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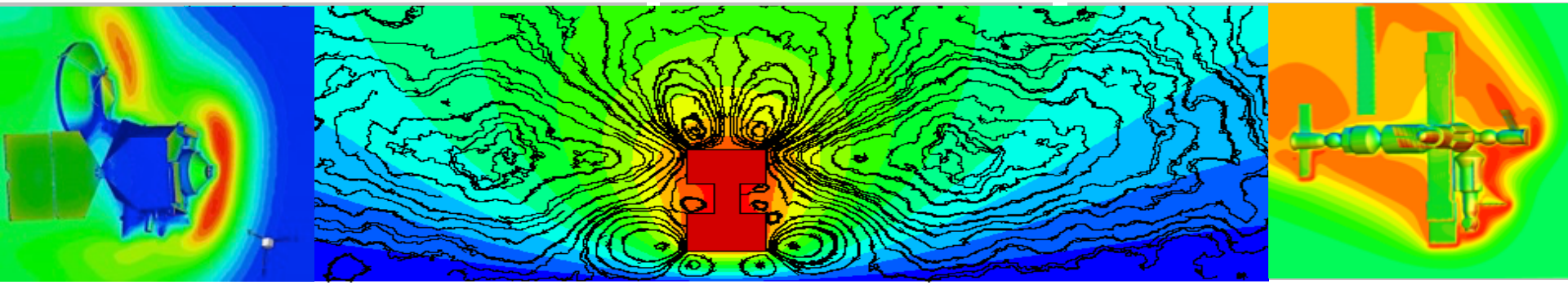

DSMC Simulations of Gas Flows

M. Gallis, T. Koehler, S. Moore, S. Plimpton, A. Stagg, J. Torczynski

Presented by: Michael A. Gallis

Engineering Sciences & Computing Research Centers
Sandia National Laboratories, Albuquerque NM, U.S.A.

U.S. DEPARTMENT OF ENERGY | NNSA

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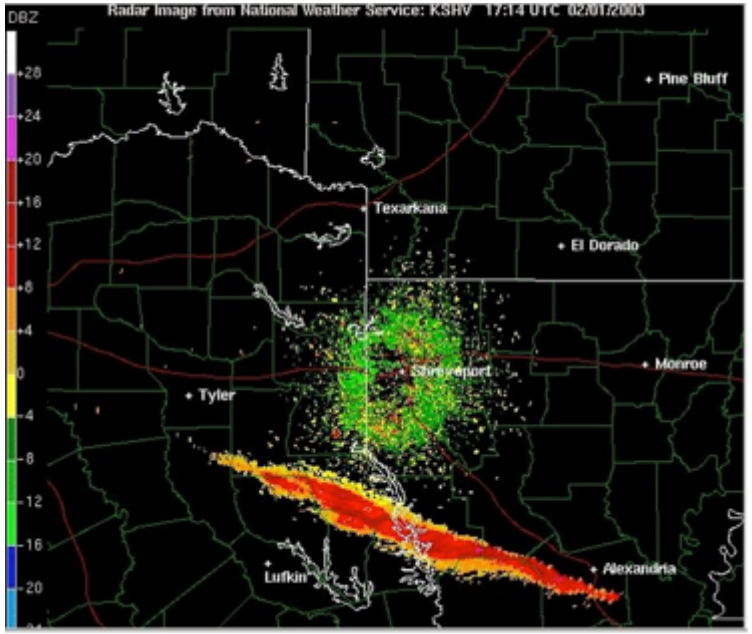
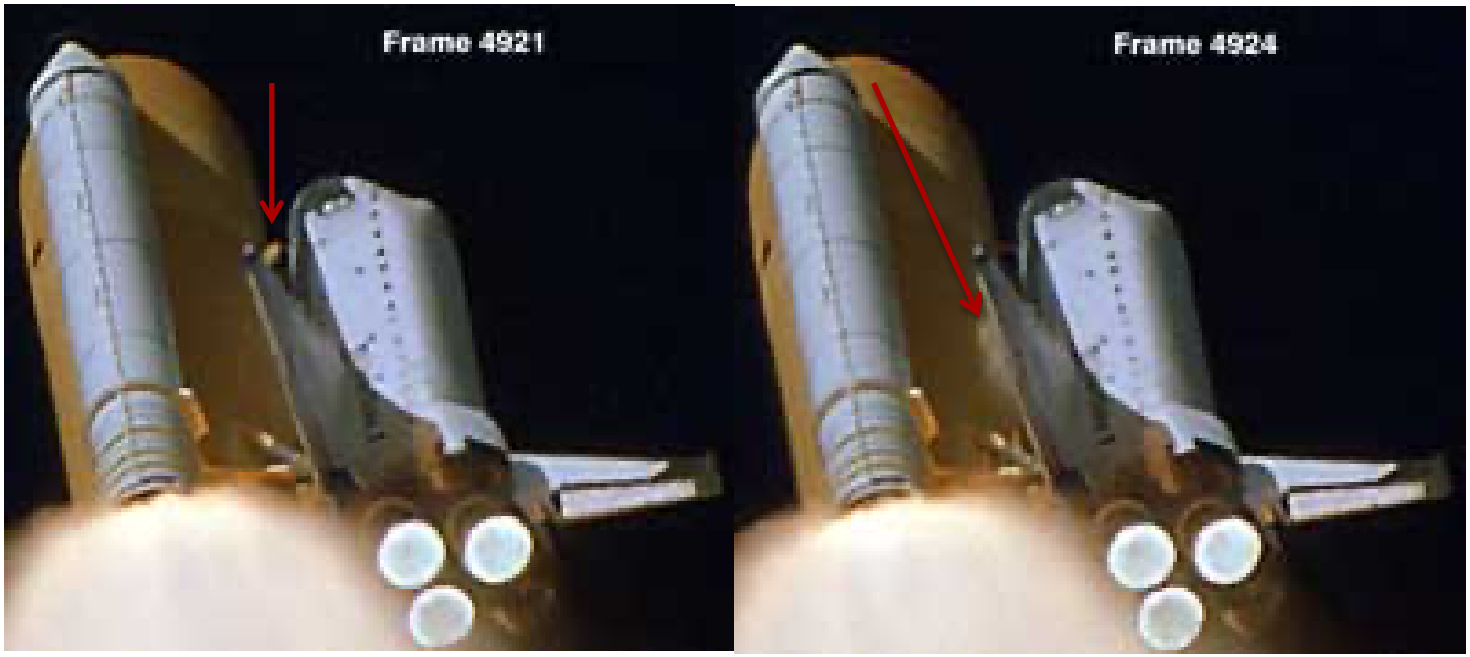
The Columbia Accident

On February 1st 2003 STS-107 with Shuttle orbiter Columbia disintegrated over Texas, minutes before it was scheduled to land.

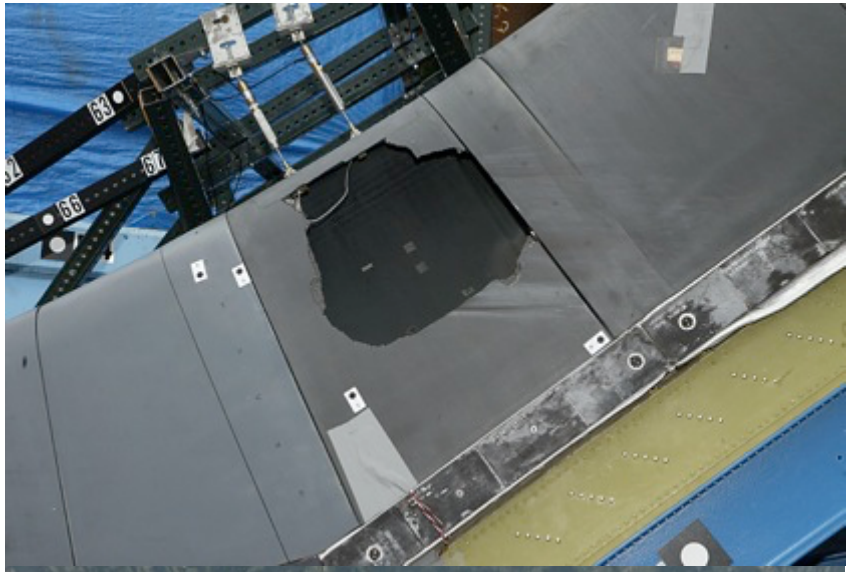


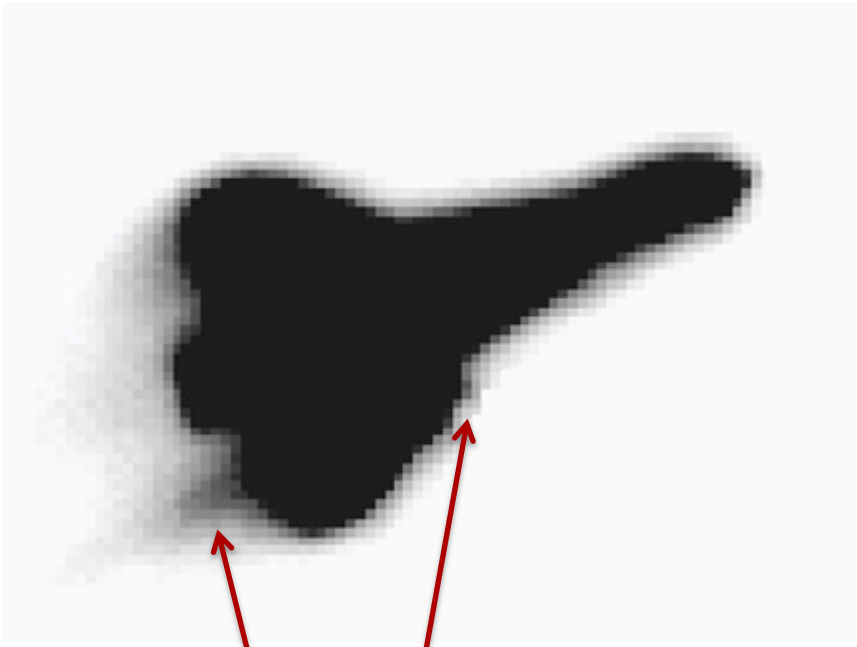
Foam impact during launch



During the ascent phase a piece of foam insulation broke off from the shuttle's propellant tank damaging (?) the shuttle's left wing.

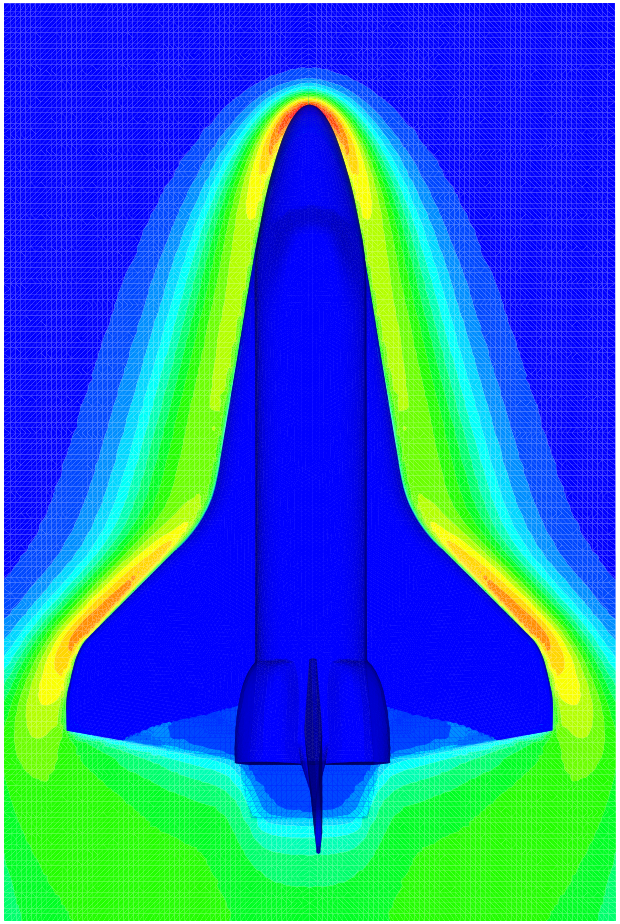
Damage Scenario Investigated

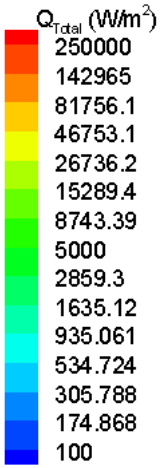


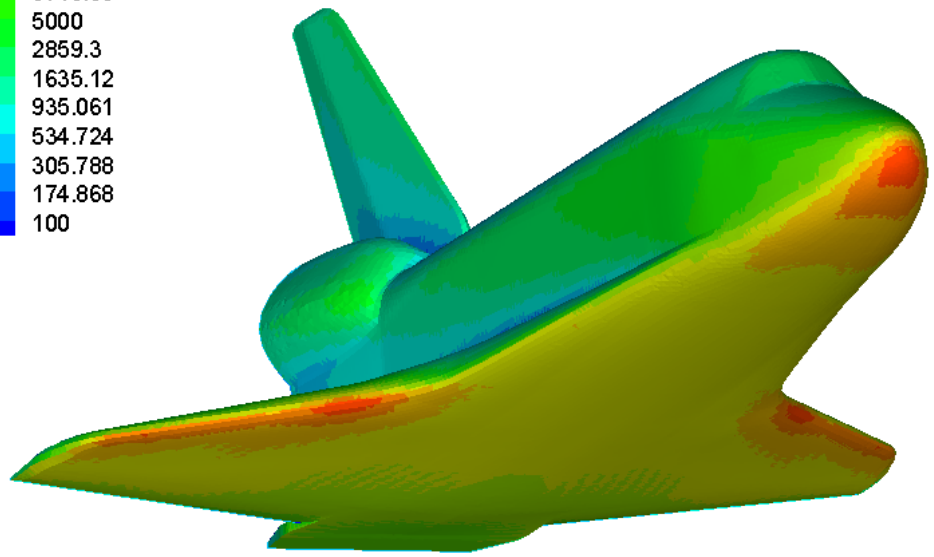


The resulting hole allowed overheated gases to burn through the wing cavity, compromise its structural integrity, leading to a loss of the vehicle during descent

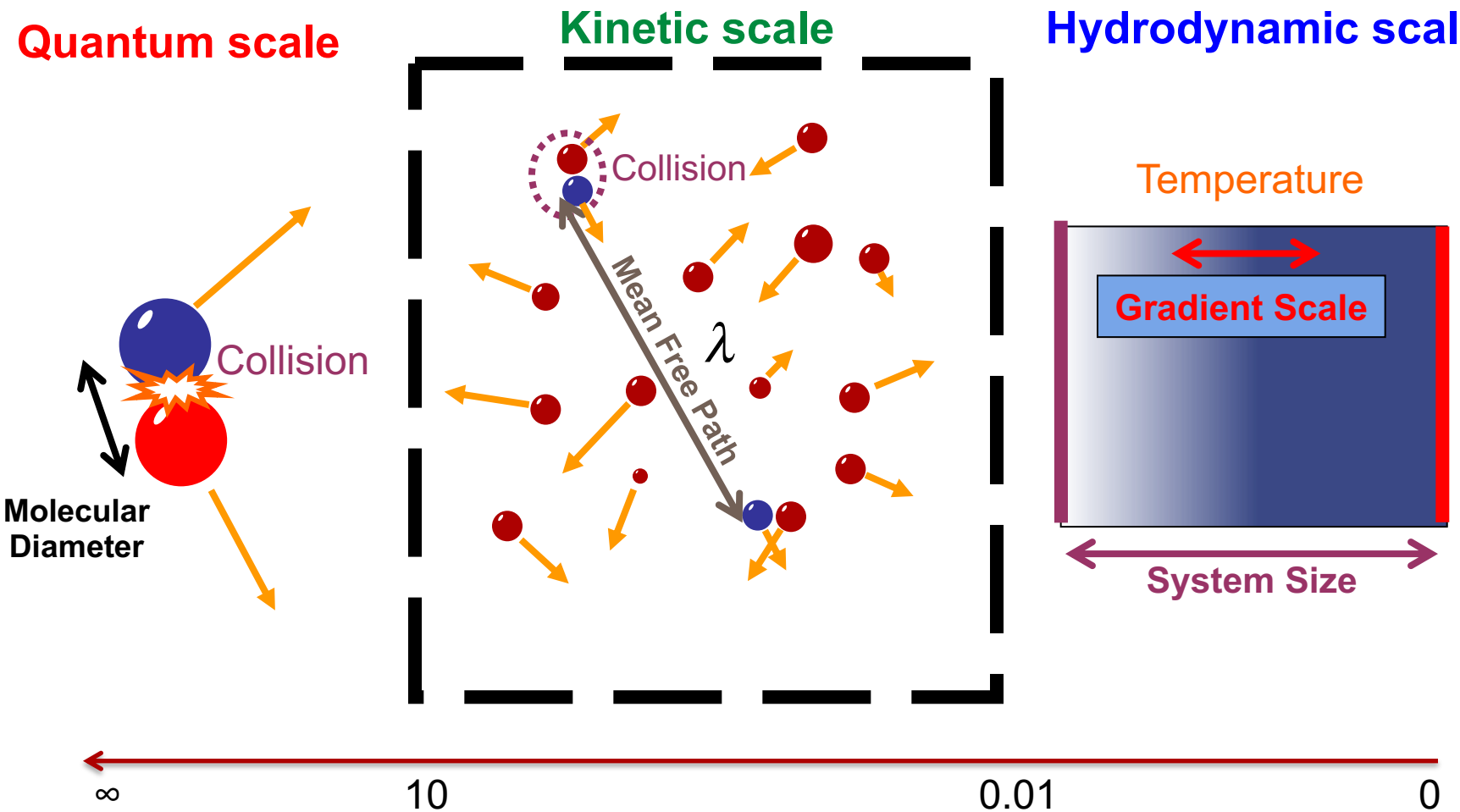
Temperature and Heating Profile







Length Scales for Dilute Gases



$$Kn = \frac{\lambda}{L} = \frac{\lambda}{T}\frac{dT}{dx}$$

Boltzmann Equation and the Direct Simulation Monte Carlo Method (DSMC)

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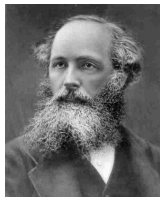
Ludwig Boltzmann

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \frac{\partial f}{\partial \mathbf{x}} + \frac{\mathbf{F}}{m} \cdot \frac{\partial f}{\partial \mathbf{v}} = \int_{-\infty}^{\infty} \int_{0}^{4\pi} \left(f^* f_1^* - f f_1 \right) \left| \mathbf{v} - \mathbf{v}_1 \right| \sigma \, d\Omega \, d\mathbf{v}_1$$

molecular motion and force-induced acceleration

pairwise molecular collisions (molecular chaos)



James Clerk Maxwell

$f(\mathbf{r},\mathbf{c},t)d^3rd^3c \rightarrow$ Expected number of molecules at time t in at $\mathbf{r} + d^3r, \mathbf{c} + d^3c$

$$n(\mathbf{r},t) = \int f(\mathbf{r},\mathbf{c},t)d^3c$$

The velocity distribution function can be replaced by a particle-based distribution function like the Klimontovich distribution function:

$$f(\mathbf{x},\mathbf{v},t) = \sum_{i=0}^{N} \delta^3(\mathbf{x} - \mathbf{x}_i(t))\delta^3(\mathbf{v} - \mathbf{v}_i(t))$$

Substituting into the Boltzmann equation we have 2 N differential equations:

$$d\mathbf{x}_i / dt = \mathbf{v}_i \qquad d(m_i \mathbf{v}_i) / dt = \mathbf{F}(\mathbf{x}_i) + \mathbf{C}(\mathbf{v}_i)$$

molecules move **molecules collide**

Boltzmann Equation and the Direct Simulation Monte Carlo Method (DSMC)

Sandia National Laboratories

Ludwig Boltzmann

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \frac{\partial f}{\partial \mathbf{x}} + \frac{\mathbf{F}}{m} \cdot \frac{\partial f}{\partial \mathbf{v}} = \int_{-\infty}^{\infty} \int_{0}^{4\pi} \left(f^* f_1^* - f f_1 \right) \left| \mathbf{v} - \mathbf{v}_1 \right| \sigma \, d\Omega \, d\mathbf{v}_1$$

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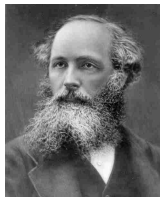

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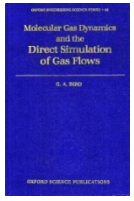
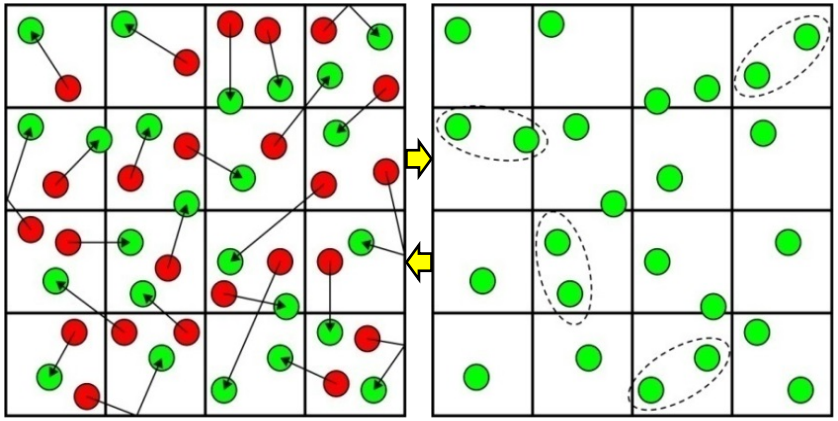


Graeme Bird (1963, 1994)



molecules move **molecules collide**

DSMC is a physical, statistical, molecular-level simulation method

Direct Simulation Monte Carlo

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How DSMC works

DSMC molecule-simulators **statistically** represent a large number of real molecules ($O(10^{10})$-$O(10^{15})$)

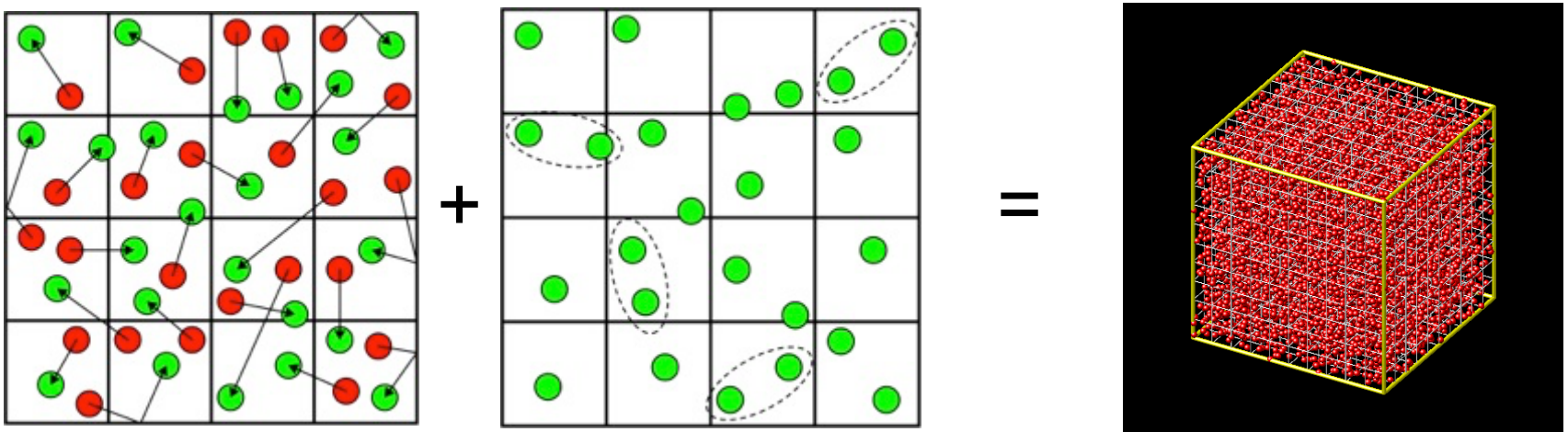
Computational molecules move ballistically, collide statistically, and interact statistically with surfaces **like real molecules**

Molecular movement, surface-interaction, and collision are implemented **sequentially** in the algorithm

Cell-based molecular statistics ("moments") are sampled and averaged over many time steps for steady flow

DSMC is inherently a transient method

Steady state is the ensemble average of unsteady state moves



Stochastic binary collisions

Deterministic ballistic move

DSMC vs. Boltzmann Equation

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- Instead of solving Newton's laws of motion (Molecular Dynamics), DSMC replaces explicit intermolecular forces with stochastic collisions
- It has been shown that DSMC is equivalent to solving the Boltzmann equation (Nambu 1980, Babovsky 1989, Wagner 1992)
- DSMC has been shown to reproduce exact known solutions (Chapman-Enskog, Moment Hierarchy) of the Boltzmann equation (Gallis et al. 2004, 2006) for non-equilibrium flows
- In fact, DSMC is superior to solving the Boltzmann equation
  - DSMC can model complicated processes (e.g., polyatomic molecules, chemically reacting flows, ionized flows) for which Boltzmann-type transport equations are not even known (Struchtrup 2005)
  - DSMC includes fluctuations, which have been shown to be physically realistic (Garcia 1990) but which are absent from the Boltzmann equation

The objective of DSMC is to simulate complicated gas flows using only collision mechanics of simulated molecules in the regime described by the Boltzmann equation

Navier-Stokes vs. Boltzmann Equation

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- The Navier-Stokes equations for gases can be derived from the Boltzmann equation assuming:
  - Near-equilibrium conditions
  - Local Thermodynamic Equilibrium (LTE)
  - Continuum medium
- Conservations equations (mass, momentum, energy) can be derived as averages of molecular properties
- Transport is given by averaging molecular fluxes. Under LTE Newton's, Fourier's and Fick's laws are obtained

George Stokes

Claude Navier

The Need for Molecular-Level Treatment
Non-equilibrium effects

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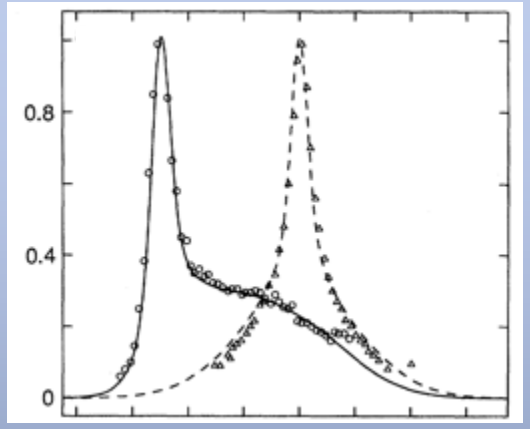
Non-equilibrium effects:

- Non-Maxwell, Chapman-Enskog velocity distribution functions
- Non-linear transport properties
- Non-Boltzmann internal energy, no energy equipartition
- Non-Arrhenius chemical reactions
- Non-continuous temperature and velocity profiles (Knudsen layers close to walls)

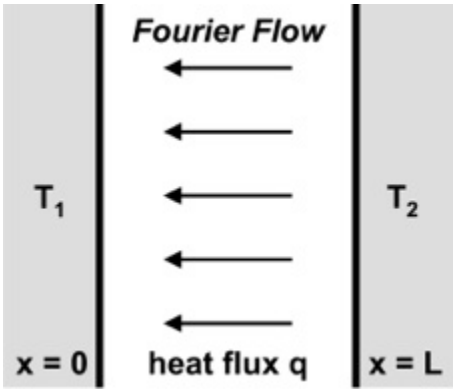


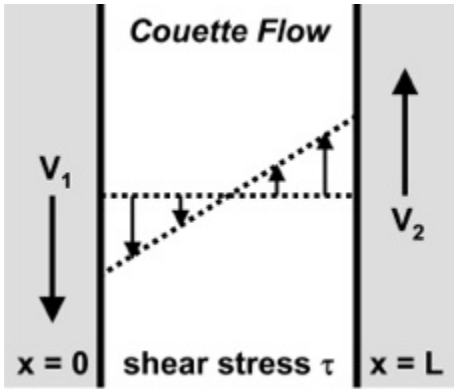
Non-equilibrium velocity distribution functions in the front a Mach 25 normal shock of helium
Pham-Van-Diep, *et al.* , *Science*, 1989

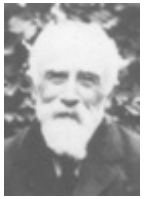
- Can be caused by:
  - Reduced collisionality (low density)
  - Strong gradients even in near-continuum conditions

Quantifying Non-Equilibrium
Fourier and Couette Flow

Joseph Fourier







Maurice Couette

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

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

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)

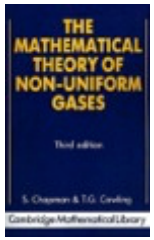
Verify DSMC accuracy at arbitrary heat flux, shear stress

- Thermal conductivity, viscosity; velocity distribution

Near-Equilibrium: Chapman-Enskog (CE) Theory

Sydney Chapman

David Enskog



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

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

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

$$K = -(5/4)k_Bc_m^2a_1 \qquad \mu = (1/2)mc_m^2b_1$$

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

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

- Chapman and Enskog analyzed Boltzmann collision term
  - Perturbation expansion using Sonine polynomials
  - Near equilibrium, appropriate in continuum limit
- Determined velocity distribution and transport properties
  - Thermal conductivity K, viscosity μ, mass self-diffusivity D
  - Prandtl number Pr from "infinite-to-first" ratios K_∞/K_1, μ_∞/μ_1
  - 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

Extracting CE Parameters from DSMC

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

$$\tau = \mu_{eff}\left(\frac{\partial V}{\partial x}\right) \qquad \frac{b_k}{b_1} = \sum_{i=1}^{k}\left(\frac{(-1)^{i-1}(k-1)!(5/2)!}{(k-i)!(i-1)!(i+(3/2))!}\right)\left(\frac{\left\langle \tilde{c}^{2(i-1)}\tilde{c}_x\tilde{c}_y\right\rangle}{\left\langle \tilde{c}_x\tilde{c}_y\right\rangle}\right) \qquad c_m = \sqrt{\frac{2k_BT}{m}}$$

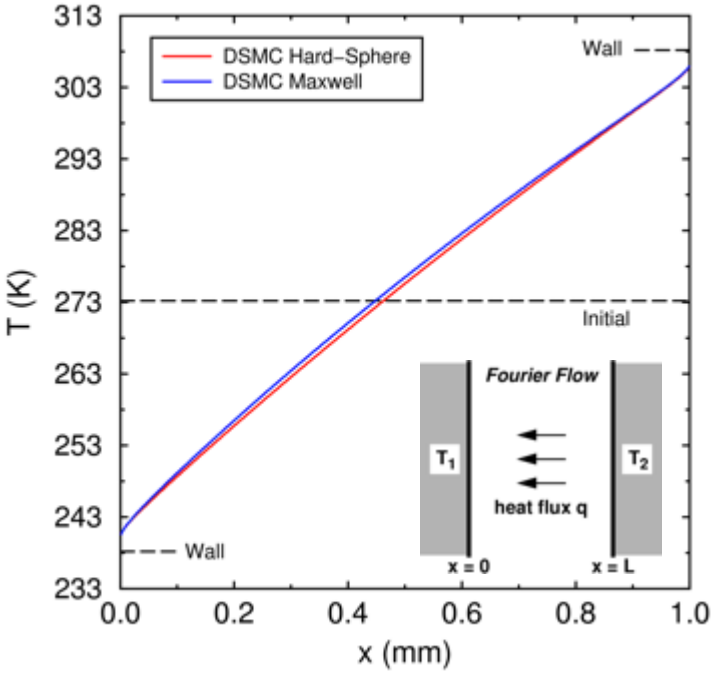
DSMC moments of velocity distribution function

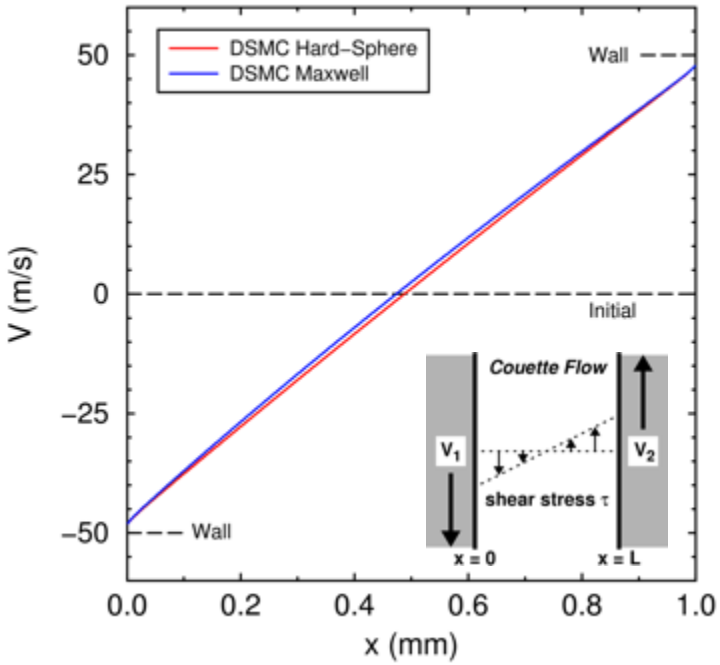
- Temperature T, velocity V
- Heat flux q, shear stress τ
- Higher-order moments

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

- Thermal conductivity and viscosity: K_{eff} and μ_{eff}
- Sonine-polynomial coefficients: a_k/a_1 and b_k/b_1
- Applicable for arbitrary Kn_L, Kn_q, Kn_τ

Temperature and Velocity Profiles



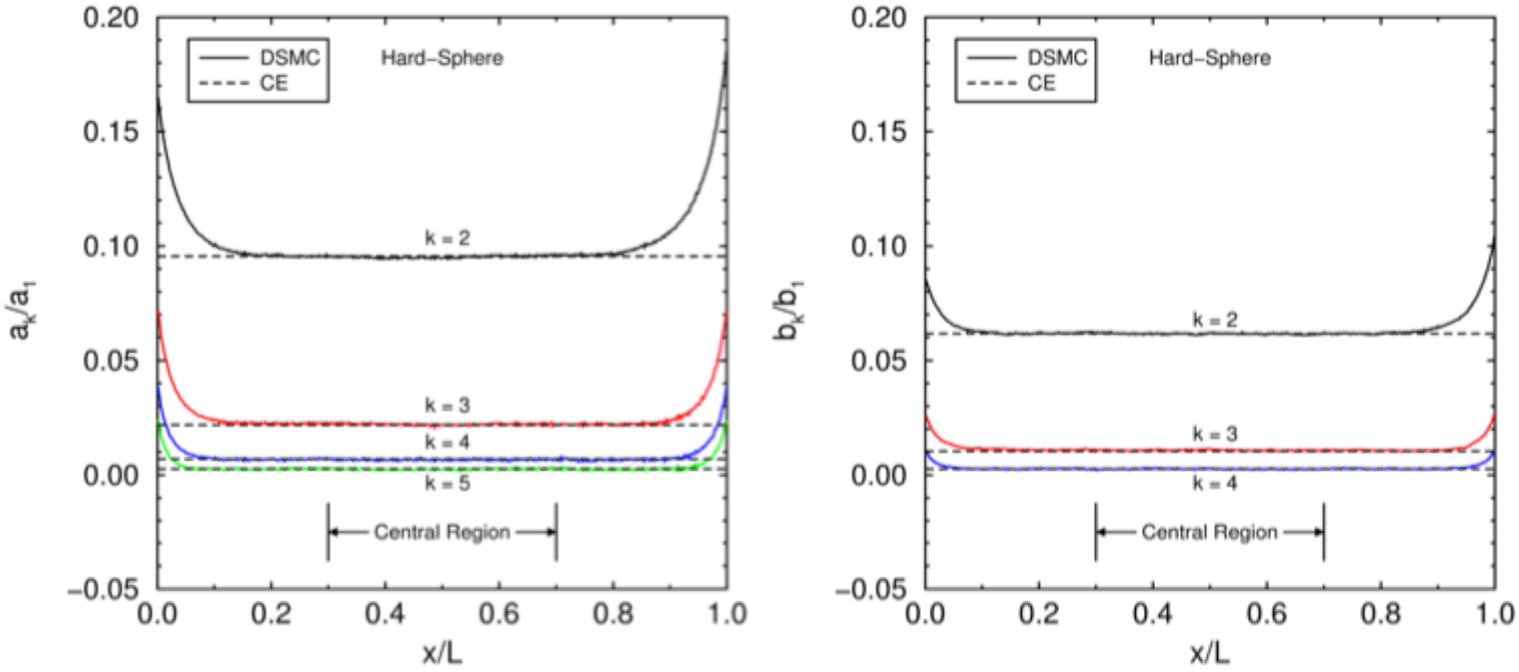


Low heat flux and shear stress: $Kn_q = 0.006$, $Kn_\tau = 0.003$

- Argon-like: initial T = 273.15 K, p = 266.644 Pa, λ = 24 μm
- Walls: L = 1 mm = 42λ, ΔT = 70 K, ΔV = 100 m/s
- $N_c = 120$, Δt = 7 ns, Δx = 2.5 μm, ~10^9 samples/cell, 32 runs

Small velocity slips, temperature jumps, Knudsen layers

DSMC Reproduces Infinite-Approximation Chapman-Enskog Velocity Distribution

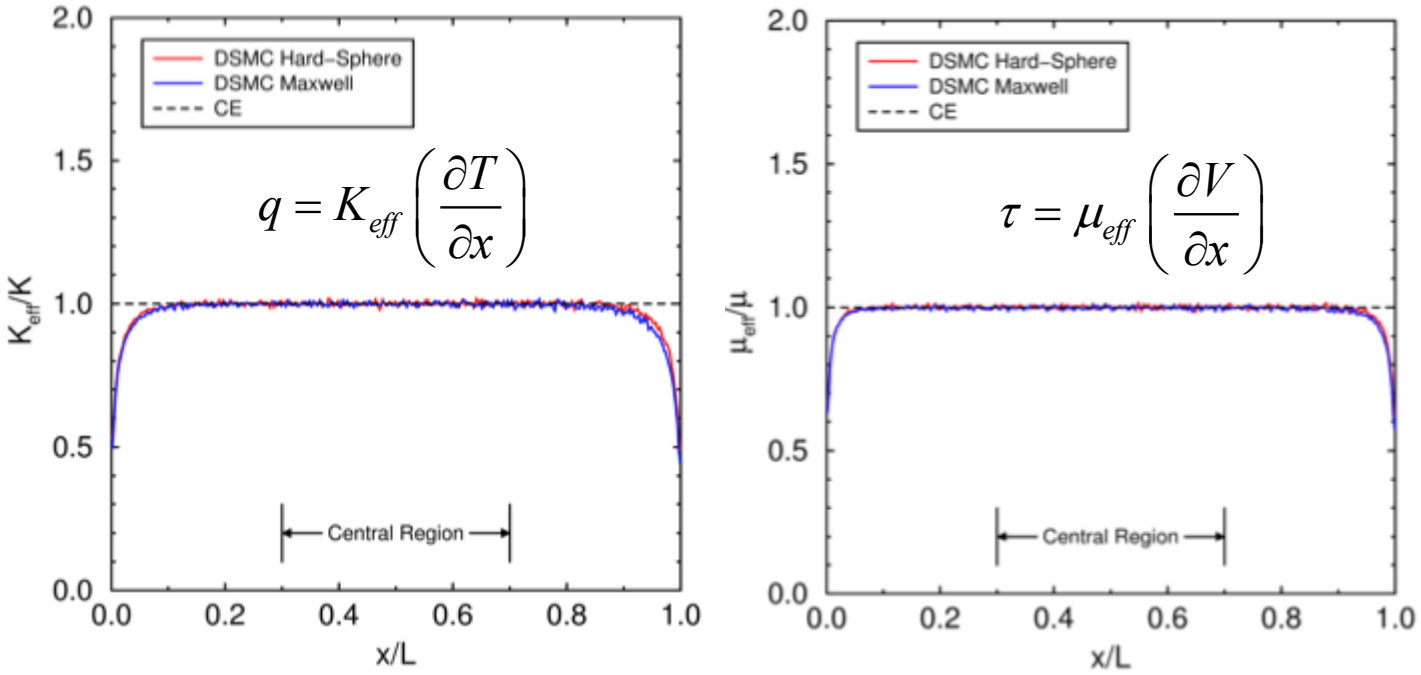


Sonine polynomial coefficients for temperature (left) & velocity (right) gradients

- Hard-sphere values are shown, other interactions have similar agreement
- Higher-order (k > 5) coefficients (not shown) also have similar agreement

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.

DSMC Reproduces Infinite-Approximation Chapman-Enskog Transport Coefficients



Thermal conductivity (left) and viscosity (right) away from walls

- Maxwell and hard-sphere results bound most gases
- Agreement with Chapman-Enskog theory verifies DSMC

Moment-Hierarchy Method

$$M_{k_1k_2k_3} = \int \tilde{c}_x^{k_1}\tilde{c}_y^{k_2}\tilde{c}_z^{k_3}\tilde{f}[\tilde{\mathbf{c}}]d\tilde{\mathbf{c}} = \left\langle \tilde{c}_x^{k_1}\tilde{c}_y^{k_2}\tilde{c}_z^{k_3}\right\rangle$$

$$J_{k_1k_2k_3} = \int \tilde{c}_x^{k_1}\tilde{c}_y^{k_2}\tilde{c}_z^{k_3}J[\tilde{\mathbf{c}}\,|\,\tilde{f},\tilde{f}]d\tilde{\mathbf{c}}$$

$$J_{k_1k_2k_3} = \text{Bilinear}\left[\left\{M_{k_1k_2k_3}\right\}\right]$$

$$M_{k_1k_2k_3}[\text{Kn}_q,\text{Kn}_\tau] = \sum_{j=0}^{k_1+k_2+k_3-2} \mu_{k_1k_2k_3}^{(j)}[\text{Kn}_\tau]\text{Kn}_q^j$$

$$K_{\text{eff}}/K = F_K[\text{Kn}_\tau] = 1 - c_K\text{Kn}_\tau^2 + \text{O}[\text{Kn}_\tau^4]$$

$$\mu_{\text{eff}}/\mu = F_\mu[\text{Kn}_\tau] = 1 - c_\mu\text{Kn}_\tau^2 + \text{O}[\text{Kn}_\tau^4]$$

$$a_k/a_1 = (-1)^{k-1}\sum_{j=1}^{k-1} A_{kj}\text{Kn}_q^{2j}$$

$$b_k/b_1 = (-1)^{k-1}\sum_{j=1}^{k-1} B_{kj}\text{Kn}_q^{2j}$$

Moment-Hierarchy (MH) normal solution

- Solve Boltzmann eqn. recursively for Maxwell molecules
- MH solution extends CE solution to finite Kn_q and Kn_τ
- Collision-term moments bilinear in distribution moments

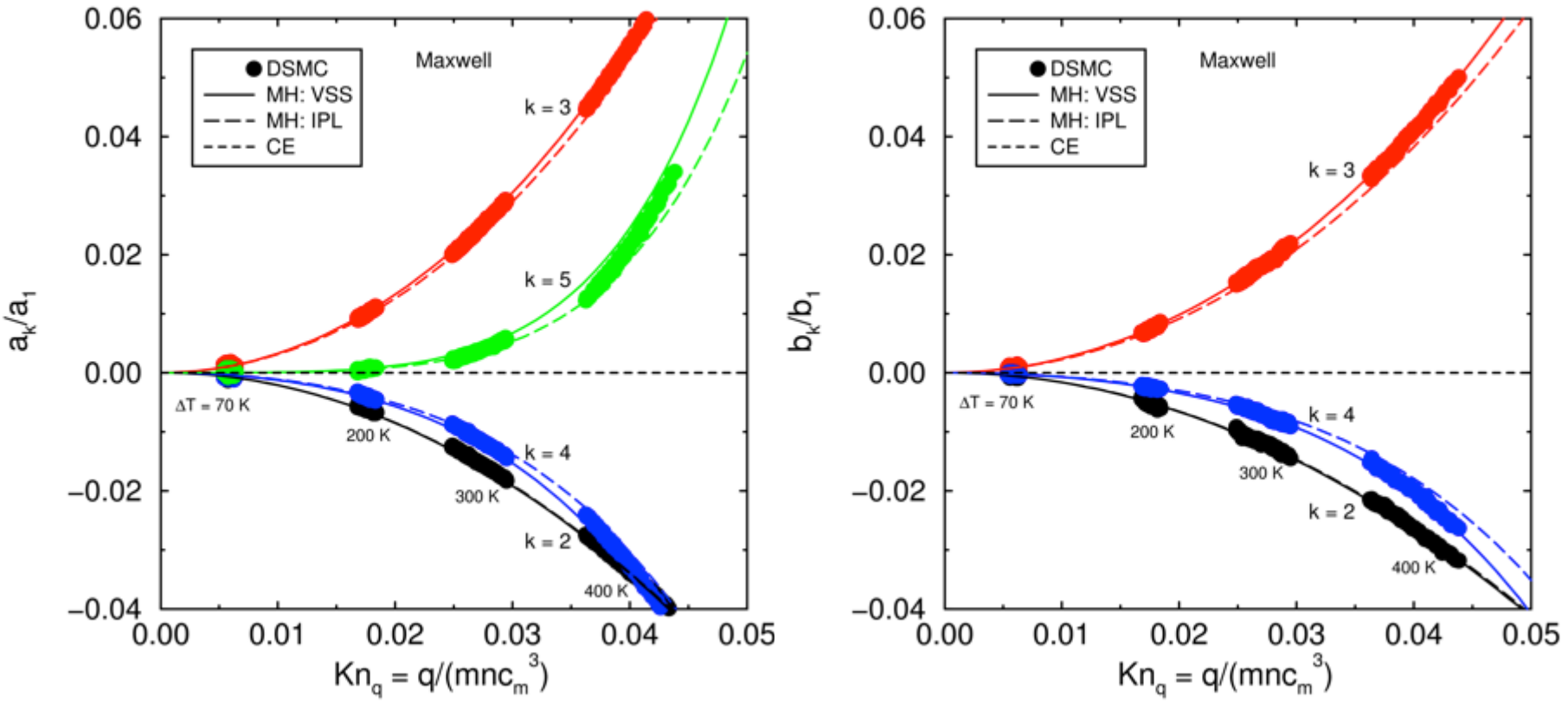
Andres Santos

Compare MH and DSMC for Maxwell molecules

- Dependence of K, μ, a_k/a_1, b_k/b_1 on Kn_q and Kn_τ

Gallis M. A., Torczynski J. R., Rader D. J., Tij M., Santos A., "Normal Solutions of the Boltzmann Equation for Highly Nonequilibrium Fourier and Couette Flow", *Phys. Fluids, 18, 017104,* 2006.

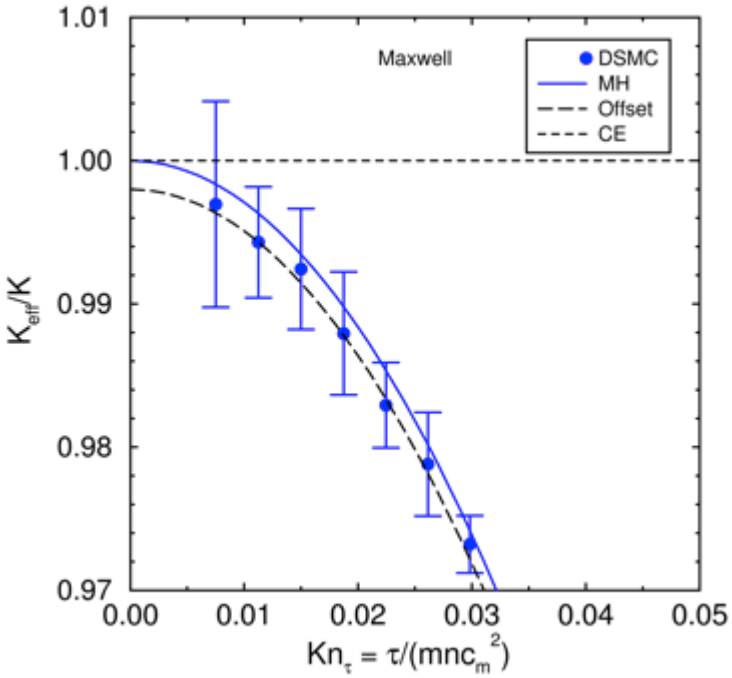
Maxwell Normalized Sonine Coefficients

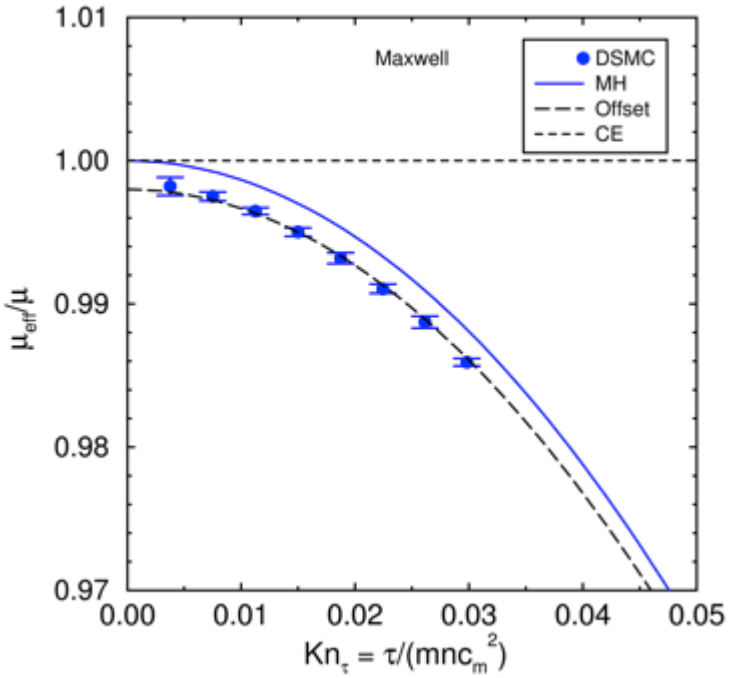


DSMC and MH Maxwell normal solutions for a_k/a_1 and b_k/b_1

- Four DSMC simulations: ΔT = 70, 200, 300, 400 K
- MH: VSS-Maxwell (solid) and IPL-Maxwell (dashed) differ
- DSMC and MH VSS-Maxwell normal solutions agree

Maxwell Normal Transport Coefficients





DSMC and MH Maxwell normal solutions for K and μ

- Finite Kn_τ (shear stress), low Kn_q (heat flux)
- Eight DSMC simulations: ΔV = 100, …, 800 m/s
- Thermal conductivity from viscous heating, larger errors
- Offset MH by DSMC discretization error

Agree to within DSMC discretization error

DSMC Numerical Error

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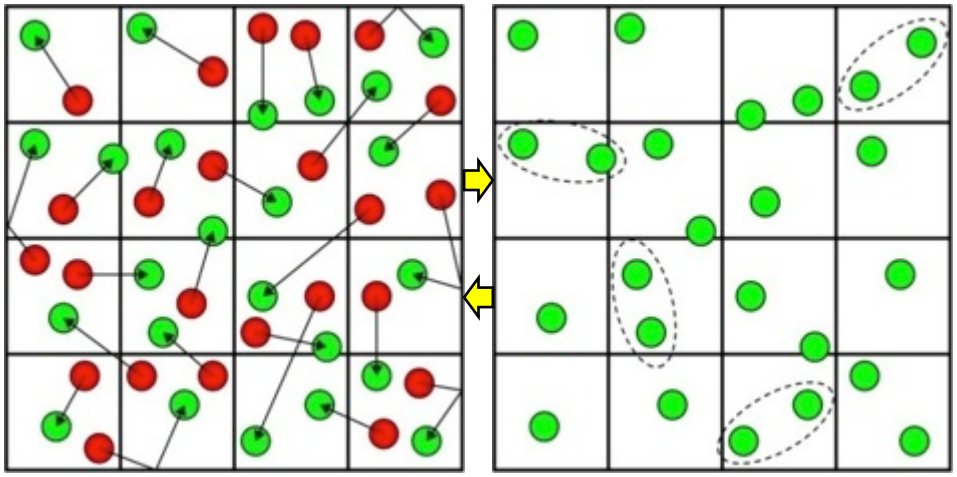
Traditional DSMC rule-of-thumb guidelines:

- Take enough samples to drive statistical error down to "acceptable" level
- Keep time step smaller than ~1/4 mean collision time
- Keep cell size smaller than ~1/3 mean free path
- Use a minimum of ~20 particles per cell

These guidelines give 2% error, which is similar to the uncertainty in measured transport properties for most gases

- DSMC is subject to the same constraints as other numerical methods.
- DSMC is correct to the limit of vanishing discretization.

DSMC Numerical Error



molecules move molecules collide

Four parameters control DSMC error:

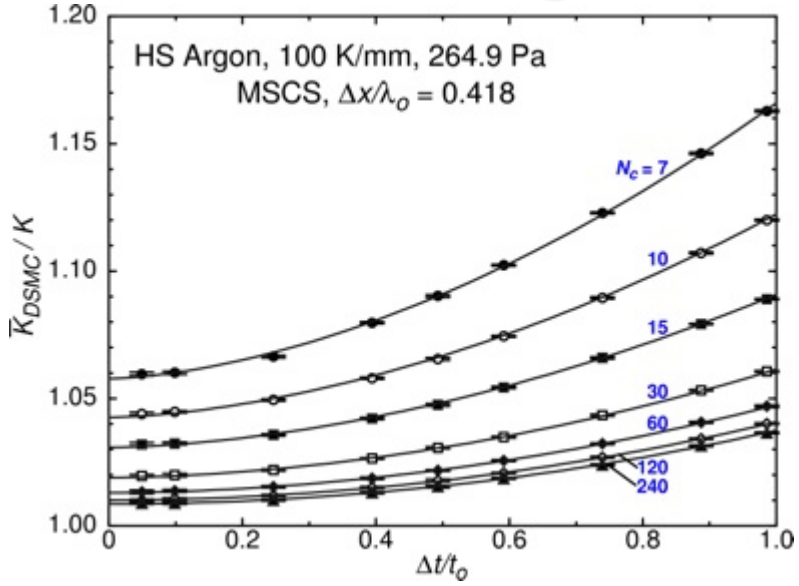
Statistical error (1)

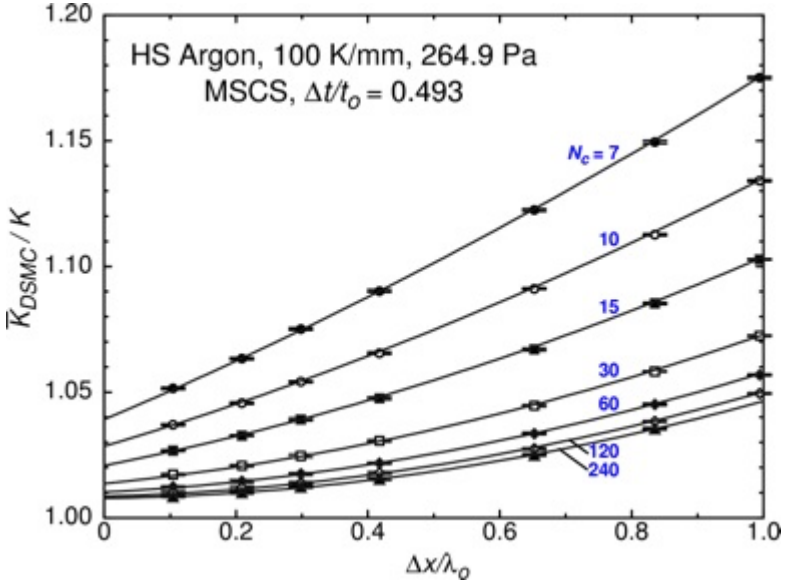
Samples per cell (S_c)

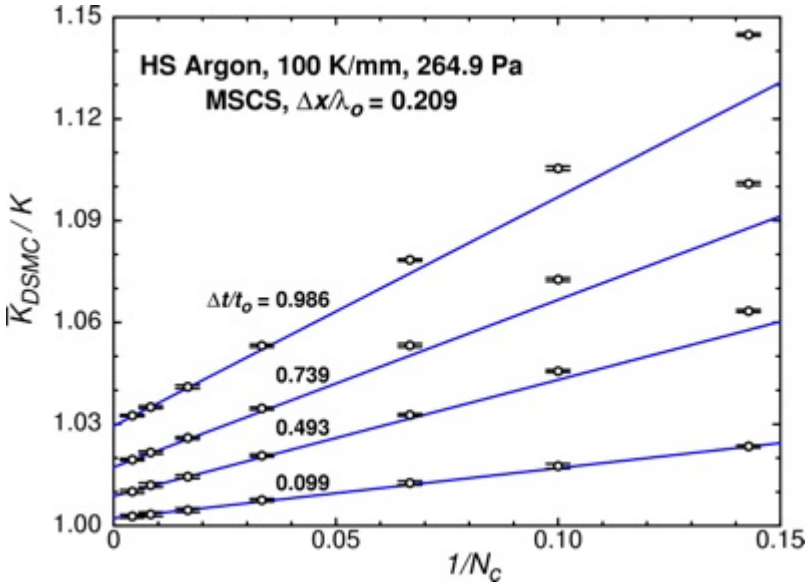
Discretization error (3)

- Particles per cell (N_c)
- Cell size (Δx)
- Time step (Δt)

DSMC Convergence







- Curves are best fits
- Error bars represent 95% confidence intervals
- Quadratic convergence for Δx, Δt
- First-order convergence $O(1/N_c)$, as $N_c \to \infty$
- Higher-order for long time steps

Functional Form of Error

Functional form that represents DSMC data

- *Ad hoc* series expansion in Δx, Δt, and $1/N_c$
- Perform least-squares fitting of entire data set

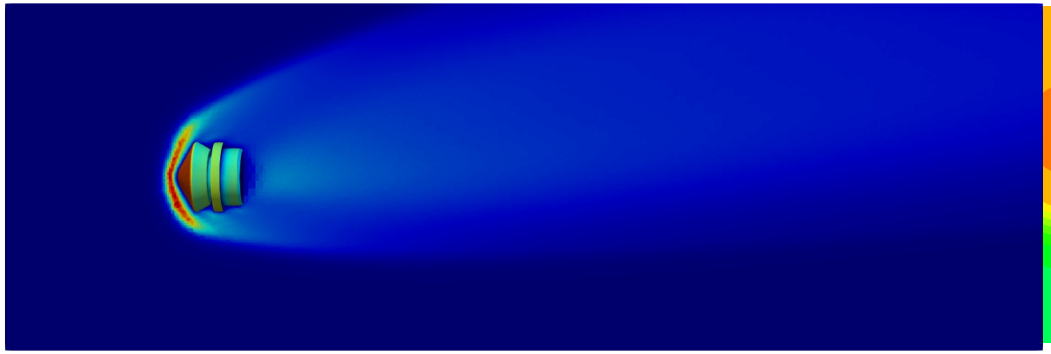
$$\frac{K_{DSMC}}{K} = 1.0000 + 0.0286\Delta\tilde{t}^2 + 0.0411\Delta\tilde{x}^2 - 0.0016\Delta\tilde{x}^3 - 0.023\Delta\tilde{t}^2\Delta\tilde{x}^2 +$$
$$-\frac{0.111}{N_c} + \frac{1}{N_c}\left[1.22\Delta\tilde{x} - 0.26\Delta\tilde{x}^2 + 0.97\Delta\tilde{t}^{3/2} + \ldots\right] + 0.95\frac{\Delta\tilde{t}^2}{N_c^2} + \ldots$$

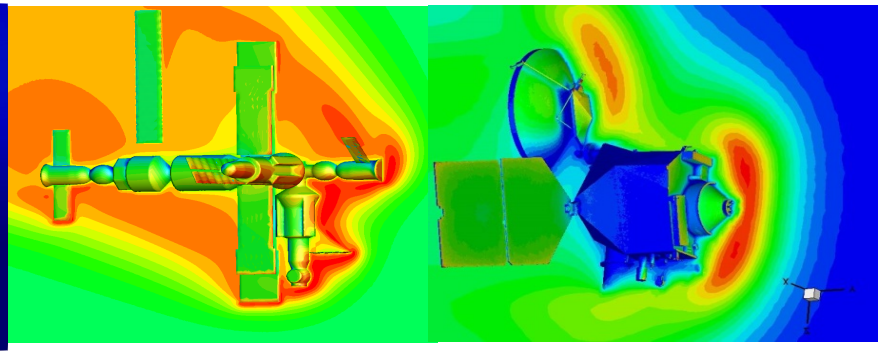
Cross terms show convergence behavior is complex

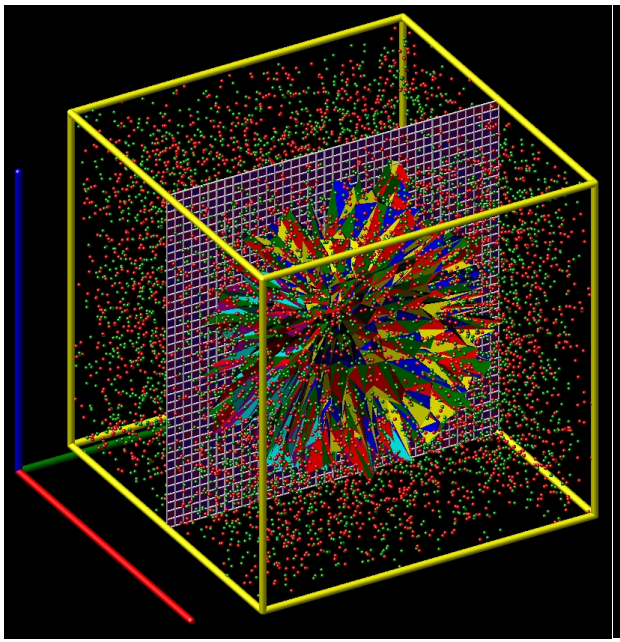
Rader D. J., Gallis M. A., Torczynski J. R., Wagner W., "DSMC Convergence Behavior of the Hard-Sphere-Gas Thermal Conductivity for Fourier Heat Flow", *Phys. Fluids*, 18, 077102, 2006.

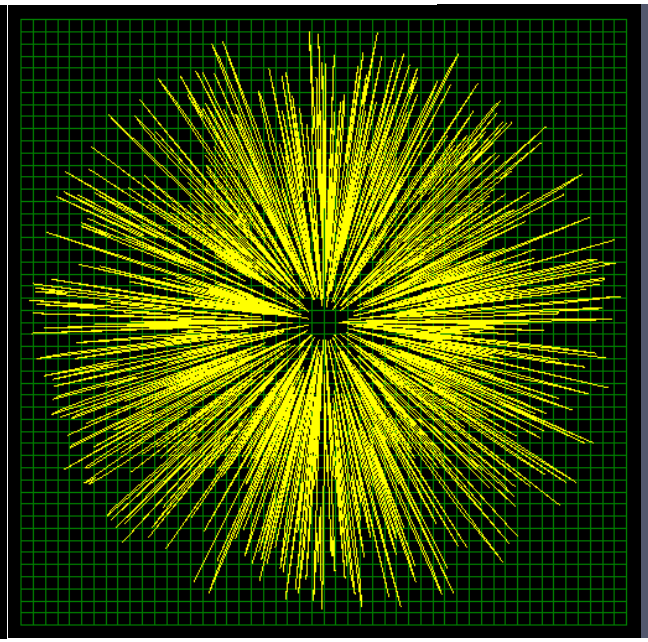
Sandia DSMC code SPARTA

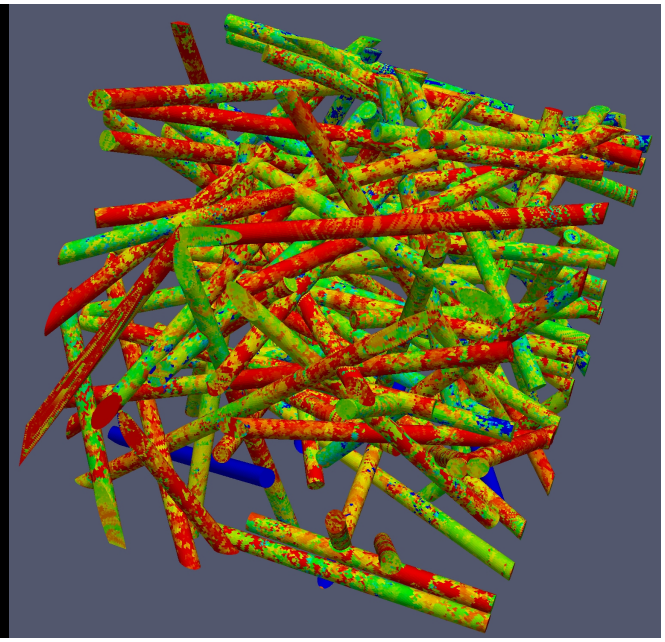
Sandia National Laboratories











Developing an Exascale DSMC Code

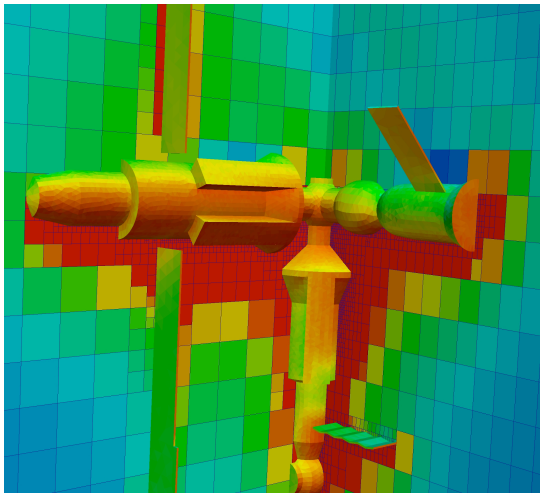
Sandia National Laboratories

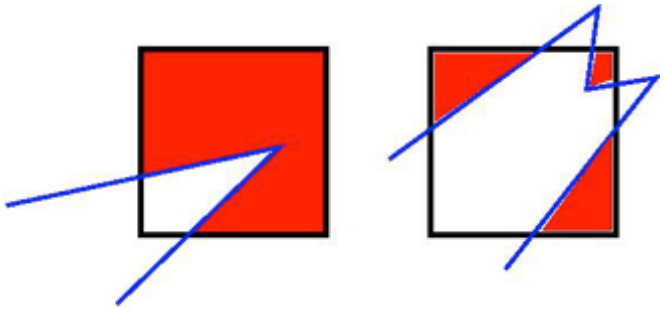
SPARTA = Stochastic PArallel Rarefied-gas Time-accurate Analyzer

General features

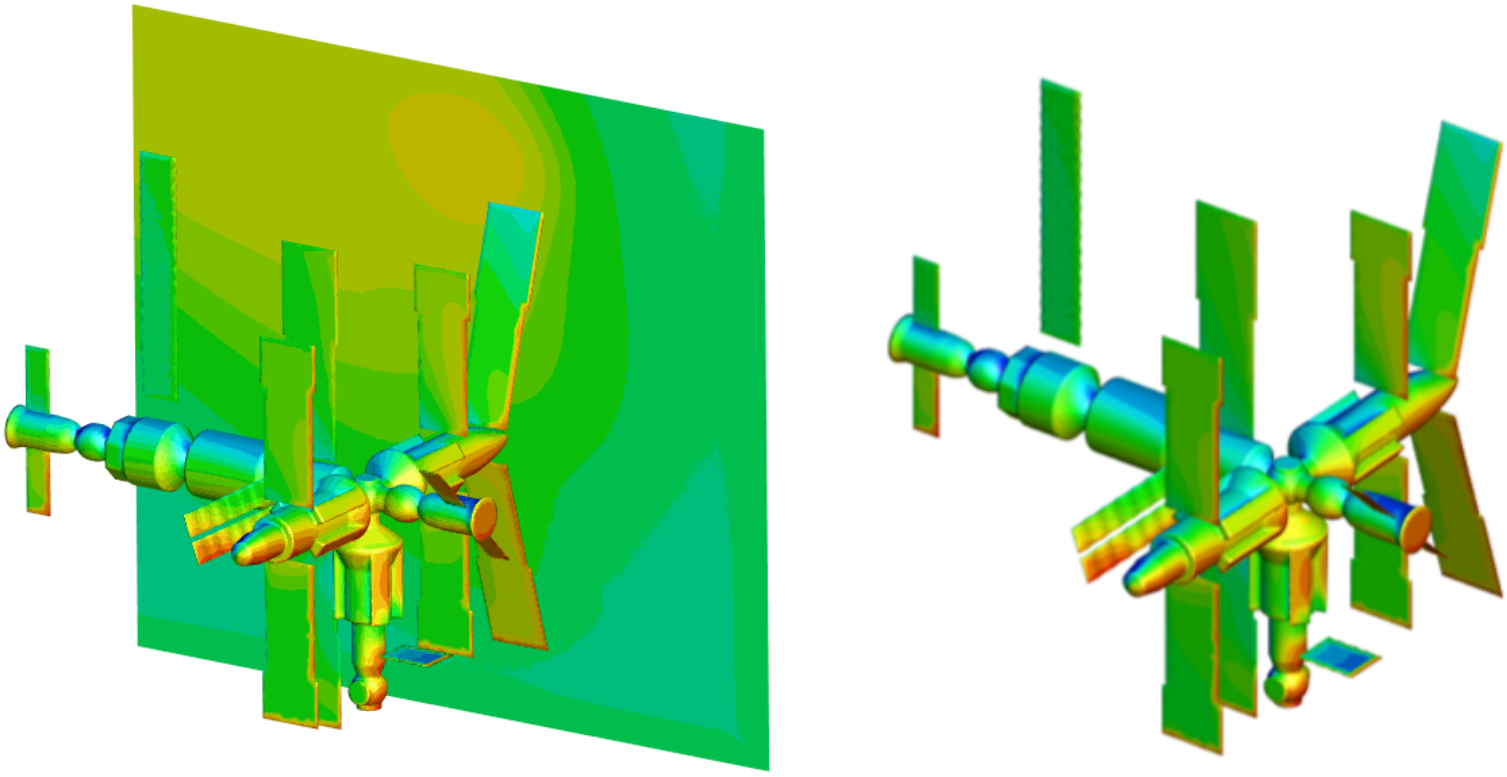
- 2D or 3D, serial or parallel
- Cartesian, hierarchical grid
  - Oct-tree (up to 16 levels in 64-bit cell ID)
  - Multilevel, general NxMxL instead of 2x2x2
- Triangulated surfaces cut/split the grid cells
  - 3D via Schwartzentruber algorithm
  - 2D via Weiler/Atherton algorithm
  - Formulated so can use as kernel in 3D algorithm
- C++, but really object-oriented C
  - Designed to be easy to extend
  - New collision/chemistry models, boundary conditions, etc.

  - Code available at http://sparta.sandia.gov





Simulation of Complicated Shapes



Mir Space Station

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

SPARTA simulation: reacting gas flow through TPS material

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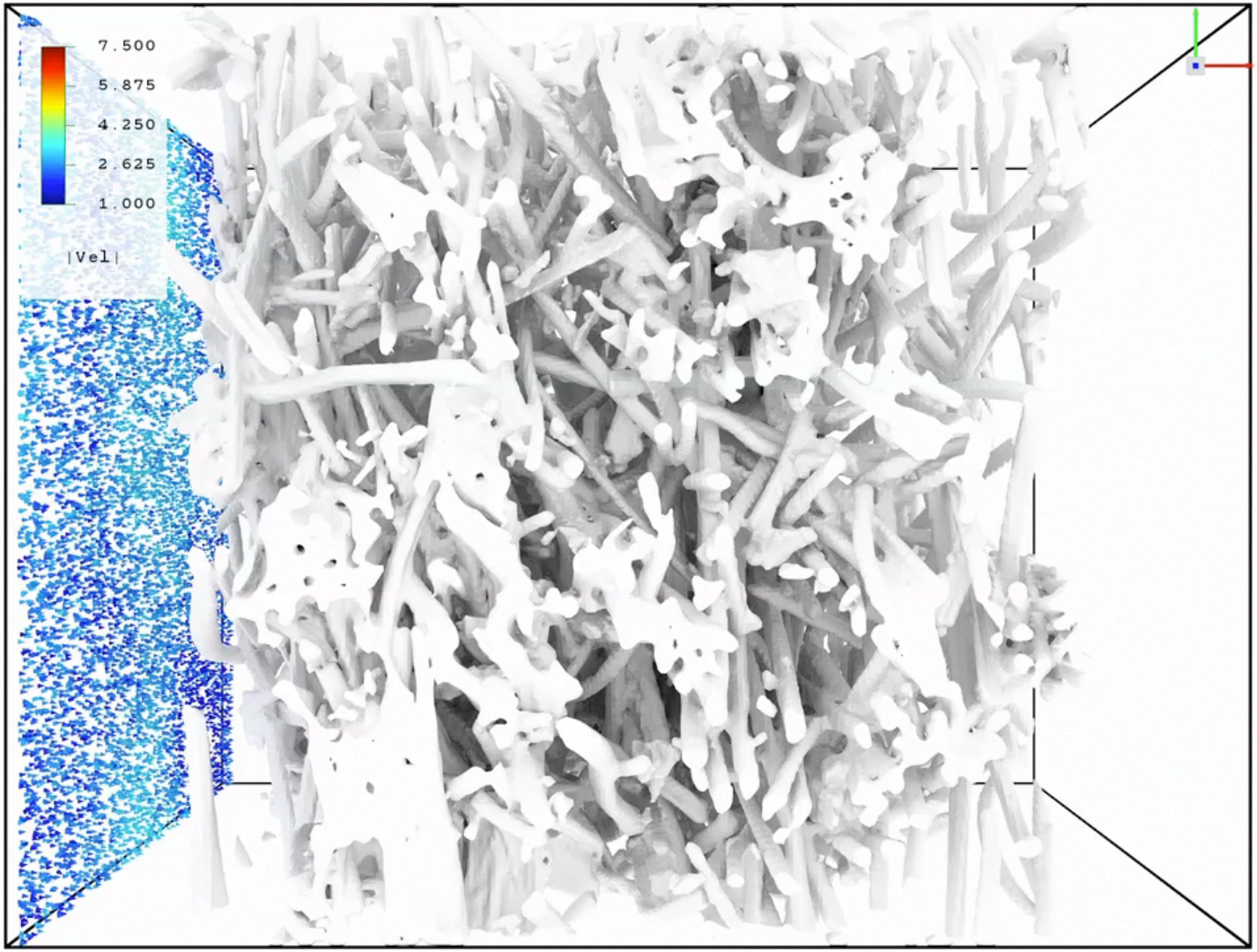
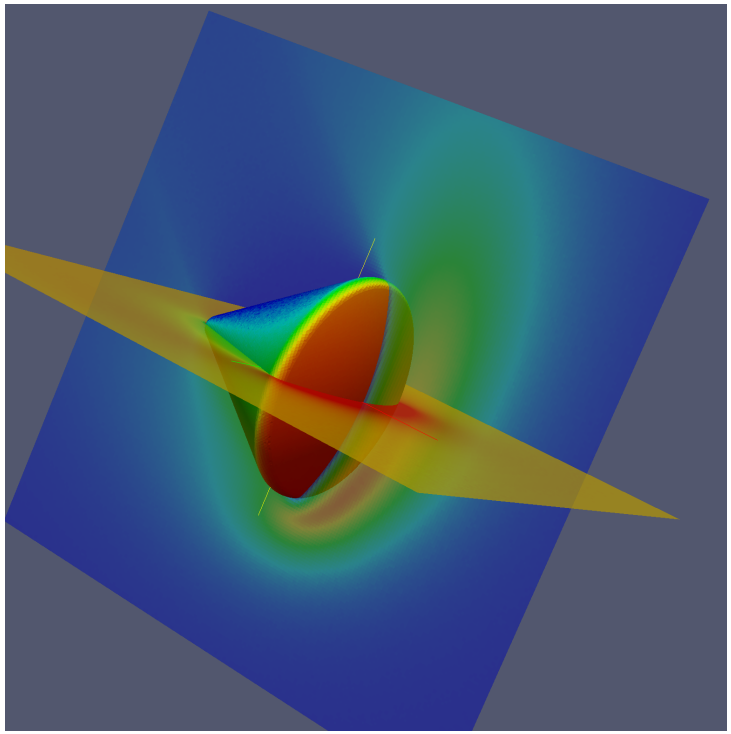


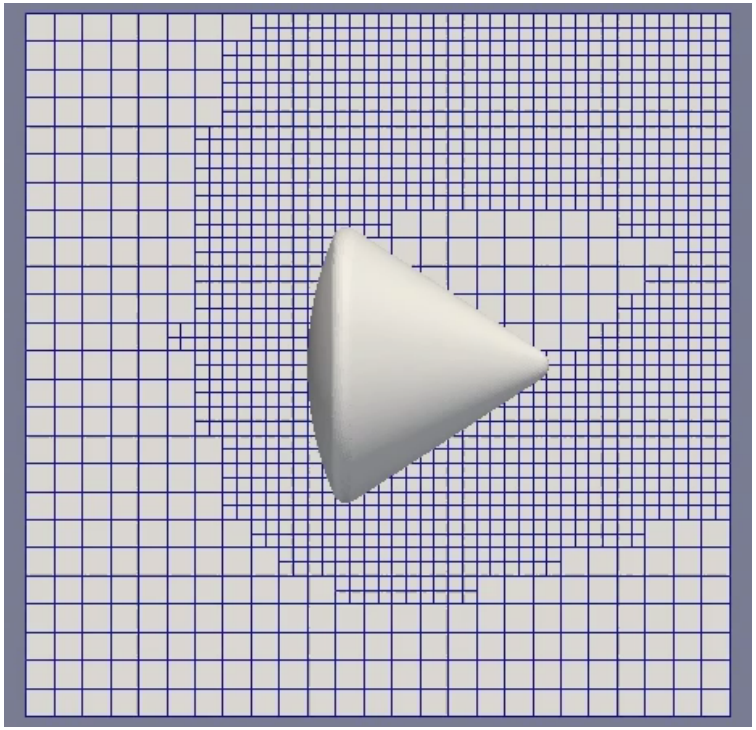
Adaptive Gridding

Sandia National Laboratories

Adaptive adaptation allows more efficient calculations

- Time: 6 levels of adaptation vs uniform grid: 4.33x speedup
- Memory:
  - 6 levels of adaptation runs on 1 64 GB 16 core Linux
  - uniform grid required a 1TB 120 code Linux





Example of multiple-level grid generation in 3D

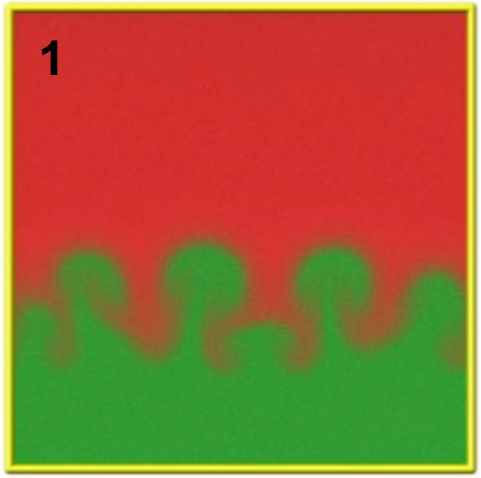
In-Situ Visualization in DSMC-SPARTA

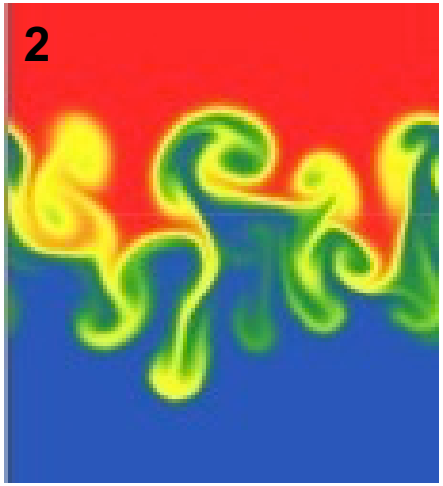
Sandia National Laboratories

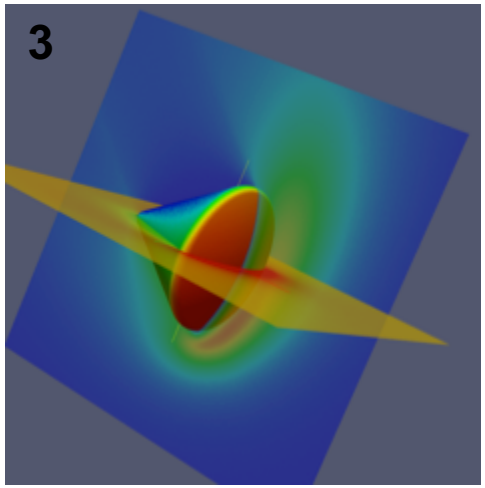
Options

1. Use built-in jpeg libraries to color molecules in cells
2. Use built-in jpeg libraries to color cell according to some variable (e.g. density)
3. Link with Paraview *in-situ* (Catalyst) to provide high quality engineering analysis software.

Quantitative data can be obtained from these plots in some cases (mixing problems) using image processing software.







Aiming for MPI+X via Kokkos

Sandia National Laboratories

- What is Kokkos:
  - Programming model in development at Sandia
  - C++ template library
  - Open-source
  - Stand-alone
- Goal: write application kernels only once, and run them efficiently on a wide variety of hardware platforms
- Two major components:
  - Data access abstraction via Kokkos arrays optimal layout & access pattern for each device: GPU, Xeon Phi, etc.
  - Parallel dispatch of small chunks of work auto-mapped onto back-end languages: CUDA, OpenMP, etc.

Efficient Communication & Load Balancing

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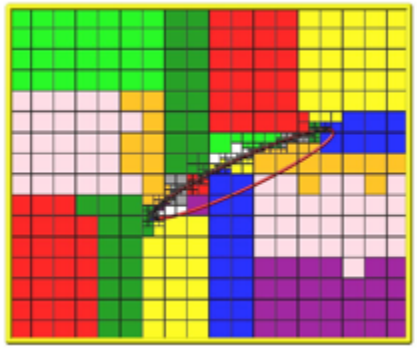
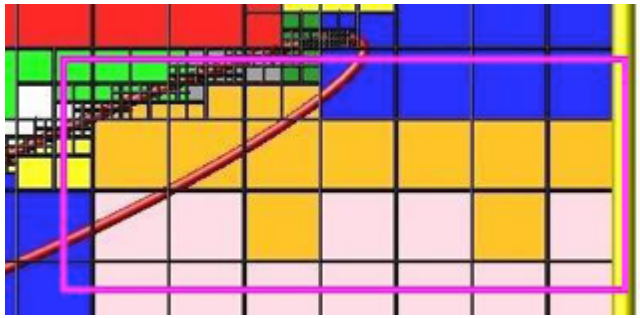
To achieve maximum efficiency:

- One communication per step
  - Multiple passes if needed (or can bound molecule move)
- Communication with modest count of neighbor processors

- One processor = compact clump of cells via load balancing
  - Ghost region = nearby cells within user-defined cutoff
  - Store surface information for ghost cells to complete move





Example:
1B cells on1024 BG/Q node
Worst case: move all cells
Balance time = 15 s:
(RCB=2, move=12, ghosts=1)

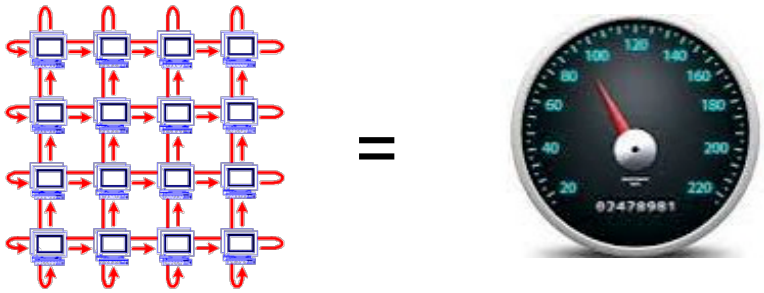
- Balance across processors, static or dynamic
- Geometric method: recursive coordinate bisection (RCB)
- Weighted by cell count or molecules or CPU

Parallel Efficiency: The Competitive Advantage

- The advantages of DSMC come at a cost
- DSMC is computationally efficient but computationally intense
- Its successful application to real problems depends heavily on its parallel performance

- 1000x speedup required for some problems of interest
- Monte Carlo methods usually have good parallel performance
  - The workload depends mainly on the molecules within a cell
  - Relatively less need to communicate information between cells
  - Trivial to parallelize in velocity space

The necessary speedup can be achieved without any loss of accuracy or convergence characteristics through parallel computing



SPARTA Benchmarking

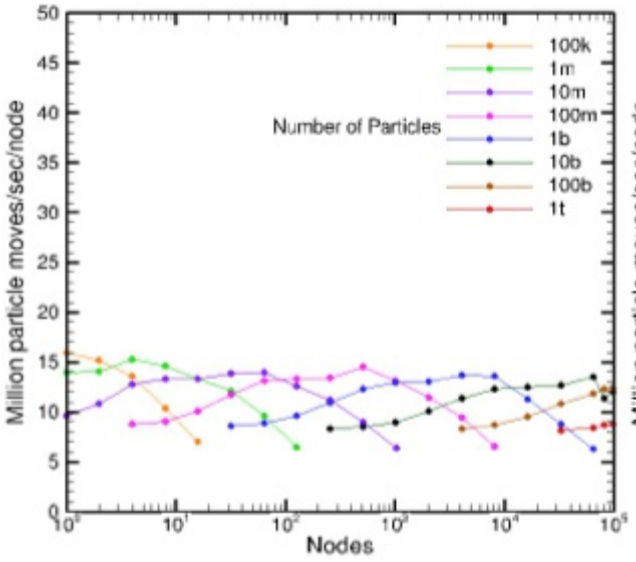
Sandia National Laboratories

- Flow in a closed box
  - Stress test for communication
    - No preferred communication direction
  - 3D regular grid, 10^4-10^{11} (0.1 trillion) grid cells
  - 10 molecules/cell, 10^5-10^{12} (1 trillion) molecules
- Effect of threading
  - 2 threads/core = 1.5 speed
  - 4 threads/core = 2x speed

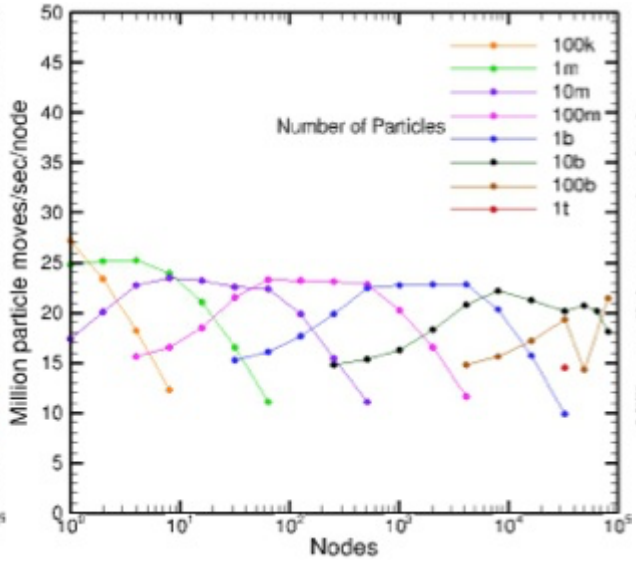
SPARTA Benchmarking

Sandia National Laboratories

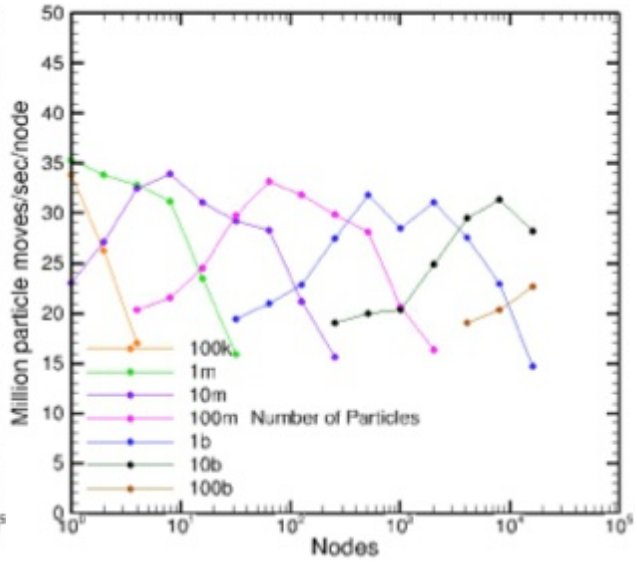
16 cores/node
1 task/core



16 cores/node
2 tasks/core

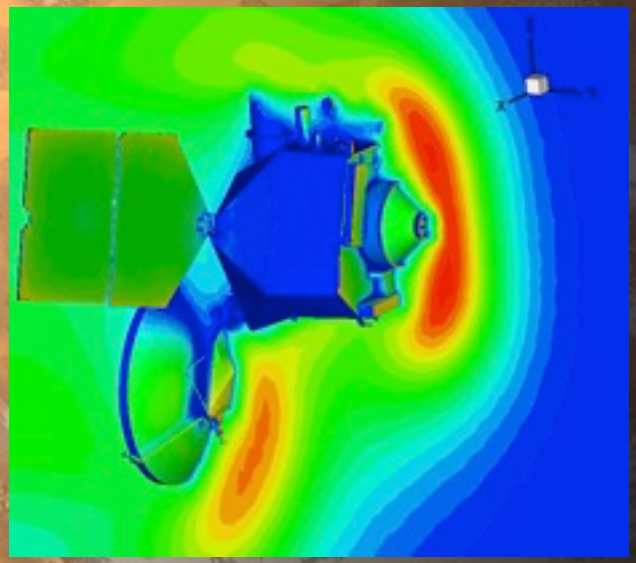


16 cores/node
4 tasks/core

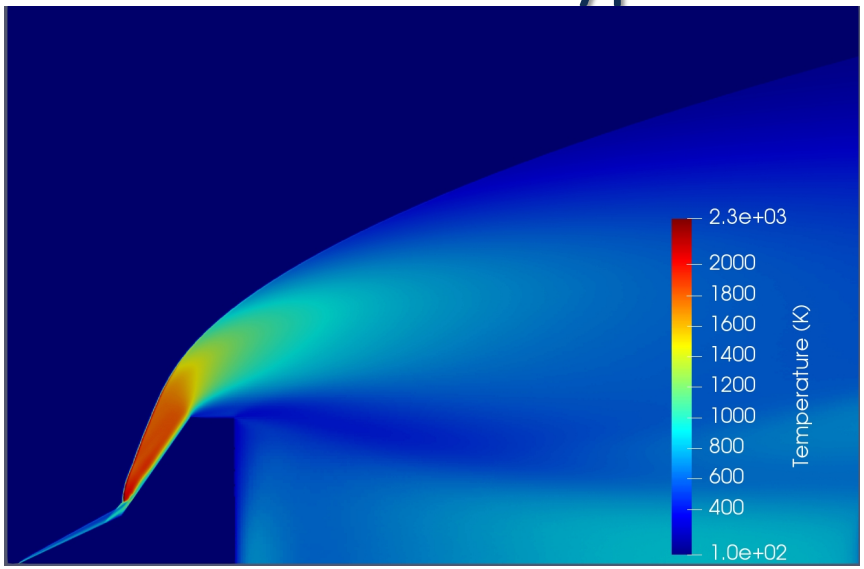


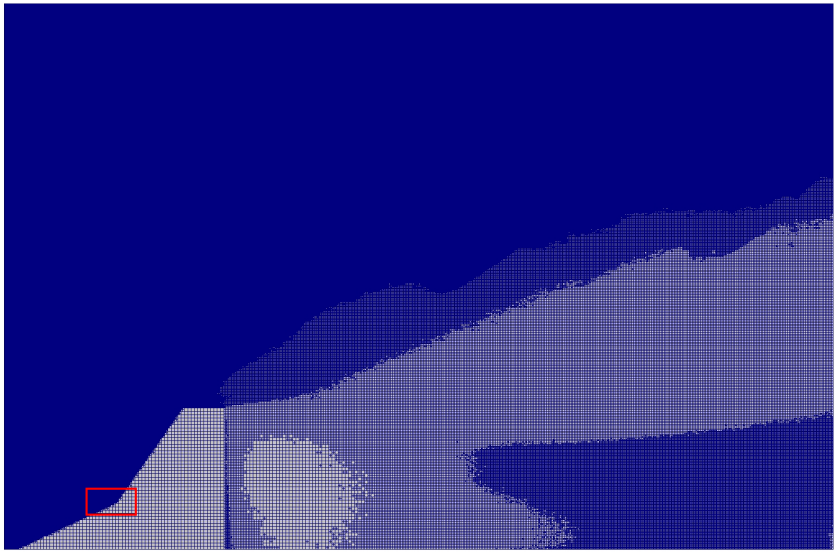
- Weak scaling indicates, 10% peak performance reduction from 1 to 10^6 cores
- 2 tasks/core gives 1.5x speedup, 4 tasks/core gives 2x speedup
- A total of 1 trillion molecules can be simulated on one third of the BG/Q
- Maximum number of tasks is 2.6 million

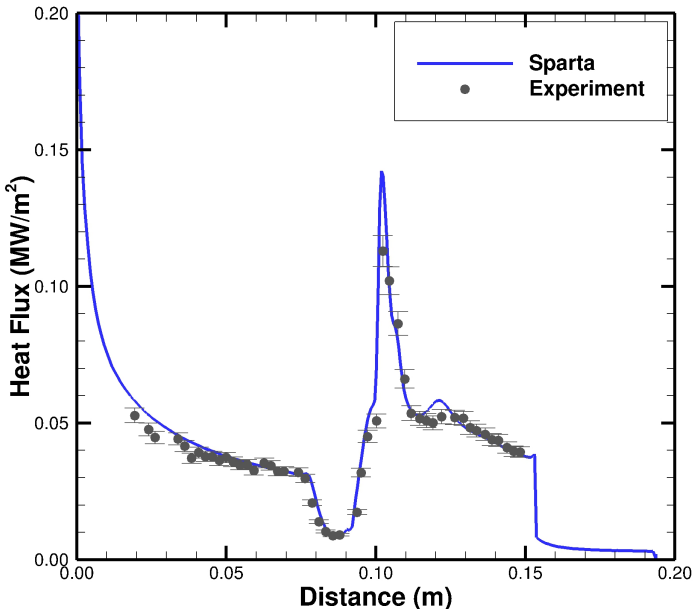
The Mars Reconnaissance Orbiter mission

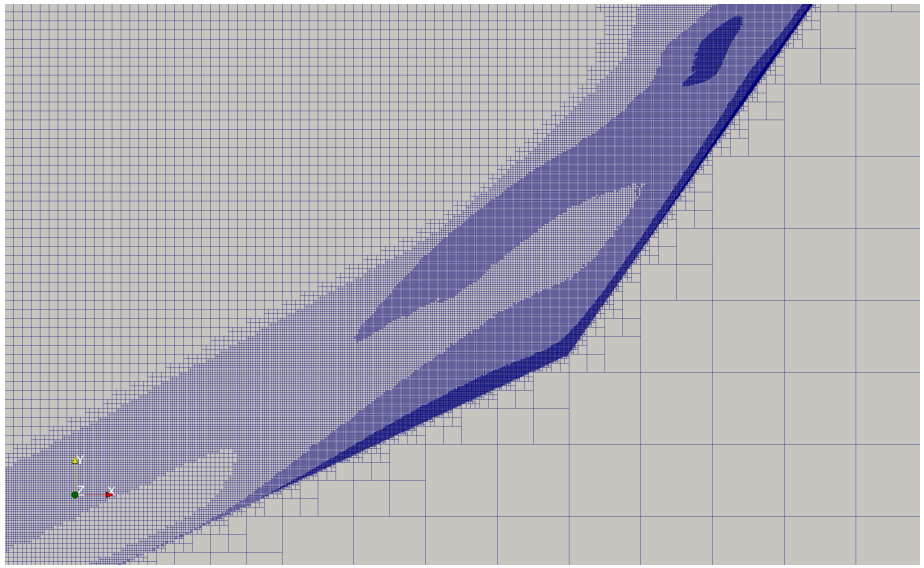


Validation for Hypersonic Flow





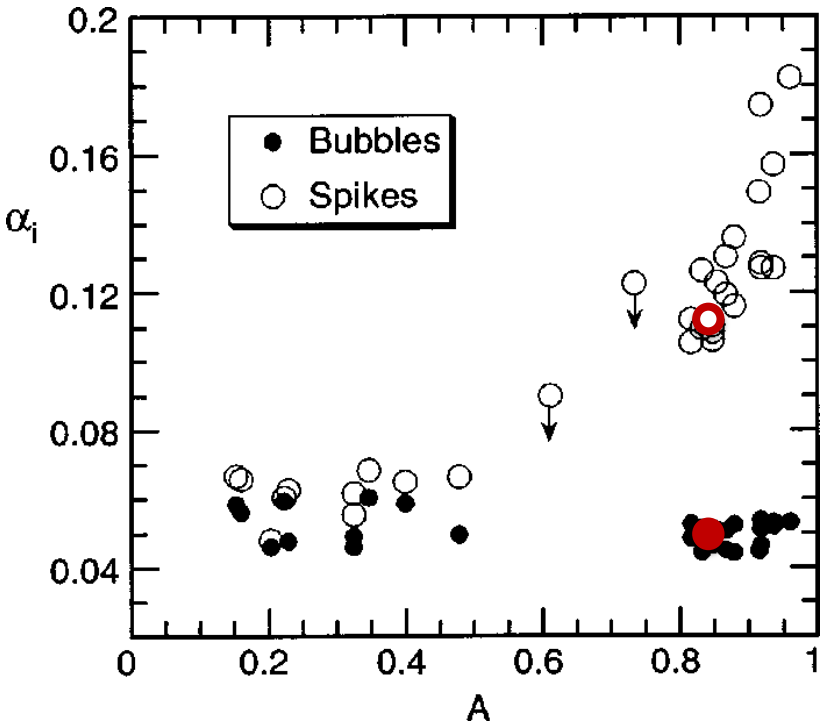


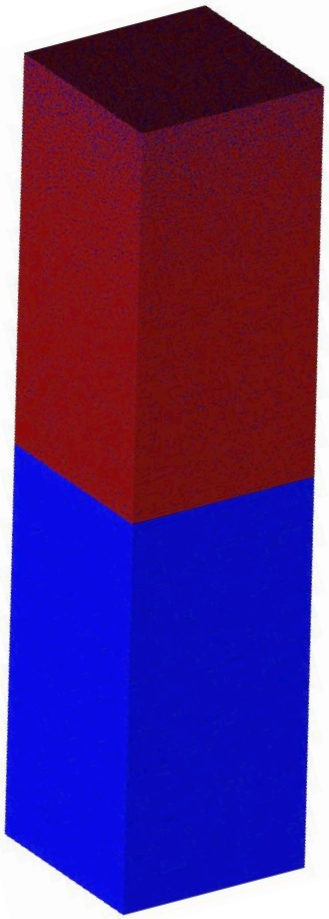


Rayleigh-Taylor Instability

Typical 3D DSMC simulation characteristics:
Physical Domain: 1 mm x 1 mm x 4 mm

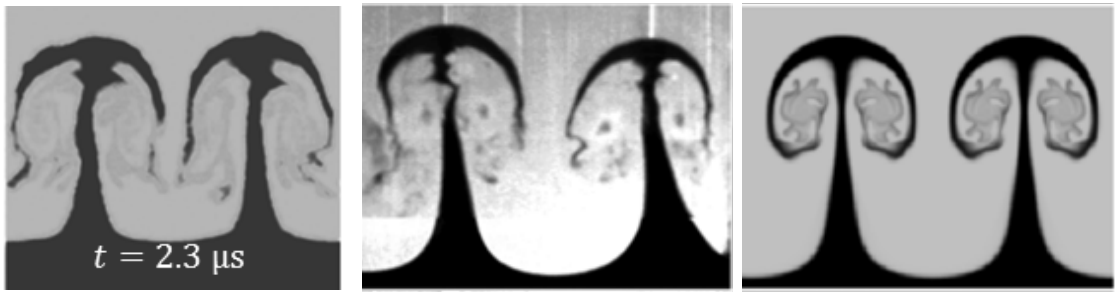
Cells: 62.5 billion
Particles: 1.2 trillion
Cores: ½ million



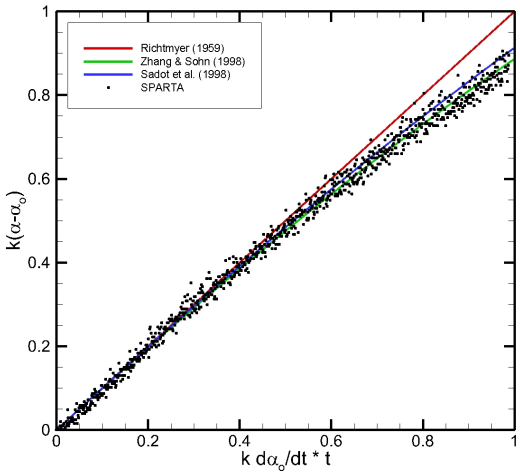


Run time: 90 hrs (5400 CPU years)
Time steps: 200,000 × 0.1 ns = 20 μs

Richmyer-Meshkov Instability
Baroclinic Creation of Vorticity



DSMC Experiment (Morgan et al., JFM, 2012) Navier-Stokes



Nondimensional amplitude for an initially small perturbation compared to theoretical & empirical models (Gallis et al., Physics of Fluids 2015)

The concentrated vorticity causes the interface to develop into mushroom-like shapes with spirals of the light gas circling the centers of vorticity.

The spirals break, and strong mixing appears, while the stems of the mushroom get thinner.

Finally, the shaded vortices interact with the stems of the mushrooms.

Turbulence at the Molecular Level

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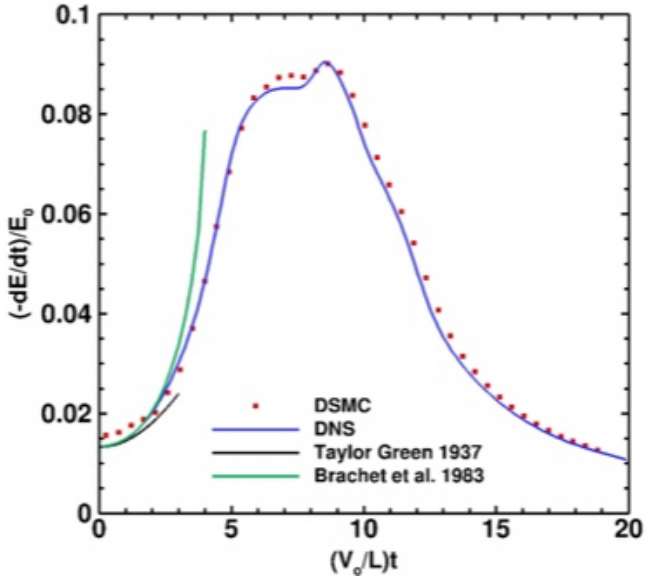
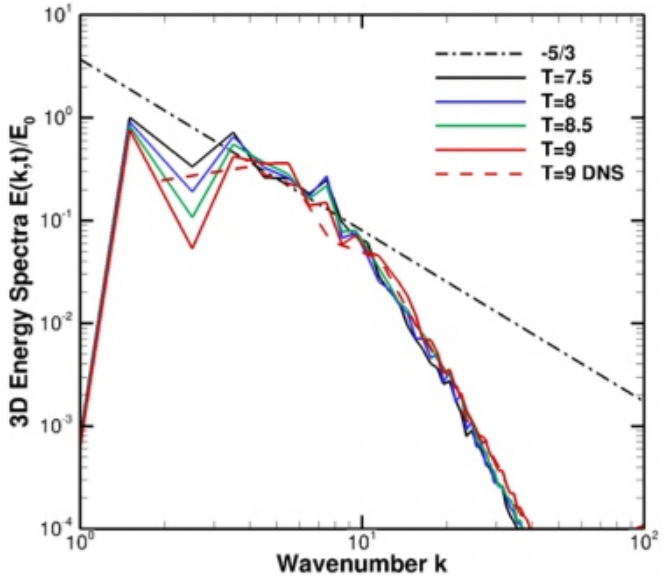
Taylor-Green (TG) vortex flow is a generic turbulent flow

- Incompressible TG flow is used in validation of codes and evaluation of subgrid-scale models
- Initial condition contains only a single length scale (single wave number)

Turbulent energy cascade can be observed numerically in TG flow

- Flow undergoes a rapid buildup of a fully turbulent dissipative spectrum
- Late-time flow exhibits basic features of isotropic, homogeneous turbulence

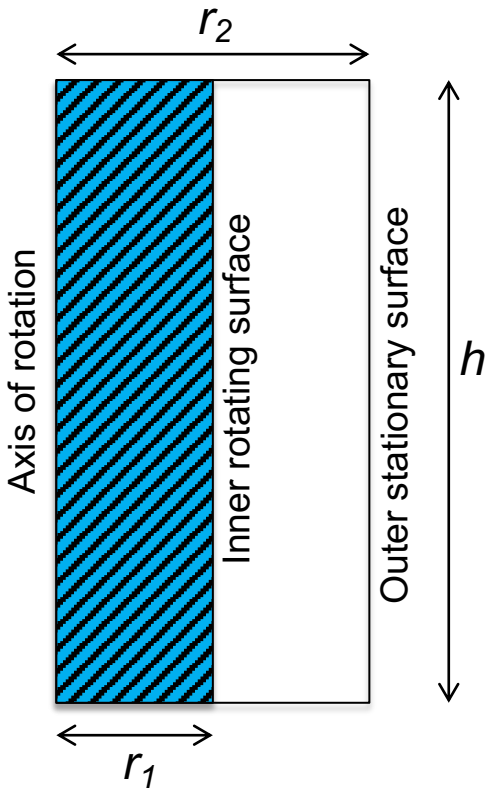




Incompressible TG flow has been successfully simulated at the molecular level.

Taylor-Couette Flow: Problem Description

- From G.A. Bird, *Molecular Gas Dynamics and the Direct Simulation of Gas Flows*, 1994, § 15.4, pg. 378
- Domain Definition: and
- Here: r_1 = 0.5 m and r_2 = 1.
  - Concentric cylinders
  - Boundary conditions:
    - Cylinder walls are diffusely reflective
    - Top/bottom of domain periodic
    - Initial conditions:
    - Stationary and uniform gas with density such that → Kn = 0.02
    - At t = 0 s, inner cylinder rotates with
      - For argon: 2071 rad/s

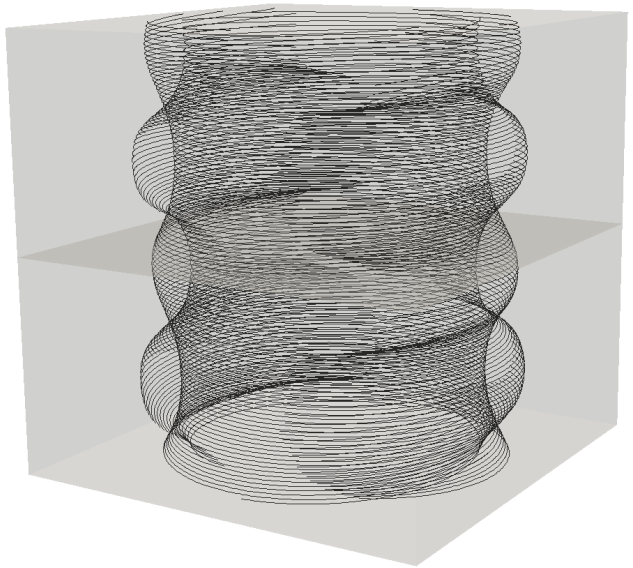


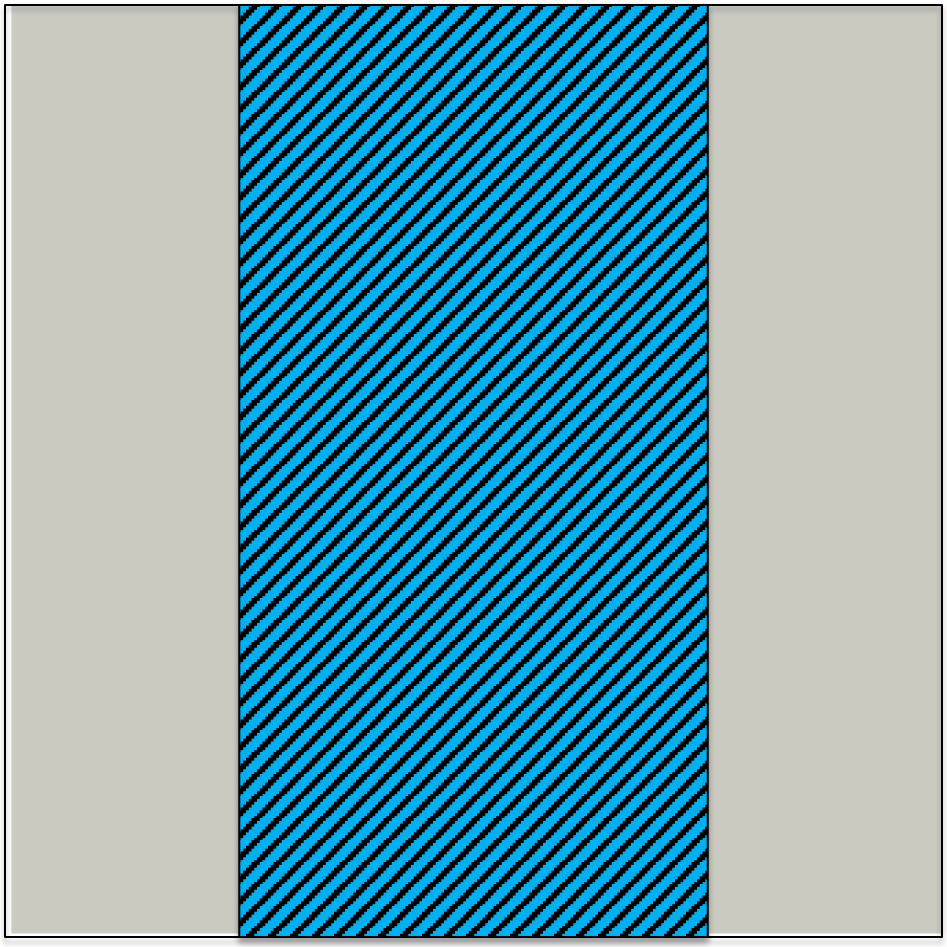
- Taylor Number: $$Ta = 4\rho^2\omega^2 r_1^4 \Big/ \mu^2 \left\{1-\left(\frac{r_1}{r_2}\right)^2\right\}^2 = 521{,}600$$
  - Exceeds critical value of 33,110 → flow instabilities/vortices

SPARTA Results:
3D Axisymmetric with Periodic BCs

Sandia National Laboratories

- Streamline projections onto a slice of the domain show four counter-rotating vortices develop
- Vortex centers are not at equal heights on opposite sides of the slice
- Wavy 3D structure in streamlines is observed when full domain is shown



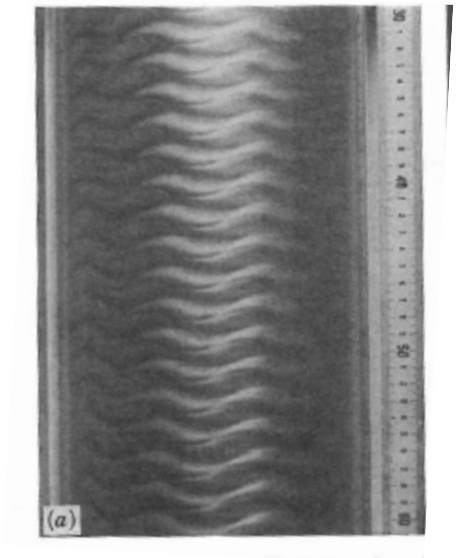


Taylor-Couette Instability in Literature

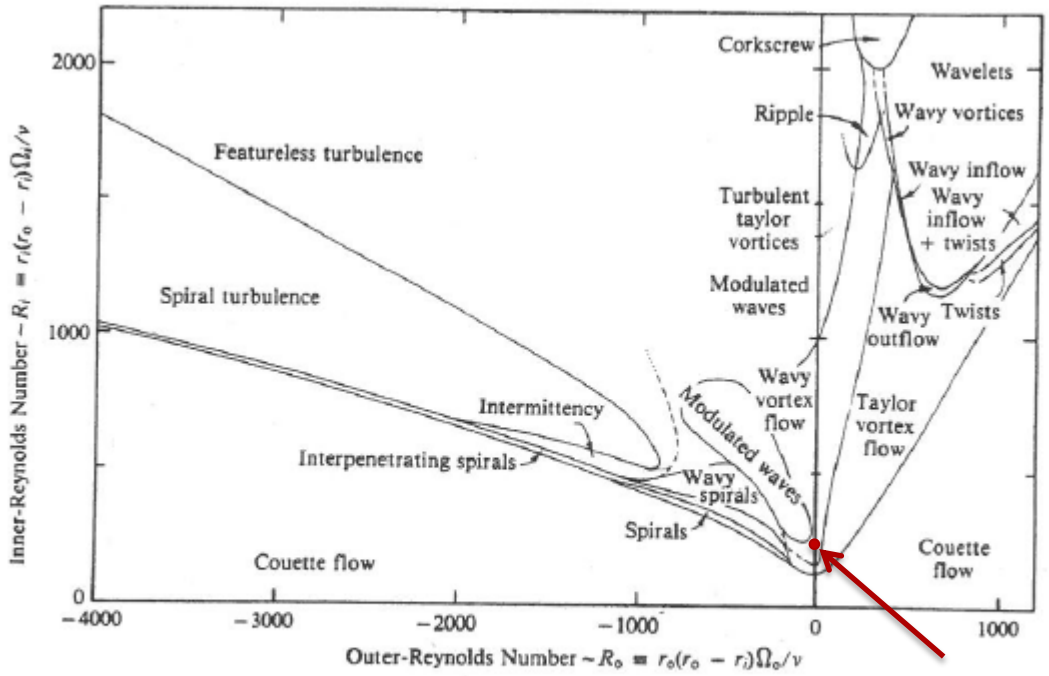
Inner Reynolds Number : $\mathrm{Re}_i = r_i(r_o - r_i)\omega_i / \nu$

Outer Reynolds Number : $\mathrm{Re}_o = r_o(r_o - r_i)\omega_o / \nu$

Here, $\omega_o = 0$ rad/s and $\nu = 2.1117\ m^2/s$ $\rightarrow \mathrm{Re}_o = 0, \quad \mathrm{Re}_i = 259$



Wavy Taylor Vortices



$\mathrm{Re}_o = 0, \quad \mathrm{Re}_i = 259$

Images from Ronald L. Panton, Incompressible Flow, 2nd Edition, §22.13, pg. 737-738

Conclusions

- DSMC is a fundamental form of computational fluid dynamics, originating from an interest in high altitude flow.
- It contains all the physics without having to make assumptions about local thermodynamic equilibrium or the macroscopic nature of the flow.
- DSMC contains thermal fluctuations, absent from most CFD techniques.
- DSMC is computationally intensive but enabled by massively parallel processing.