Modeling the Flow of Rarefied Gases at NASA

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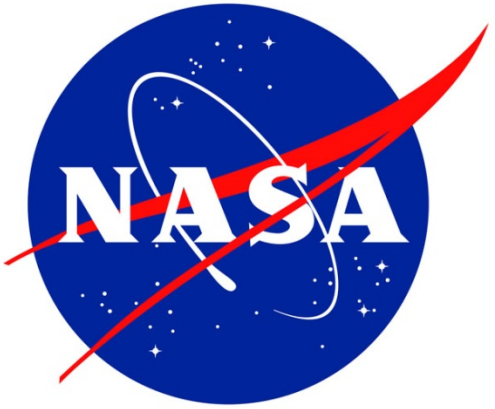
At modest temperatures, the thermal energy of atmospheric diatomic gases such as nitrogen is primarily distributed between only translational and rotational energy modes. Furthermore, these energy modes are fully excited such that the specific heat at constant volume is well approximated by the simple expression $C_v = \frac{5}{2} R$. As a result, classical mechanics provides a suitable approximation at such temperatures of the true quantum mechanical behavior of the inter-molecular collisions of such molecules. Using classical mechanics, the transfer of energy between rotational and translation energy modes is studied. The approach of Lordi and Mates is adopted to compute the trajectories and time dependent rotational orientations and energies during the collision of two non-polar diatomic molecules. A Monte-Carlo analysis is performed collecting data from the results of many such simulations in order to estimate the rotational relaxation time. A Graphical Processing Unit (GPU) is employed to improve the performance of the Monte-Carlo analysis. A comparison of the performance of the GPU implementation to an implementation on traditional computer architecture is made. Effects of the assumed inter-molecular potential on the relaxation time are studied. The seminar will also present highlights of computational analyses performed at NASA Johnson Space Center of heat transfer in rarefied gases.



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Outline

- Highlights of Rarefied Gas Dynamics Modeling at NASA JSC
  - Background
  - Direct Simulation Monte Carlo (DSMC) and example applications
  - On-orbit Plume Modeling
  - Application of a Coupled CFD/DSMC Technique for High Fidelity Plume Modeling
- Application of Molecular Dynamics Trajectory Simulations on a GPU Architecture to Evaluate Translation-Rotational Energy Exchange in Diatomic Molecules
  - Background
  - Problem Description
  - Governing Equations
  - Numerical and Computational Details
  - Results
    - Single Trajectory Animation
    - Examples of Energy Dependence on Input Trajectory Parameters
    - CPU vs. GPU performance
  - Future Work

Background: NASA's need to model RGD flows

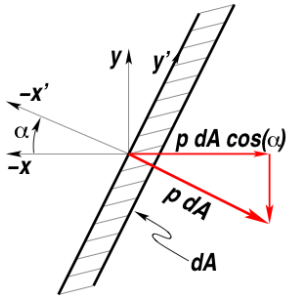
- NASA has numerous programs that require detailed information about the low density flow environments encountered by its spacecraft.
  - Knowledge is required during the entire lifecycle from preliminary design through mission operations.
  - A wide range of fidelity is desired from simple engineering tools to state-of –the-art high fidelity simulation.
  - Modeling tools are developed and applied in collaboration with the best available experimental data.
  - Environments are used to assess aerodynamic heating and mechanical loads and used in the design of the spacecraft, the design of mission operations, and to assist during anomaly investigations.
  - Applications include aero-braking (Mars robotic missions), plume impingement modeling (International Space Station), and Orion re-entry aerothermodynamics database development.
- Serve as Johnson Space Center technical lead for rarefied gas dynamic environments (RGD)
  - Role includes responsibility for tool development, application of tools to analyses of importance to NASA JSC, and leadership of a small team (~5 members) focused on this technical discipline

Rarefied Gas Dynamic Capabilities: Overview

- NASA-JSC has a world class capability in RGD (Kn = λ/L_{ref} > ~0.01) analysis and engineering assessments in terms of both tools and skilled personnel

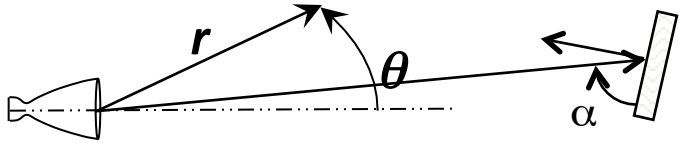
- Tools
  - RPM (RCS Plume Model)
    - Plume impingement model
  - DAC (DSMC Analysis Code)
    - Premier NASA DSMC code.
  - FREEMO
    - Free molecular aerodynamics

Free Molecular Aerodynamics



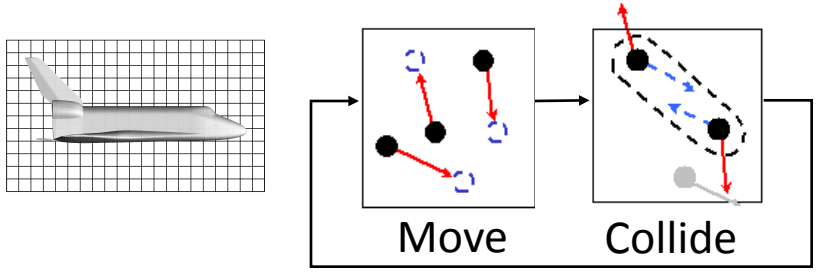
$$C_p = \cos^2\alpha\left\{\left[\frac{1}{S_v}\left(\frac{1}{\sqrt{\pi}}+\frac{1}{2S_v}\sqrt{\frac{T_r}{T_i}}\right)e^{-S_v^2}\right] + \left[\left(1+\frac{1}{2S_v^2}+\frac{\sqrt{\pi}}{2S_v}\sqrt{\frac{T_r}{T_i}}\right)\times\left[1+\mathrm{erf}(S_v)\right]\right]\right\}$$

Plume Modeling



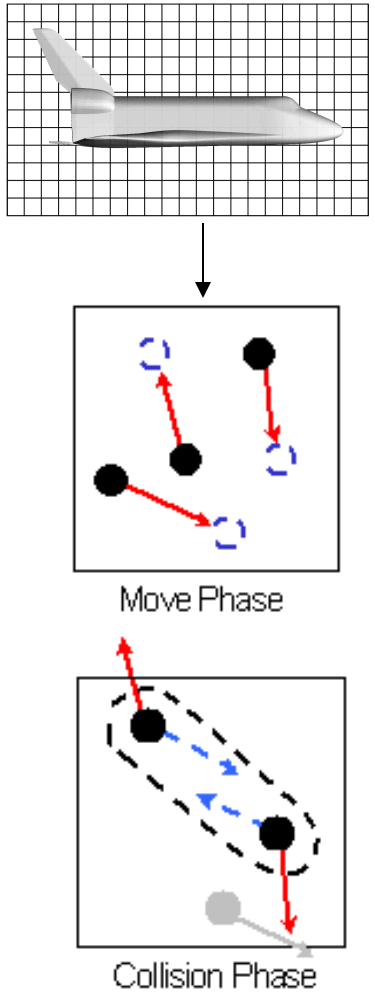
$$\rho = \rho(r,\theta) = f(r)g(\theta); \quad u = u_{\lim} = \sqrt{2\gamma T/(\gamma-1)}$$
$$\dot{q} = c_h q = (c_{ho}\sin^2\alpha)\ (\tfrac{1}{2}\rho u^3)$$

DSMC (Molecular Based Simulation)



DSMC: Direct Simulation Monte Carlo

- Results shown to be equivalent to solutions of the Boltzmann equation.
- Simulated molecules tracked through space and time.
  - Each simulated molecule represents many real molecules.
- Network of flow field cells used to group neighboring molecules into collision pairs.
- Move and collision phases decoupled and treated as distinct computational steps.
  - Move step is deterministic.
  - Collision step is a Monte-Carlo simulation of kinetic theory based collision statistics.
- Statistical sampling of the ensemble of molecules provides macroscopic properties.
- Fundamental requirements on simulation parameters must be satisfied to achieve an accurate result.

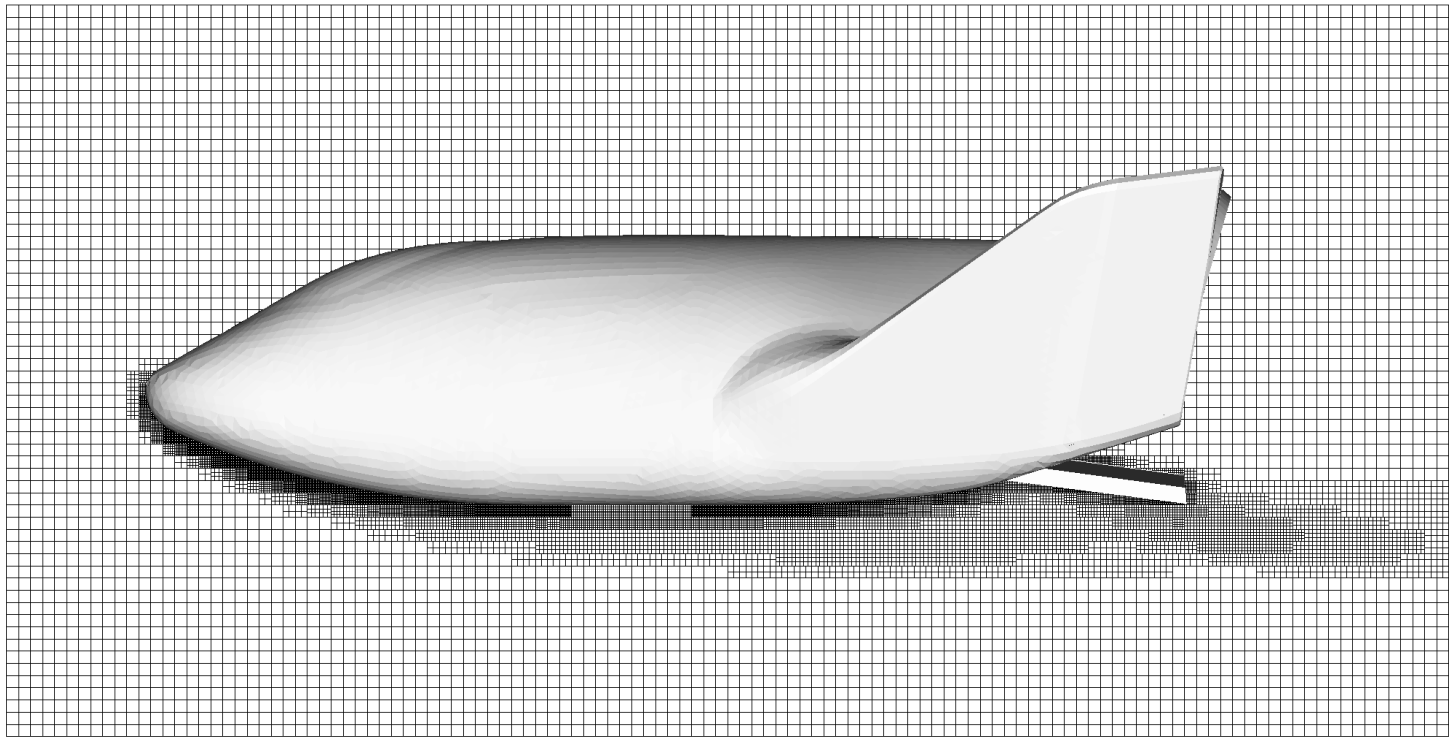


DSMC Analysis Code (DAC)
JSC's State-of-the-Art DSMC Implementation

- The Aeroscience and Applied CFD Branch at NASA Johnson Space Center is the developer and owner of this software package.
  - Co-Winner of NASA's 2002 Software of the Year
- Combined the successful techniques of previous implementations with new and innovative features, while automating much of the process.
- Geometric and boundary condition flexibility and gas chemistry options allow a wide variety of rarefied problems to be analyzed.
  - Including on-orbit plumes
- Provides automatic flow field discretization and solution adaptation such that fundamental simulation constraints are satisfied.
- Enabling feature of DAC is its ability to easily and efficiently utilize a large number of processors on a single problem.
  - Automatically performs domain decomposition
  - Re-partitions domain decomposition during runtime to maintain load balancing
  - A halted run can be restarted on a different number of processors
- The above features provide "ease of use" as well as versatile capabilities.

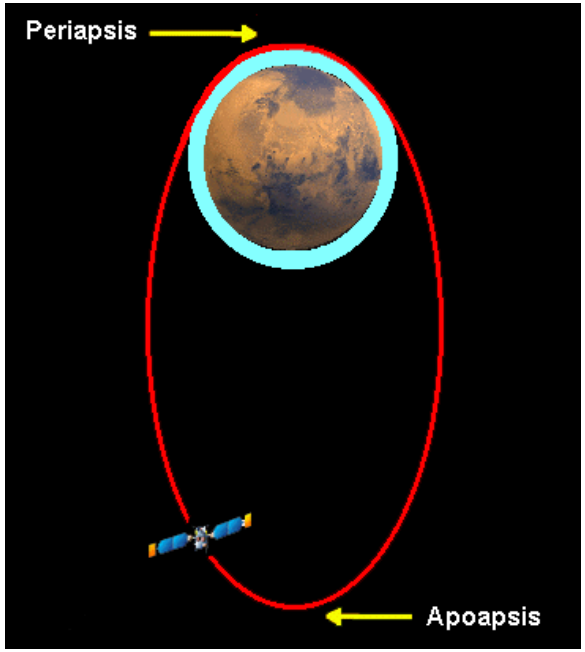
Volume Geometry Created by DAC Preprocessor

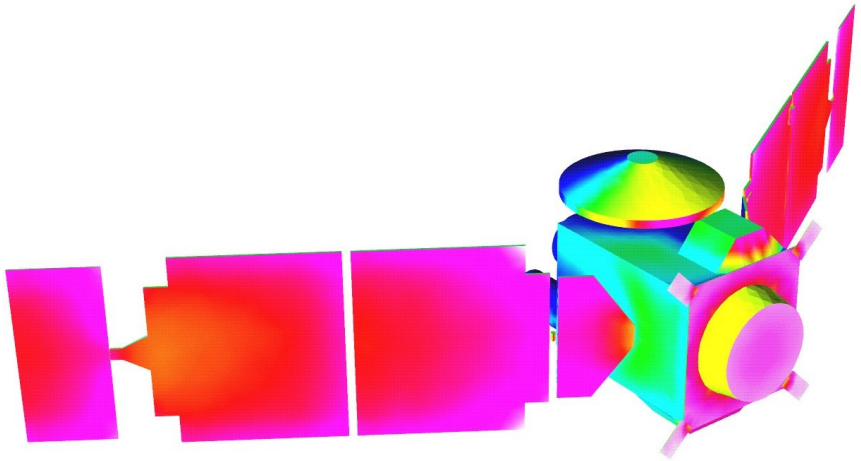
- A 2-level embedded Cartesian grid system, that is completely uncoupled from the surface representation, is automatically generated by the software.
- Relieves the user of this traditionally time consuming task, and insures that the fundamental constraints that govern the accuracy of the simulation are satisfied.
- Cells are used to group neighboring molecules and also act as flow field sampling zones.



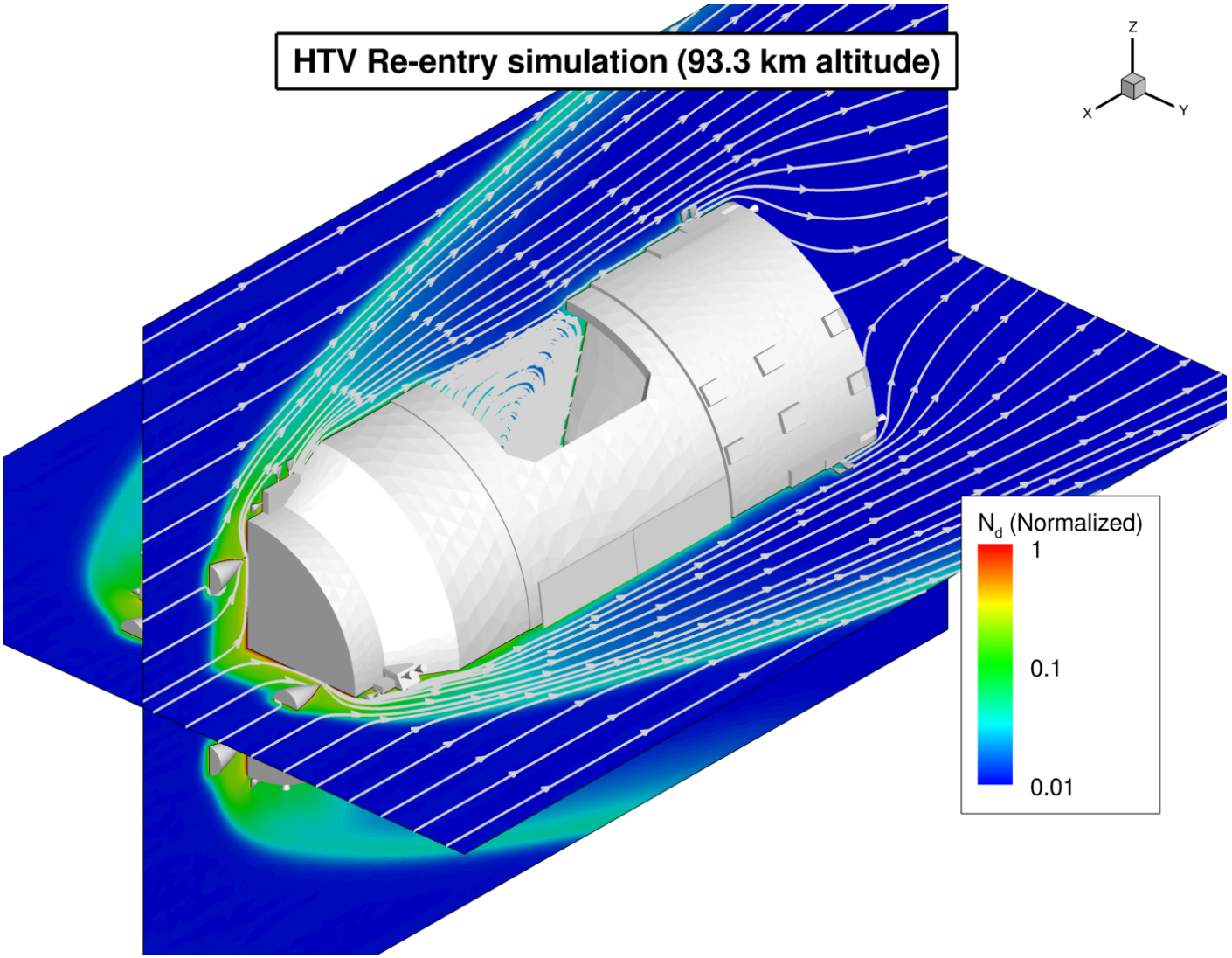
Mars Aerobraking

- Aerobraking
  - Exploration Applicability (exclusively robotic since manuevers require many aeropasses)





Japanese HTV Re-entry Simulation



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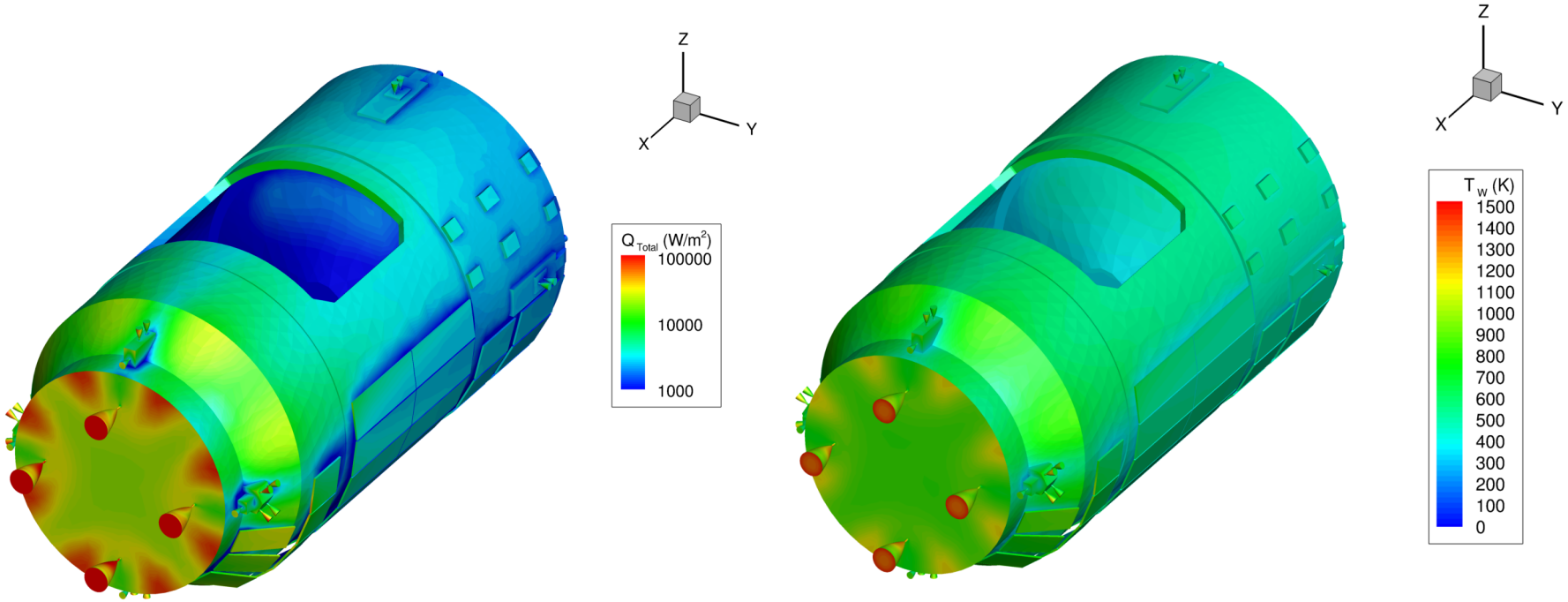
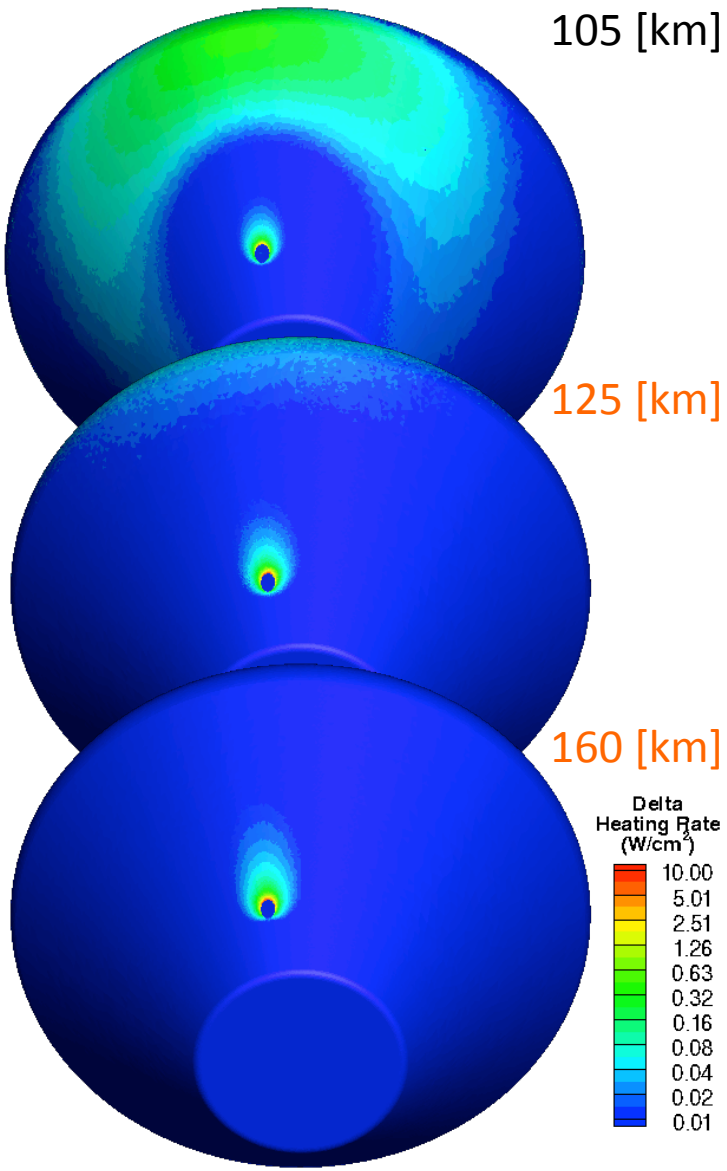


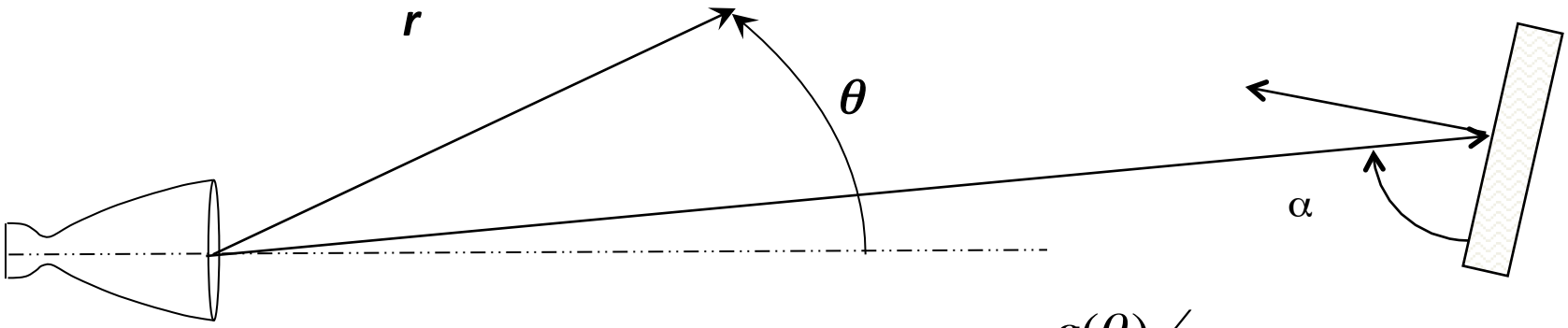
Orion: Plume increment to aerodynamic heating



Delta Heating = $q_{RCS\ DAC} - q_{SOML\_DAC}$

- 105 [km] near the rarefied / continuum transition point – sees the most pronounced farfield influence
- Farfield influence diminishes rapidly with increasing altitude
  - 125 [km] solution shows very limited farfield influence (sliver near the shoulder)
  - Believe the same trend applies to the other jets
- Local influence increases with increasing altitude
- No influence on the apex

Engineering Approach Illustration: Single Axi-symmetric Plumes Impinging Simple Targets



Source flow approximation: $\rho = \rho(r,\theta) = f(r)g(\theta) = g(\theta)/r^2$

Conservation of energy: $u = u_{\lim} h(\theta) = \begin{cases} \sqrt{2\gamma T/(\gamma-1)} & \theta \le \theta_V \\ \sqrt{2\gamma T/(\gamma-1)}\,(1-\chi\theta) & \theta > \theta_V \end{cases}$

Surface pressure: $p = c_p q = \frac{1}{2} c_p \rho u^2$

$c_p = c_{po} + c_{p1}\sin\alpha + c_{p2}\sin^2\alpha$

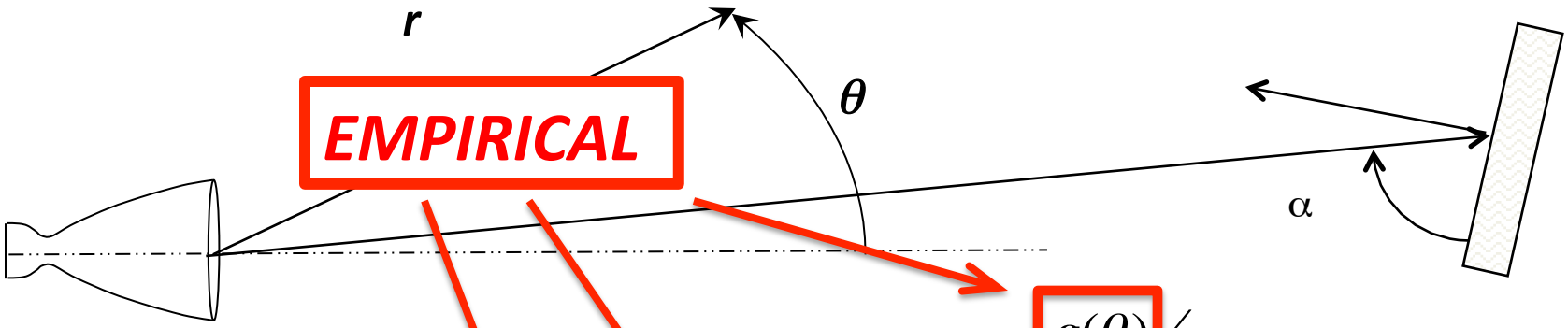
Relations for $c_{po}, c_{p1}, \& c_{p2}$ exist to bridge between continuum and free molecular flow.

$$c_p = \frac{2}{\gamma M}\left\{\left[\frac{(\gamma+1)^2 M^2}{4\gamma M^2 - 2(\gamma-1)}\right]^{\gamma/(\gamma-1)}\left[\frac{1-\gamma+2\gamma M^2}{\gamma+1}\right]-1\right\}\sin^2\alpha \xrightarrow[M=\infty,\gamma=1.4]{} 1.82\sin^2\alpha$$ Continuum (Mod. Newt)

$$c_p = \frac{1+\varepsilon}{2}\left\{\frac{2\sin\alpha\, e^{-S^2\sin^2\alpha}}{\sqrt{\pi}\,S} + \left(\frac{1}{S^2}+2\sin^2\alpha\right)\left[1+\mathrm{erf}(S\sin\alpha)\right]\right\}$$

$$+\frac{1-\varepsilon}{2}\sqrt{\frac{T_r}{T_i}}\left\{\frac{e^{-S^2\sin^2\alpha}}{S^2}+\frac{\sqrt{\pi}\sin\alpha}{S}\left[1+\mathrm{erf}(S\sin\alpha)\right]\right\} \xrightarrow[S=\infty,\,\varepsilon=1]{} 4\sin^2\alpha$$ Free Molecular

Engineering Approach Illustration: Single Axi-symmetric Plumes Impinging Simple Targets



EMPIRICAL

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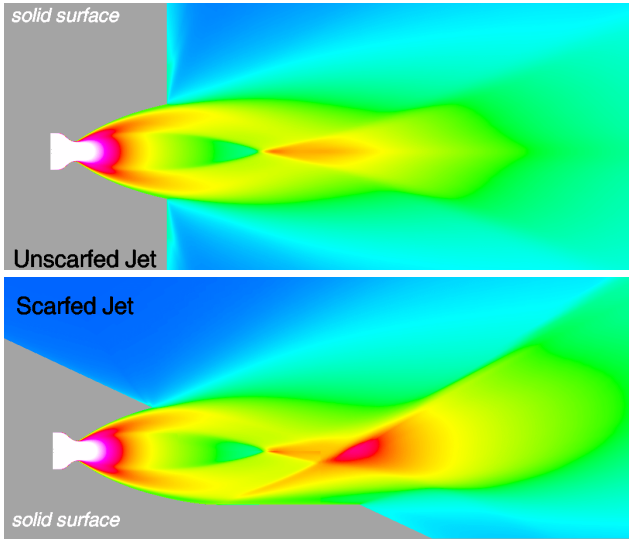
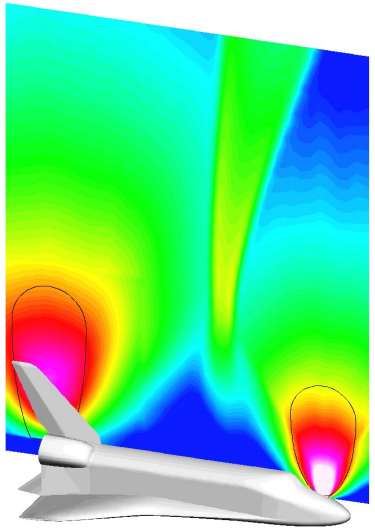
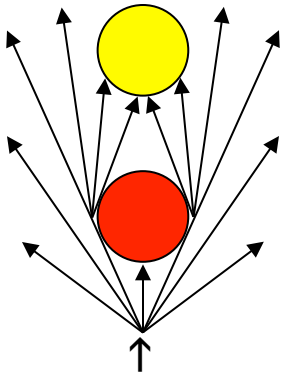
What about more complicated situations?

- Complex Plumes
  - Scarfed Jets
  - Multiple Jets

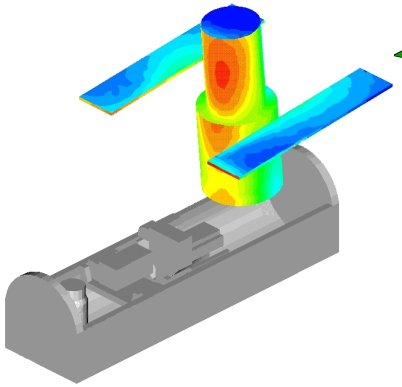


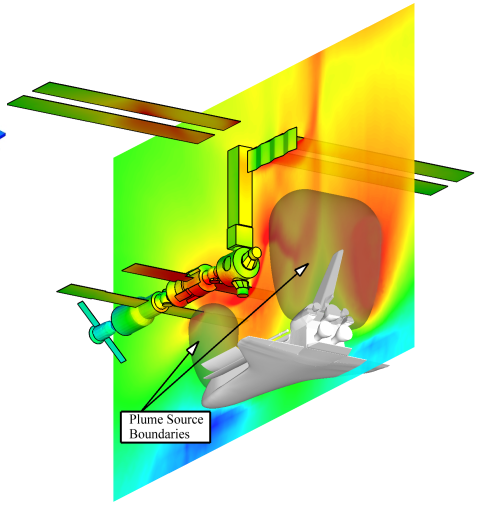


- Complex Interactions
  - Wakes
  - Shadowing an assumption
- Complex geometry
  - Molecules strike more than once



Flow Turning

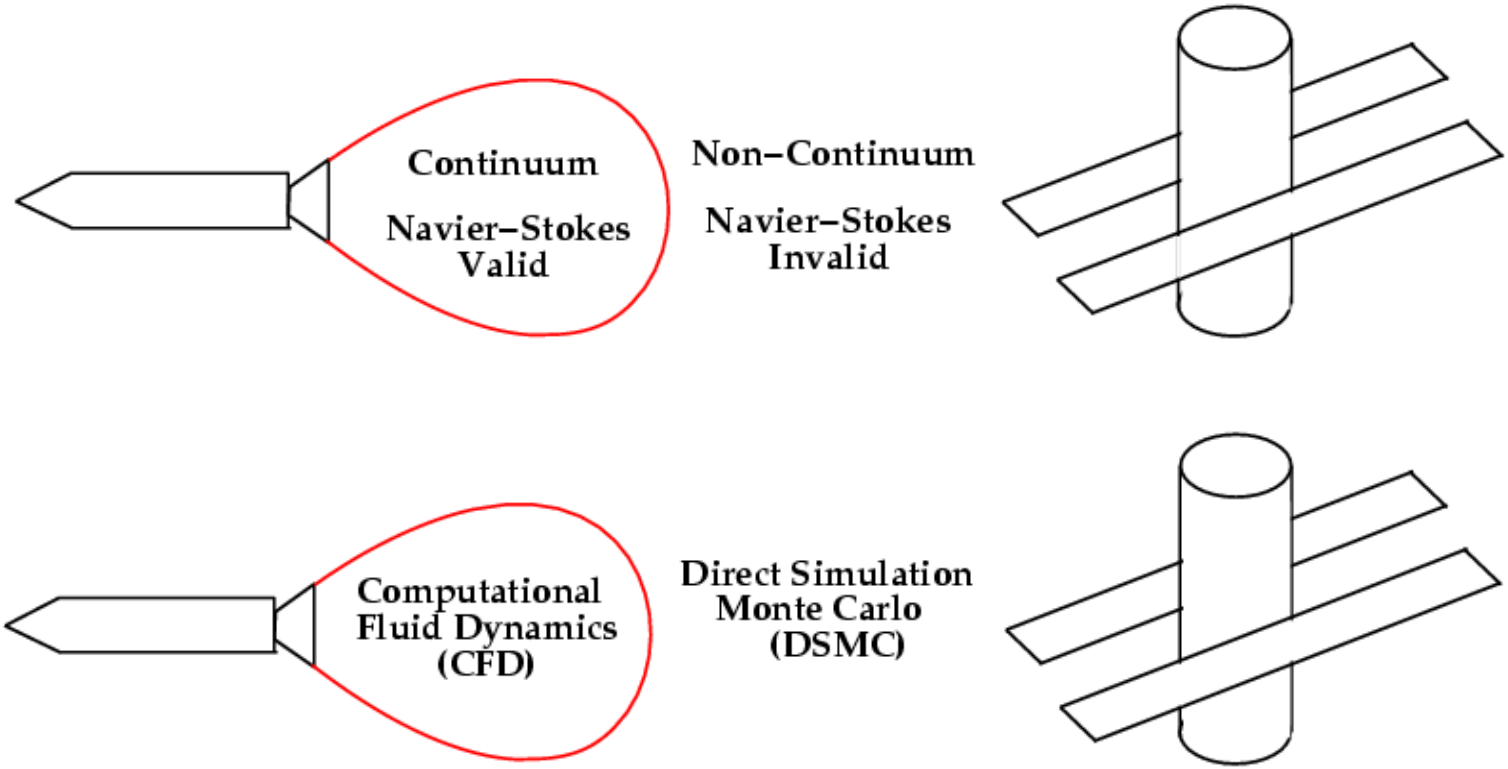




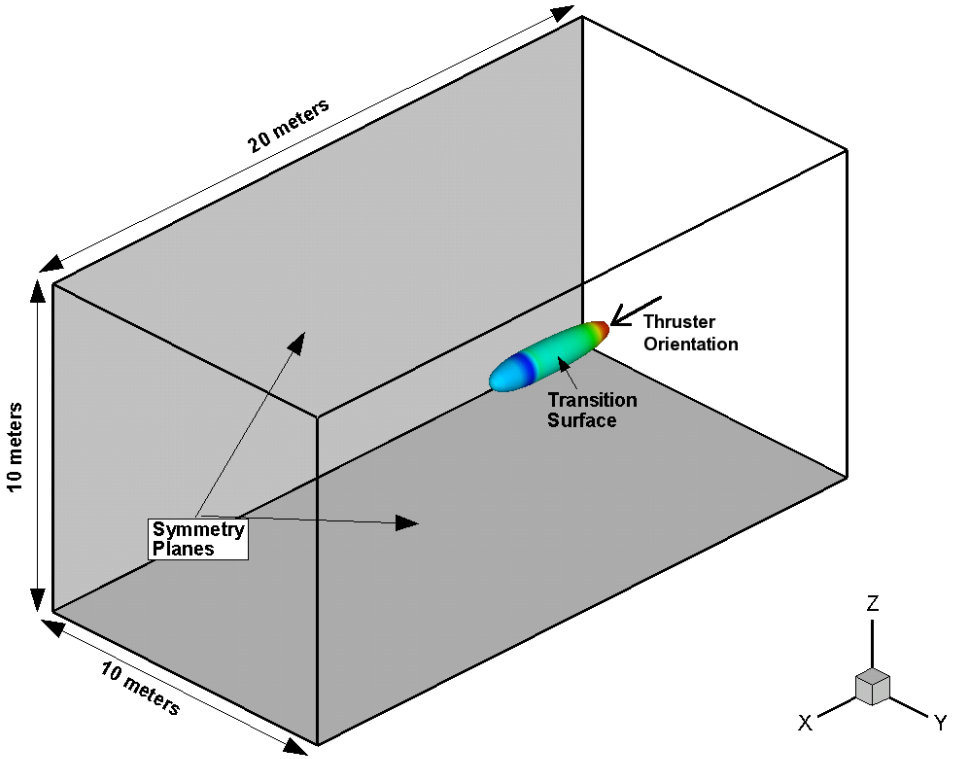
How we handle these complicated cases.

- Add additional variables for curve fits
  - For scarfed jets, we add the clocking angle, ϕ.
    - $g(\theta) \Longrightarrow g(\theta,\phi)$; $h(\theta) \Longrightarrow h(\theta,\phi)$
  - Fancy curve fits for dual jets
    - Curve fit to determine if in or out of interaction regime.
    - Curve fit for dynamic pressure "amplification" factor if in interaction regime.
  - Semi-Empirical
- In both these cases, insight from either experiment or high fidelity modeling is used to fine tune the models/develop the fits.
- Table look ups
  - Empirical basis $\Longrightarrow$ data for table has to come from somewhere.
    - Experiment
    - High Fidelity Modeling of flow field (CFD and, possibly, DSMC)
- High fidelity modeling of plume AND impingement (CFD and DSMC)
  - Computationally expensive $\Longrightarrow$ each case is a different high fidelity run.

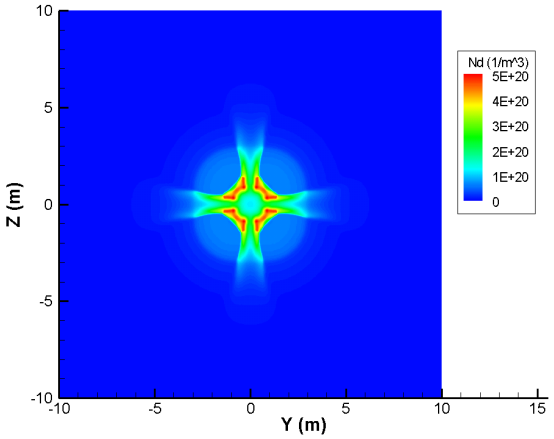
Decoupling the Continuum & Rarefied Domains
An illustration



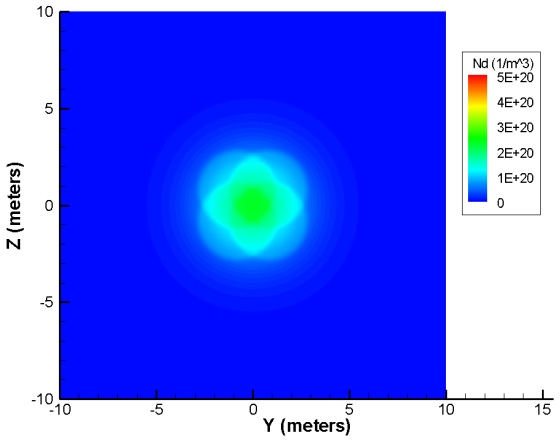
Example Plume Simulation
JAXA HTV Firing Four R4D Engines



DSMC, X = 10



Superposition, X = 10



Background: Rotational Relaxation

- Diatomic gases such as nitrogen and oxygen have three "modes" of thermal energy: translational, rotational, and vibrational.
- Except at very low temperatures, the translational and rotational modes are fully excited and can be analyzed to good approximation using classical rather than quantum mechanics.
- The vibrational mode, because of the large spacing of vibrational quantum levels, is completely unexcited at room temperature and slowly move towards full excitation as the temperature rises through the range of 1000's of Kelvin.
  - Why air's specific heat $\boldsymbol{C_v}$ increase above the ***5/2 R*** value as temperature increases.
- Molecular collisions transfer energy in a gas between these modes. When there are sufficient collisions the gas is in "thermodynamic" equilibrium.
  - The translation, rotational, and vibrational temperature are equal.
- Rate equations (Jeans, Landau-Teller) are often used to model the rate of change of these temperatures towards equilibrium.

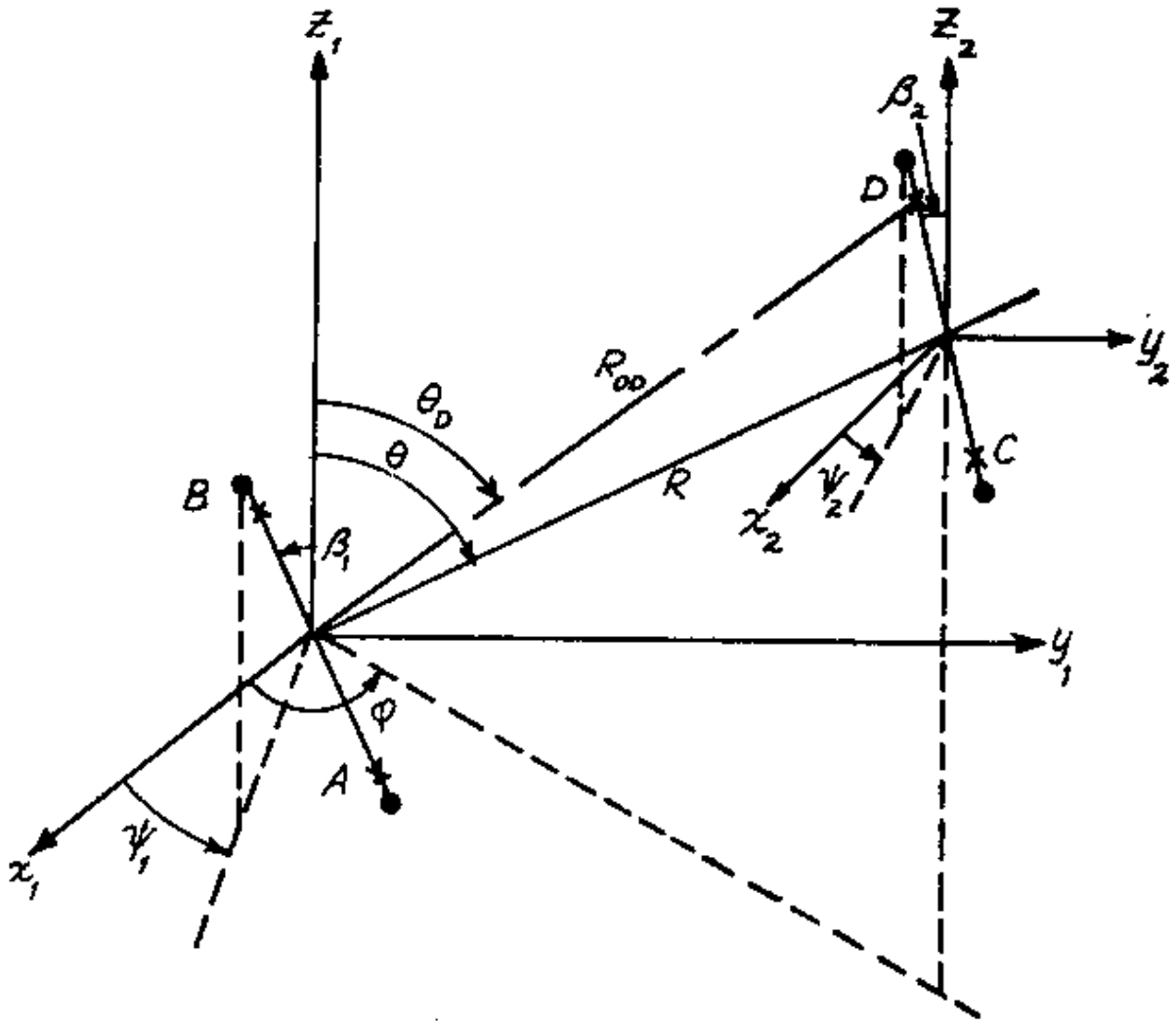
$$\frac{dT_i}{dt} = \frac{T - T_i}{\tau_i}$$

- Relaxation time is an input to these equations and is determined by a mix of theory and experiment.

Background: Rotational Relaxation concluded

- Experimental techniques to measure relaxation time vary widely
  - Attenuation and absorption of sound at given frequencies as a function of temperature.
  - Coherent Anti-Raman Spectroscopy (CARS)
- Theoretical techniques include molecular dynamic trajectory simulations
  - Many simulations are performed in a Monte Carlo framework to "integrate" the results over many independent variables which must be "chosen" as initial conditions to the trajectory simulation.
    - Impact parameter
    - Initial orientations
    - Relative velocity
    - Etc, etc, …
  - Computational chemists perform such simulations with ab initio determinations of the potential energy surfaces to get chemical reaction rates → very expensive
- Current work follows technique of Lordi and Mates
  - Pure use of classical mechanics

Problem Description



Governing Equations

- Seven positions or angles are needed describe the orientation of the molecules with respect to one another

$$R,\ \theta,\ \phi,\ \beta_1,\ \psi_1,\ \beta_2,\ \psi_2$$

- Hamiltonian mechanics are used to derive the equations of motion
  - Have 7 generalized coordinates (q_i) and 7 generalized momenta (p_i)
  - System of 14 ordinary differential equations to be integrated in time

$$H = T + V$$

$$\dot{q}_i = \frac{\partial H}{\partial p_i}$$

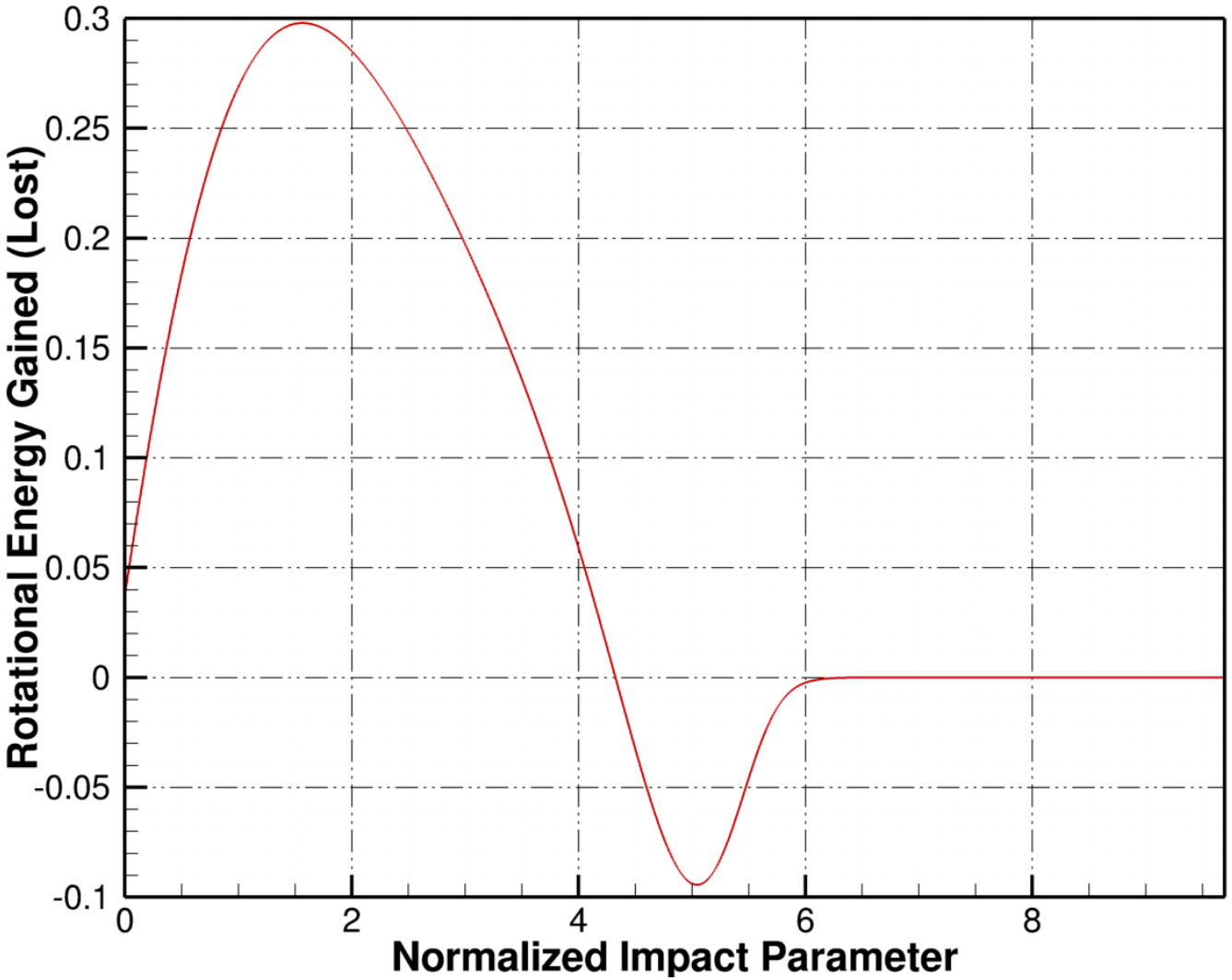
$$\dot{p}_i = -\frac{\partial H}{\partial q_i}$$

- Conservation of total system angular momentum is employed to reduce the equation set from 14 to 12.
- Potential function, V, is composed of three exponential functions of distance
  - Single attractive potential at molecule center
  - Two repulsive potentials along molecule axis separated by d^*

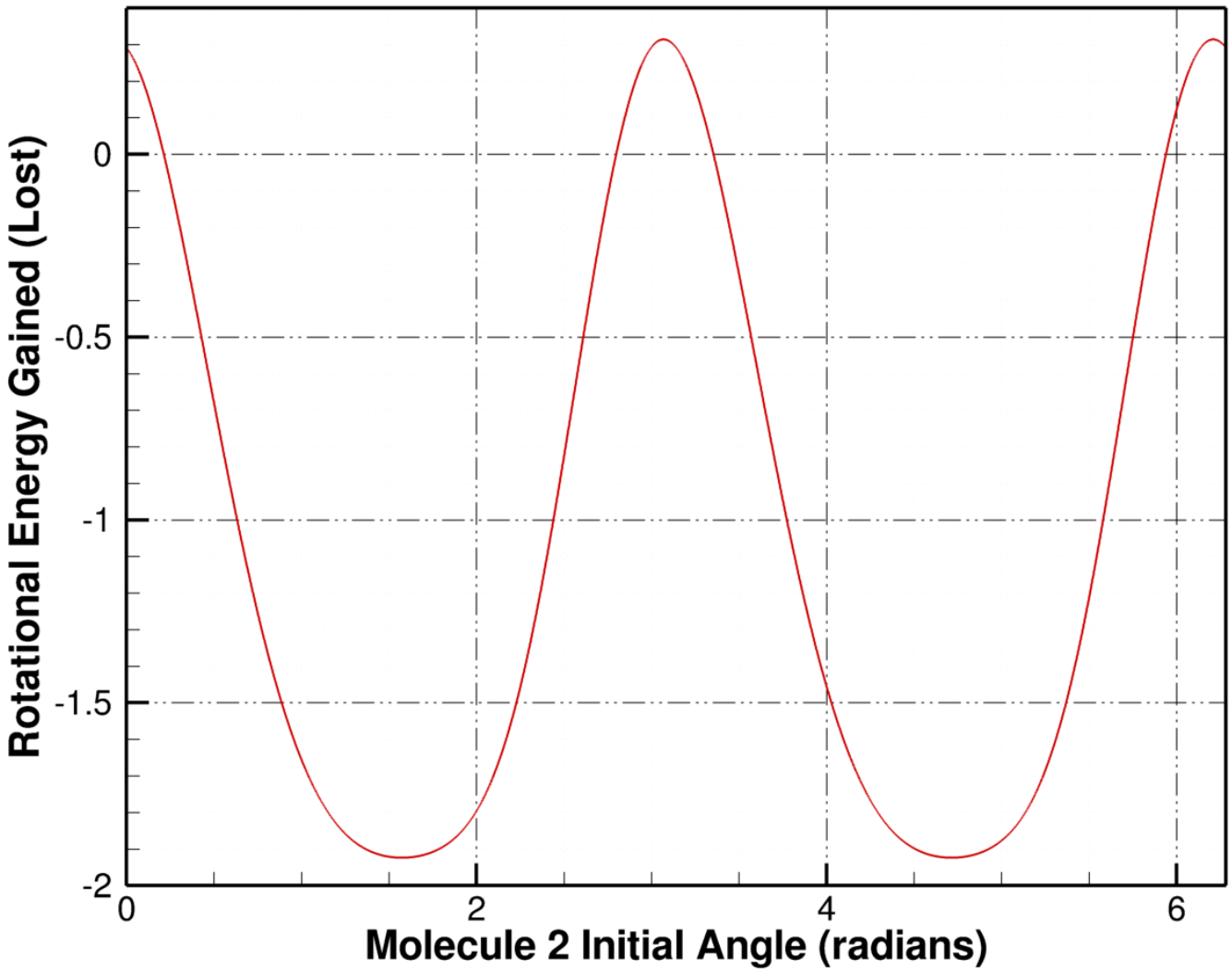
Numerical and Programming Considerations

- Equations of motion integrated in time using standard 4th order Runge-Kutta.
- Hamiltonian checked to insure it remains constant during integration
  - Any change mitigated by reducing the time step
- Simulation developed in C with CUDA GPU API elements as an option
- If performing a single trajectory calculations, the time history of the generalized co-ordinates may be output to allow an animation to be created
  - Animation facilitated by converting molecular orientations into YPR Euler angle sequences.
  - Tecplot macro developed to loop through time steps and render individual frames of the trajectory
  - At each loop iteration the macro calls a FORTRAN application to read in the two unstructured grids for the molecules (created in GRIDGEN) and position and orient the molecules appropriately.
- Code can be run for large number of trajectories
  - CPU or GPU implementations chosen at compile time via C preprocessor directives.

Result: Energy transfer as a function of initial impact parameter



Result: Energy transfer as a function of initial molecule orientation



CPU vs. GPU performance

- 3840 trajectories simulated with both the CPU and GPU implementations
- Results were identical
- CPU time: 472.53 sec.
- GPU time: 7.575 sec.
- Ratio: 62.4 !!

Future Work

- Complete Monte Carlo Analysis to obtain the rotational relaxation time as a function of translational temperature and perhaps other variables.
- Explore more complex and realistic intermolecular potential energy functions.
- Explore optimizations of both the CPU and GPU implementations of the analysis code.