DSMC Method for Nanoscale and Microscale Gas Flow

Combustion Research and Flow Technology, Inc. (CRAFT Tech)
Pipersville, PA 18947 and Huntsville, AL 35801

Doug VanGilder , Ashvin Hosangadi, Judy Busby, and John Papp

Outline

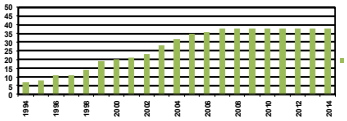
- Who is CRAFT Tech
- What is DSMC
- How is this related
- Channel flow example
- Future possibilities

January 29, 2008

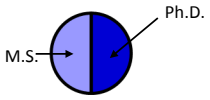
CRAFT Tech Background

- **AeroSpace R&D Business started in 1994**
  - Principals migrated from Propulsion Sciences Division of SAIC which Dash (VP/Mgr) started in 1980
  - Company has grown from 7 to 38

EMPLOYEE GROWTH



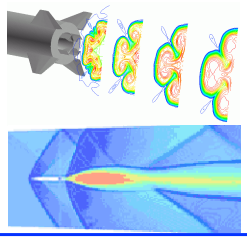
- **Specialty -"high-fidelity" CFD for complex problems**
- **Broad range of problems areas addressed from "sea to space"**
- **Propulsion, Combustion, AeroAcoustics, Aerodynamics are key areas - advanced R&D in these areas supported by DoD/DoE/ NASA**
- **High-tech staff, many have worked together for 25+ years**



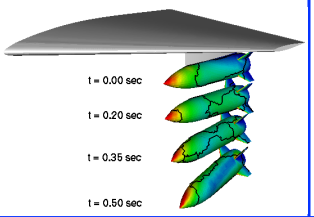
- **Business areas encompass:**
  - Consulting
  - Design optimization
  - Code licensing and customization
- **Facilities**
  - Large In-house Linux cluster with over 2000 cores with high speed Infiniband communication for general consulting

DOD CFD Applications

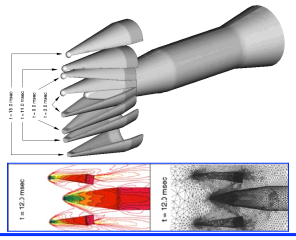
Plumes with Chemistry & Particles



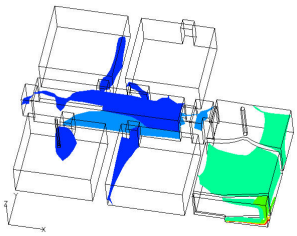
Cavity Dispense - UNS CFD & 6DOF



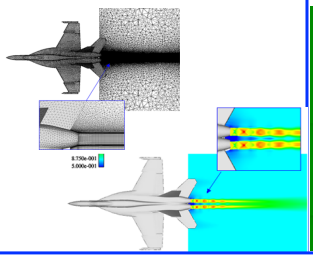
Shroud Dispense at High Velocities



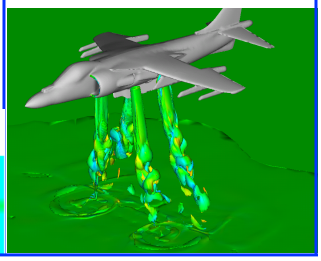
Particle/Pollutant Spread in Facility



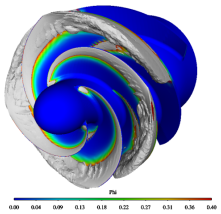
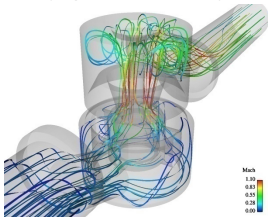
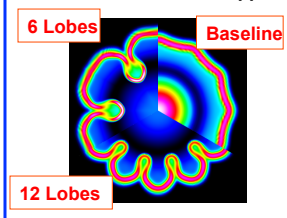
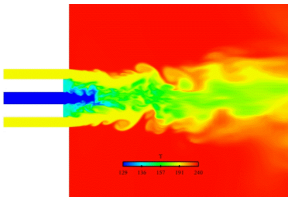
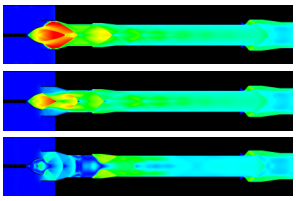
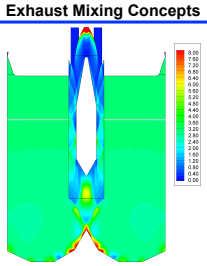
Jet Noise Reduction for High-Speed AC



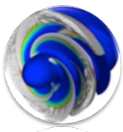
VSTOL Naval Carrier Landing



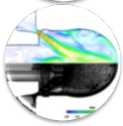
NASA CFD Application

Cryogenic Turbopump Modeling	Cryogenic Valve Analysis	Jet Noise Prediction Support
 LOX Pump	 Pressure Regulator	 Exhaust Mixing Concepts
 Trans-critical liquid Nitrogen Jet	 Shutdown of Rocket Engine in Test Facility	 Simulation of Rocket Engine Firing in Water-Cooled Test Facility

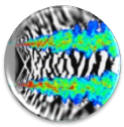
CRAFT Tech Products and Services



CRUNCH CFD®: Unstructured Navier-Stokes Solver for all Flow Regimes with Models for Non-Ideal/Real Fluids, Combustion, and Cavitation

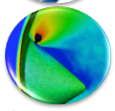


CRISP CFD®: Unstructured Grid Adaptation Tool with Error Quantification



CRAFT CFD®: Structured Navier-Stokes Solver with Fifth Order Accuracy for Aero-Acoustics and Advanced Non-Equilibrium Thermo-Chemistry for Hypersonics and Aero-Propulsion

AEGIS: Coupling Tools for Hybrid Continuum/Non-Continuum (DSMC) Analysis



HAMMRS: Steady and unsteady stand-alone Direct Simulation Monte Carlo solver for pure rarefied flows or coupled DSMC/Navier-Stokes solver for one-way continuum to rarefied hybrid rarefied/continuum flows.

Continuum or Rarefied Flow

Discrete Particle Or Molecular Model

Boltzmann Equation

Collisionless Boltzmann Equation

Continuum Model

Euler Equations

Navier-Stokes Equations

Conservation Equations Do NOT form a closed set

→ 0 0.01 0.1 1 10 100 →

Free Molecular Limit

Local Knudsen Number

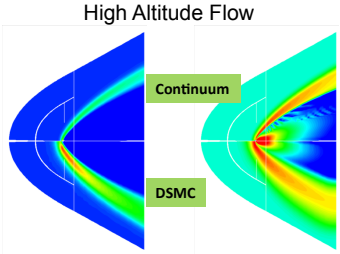
Kn = l / L

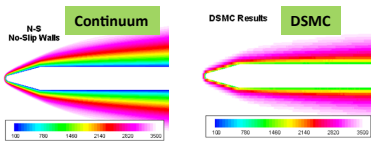
*From moments of the distribution and Boltzmann equation, one can obtain the conservation equations

Modeling Approach

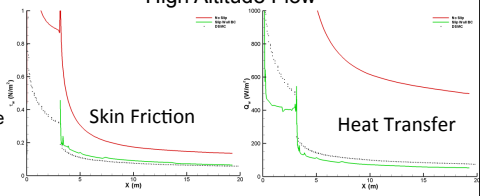
- **When Knudsen numbers get large Fully continuum simulation produces erroneous results**
  - Slip effects become important and flow does not equilibrate thermodynamically
  - Over-predicts near wall features such as skin friction and heat transfer
- **Fully rarefied (DSMC) computationally intractable in low Knudsen number regions**
- **Most engineering applications have a combination of Continuum and Rarefied regions in their domain**
- **CRAFT Tech utilizes hybrid approach**
  - Continuum model within continuum regions (typically Navier-Stokes) with possible enhancements to extend range to more rarefied regimes
  - Rarefied model within rarefied regions (typically Direct Simulation Monte-Carlo)
  - Coupling occurs across interface surface or region
  - Mitigates numerical inefficiencies, i.e., no longer inefficiently applying DSMC in high density regions or inappropriate continuum models in rarefied regions
  - Modeling of important physical phenomena must be consistent across interface

High Altitude Flow



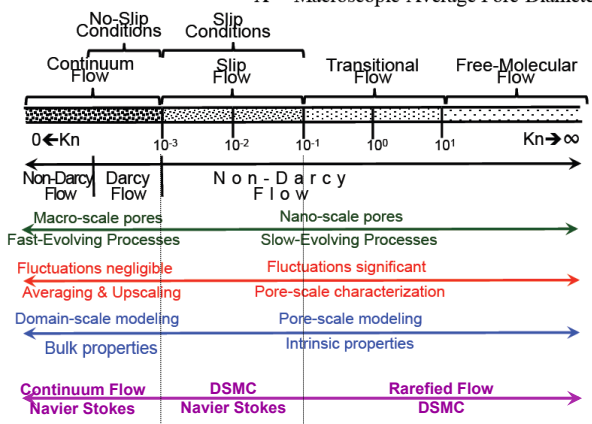


High Altitude Flow



Rarefied Gas ~> Unconventional Wells

Knudsen Number: $Kn = \frac{\lambda}{\Lambda} = \frac{\text{Mean Free Path of Fluid Molecules}}{\text{Macroscopic-Average Pore-Diameter}}$



- **Can use either DSMC or N-S (with slip effects) between 10^{-3} – 10^{-1}**
- **Continuum model requires adequate slip boundary treatment in this region**
- **Cost is cheaper the higher the Knudsen number at which Continuum/ DSMC interface occurs**

Direct Simulation Monte Carlo

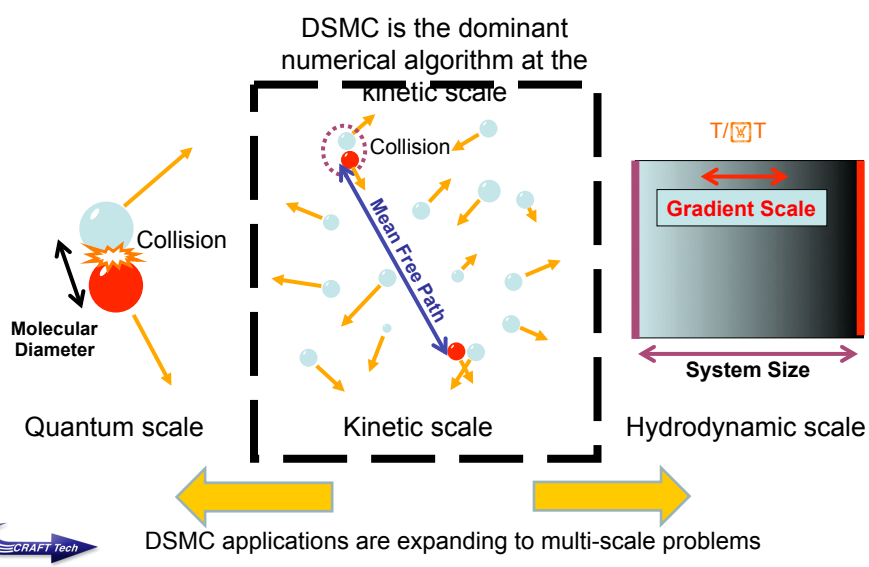
Development of DSMC

- DSMC developed by Graeme Bird (late 60's)
- Popular in aerospace engineering (70's)
- Variants & improvements (early 80's)
- Applications in physics & chemistry (late 80's)
- Used for micro/nano-scale flows (early 90's)
- Extended to dense gases & liquids (late 90's)
- Mature Tech for Various Applications (post-2000)
  - Plume expansion/impingement (& hybrid)
  - Vapor deposition
  - Multi-phase (particulates)

DSMC: Direct Simulation Monte Carlo

- **Particle-based technique for simulating rarefied fluid flows**
  - Knudsen number~0.1 or greater => rarefied flow
- **Simulation molecules ~ large number of real molecules => probabilistic simulation to solve Boltzmann equation.**
- **Intermolecular collisions and molecule-surface collisions calculated using probabilistic models**
  - **Unlike Lattice-Boltzmann methods where collision model is linearized using relaxation rate and equilibrium distribution**
- **Fundamental assumption:**
  - Molecular movement and collision phases can be decoupled over time periods that are smaller than the mean collision time

Physical Scales for Dilute Gases

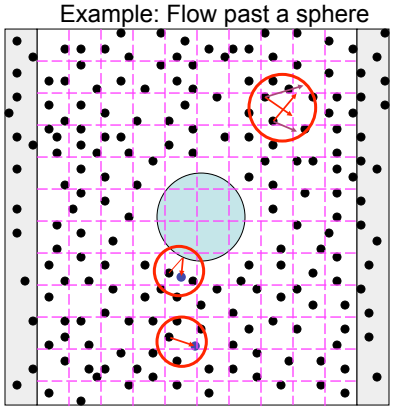


DSMC applications are expanding to multi-scale problems

DSMC Algorithm

- Initialize system with particles
- Loop over time steps
  - Create particles at open boundaries
  - Move *all* the particles
  - Process any interactions of particle & boundaries
  - Sort particles into cells
  - Sample statistical values
  - Select and execute random collisions

Example: Flow past a sphere

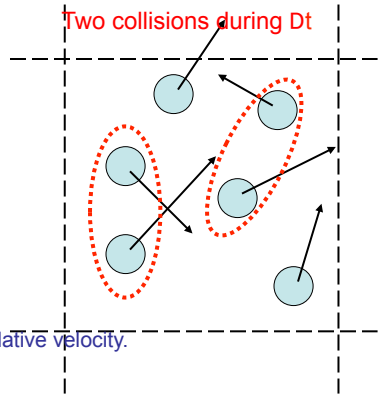


G.A. Bird, *Molecular Gas Dynamics and Direct Simulation of Gas Flows*, Clarendon, Oxford (1994)
F. Alexander and A. Garcia, *Computers in Physics*, **11** 588 (1997)

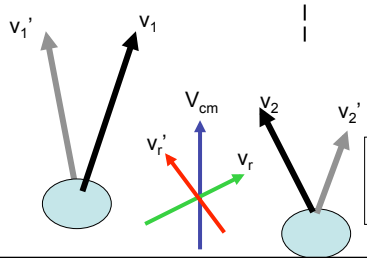
DSMC Collisions

- Sort particles into spatial collision cells
- Loop over collision cells
  - Compute collision frequency in a cell
  - Select random collision partners within cell
  - Process each collision

Two collisions during Dt



Probability that a pair collides only depends on their relative velocity.



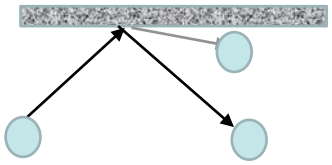
Direction of v_r' is uniformly distributed in the unit sphere

Surface Model

- Specular
- Diffuse

Requires accommodation coefficient which represents a probability a molecule will reflect with full thermal accommodation

  - Zero is pure specular
  - One is 100% thermally accommodated to wall temperature



- Cercignani-Lampis & Lord (CLL)

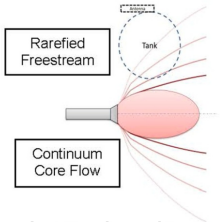
Requires independent accommodation coefficients for normal and tangential reflection accommodation as well as for rotational accommodation

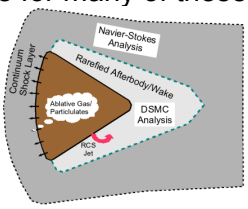
- Chemically-reacting

  eg.Sticking, dissociation, etc.

Hybrid Examples

- High altitude problems of interest typically involve some type of hybrid continuum/rarefied analysis
  - Flow-field contamination on critical components (solar arrays)
  - Hard body heating from thruster firing
- One-way hybrid coupling adequate for many of these applications

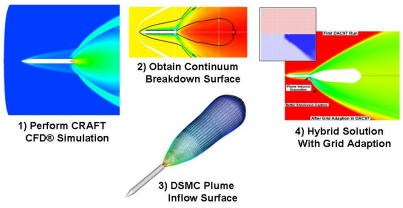


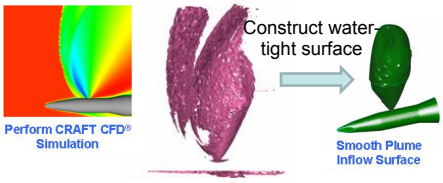


- Hybrid analyses burden typical DSMC methodologies
  - Up to 4 orders of magnitude differences in number density possible
  - Grid structure for sampling and collisional statistics is stressed
- DSMC code development for hybrid simulations must account for these issues

Steady-State Hybrid Interfacing

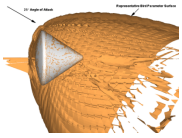
- **For steady-state applications hybrid interfacing essentially involves four steps**
  - Perform continuum simulation
  - Identify breakdown and create interface surface
  - Interpolate continuum solution onto interface surface
  - Perform hybrid simulation with interface surface as outgassing boundary condition
- **Caveats**
  - Most accurate implementation requires water-tight interface
  - Most efficient interface should only encompass flow within breakdown regime which may be complex and discontinuous
  - Generalized surface creation characterized by basic geometric shapes can either capture too much continuum regime leading to extensive simulation times or capture too much non-continuum regime leading to inaccuracies of non-continuum inflow conditions





Divert Jet

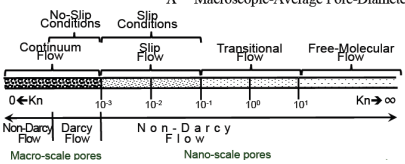
Re-Entry Vehicle

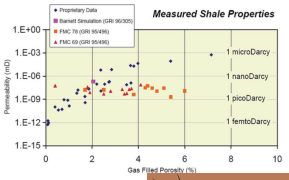


Application to Nano-Porous Unconventional Reservoirs

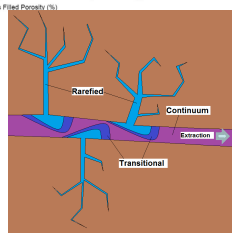
- Flow within pores although under high pressure, i.e. small mean-free-path, are within non-continuum regime because geometric length scale is small
- For rarefied flow bulk continuum transport properties (diffusion, viscosity, etc.) are no longer valid requiring rarefied physical models
- Variation of length scale through extraction region also means there is mixture of continuum and rarefied regions
- Successfully modeling of system requires hybrid analysis

Knudsen Number: $Kn = \frac{\lambda}{\Lambda} = \frac{\text{Mean Free Path of Fluid Molecules}}{\text{Macroscopic-Average Pore-Diameter}}$





Taken from Prof. Ozkan's Presentation



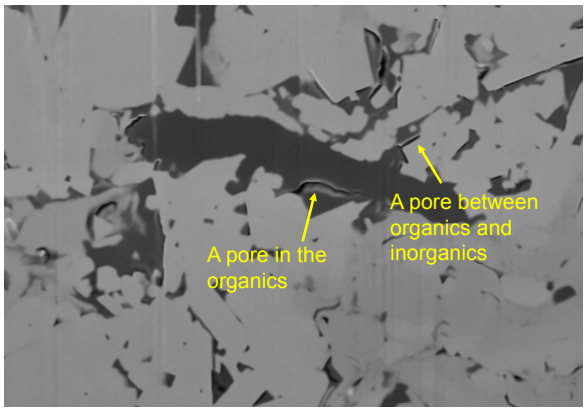
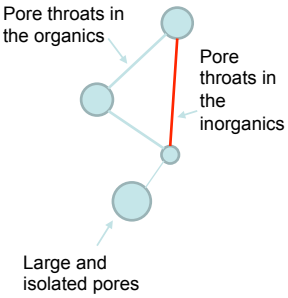


Illustration of Network Model and Upscaling

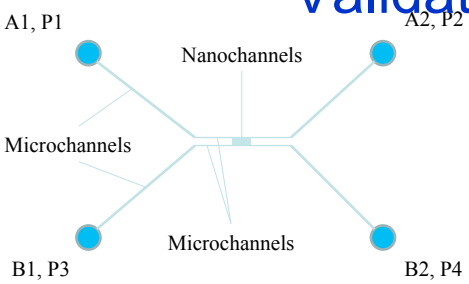


DSMC – small pores (Kn > 0.1)
- Transport law (rate vs. pressure drop) in simple organic and inorganic pores

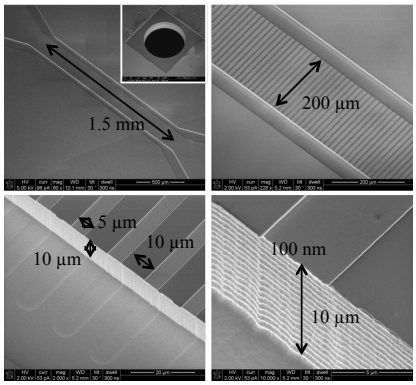
LBM – large pores (Kn < 0.1)
- Transport law (rate vs. pressure drop) in simple organic and inorganic pores

Pore network model that incorporates pore type, pore size, and pore connectivity → Upscaled permeability

Test Case: Experimental Validation



Conduct flow rate measurements across the nanofluidic channels to validate the model prediction.



Test Case: Channel Flow

Inlet:
λ = 60nm
P/Po = 3.6
Local Kn = 0.1

- The speed of gas flow is very high (hundreds of meters per second)
- In reality, the flow of gas is much slower – maybe a few millimeters per second or less
- Can we use the set up below?

Outlet:
λ = 216nm
P/Po = 1
Local Kn = 0.36

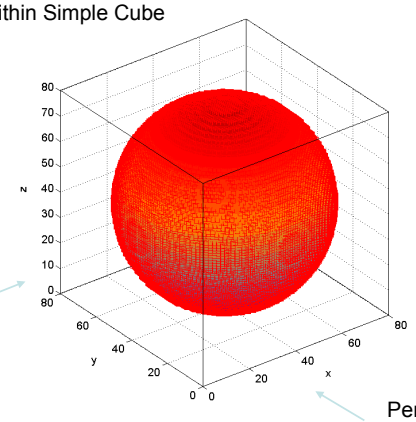
Inlet:
λ = 60nm
P/Po = 1.0001
Local Kn = 0.1

Low speed – there will be a lot of thermal noise and longer time is needed for averaging – is it possible?

Outlet:
λ = 60nm
P/Po = 1
Local Kn = 0.1

Test Case: Flow Past Sphere

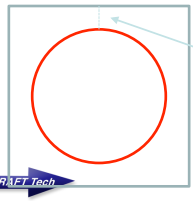
Sphere Geometry – within Simple Cube



Pressure boundary on yz faces

Pressure boundary on yz faces

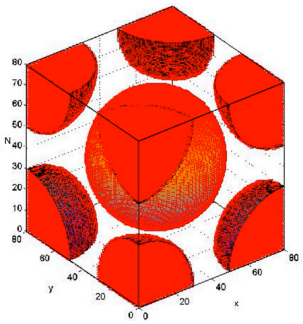
Periodic boundary for the particles on xy and xz faces?



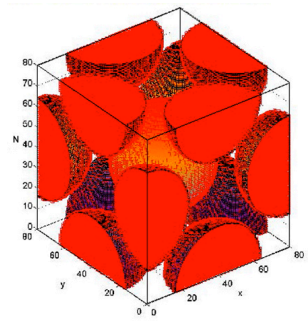
Kn = 2λ / (H – d) = 0.1

- Pure DSMC – high computational cost
- Hybrid (continuum + DSMC) possible? Kn is only high in the gaps between the particle and the boundary

Sphere(s) Geometric Configurations



*BCC (start with this one)



FCC

- Complex geometry can be handled by "cutting" computational cells using GTS library within CRAFT Tech's DSMC code

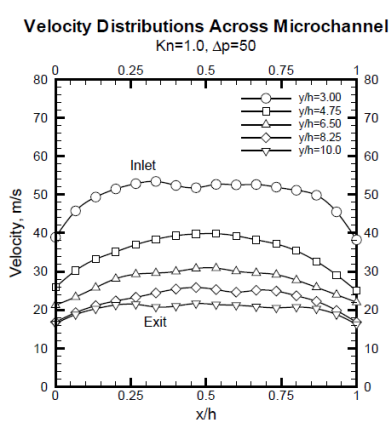
Flow Characteristics for DSMC

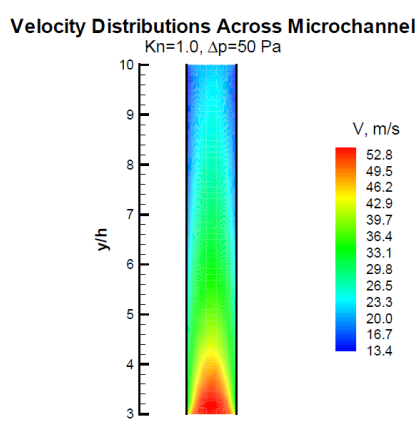
- Diffusion dominated low speed flow
- Wall interactions play significant role in molecule scattering
  - Geometric complexity can be modeled
  - Surface structure (roughness) and temperature affects reflection properties when molecules collide with wall
- Statistical scatter major obstacle for low-speed (subsonic flow) -- numerical diffusion errors
  - Flow velocity on scale of "noise"
    - Thermal velocity much higher than characteristic flow velocity
  - Affects accuracy of low speed flux calculation and introduces numerical/artificial diffusion
- Two-way coupling affected by numerical diffusion errors (& un-smooth DSMC solutions)
- Multi-phase flow (gas bubbles in liquid) area of research

Objectives

- DSMC and hybrid DSMC/Continuum technology can potentially be applied to modeling nano-porous unconventional reservoirs with additional technology development
- Characterize pores of different scales with DSMC or hybrid DSMC/Continuum procedures
  - Demonstrate that this more fundamental approach provides more accurate permeability factors for given pressure drops in these channels
- Integration into fast running system tools can potentially be achieved by using DSMC calculations to provide calibration of permeability as a function of porosity and pore size

DSMC Example: Low Velocity 2D Pipe Flow





Subsonic Channel Flow DSMC Simulations Knudsen Number Effects

J. Papp, D. VanGilder, and A. Hosangadi

Combustion Research and Flow Technology, Inc. (CRAFT Tech)
6210 Keller's Church Road, Pipersville, PA 18947

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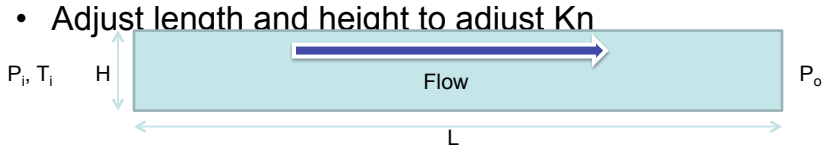
Simulation Conditions

- P_i/P_o of 3.6 kept constant
- Mean free path of ~60nm is kept constant
- Flow/wall temperature of 273K kept constant
- Computational grid always 200 (length) X 20 (height) cells
- Ratio of real to simulated molecules adjust to maintain correct collisional statistics in each cell
- Adjust length and height to adjust Kn



Kn	0.01	0.05	0.10	0.15	0.20
Height (m)	6.0042e-6	1.2009e-6	6.0043e-7	4.0028e-7	3.0021e-7
Length (m)	1.3646e-4	2.7292e-5	1.3646e-5	9.0974e-6	6.8230e-6

Analytic Channel Flow†

- Pressure Ratio

$$\frac{P(x)}{P_o} = -6\sigma Kn_o + \sqrt{(6\sigma Kn_o)^2 + \left(P^2 + 12\sigma Kn_o P\right)\left(1 - \frac{x}{L}\right) + \left(1 + 12\sigma Kn_o\right)\left(\frac{x}{L}\right)}$$

- Velocity

$$u(x,y) = \frac{1}{2\mu}\frac{dp}{dx}\left(y^2 - \frac{H^2}{4} - \sigma H^2 Kn\right)$$

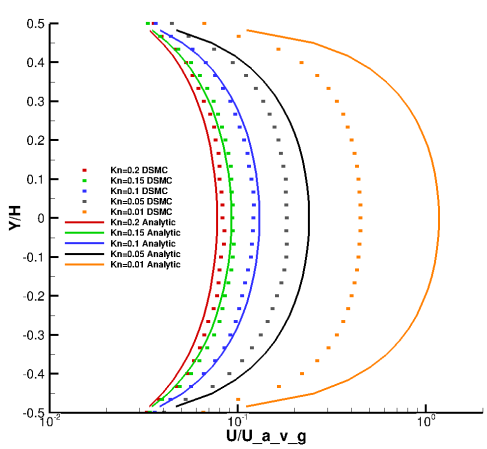
- Definitions

subscript 'o': Outflow condition
σ: Accommodation coefficient (0 = specular; 1 = diffuse)
μ: Viscosity
H: Channel height
L: Channel Length

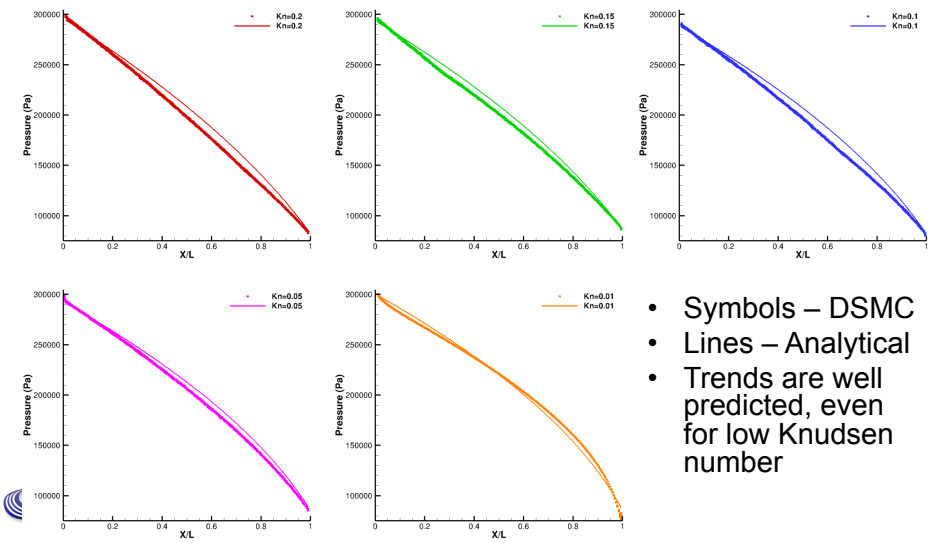
† Arkilic, E.B., Breuer K. S., and Schmidt, M. A., "Gaseous flow in microchannels", *ASME FED 1994; 197*, pp. 57-65

DSMC Channel Flow

- Symbols – DSMC
- Lines – Analytical
- Average velocity is area weighted for lowest Kn number (662.971 m/s)
- Agreement for Kn > 0.1 is within 10% of analytical
- Good prediction of slip velocity



DSMC Channel Flow



- Symbols – DSMC
- Lines – Analytical
- Trends are well predicted, even for low Knudsen number

Low Speed Channel Flow

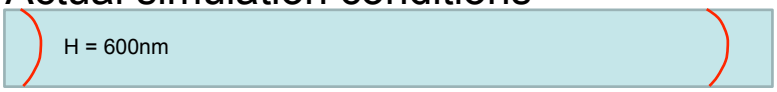
- Proposed conditions

Inlet:
λ = 60nm
P/Po = 1.0001
Local Kn = 0.1

Low speed – there will be a lot of thermal noise and longer time is needed for averaging – is it possible?

Outlet:
λ = 60nm
P/Po = 1
Local Kn = 0.1

- Actual simulation conditions



Inlet:
λ = 60nm
P/Po = 1.001
Local Kn = 0.1

Kn	0.10
Height (m)	6.0043e-7
Length (m)	1.3646e-5

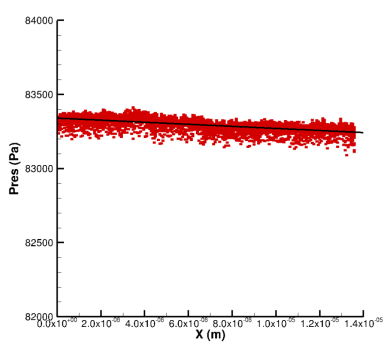
Outlet:
λ = 60nm
P/Po = 1
Local Kn = 0.1

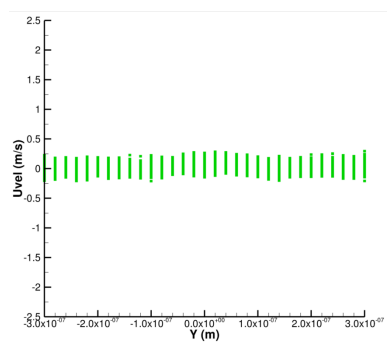
Low Speed Channel Flow

- Simulation issues
  - Current subsonic boundary condition is not self adjusting based on pressure ratio
  - Had to gradually modify inflow/outflow pressure to get desired pressure ratio
  - Each modification required restarting samples
- Simulation summary
  - Utilizing 48 cores
  - 200x30 cells and 730,000 molecules resulting in approx 121 molecules per cell and < 2% forced collisions
  - Once inflow/outflow pressure determined required 24 hours to reach steady state and another 24 hours for final sampling

Low Speed Channel

- Average conditions
  - Mass flow rate: 1.35×10^{-15} kg/s
  - Average flux velocity: 2.15 mm/s





DSMC Issues and Technology Upgrades

- DSMC is being used for small length scale problems such as MEMS devices
- Computationally-intensive to get significant samples to diminish errors
- Assumptions about surface/wall collisions needed
- Various modifications to basic DSMC scheme to address statistical shortcomings
  - *Information Preservation (used for MEMS)
    - Splits out collective and individual molecule velocities
  - Low diffusion (LD) particle method (near-continuum regimes)
    - Coincident Lagrangian and Eulerian cells
- A few recent references describe these efforts

DSMC: Related References for Minimizing Statistical Error

- **Statistical Simulation of Low Speed Rarefied Gas Flows**
  - Fan, Shen (Inst. Of Mechanics Beijing, China)
  - Information preservation (IP) method that modifies how molecules' velocities are modeled (ie. 2 components: collective (ave.) & individual ("peculiar")
- **A Direct Simulation Method for Subsonic Microscale Gas Flows**
  - Sun, Boyd (Univ. Michigan), Candler (Univ. Minnesota)
  - Applied to MEMS devices
  - Uses Information preservation (IP) method
- **A hybrid continuum/particle approach for modeling subsonic, rarefied gas flows**
  - Burt, Boyd (U. Michigan)
  - Couples IP & N-S
- **A low diffusion particle method for simulating compressible, inviscid flows**
  - Burt, Boyd (U. Michigan)
  - Particles have individual velocities as well as collective/average quantities
  - Mixed Eulerian and Lagrangian grids (coincident) used to update molecules
- **All-Particle Multiscale Computation of Hypersonic Rarefied Flows**
  - Jun, Burt, Boyd (U. Michigan)
  - Combines low diffusion (LD) with DSMC to avoid CFD/DSMC coupling

Future Work

- Continue Validation effort for Micro-channel
  - Low-speed simulation
  - Comparison of velocity profile with LB channel flow simulation at Kn = 0.1
  - Presentation at UREP review meeting in November
- Near term goals
  - 3D simulations for sphere configurations (Simple Cubic)
  - Comparison with LB at Kn = 0.1
  - Present at UREP review meeting in May?
- Longer term objectives and future goals
  - Nanofluidics validation (w/ experiment)
  - Develop framework for modeling geometric complexity of multi-pore configuration
  - Couple with Lattice-Boltzmann procedure for a unified framework across complete range of Knudsen numbers
  - Fluid-surface interaction?
  - Filtration of molecules of different sizes?
  - Multi-phase Extensions?
  - Upscaling?