of chemical reactions in DSMC**
  - Specify the reaction probability P_R of a colliding pair based on their kinetic parameters
  - Redistribute the post-reaction collision energy into the translational and internal modes of the product species
- **In DSMC, P_R is usually a function of the translational and internal energies as well as the reaction activation energy**
- **The total collision energy (TCE) model is the most widely used DSMC chemistry model. Its P_R functional form assumes**

$$P_R^{TCE} = \begin{cases} 0 & \text{if } E_c \le E_a \\ C_1 \dfrac{(E_c - E_a)^{C_2}}{E_c^{C_3}} & \text{if } E_c > E_a \end{cases}$$

Chemistry Modeling

- **The rate of change in the number density of species A due to the bimolecular reaction $A + B \rightarrow C + D$ with reaction rate coefficient $k(T)$ can be expressed as**

$$\frac{dn_A}{dt} = -n_A n_B k(T) = -n_A n_B \overline{\sigma_T c_r P_R}$$

- **Note that the reaction probability can be written in terms of the reaction cross-section, $P_R = \sigma_R/\sigma_T$**
- **The RHS of the above can be approximated as $n_A n_B \overline{\sigma_T c_r P_R} \approx N_{A,B} \overline{P_R}$ where $N_{A,B}$ is the bimolecular collision rate**
- **Assuming $\sigma_T = \sigma_{VHS}$ and that E_c and molecular velocities follow continuum Boltzmann distributions, the equations can be calculated analytically where the modified Arrhenius form $k(T) = \Lambda T^{\eta} exp(-E_a/k_B T)$ is used. Then…**

Chemistry Modeling

- **By inspection we can obtain the constants to get**

$$P_R^{TCE} = \left[\frac{(1+\delta_{AB})\Lambda\sqrt{\pi}T_{ref}^{\eta}}{2\sigma_{ref}\left(k_B T_{ref}\right)^{\eta-1+\omega}} \frac{\Gamma(\overline{\varsigma}+5/2-\omega)}{\Gamma(\overline{\varsigma}+3/2+\eta)} \left(\frac{m_r}{2k_B T_{ref}}\right)^{1/2} \right] \frac{(E_c - E_a)^{\eta+\overline{\zeta}+0.5}}{E_c^{\overline{\zeta}+1.5-\omega}}$$

- **A slight modification is required for recombination reactions, and statistical mechanics can be used to formulate the reverse reaction rate from the forward rate**
- **Possible issues in practical DSMC applications:**
  - Accurate only near equilibrium
  - Probability may exceed unity under high temperature conditions
  - Limited range for η due to singularities in equation
  - TCE rates deviate from exact rates when discrete ro-vibrational levels are used
    - This can be corrected with an empirical procedure

Chemistry Modeling

- **Other phenomenological models have been proposed to better reproduce available data on nonequilibrium reacting flows or to be alternatives to the TCE framework**
  - Vibrationally Favored Dissociation (VFD) Model
    - Captures coupled vibration-dissociation behavior
  - Generalized Collision Energy (GCE) Model
    - Allows favoring of different energy modes
  - Maximum Entropy (ME) Chemical Reaction Model
    - Reaction probability linked to collision energy distribution
  - Extended Bias (EB) Dissociation Model
  - Quantum-Kinetic (QK) Model
    - Does not rely on previous $k(T)$ knowledge
  - Macroscopic Chemistry Method (MCM)
    - Instead of a per collision basis, #of reactions are based on the cell-wise macroscopic parameters

Numerical error in DSMC

Four parameters control DSMC numerical error:

- Sample size per cell (M_c) → statistical error
- Simulators per cell (N_c)
- Cell size (Δx)
- Time step (Δt)

(Simulators per cell, cell size and time step → discretization error)

Early DSMC users followed rule-of-thumb guidelines:

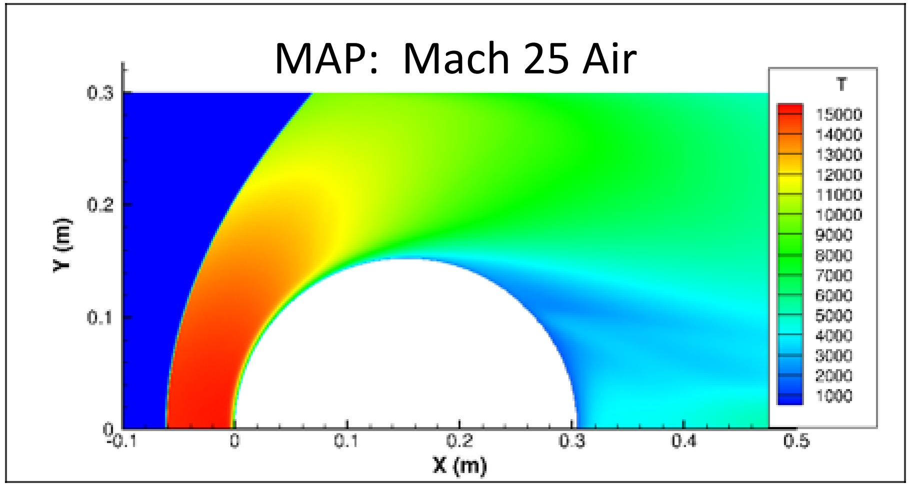
- Sample enough to drive statistical error down
- Keep time step smaller than ~1/4 mean collision time
- Keep cell size smaller than ~1/3 mean free path
- Use a minimum of ~10-20 simulators per cell

MAP[1] (Multiphysics Algorithm with Particles)

- **MAP is a 0D/2D/Axi/3D adaptive Cartesian implementation**
- **Dynamic adaptation**
  - Flow field grid – fraction of the local mean free path
  - Time step – local mean collision time or transit time
  - Surface temperature – radiative equilibrium
- **Grid**
  - Morton Octree Cartesian grid for the flow field
  - Unstructured surface grid separate from flow field
- **Gas model**
  - Internal degrees of freedom – rotational, vibrational, electronic
  - Chemistry – gas phase and surface

[1]D.S. Liechty, *Journal of Spacecraft and Rockets*, **52**(6), 1521-1529 (2015)
https://software.nasa.gov/software/LAR-18801-1

MAP: Application to Hypersonic Flow



- **A 12-inch cylinder[1] (2-D) is the baseline for the current study**
  - Kn reduced to 0.0005 to reduce rarefaction effects (~55km)
  - Oxygen and Air mixtures simulated at nominal Mach numbers of 10 and 25
  - Focus of present study is transport properties…
    - Chemically frozen flow – species based on nominal post-shock compositions
    - Thermal equilibrium – single temperature for CFD, collision numbers of one for DSMC
  - Both calibrated VSS and standard high temperature air VHS provided with DAC are used for DSMC

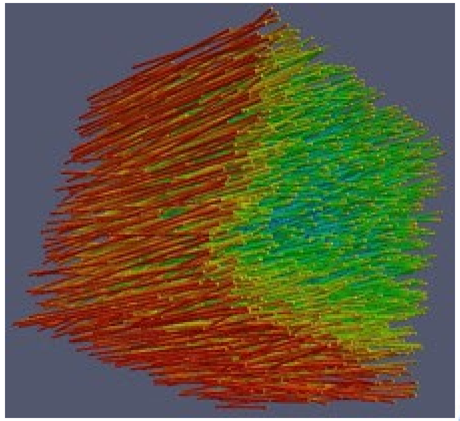
[1]A.J. Lofthouse, L.C. Scalabrin, I.D. Boyd, AIAA Paper 2007-3903

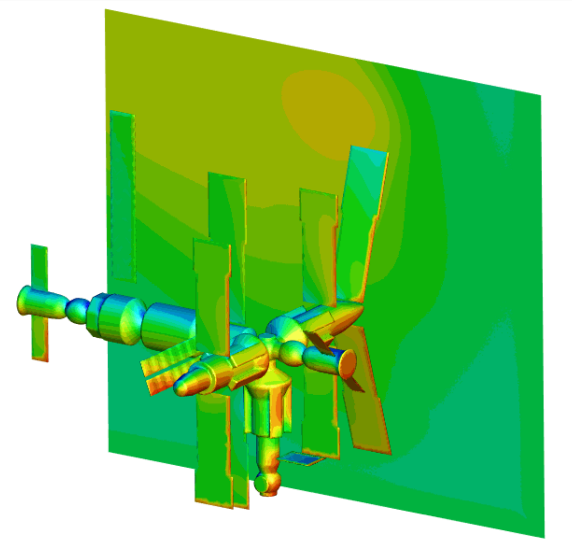
MAP: Application to Hypersonic Flow (2)

- **Comparisons made between CFD, DSMC (VHS), and DSMC (VSS)**
  - Flow field structure/Temperature
  - Surface heating
  - Surface shear stress (x- and y-components)
  - Mixture viscosity
  - Mixture thermal conductivity
- **In general, good agreement between CFD and DSMC (VSS)**
  - Some assumptions have to be accounted for with thermal conductivity, but agreement is shown given the adjustments
- **Some differences between DSMC (VHS) and DSMC (VSS)**
  - Flow field structure/Temperature show good agreement
  - Surface quantities agree at Mach 10, but not at Mach 25
  - Differences in transport properties

SPARTA[1] (Stochastic PArallel Rarefied-gas Time-Analyzer)

- 2D, 2D axisymmetric or 3D, serial or parallel
- Cartesian, hierarchical grid
  - Oct-tree (up to 16 levels in 64-bit cell ID)
- Triangulated surfaces cut/split the grid cells
  - In-situ visualization, adaptive gridding, load balancing
- Aiming for next generation MPI
  - Exascale capable
  - Write application kernels only once, and
  - Run them efficiently on a wide variety of platforms:
    - GPU, Xeon Phi, etc.
  - Has been used to run the largest (we think!) DSMC models up-to-date, with up to **100 billion particles and billions of grid cells. Can also handle billions of surface elements**
- **Open-source** code available at http://sparta.sandia.gov
  - Product of collaboration between National Labs, NASA, academia and industry.
  - 5000+ downloads, 200+ users worldwide.

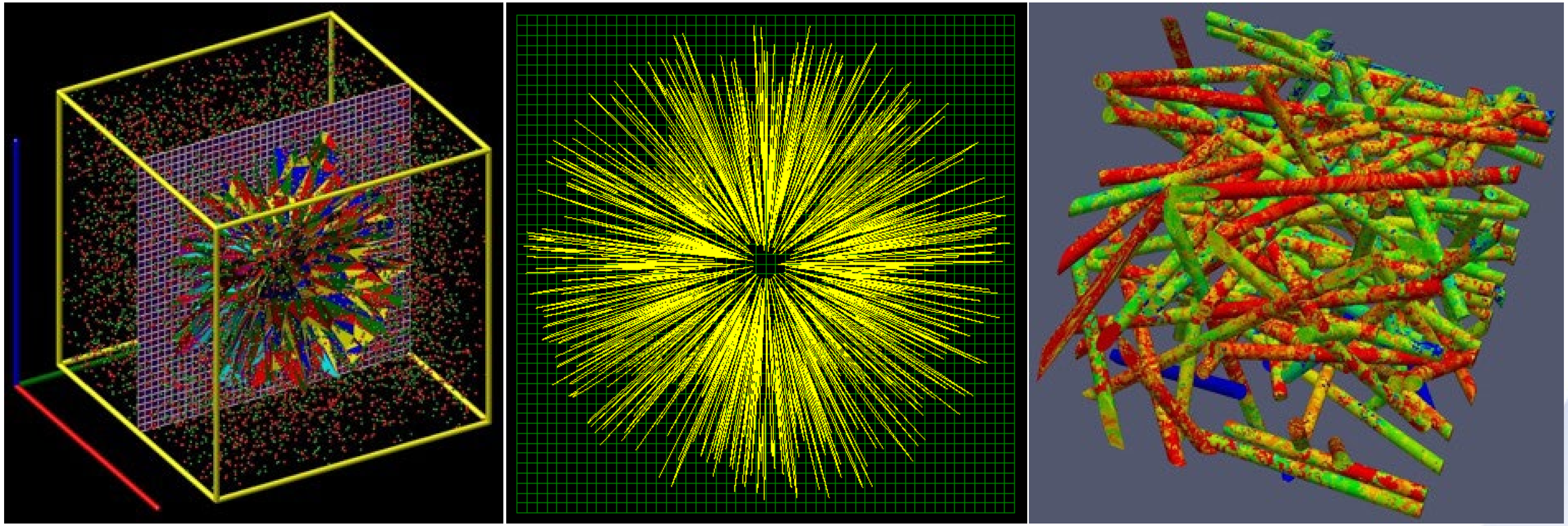




[1]Plimpton, S. J., Moore, S. G., Borner, A., Stagg, A. K., Koehler, T. P., Torczynski, J. R., & Gallis, M. A. (2019). Direct simulation Monte Carlo on petaflop supercomputers and beyond. *Physics of Fluids*, *31*(8), 086101.

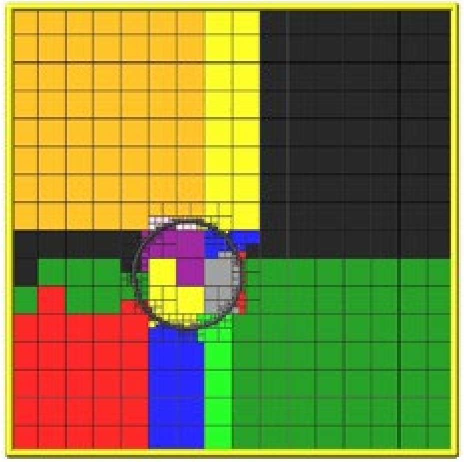
SPARTA: Simulation of Complicated Shapes

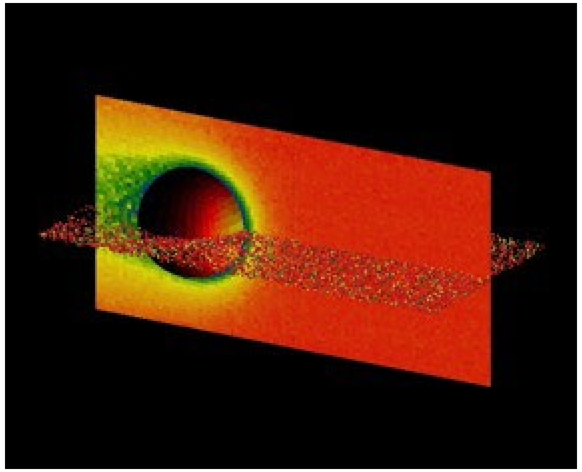
- SPARTA now computes all the cut cell volumes, identifies any split cells, colors all grid cells as inside, outside, or cut/split.
- Each surface in a split cell is tagged by which split volume it belongs to, which will be needed for tracking particles into the split cells.
- Infinitely thin surfaces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



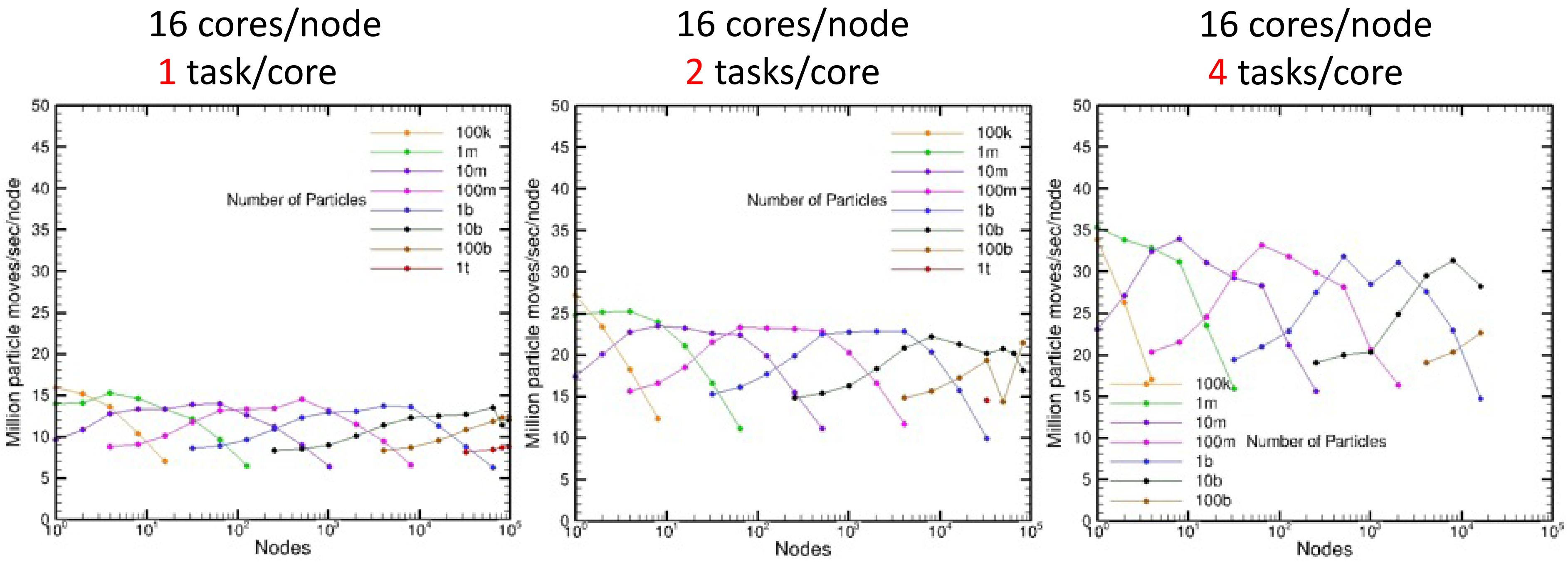
SPARTA: Some other features of interest

- Create/adapt grid on the fly
- Efficient communication & Load Balancing
  - One comm per step
  - Static or dynamic load balancing
  - Weighted by cell, particles or CPU time
- In-situ visualization
  - Not a replacement for interactive viz, but ...
  - Quite useful for debugging & quick analysis
  - At end of simulation (or during), instant movie
  - Images are ray-traced quality





SPARTA: Benchmarking



- Flow in a 3D closed box
- Weak scaling indicates, 10% peak performance reduction from 1 to 10^6 cores
- 2 tasks/core gives 1.5x speedup, 4 tasks/core gives 2x speedup
- A total of 1 trillion molecules can be simulated on one third of the BG/Q cluster
- Maximum number of tasks is 2.6 million

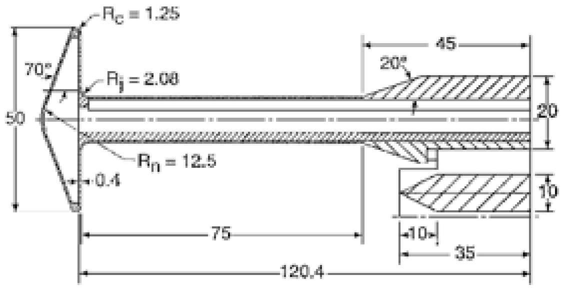
Other DSMC codes

- **DS1V, DS2V, DS3V**
  - original DSMC codes of Graeme Bird
- **DAC3D**
  - Lebeau group at NASA Johnson Space Center
  - 3-level Cartesian grids
- **MONACO**
  - Boyd group at U Michigan (now at CU Boulder)
- **MGDS**
  - Schwartzentruber group at U Minnesota
  - 3-level Cartesian grids
- **SMILE**
  - Russian group at Khristianovich Institute of TAM
- **dsmcFOAM**
  - Group at U Strathclyde, Scotland
  - open-source, built on OpenFOAM CFD package
  - body-fitted finite-element style grids
- **Others we forget?**

DSMC V&V using SPARTA

- **3 test cases (all 2D axi):**
  - 70º blunted cone (SR3)

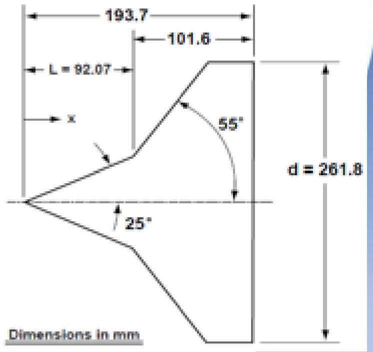
Flow conditions	Gas	Ma	T_0	P_0	Re
1	N_2	20.2	1100	3.5	1420
2	N_2	20	1100	10	4175



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

  - 25-55º biconic (CUBRC LENS)

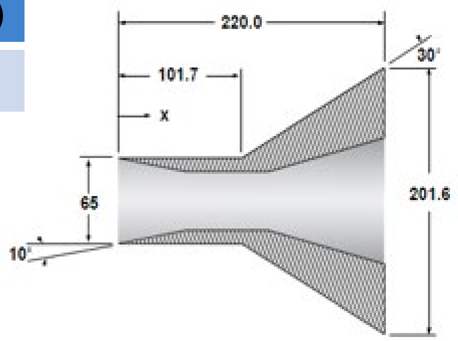
Conditions	Flow Velocity (m/s)	Number Density (m^{-3})	Flow Temperature (K)	Gas	Surface Temperature (K)
LENS Run 11	2484	$3.78x10^{21}$	95.6	N_2	297.2



    - Flow-field dimensions: 22 cm x 12 cm
    - Grids: Uniform 1000 x 1800 cells, 2-Level 957 x 440 cells second level 10x10 cells

  - Hollow cylinder flare (CUBRC LENS)

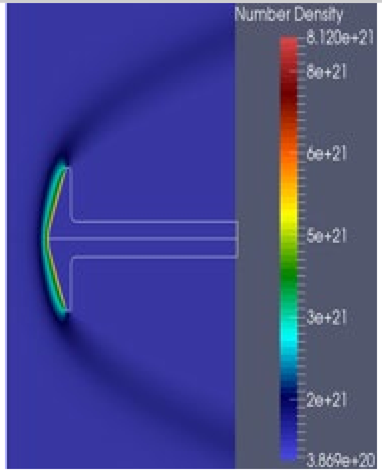
Conditions	Flow Velocity (m/s)	Number Density (m^{-3})	Flow Temperature (K)	Gas	Surface Temperature (K)
CUBRC Run 7	2072.6	$3.0x10^{18}$	42.61	N_2	297.2

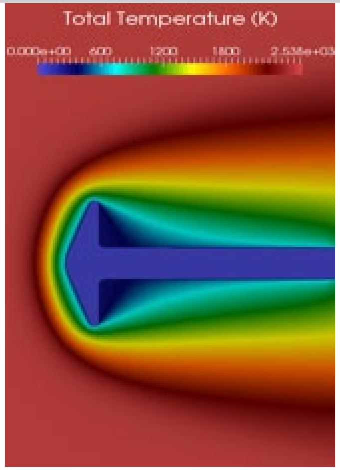


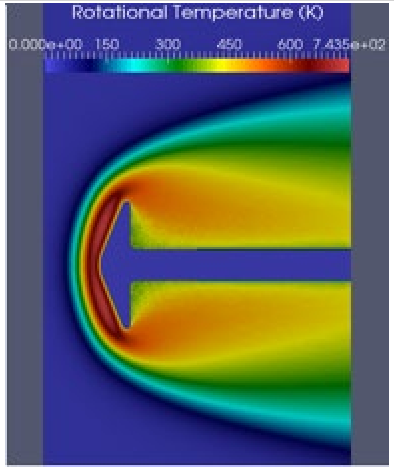
    - Flow-field dimensions: 22 cm x 50 cm
    - Grid: 2 level grid, first level 870 x 870 cells, second level 10 x 10 cells refinement of the first level, second level starts from 5 cm after the biconic's leading edge and ends at the end of the biconic's surface.

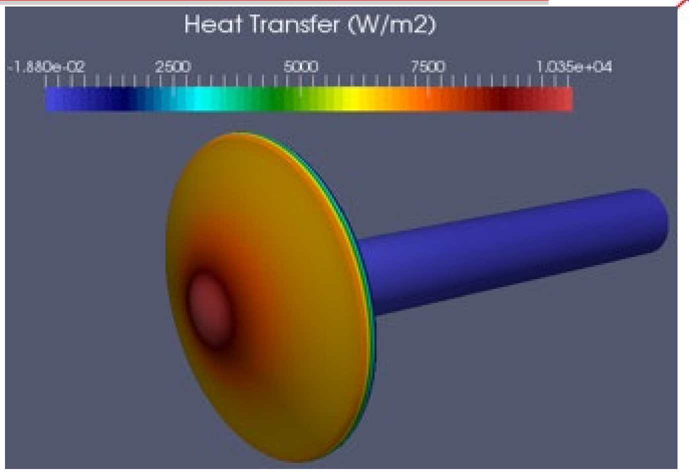
Simulations performed by A. Klothakis and I. Nikolos, *Modeling of Rarefied Hypersonic Flows Using the Massively Parallel DSMC Kernel "SPARTA"*, 8th GRACM International Congress on Computational Mechanics, Volos, Greece, July 12– 15, 2015

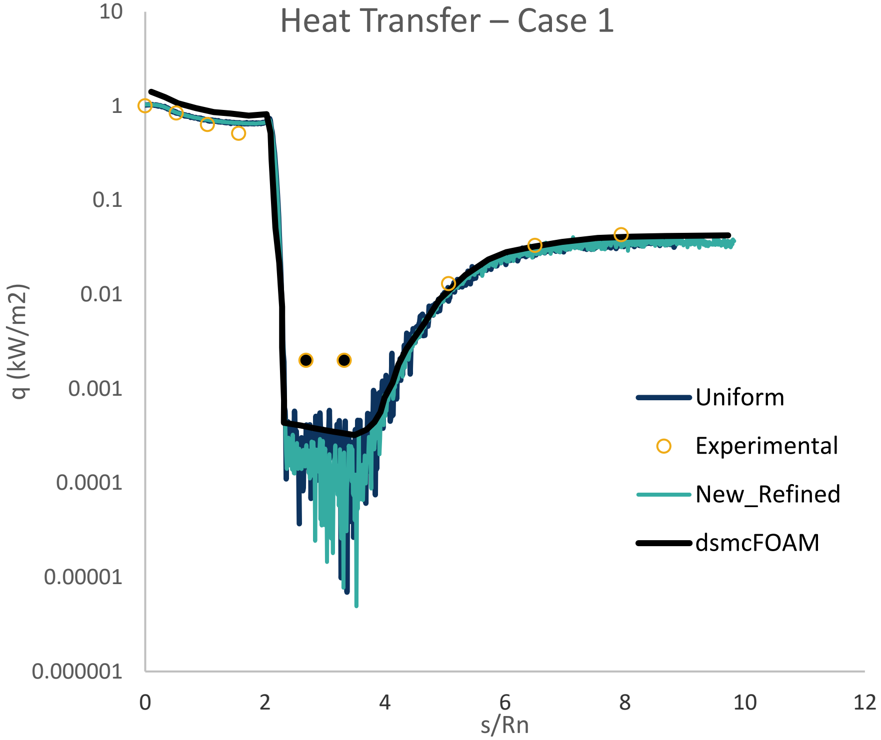
70º blunted cone

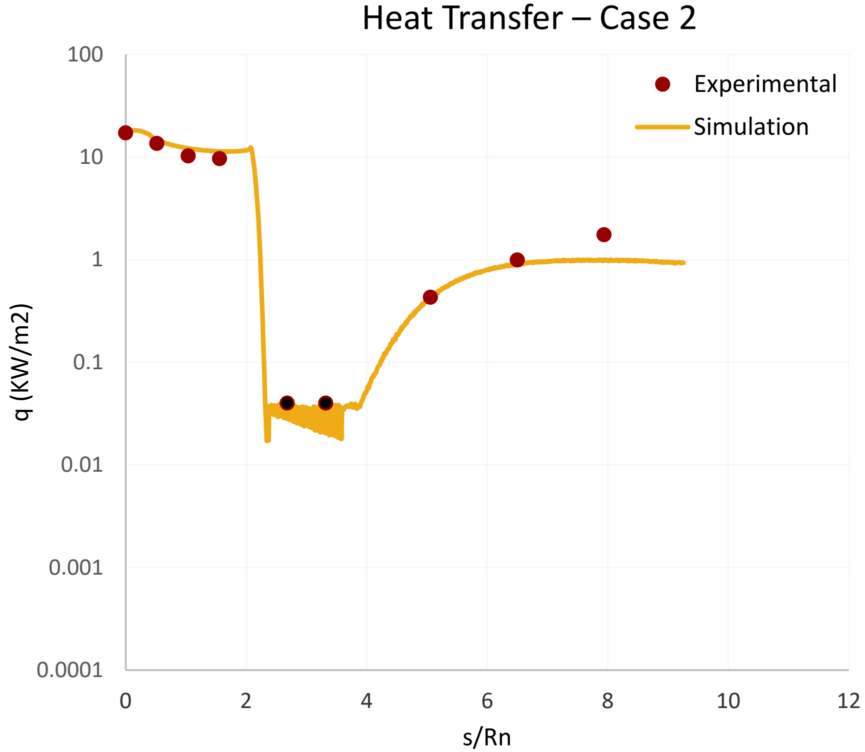




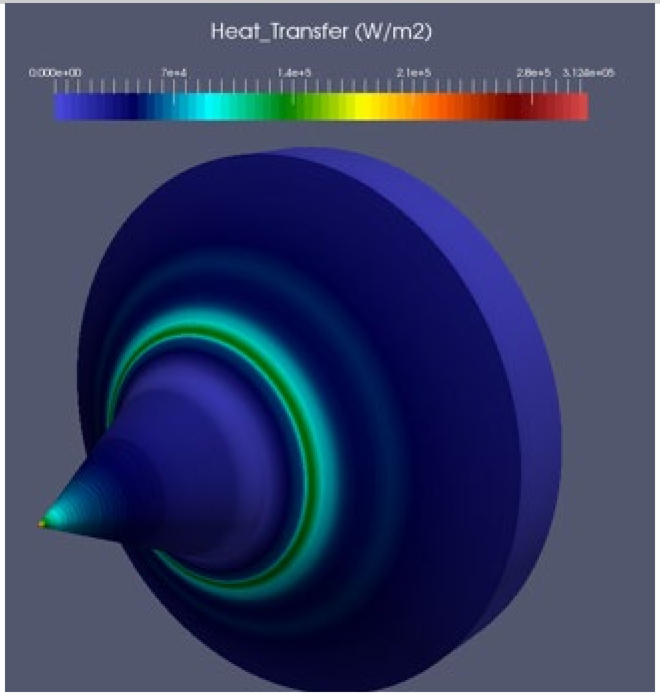


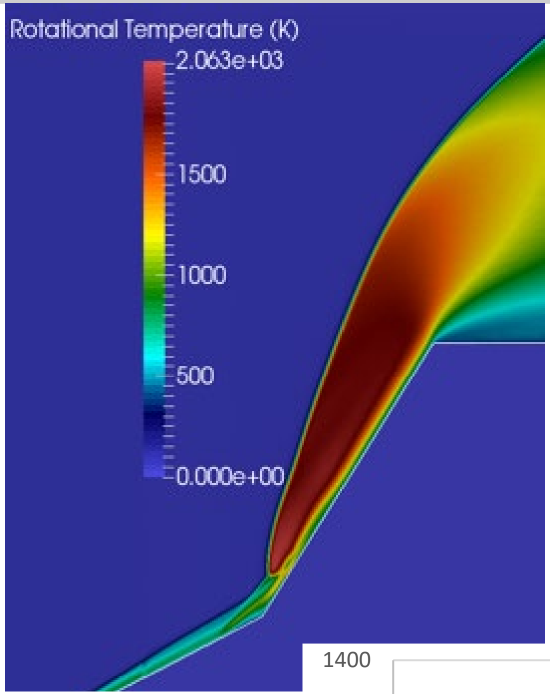


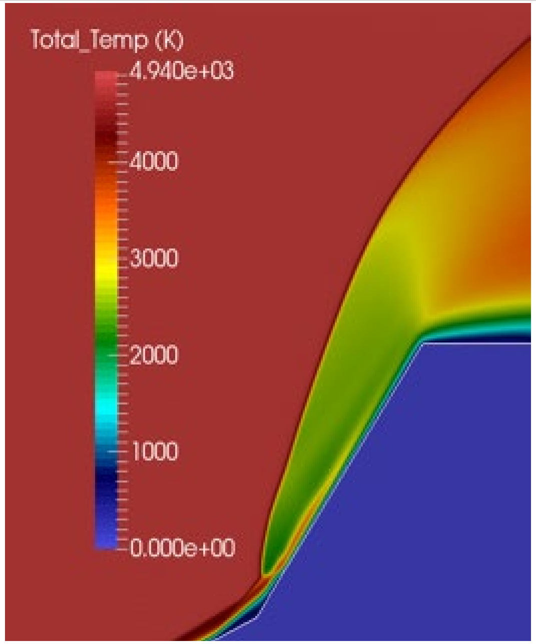


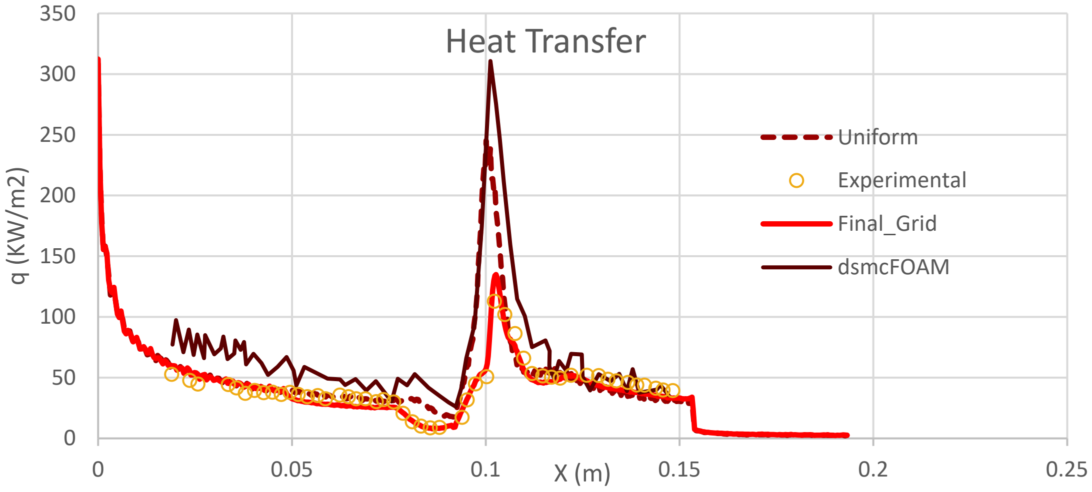


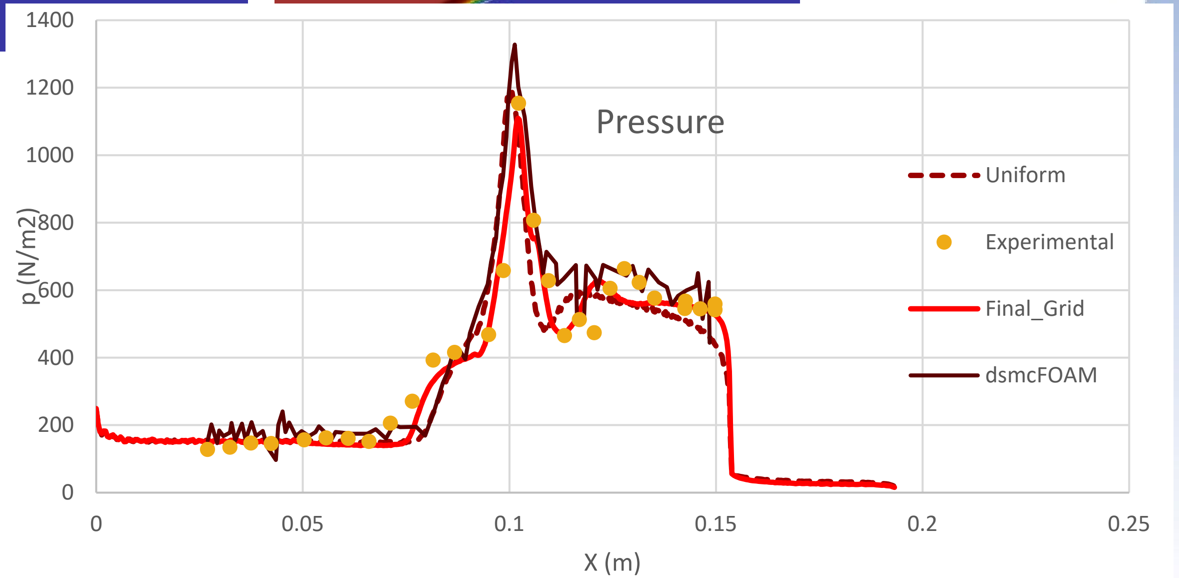
Biconic


Heat_Transfer (W/m2)

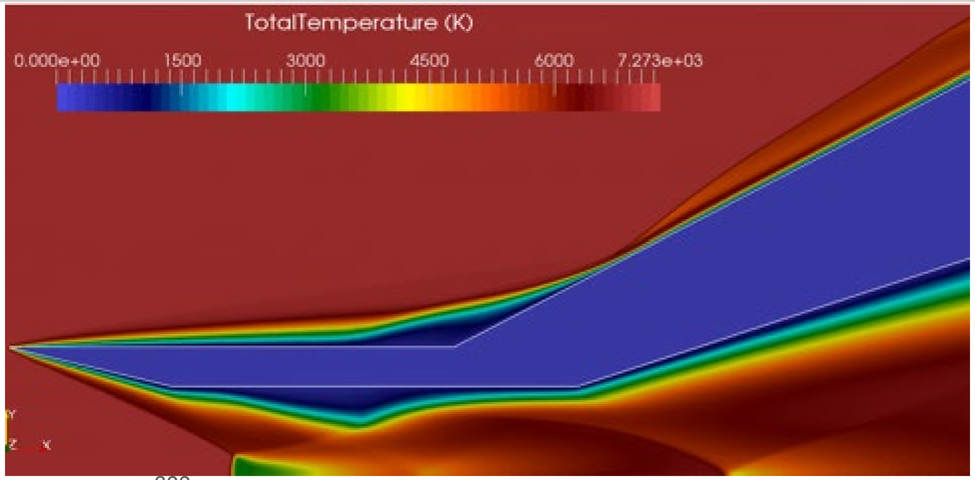

Rotational Temperature (K)
2.063e+03
1500
1000
500
0.000e+00

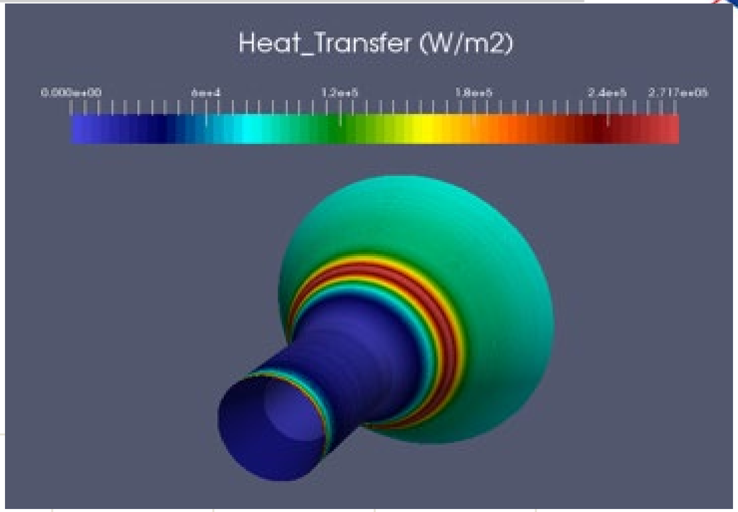

Total_Temp (K)
4.940e+03
4000
3000
2000
1000
0.000e+00

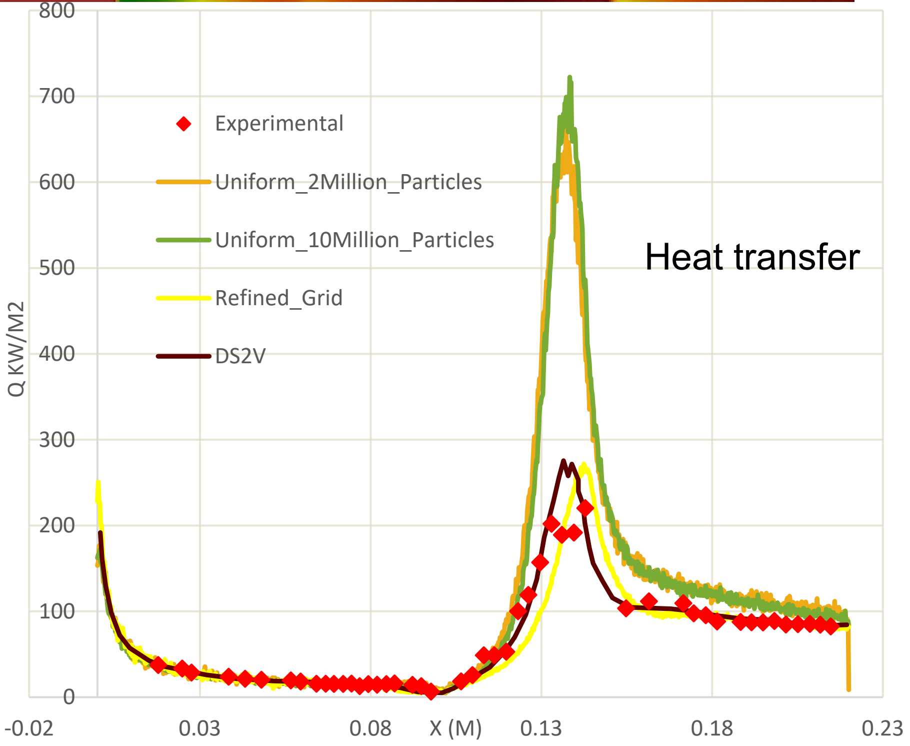

Heat Transfer
q (KW/m2)
X (m)
0
50
100
150
200
250
300
350
0
0.05
0.1
0.15
0.2
0.25
Uniform
Experimental
Final_Grid
dsmcFOAM

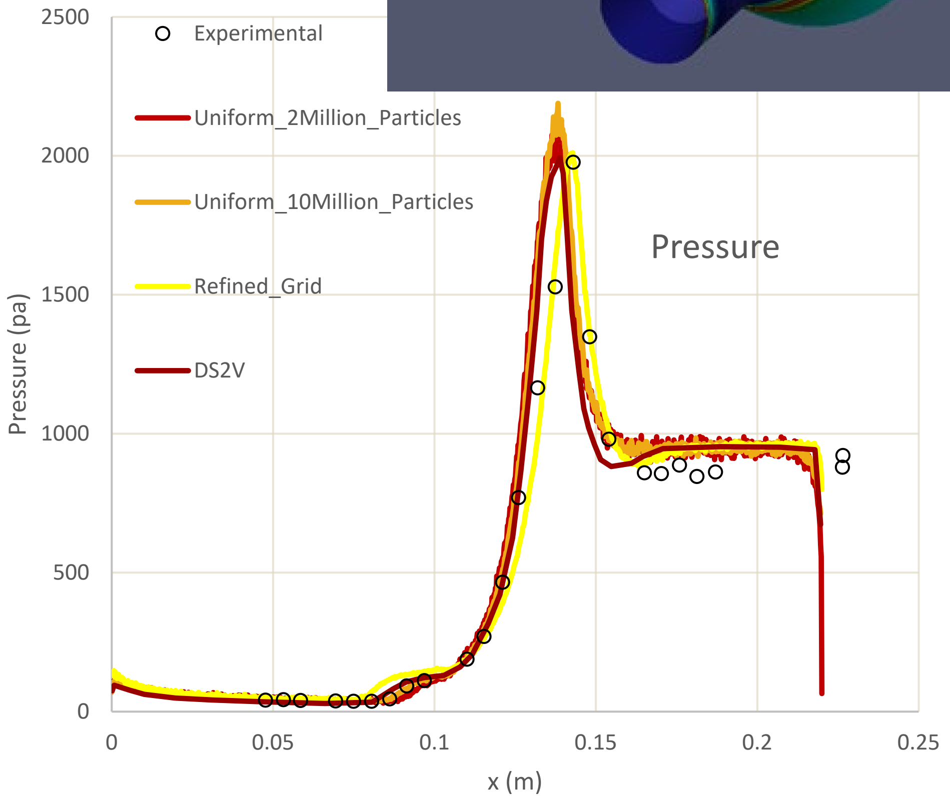

Pressure
p (N/m2)
X (m)
0
200
400
600
800
1000
1200
1400
0
0.05
0.1
0.15
0.2
0.25
Uniform
Experimental
Final_Grid
dsmcFOAM

Flared cylinder







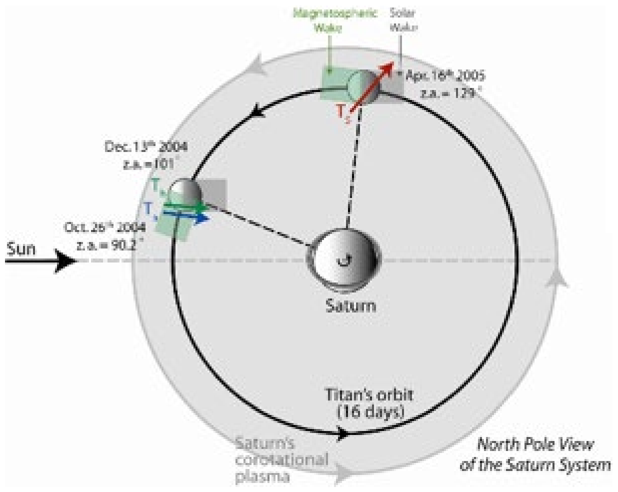


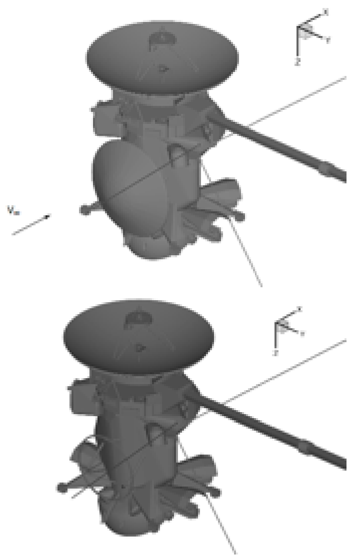
Cassini/Huygens – Discrepancy in aerodynamic performance estimates

Program: Cassini/Huygens mission to Saturn System

Issue: Factor of 3-5 difference in spacecraft aerodynamic performance during Saturn pass as estimated by different methods

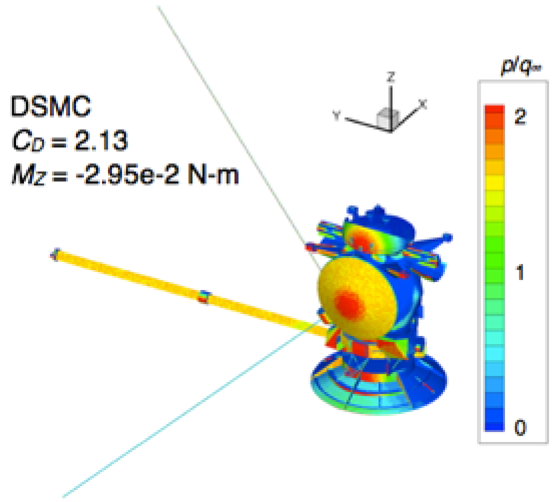
Approach: Performed free molecular and DSMC simulations to determine source of discrepancy with and without Huygens attached to Cassini (Ta vs. T5).





Computed C_D and Surface Pressure

Team	Ta	T5
INMS-DATA	2.11	2.00
INMS-FIT	---	2.00
AACS-1	2.12	1.99
AACS-2	2.13	1.99



Impact: DSMC computations for moments were within 10-15% of those measured in flight and for C_D were consistent with assumed values. Source of discrepancy not determined as fidelity of DSMC was more accurate than available input data.

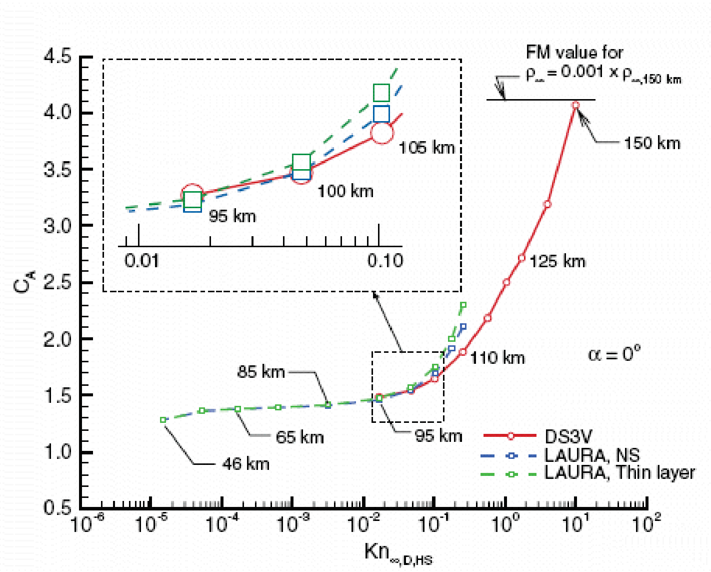
Pass	Team	Axis	Flight (N m)	DSMC (N m)	% Diff
Ta	AACS-1	Z	-0.158	-0.134	15.2%
Ta	AACS-2	Z	-0.103	-0.095	7.8%
T5	AACS-1	Y	-0.23	-0.256	11.3%
T5	AACS-1	Z	-0.44	-0.418	5.0%
T5	AACS-2	Z	-0.39	-0.35	10.3%

IRVE II – Rarefied Aerodynamic/Aeroheating

Program: Inflatable Re-entry Vehicle Experiment (IRVE) II – flight-test to demonstrate various aspects of inflatable technology.

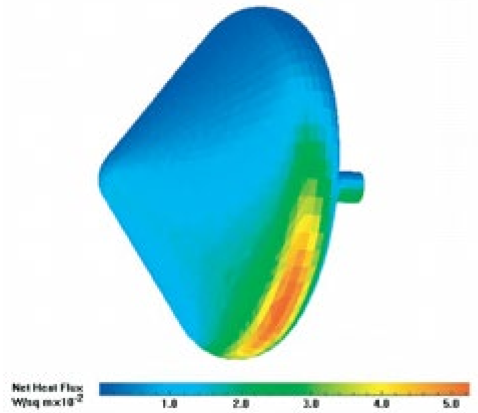
Issue: Evaluate aerodynamic characteristics of vehicle in low-velocity, rarefied trajectory. Existing aerodynamic databases for similar configurations was not appropriate for IRVE conditions, especially at deployment from launch vehicle

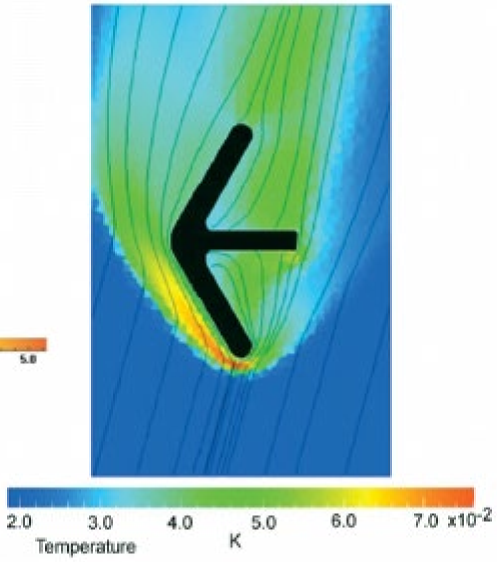
Approach: Perform free molecular and DSMC simulations, overlapping the CFD database at lower altitudes.



Impact: A very strong dependency on velocity was demonstrated. IRVE shown to be statically stable in free-molecular regime but exhibited multiple stable trim points through most of the transitional regime. For angles of incidence, local surface heating rates can be significantly higher on either the inflated aeroshell or the center body structure than that at the stagnation point at zero incidence.

Successful flight test in Aug 2009





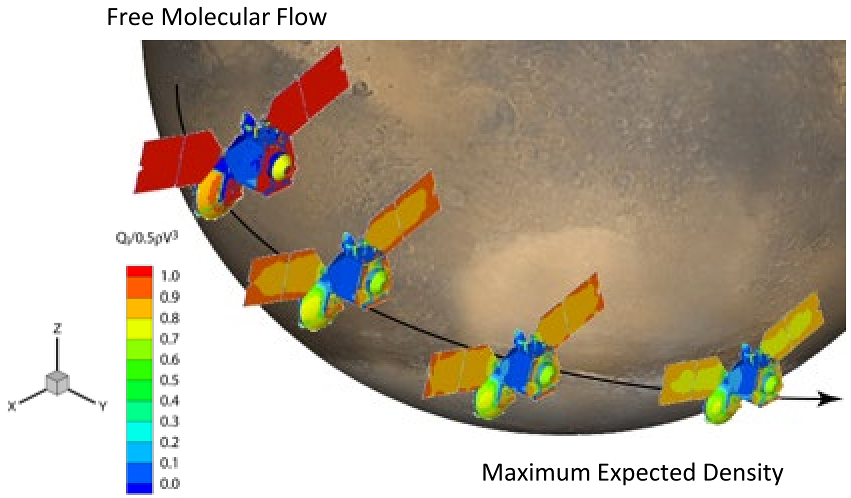
Mars Reconnaissance Orbiter (MRO) – Aero/Aeroheating Database for Aerobraking

Program: Mars Reconnaissance Orbiter (MRO)

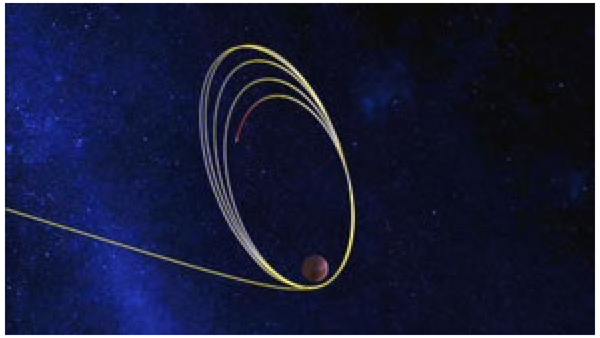
Issue: Define aerodynamic and aeroheating performance of the space craft during aerobraking at Mars

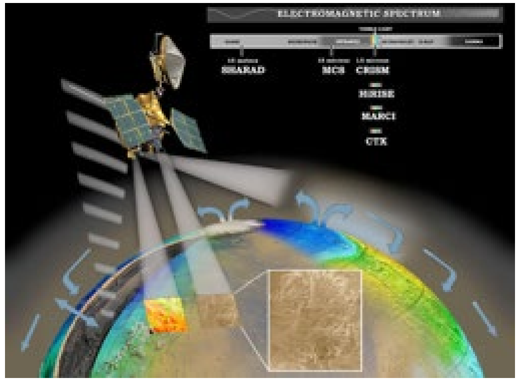
Approach: Perform free molecular and DSMC simulations at various orientations, velocities and densities.

Non-Dimensional Heating Through A Pass

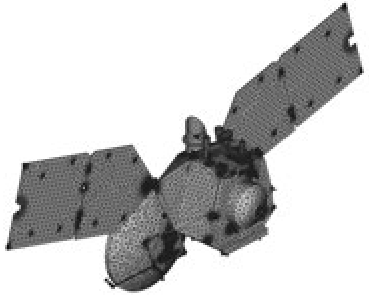


MRO Aerobraking and Science Missions





Impact: DSMC performance database applied to accomplish successful aerobraking at Mars in 2006



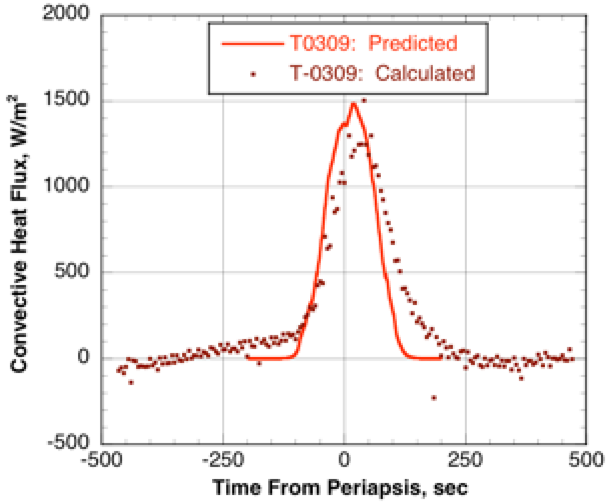
Mars Reconnaissance Orbiter (MRO) – In-Flight Operations Support

Program: Mars Reconnaissance Orbiter (MRO)

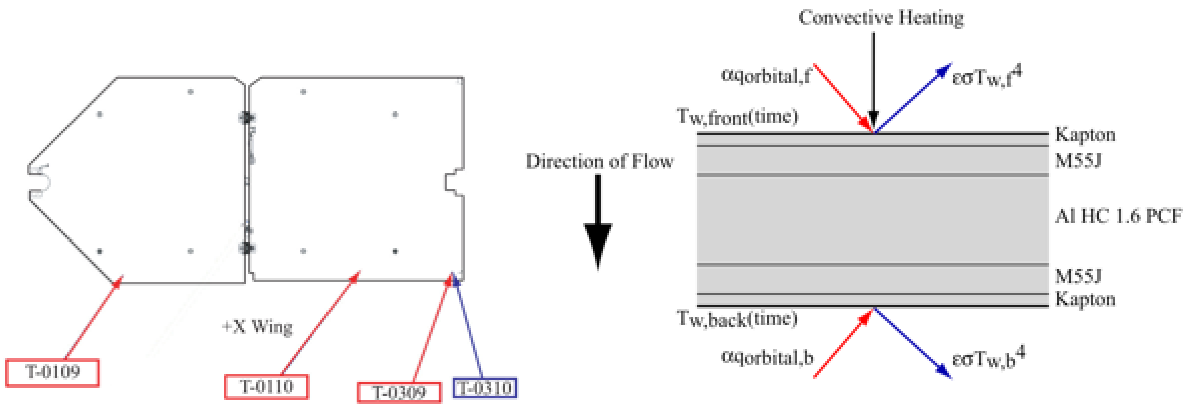
Issue: Provide support in real-time for operations portion of aerobraking mission. Determine if the space craft was experiencing expected aero/aeroheating responses.

Approach: Process data from on-board sensors – accelerometers for aerodynamics and thermocouples for aeroheating.

Comparison of Calculated In-Flight Heating with DSMC Database



MRO Thermocouple Locations and Heating Analysis



Impact: **Real-time orbit analysis allowed small corrections to be made to aerodynamic database, reducing associated uncertainties and allowing for more aggressive aerobraking maneuvers. First time that real-time aeroheating analysis had been performed on an aerobraking mission for database comparison.**

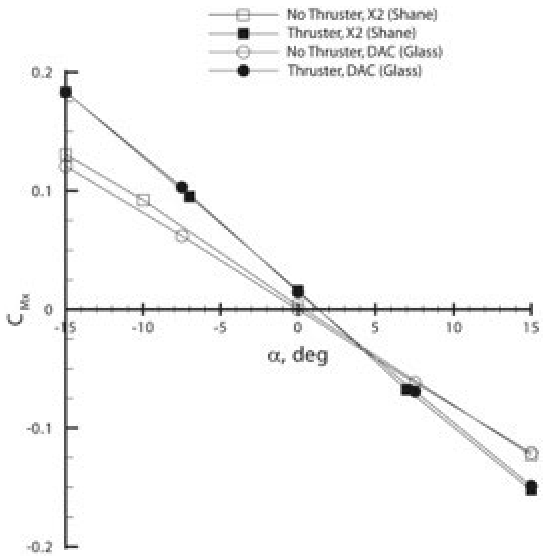
Mars Global Surveyor – Thruster Interaction Effects

Program: Mars Global Surveyor (MGS)

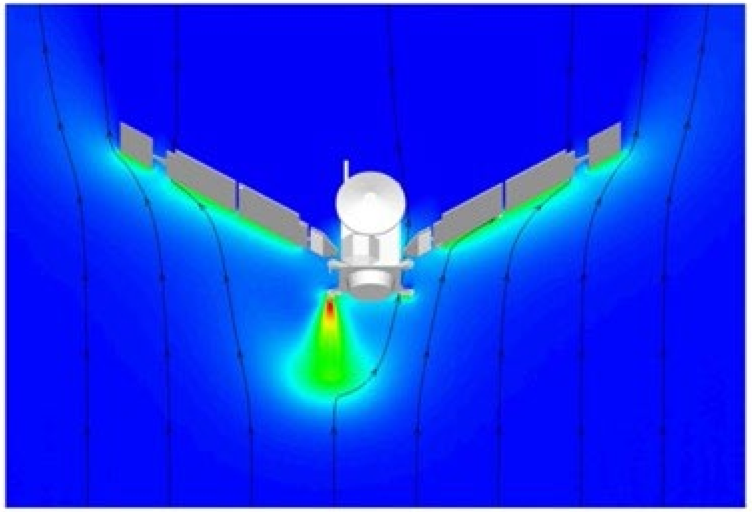
Issue: Development of thruster performance database for MGS aerobraking at Mars

Approach: Apply hybrid DSMC/continuum flow-field computational technique to model interaction of high-density thruster and low-density flow field.

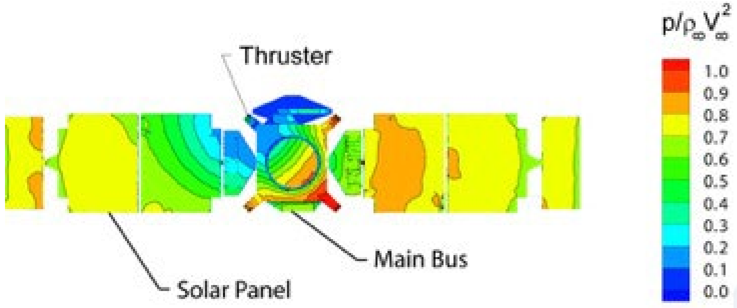
Quantification of Effects of Thruster on Pitching Moment and Code-to-Code Comparison



Flow-Field Resulting from Thruster Firing



Impact: **Thruster performance database applied to mission design, successful aerobraking performed at Mars in 1997.**



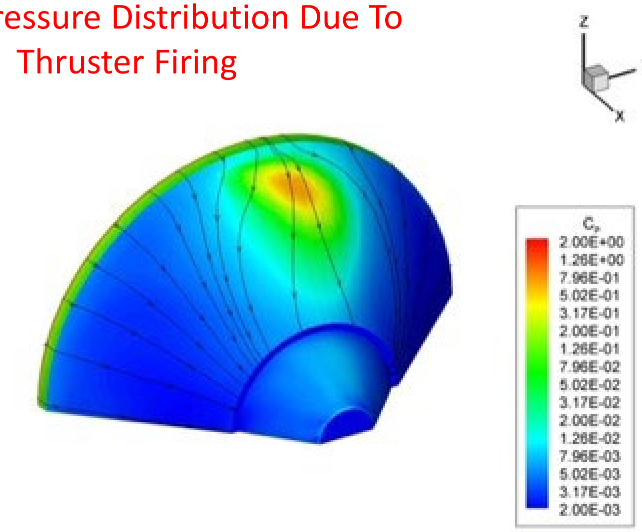
Mars Phoenix – Thruster Interaction Effects on Aerodynamics

Program: Mars Phoenix Lander

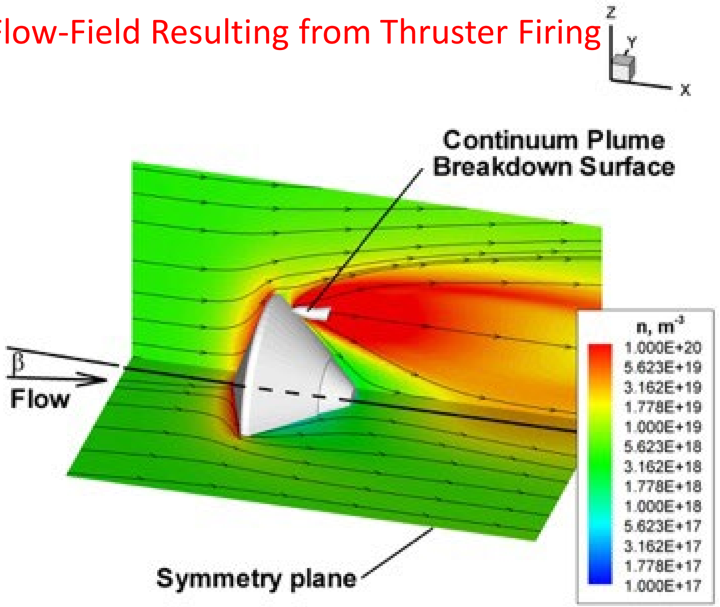
Issue: Ensure that effects of thruster firings on transitional-regime aerodynamics were within control authority of spacecraft.

Approach: Apply hybrid DSMC/continuum flow-field computational technique to model interaction of high-density thruster and low-density flow field

Surface Pressure Distribution Due To Thruster Firing



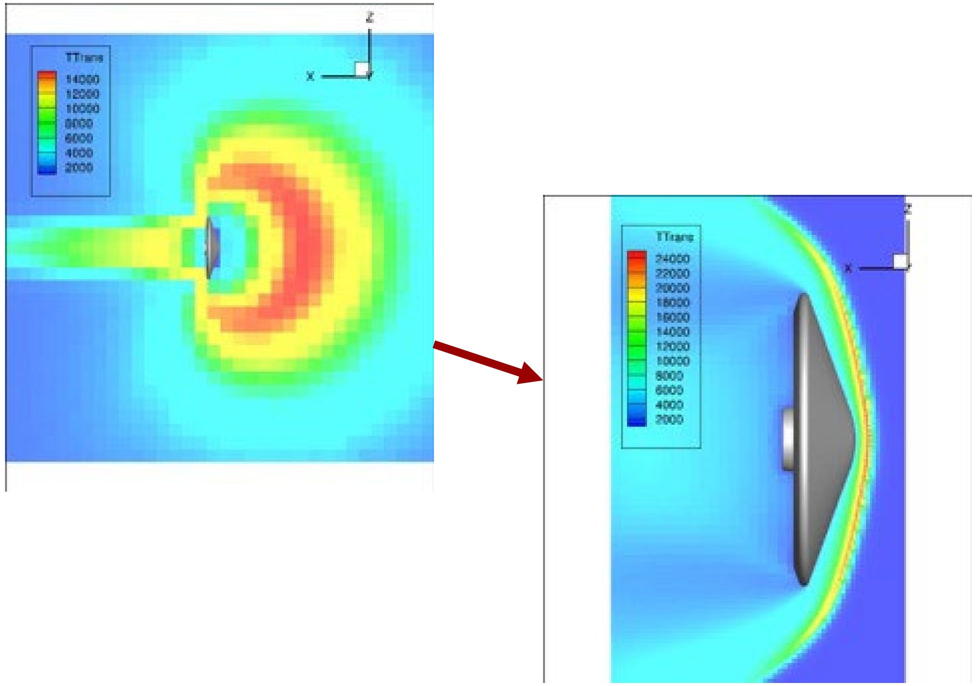
Flow-Field Resulting from Thruster Firing

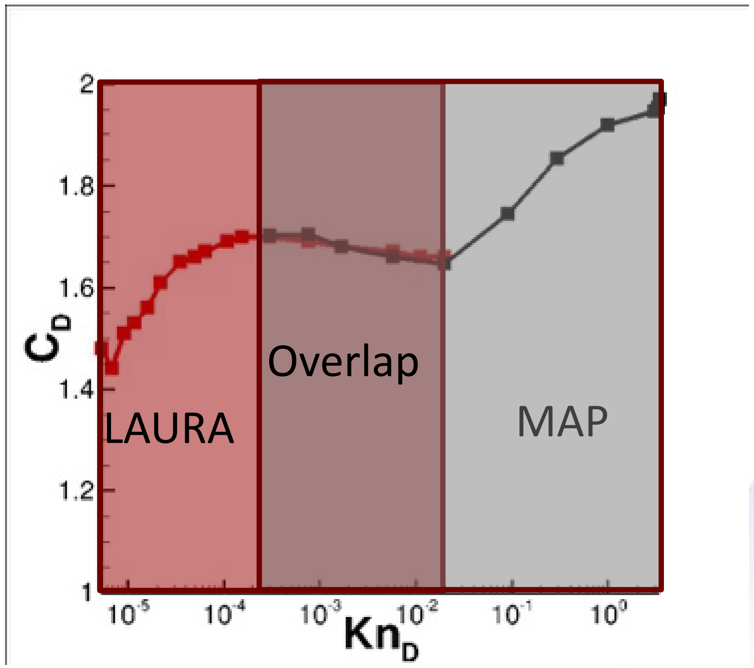


Impact: Thruster effects on aerodynamics were quantified and an increase in yawing moment was observed. It was shown that the control authority margin was sufficient in the transitional flow regime. Successful Entry, Descent & Landing at Mars in 2008

LOFTID Aerothermodynamic Database: DSMC

- **Aerodynamic/Aeroheating database provided for altitudes between 73- and 450-km (Kn = 0.0002 – 200,000) over a wide range of angles-of-attack**
- **Comparison between LAURA and MAP very good**

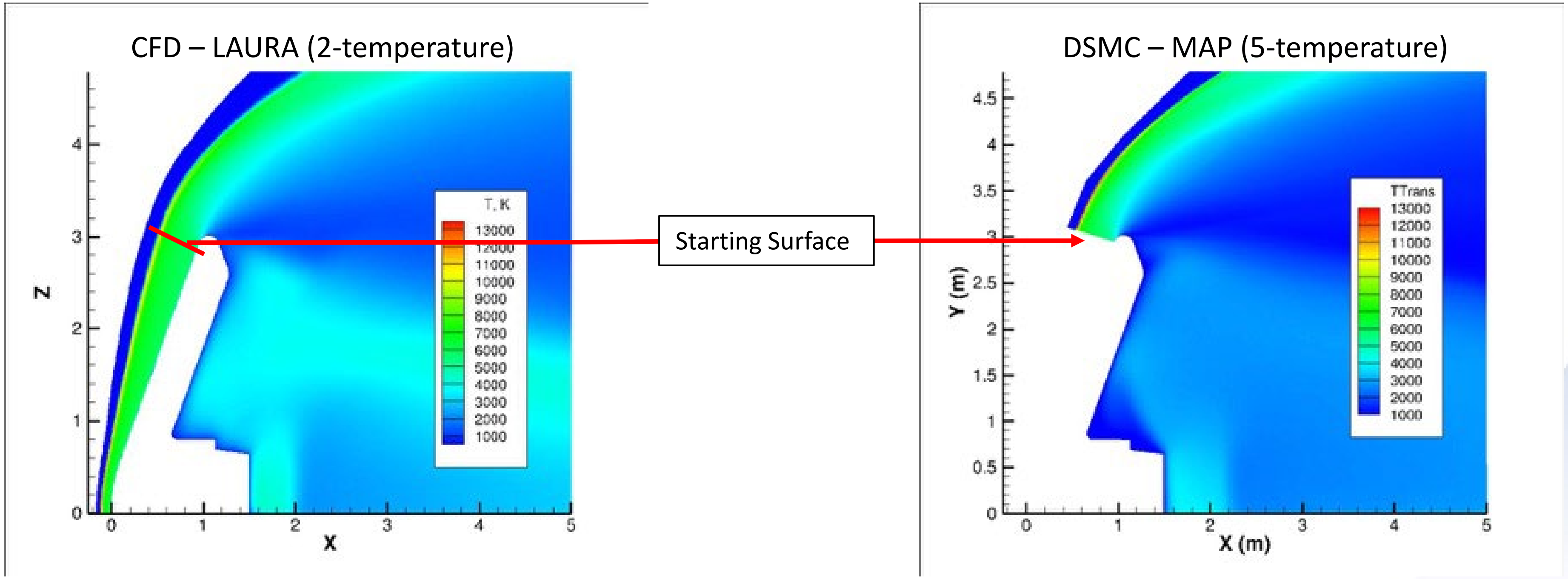




LOFTID Wake Flow: Hybrid CFD/DSMC

- **To generate valid solutions in all parts of some flow fields, hybrid DSMC/CFD solutions will need to be generated**
  - Too computationally expensive for DSMC and inappropriate for CFD for entire domain

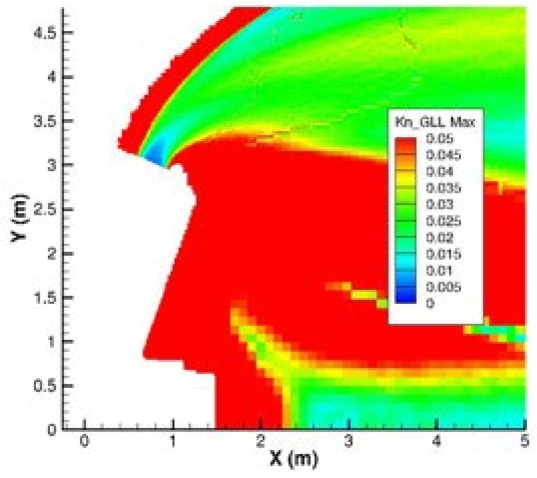
1-Way Hybrid Methodology Has Been Developed



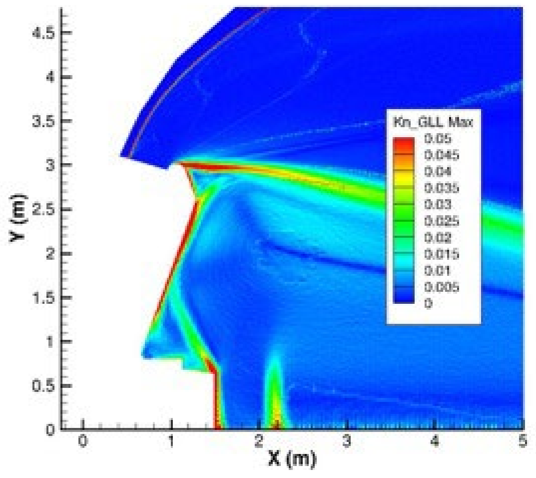
LOFTID Wake Flow: DSMC

➢ **Began looking at wake flow with DSMC because of uncertainties in grid topologies and computational methods.**
- No structured grid required.
- Developed a mostly automated 1-way hybrid CFD/DSMC solution technique.
- Found potentially large regions of continuum breakdown – even at "continuum" conditions.
- Comparisons between CFD and DSMC became much better after grid topology was addressed.

t = 728 s (Transitional)

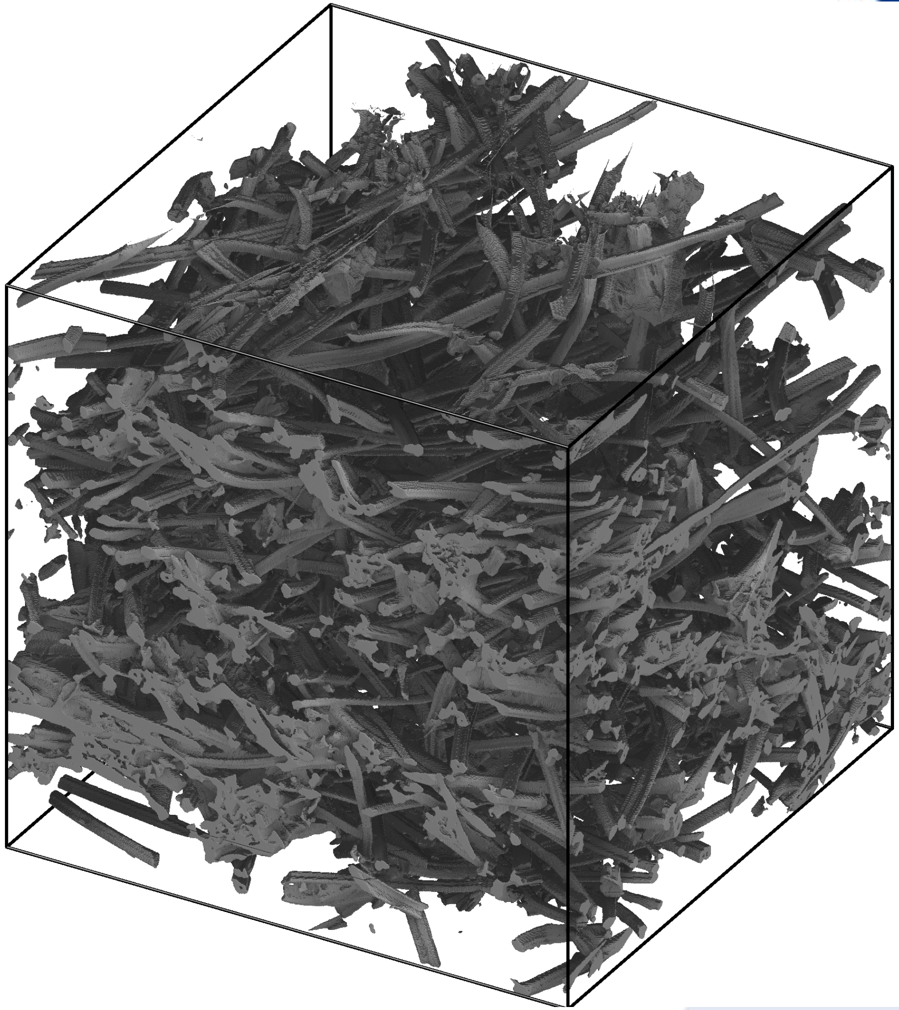


t = 776 s (Continuum)



TPS modeling using SPARTA

Flow through a FiberForm sample

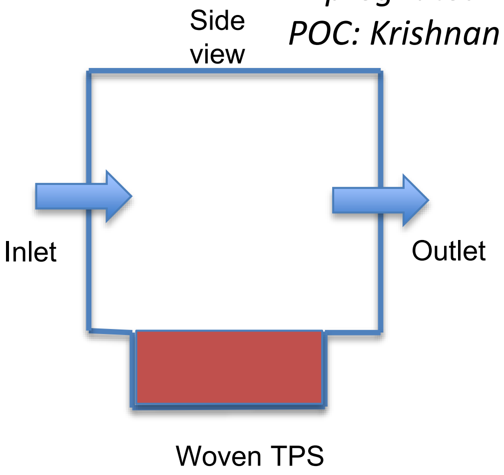


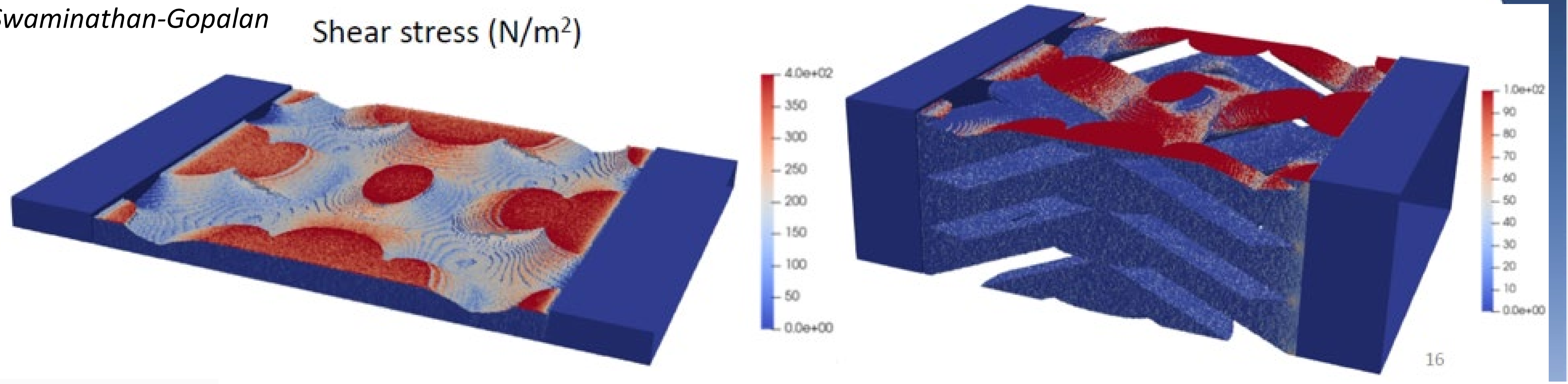
Ablation of FiberForm

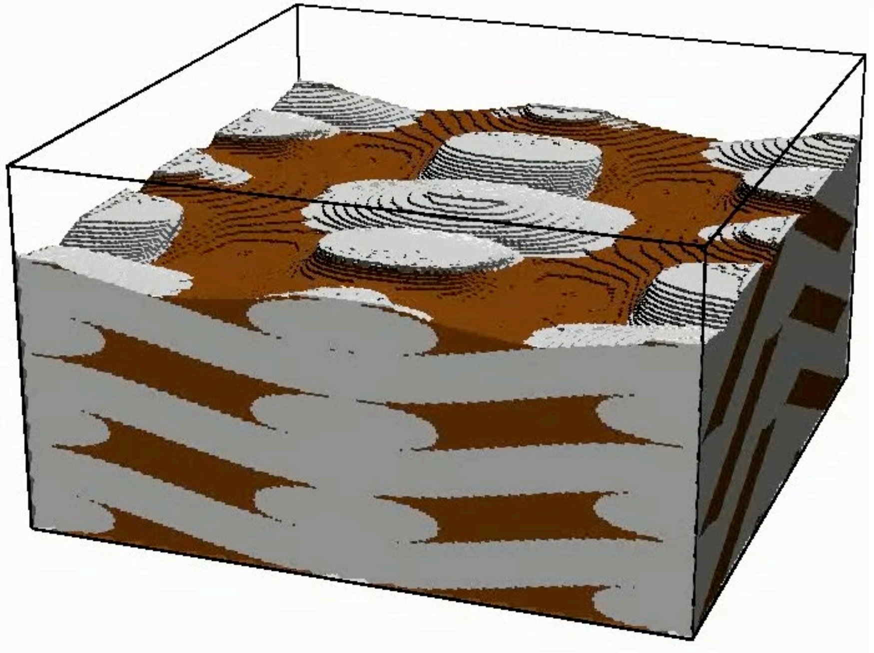
TPS modeling using SPARTA (2)

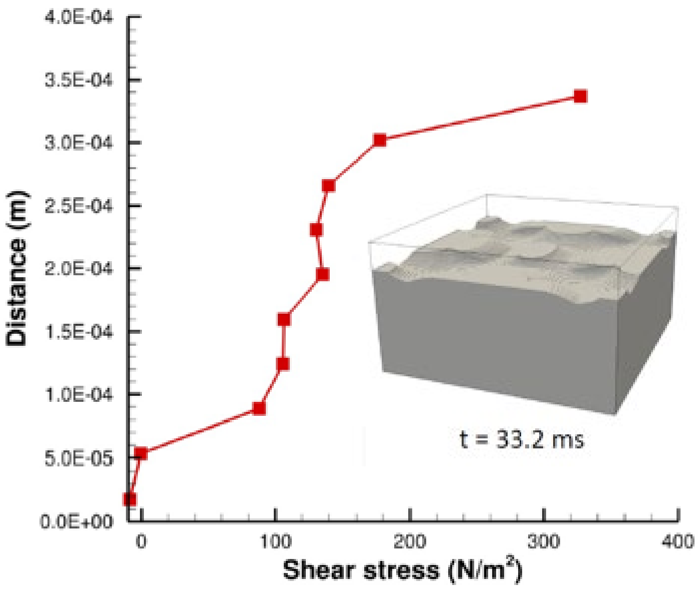
Computation of shear stresses and heating on the surface of a woven TPS material, impregnated with resin, and non-impregnated

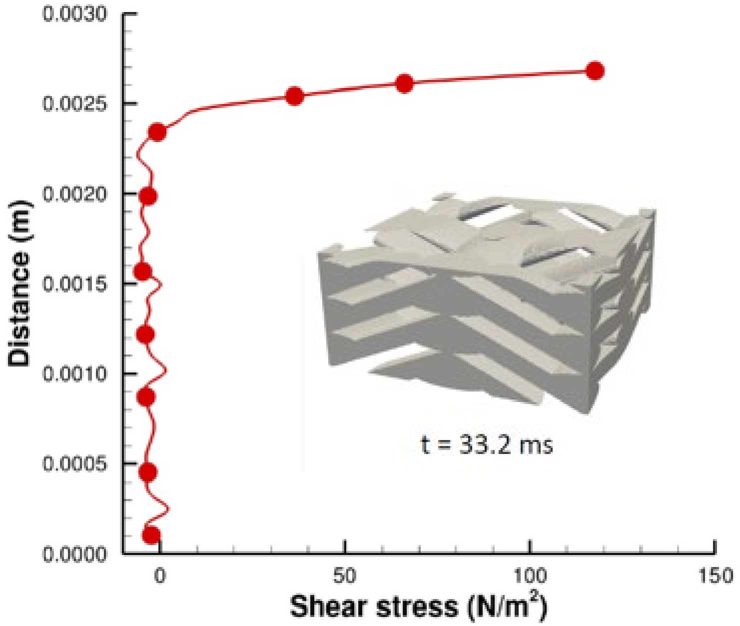
POC: Krishnan Swaminathan-Gopalan





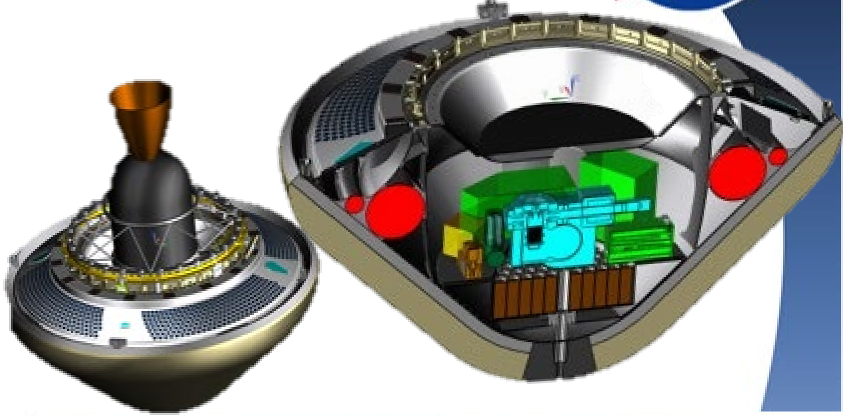


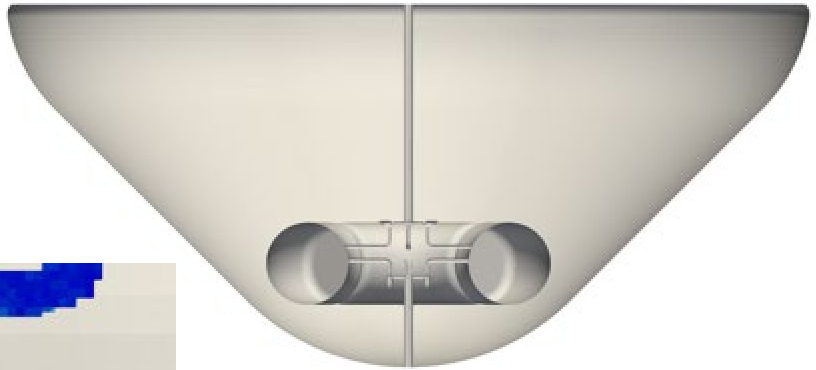


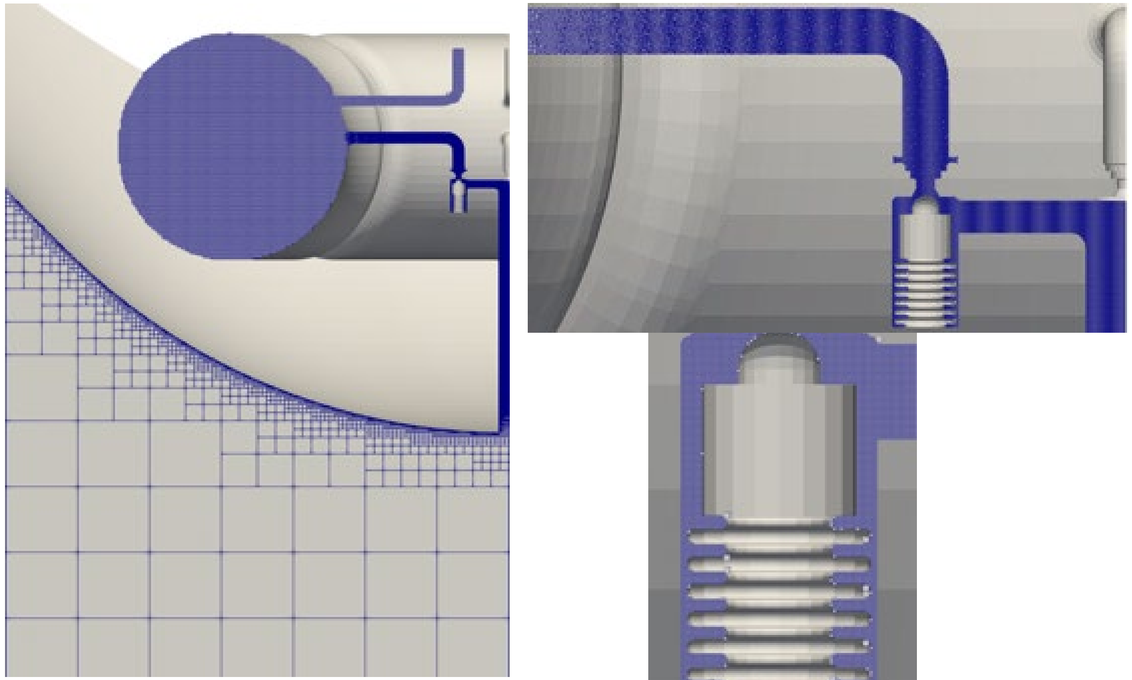


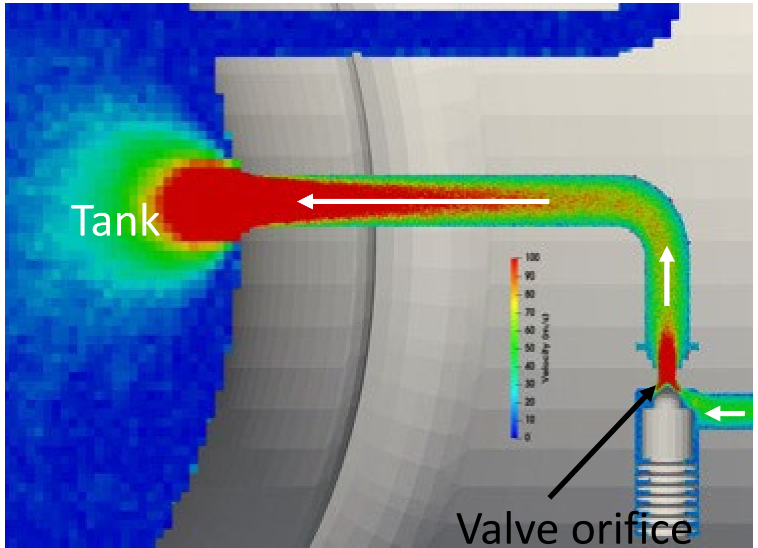
Cupid's Arrow modeling using SPARTA

- Cupid's Arrow Mission Concept: Small probe designed to sample upper atmosphere of Venus and measure noble gas abundances (JPL led – supported by ARC and Sandia)
- Ar/Xe/Kr/Ne/He are the noble gases, 15 isotopes total
- Driving Objective:
  - Is the gas acquired by the sampling system at 110 km in the Venus atmosphere while traveling at 10.5 km/s representative of the free stream?
  - Can isotopic fractionation be quantified and accurately predicted?
- Using SPARTA DSMC code (flow too rarefied for CFD to be accurate).
- First DSMC simulation to resolve internal and external flow features, spanning multiple length and time scales.
- Longest 3D run was for 30s of flight time, resolving multiple molecular time scales (20,000 cores simulation at Sandia – 2,000 cores on Pleiades – 200+ TB of RAM).









Thanks - Questions?

- Thanks to Steve Plimpton and Michael Gallis (Sandia) for a lot of the SPARTA related material used here.
- Thanks to the Entry Systems Modeling (ESM) project ((M. Wright/)M. Barnhardt PM, A. Brandis PI), under the NASA Game Changing Development (GCD) program, for funding the MAP development and SPARTA modification.

Backup