Direct Simulation Monte Carlo Calculations in support of the Columbia Shuttle Orbiter Accident Investigation

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Mathematical models for gas dynamics

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

<table>
<thead>
<tr>
<th>Euler Equations</th>
<th>Navier-Stokes Equations</th>
<th>Conservation Equations do not form a closed set</th>
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<tbody>
<tr>
<td></td>
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<td>Boltzmann Equation</td>
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<td>Collisionless Boltzmann Equations</td>
</tr>
</tbody>
</table>

0 0.01 1 100

Local Knudsen number
The Boltzmann Equation

\[ \frac{\partial}{\partial t} (nf) + \vec{v} \cdot \frac{\partial}{\partial \vec{r}} (nf) + \vec{F} \cdot \frac{\partial}{\partial \vec{v}} (nf) = \left[ \frac{\partial}{\partial t}(nf) \right]_{\text{collision}} \]

\( f \): distribution function  
\( n \): number density  
\( F \): external force

Microscopic description of gases

- The rarefied regime is described by the Boltzmann equation
- Particulate nature of gas
- Gas is described by the position, velocity, energy of an ensemble of molecules in a statistical manner
- The microscopic description describes physical processes regardless of the mathematical complexity of the problem
Direct Simulation Monte Carlo (DSMC)

Move phase (deterministic)

Collide phase (stochastic)

\[ \frac{\partial (nf)}{\partial t} + \nabla \cdot (nf) + \vec{F} \cdot \frac{\partial (nf)}{\partial \vec{v}} = 0 \]

DSMC methodology

- Physical statistical simulation of real dilute gas flow
- Millions of molecules representing real gas molecules modify their velocities and positions as they interact with each other and the boundaries
- Discretization of time and physical space
- Decoupling of the move and the collide phase
Features of DSMC

- The calculation is always unsteady. Steady state achieved as a long time state of the unsteady flow
- There are no numerical instabilities
- Fluctuations have the same physical characteristics as the real fluctuations
- Physics and chemistry models are mere additions to the molecular model (surface interactions, energy exchange, chemical reactions)

Application overview

- Ultimate goal: to provide "piecewise integration" of key scenario events to determine the plausibility or implausibility of the candidate failure scenarios
- Target of current analysis: Determine aerodynamic and heating behavior of the Shuttle Orbiter during aerobraking maneuvers
  - Provide an independent assessment of the internal plume engineering model developed by Steve Fitzgerald (NASA JSC)
- Methodology: Direct Simulation Monte Carlo method
  - DAC implementation by LeBeau (NASA JSC)
- Results: Flowfield simulations at representative re-entry trajectory points
Modeling procedure

- Geometry Modeling
  - Surface grid: Triangulated unstructured constructed from Orbiter CAD model
  - Gas phase grid: Cartesian (adapted where large gradients are present)
- 3-D DSMC Analysis
  - Code used: DAC (version 97)
  - Thermal and chemical non-equilibrium included
  - Chemistry modeling: Finite rate chemistry model of Bird

DSMC analysis of flight trajectory

- DSMC simulations were performed at two points of the entry trajectory

<table>
<thead>
<tr>
<th>DSMC Point AA</th>
<th>DSMC Point A</th>
</tr>
</thead>
<tbody>
<tr>
<td>El + 91 seconds</td>
<td>El + 197 seconds</td>
</tr>
<tr>
<td>Mach = 25.1</td>
<td>Mach = 27.0</td>
</tr>
<tr>
<td>Altitude = 350,274 ft</td>
<td>Altitude = 300,003 ft</td>
</tr>
<tr>
<td>AOA = 41 degrees</td>
<td>AOA = 40 degrees</td>
</tr>
<tr>
<td>Kn ~ 0.02</td>
<td>Kn ~ 0.001</td>
</tr>
</tbody>
</table>
Grids used for the simulations

Adapted grid in the front part of the vehicle

Adapted grid around the wing

Flowfield temperature profile (350kft)
Flowfield temperature profile (300kft)

350 kft flowfield
Surface heating
300 kft flowfield
Surface heating

Temperature profile at wing level
(350 kft)
Temperature and density profiles
6m from centerline

Wing geometry
Wing leading edge geometry

Vents
(Area = 66 in²)

Panel 1

Panel 22

Damage scenarios investigated

- What size plume can burn through wire(s) in 530 seconds from EI?:
  - Scenario A: Breach between RCC panels 9 and 10
  - Scenario B: 10 inch hole in RCC panel 8
Damage scenarios simulations

Goal: Model the effects of a damage to the leading edge

- 3-D representation of critical parts of wing leading edge
- Boundary conditions from undisturbed geometry simulations
- DSMC simulations performed with full chemical and thermal non-equilibrium included

Damage scenario A
Flow through a slit
Representative internal wing leading edge flow field

![Panel 1 and Panel 22](image)

Representative internal wing leading edge spar heating

![Panel 1 and Panel 22](image)
Damage scenario B
Panel 8, 10" hole

Number density in flowfield with streamlines

350kft
300kft
Reference heating distribution in RCC cavity

Reference pressure distribution in RCC cavity
Heating Distribution and Engineering Model Comparisons

- Plume heating model was developed based on continuum flow assumptions, leading to slightly less diffuse plume structures
- Results are favorable
  - Heating predictions within factor of 2
  - Similar predicted impingement location

Conclusions

- The Direct Simulation Monte Carlo method was used to provide 3-D simulations of the early entry phase of the Shuttle Orbiter
- Undamaged and damaged scenarios were modeled to provide calibration points for engineering "bridging function" type of analysis
- Currently the simulation technology (software and hardware) are mature enough to allow realistic simulations of three dimensional vehicles
Applications of DSMC and typical length-scales

- Hypersonics (m)
- Microelectronics manufacturing processes (cm)
- Physical, Chemical vapor deposition (cm)
- MEMS (microns)
- Non-equilibrium chemistry (atomic level)
The limitations of DSMC

- The computational load increases with the density of the flow
- Statistical error decreases as a function of the square root of the number of samples
- DSMC can carry more information than actually needed for some applications
- DSMC is an MMP empowered technology

Calculations performed

- 350 kft
  - 2 levels of adaptation
    - 1st level of adaptation: mean free path wide subcells
    - 2nd level of adaptation: 0.5 mean free path subcells
- 300 kft
  - 2 levels of adaptation
    - 2nd level of 350kft adaptation
    - 3rd level of adaptation:(0.1 mean free path subcells)
Grid 6 meters from the centerline