Particle Approaches for Modeling Nonequilibrium Flows using Petascale Computing

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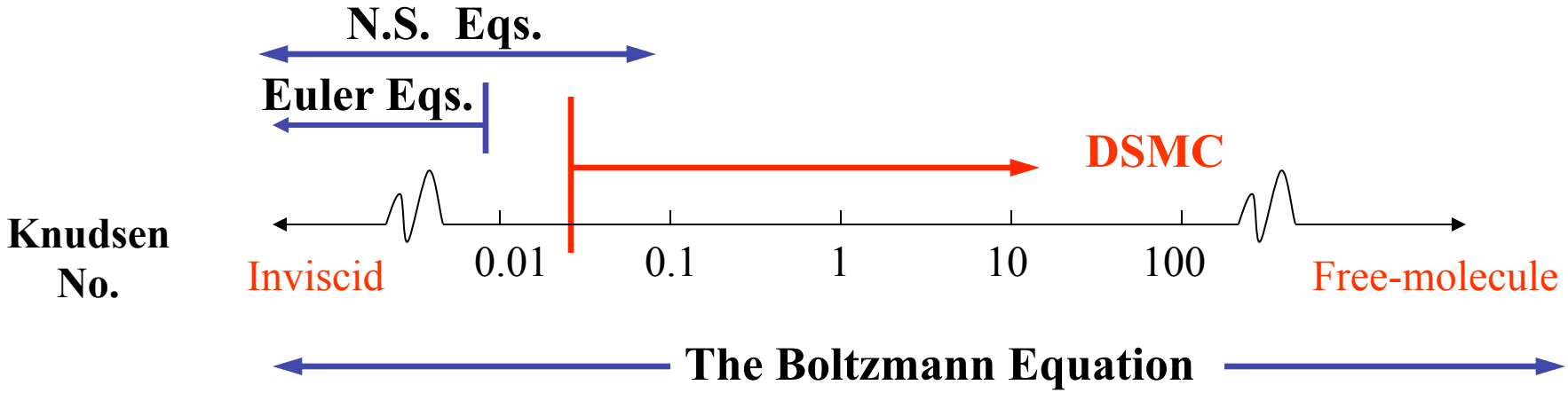
Relations of Different Flow Models

Kn = mean free path/ characteristic length



- **Boltzmann equation:**

$$\frac{\partial f_1}{\partial t} = -\vec{q}_1 \cdot \frac{\partial f_1}{\partial \vec{r}} + \int d\vec{p}_2 \int d\Omega g \sigma(\theta, g)\left(f_{1'} f_{2'} - f_1 f_2\right)$$

= **flux thru CV, ΔV1 + change due to collision in/out of CV**

- **The DSMC is a numerical method for solving the Boltzmann equation, under the assumption of a dilute, binary "gas":**

- **1 DSMC particle ~ 10^6 – 10^{18} physical gas particles**
- **During each time step, free motion and collisions are performed concurrently:**

Free motion:

$$\vec{r}_2 = \vec{r}_1 + \Delta t \cdot \vec{v} \qquad (1)$$

Collisions:

1) the number of collision pairs, *q*, is calculated:

$$q = \frac{1}{2} N \overline{N} F_N (\sigma C_r)_{\max} \Delta t / V_c \qquad (2)$$

2) the collision probability, *p*, for each pair:

$$P = \frac{\sigma C_r}{(\sigma C_r)_{\max}} \qquad (3)$$

3) the acceptance-rejection principle is used to evaluate whether a collision is to be evaluated.

4) the particle energy would be redistributed for a successful inelastic collision by:

i. Larsen-Borgnakke/FHO model for internal energy exchange, MD/QCT

ii. Chemical reactions, MD/QCT, TCE

AFOSR Gas – Surface MURI has changed this paradigm.

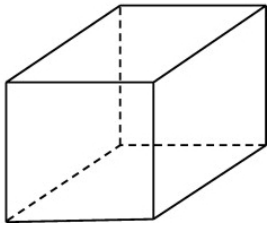
Comparison of Methodologies

	MD	DSMC
Method	**kinetic**	**kinetic**
Application	**Solid, Liquid, Gas**	**Gas** (+ drops)
Simulated Particle		
geometry	**point-size**	**sphere**
[a]F_N	**1**	**$10^6 \sim 10^{18}$**
Interactions	**Potential**	**Collision**
Time Step	**10^{-15} Sec**	**$10^{-6} \sim 10^{-9}$ Sec**
System Capabilities		
Computational Domain	**~nm**	**> mm**
# of Real Particles	**~10^6**	**> 10^{23}**
time Scale	**~1-10ns**	**> 10^{-9} s**

[a]**F_N:** the number of real atoms represented by a simulated particle.

SUGAR Framework & Parallelization Strategies

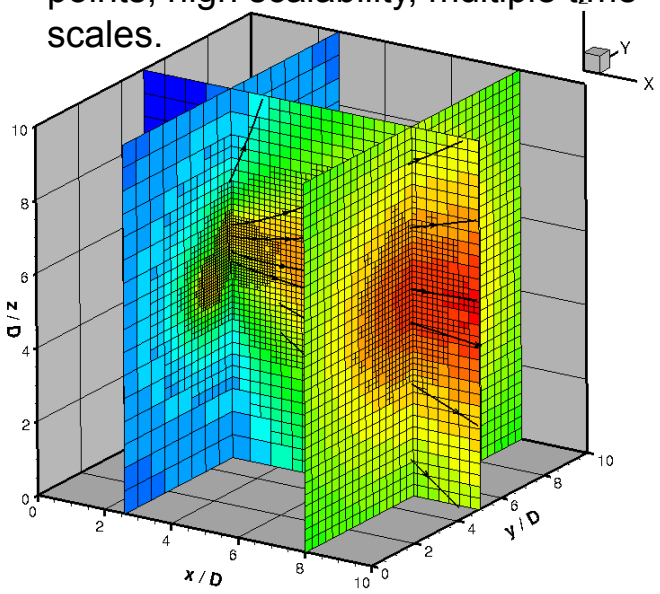
- Scalable Unstructured Gas-dynamics with Adaptive mesh Refinement (SUGAR) started as a development effort for simulating electric propulsion plumes in 2012.
- Last year, a separate effort for modeling other physical applications building on the MPI-C++ framework with OOP.
- For simulating the shock dominated flows, a major effort was added for modeling gas-surface interactions.
- Adaptive Mesh Refinement (AMR) is a robust and flexible approach for creating the computational mesh.
- Hybrid capability with OpenMP and GPGPUs is under consideration.



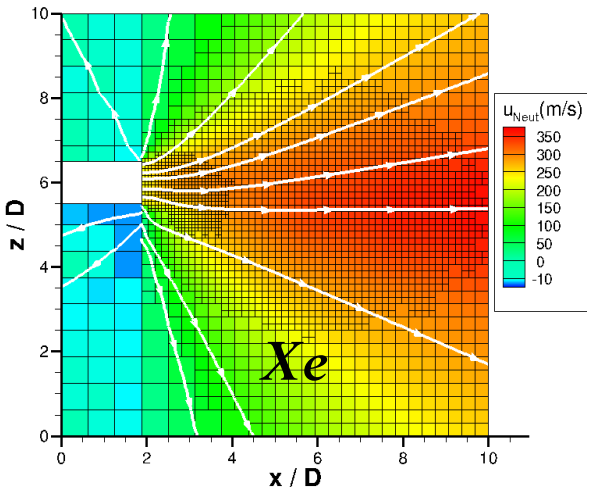
Hexahedron used in this work

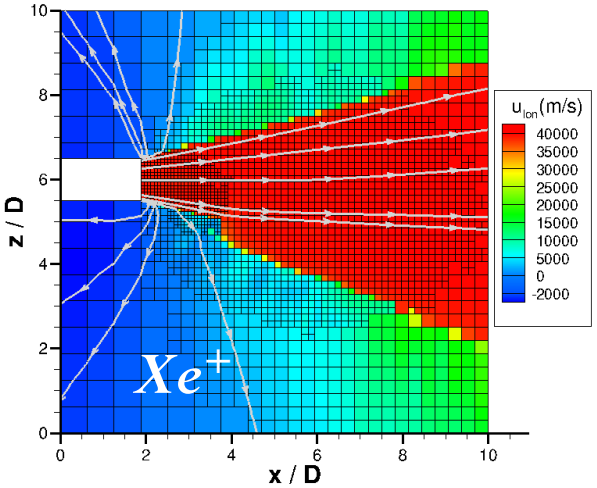
Use of Peta-scale Computing Techniques to Model Neutral and Charged Species Backflow Contamination

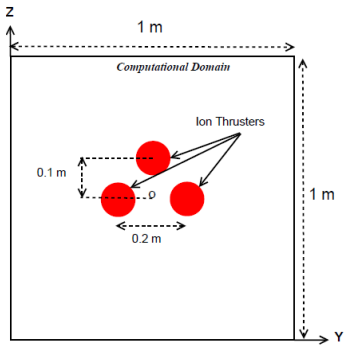
- AMR/Octree – factor of 300 fewer grid points, high scalability, multiple time scales.

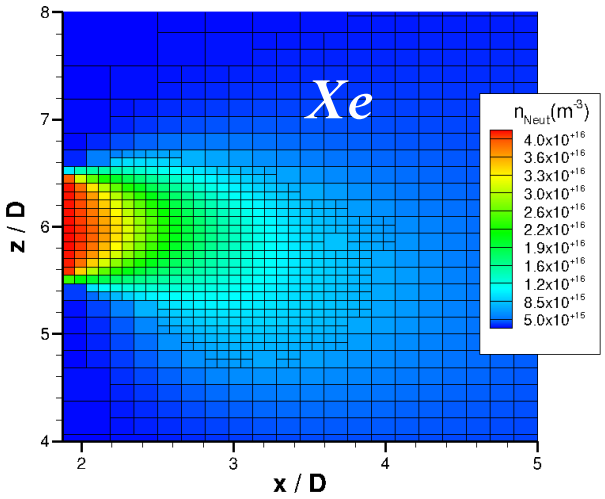


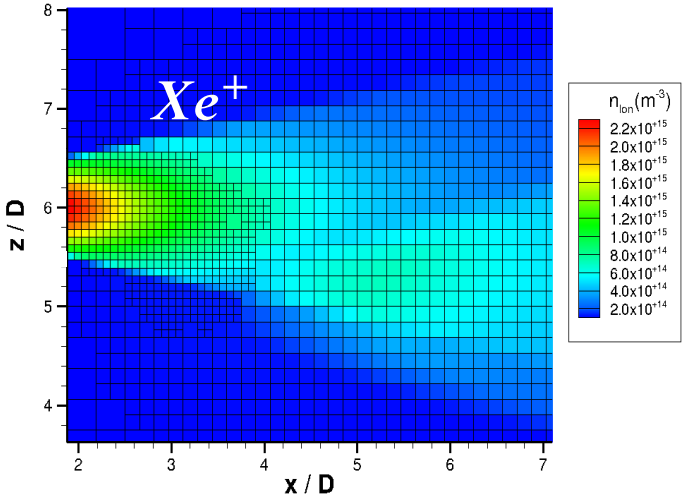
- Resolve Charge Exchange Collisions
- Backflow structure is asymmetric



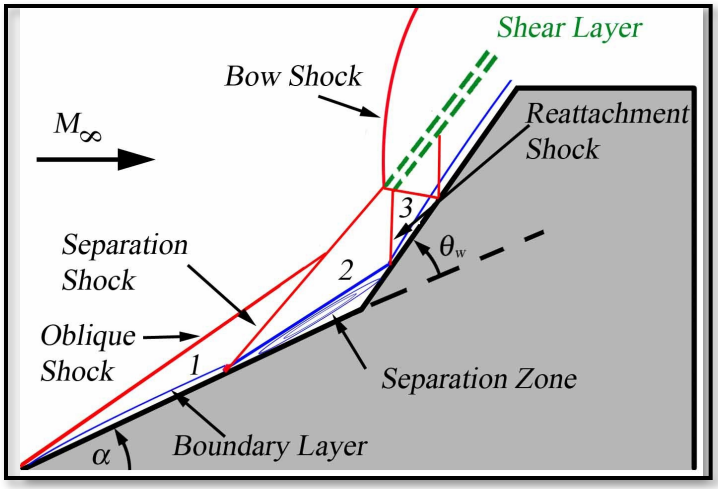








Strong Shock Interactions – HET* N_2 High Enthalpy Case



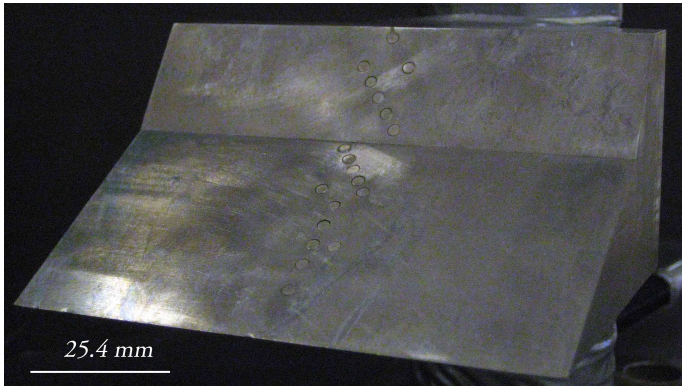


Figure 2. The experimental double wedge model used in the current study. The coaxial thermocouple gauges can be seen along the center of the model. Note: Some gauges are staggered to increase spatial resolution.

Freestream Parameters	M 7_8 (High Enthalpy)
Mach number	7.14
Static Temperature, K	710
Static Pressure, kPA	0.78
Velocity, m/s	3812
Density, kg/m^3	0.0037
Number Density, /m^3	7.96 x 10^{22}
Stagnation Enthalpy, MJ/kg	8.0
Unit Reynolds number, /m	0.4156x 10^6
Knudsen number	4.0256 x 10^{-4}

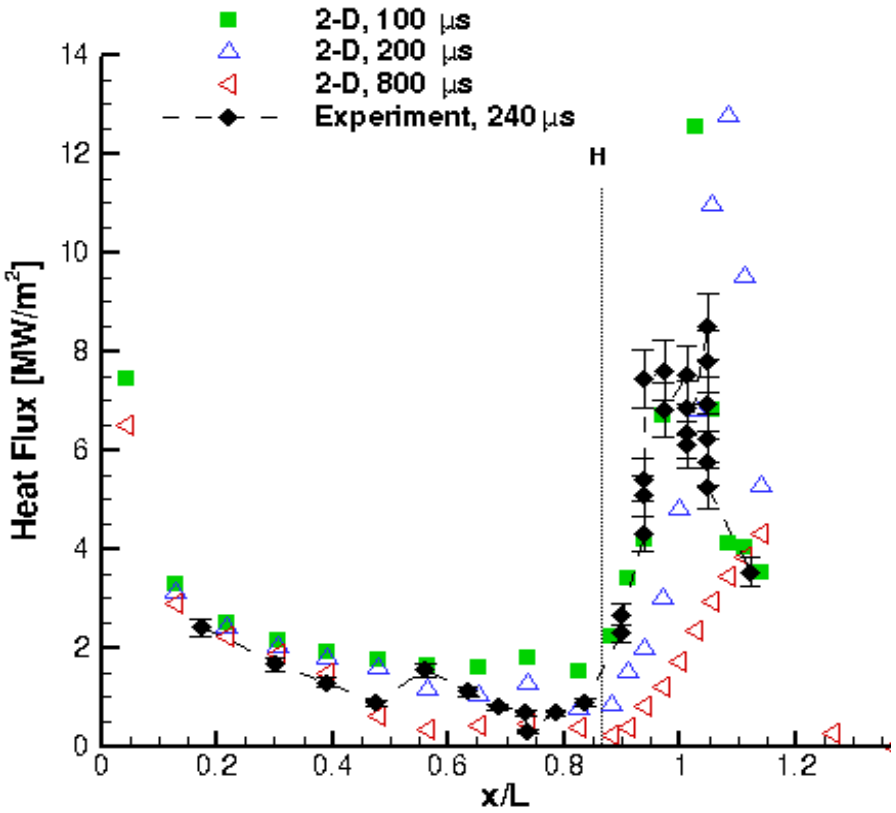
- ***Hypervelocity Expansion Tube - AIAA 2012-0284 by A.B. Swantek and J. M. Austin.**
- **Stagnation enthalpies from 2-8 MJ/kg, about a 30-/55-deg double wedge model.**

DSMC Numerical Parameters

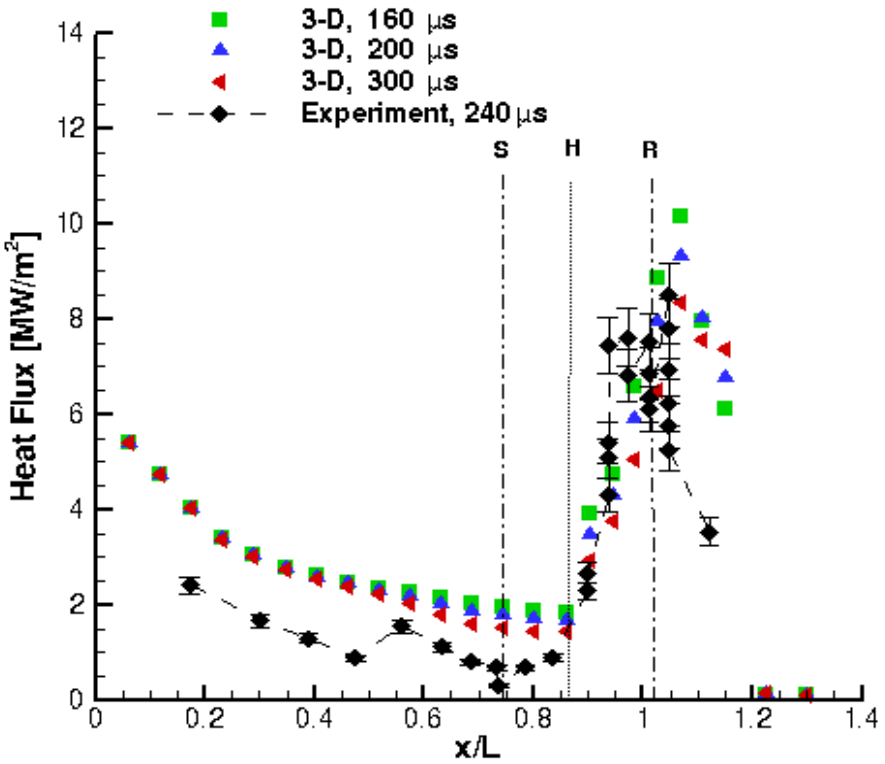
Numerical Parameter:	Nitrogen 2-D	Nitrogen 3D baseline	Nitrogen 3D fine	Air 2-D	Argon 2-D
Total number of time-steps	800,000	300,000	100,000	400,000	400,000 (ongoing)
Number of molecules per simulated particle	1.0×10^{13}	4.0×10^{13}	1.0×10^{13}	2.5×10^{12}	1.0×10^{13}
Number of cells	450 x 400	200 x 200 x 150	280 x 280 x 210	400 x 400	400 x 400
Number of simulated particles	96×10^{6}	1.86x	7.96×10^{9}	312×10^{6}	96×10^{6}
Grid adaptation	20x20	20x20x1	30x30x1	20x20	20x20
Number of processors	64	128	192	128	128
Total CPU hours	10,240	106,000	112,200	16,384	-

Comparisons of N_2 Heat-Flux for 2-D and 3-D Cases

a) Experiment vs. 2-D DSMC



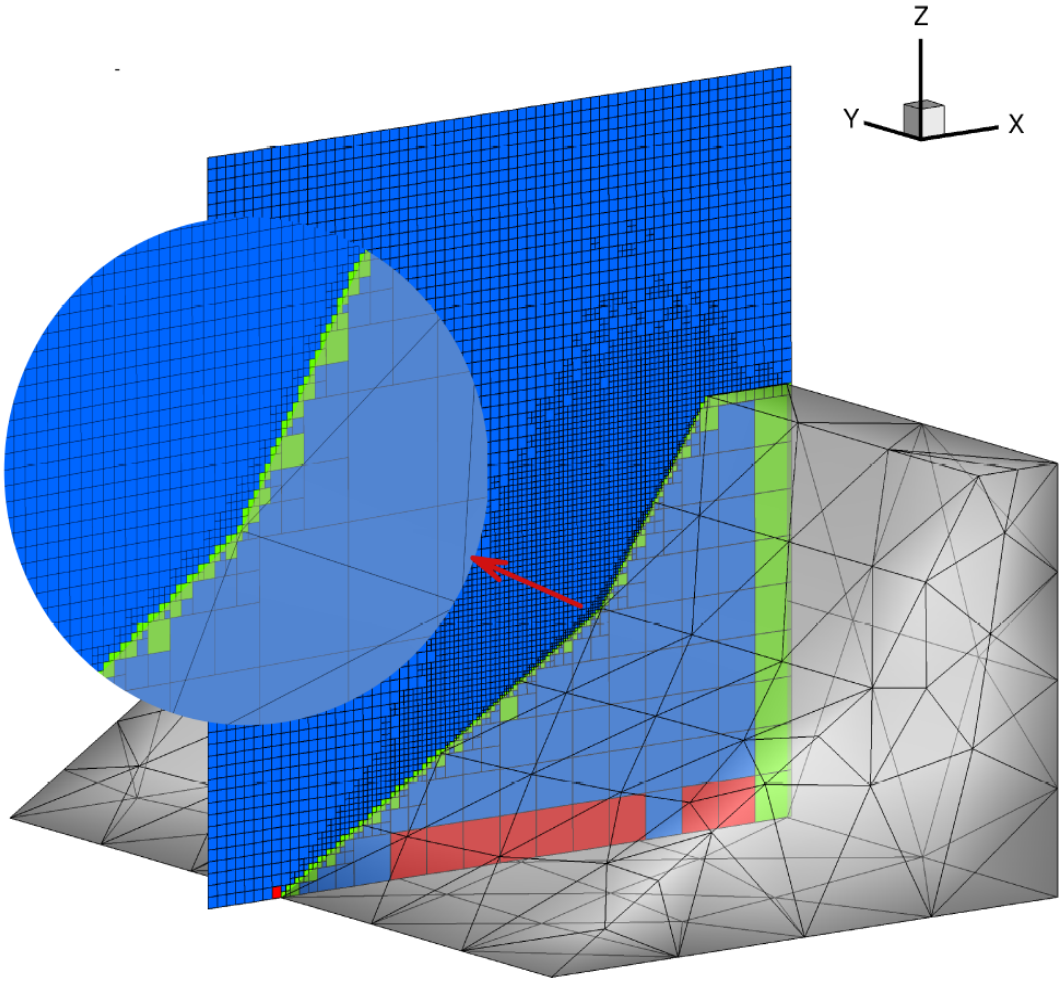
b) Experiment vs. 3D DSMC



S : Separation
H : Hinge point
R : Reattachment
L : Length of the first wedge=0.05 m

Representation of the V-Mesh

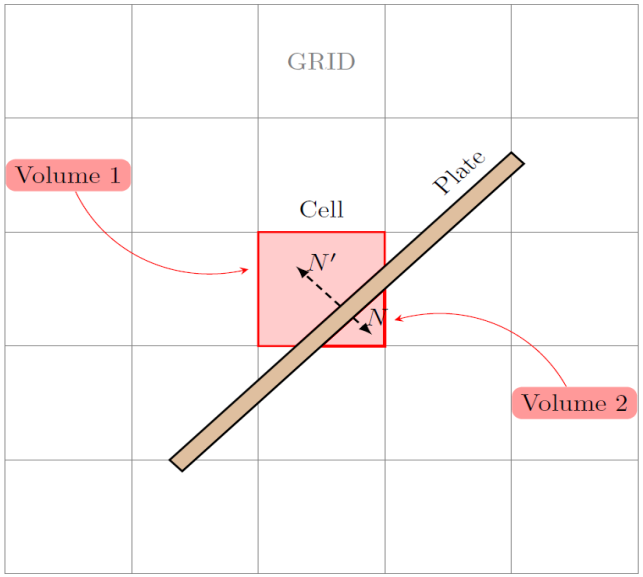
Cut-cell demonstration on V-Mesh

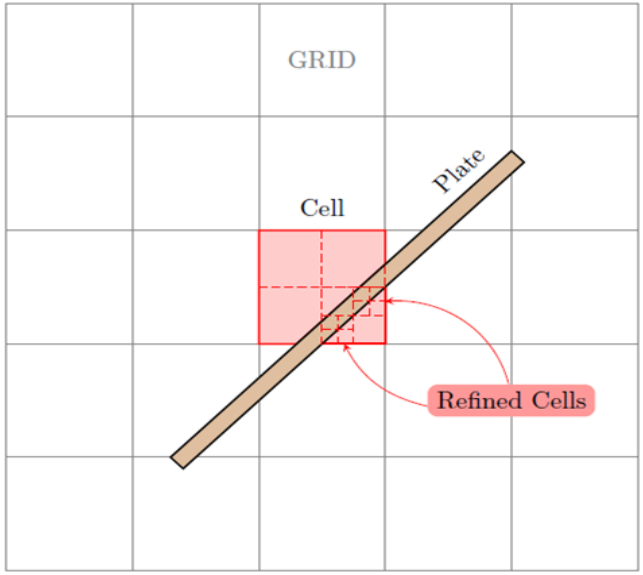


- Green Cells: Cut-cells.
- Red cells: Cells having triangular edges of the surface panels passing through them for reference frame shown.
- No split-cell.
- Fourth level of Refinement in the vicinity of the surface.

Cut-cell - Split-Cells

- **Split-Cell: Cell split into many different flow volumes.**
  - **Different volumes may have different flow properties**
  - **Algorithm calculates linked-list of polyhedrons.**



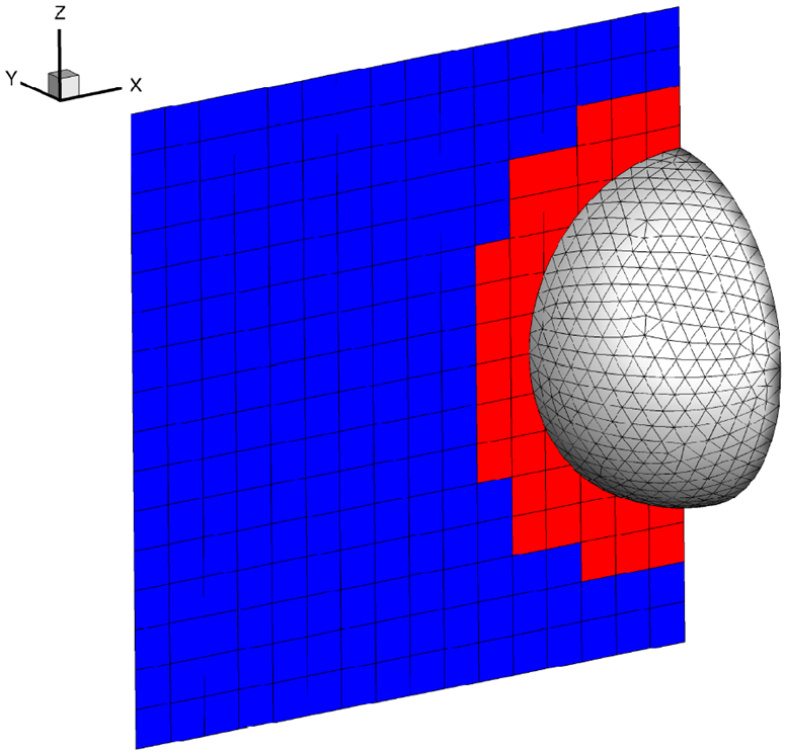


  - **Representation of a split-cell in V-Mesh is difficult.**
    - **Remedy: VTK-Polygon Class or Refinement of the split-cell.**

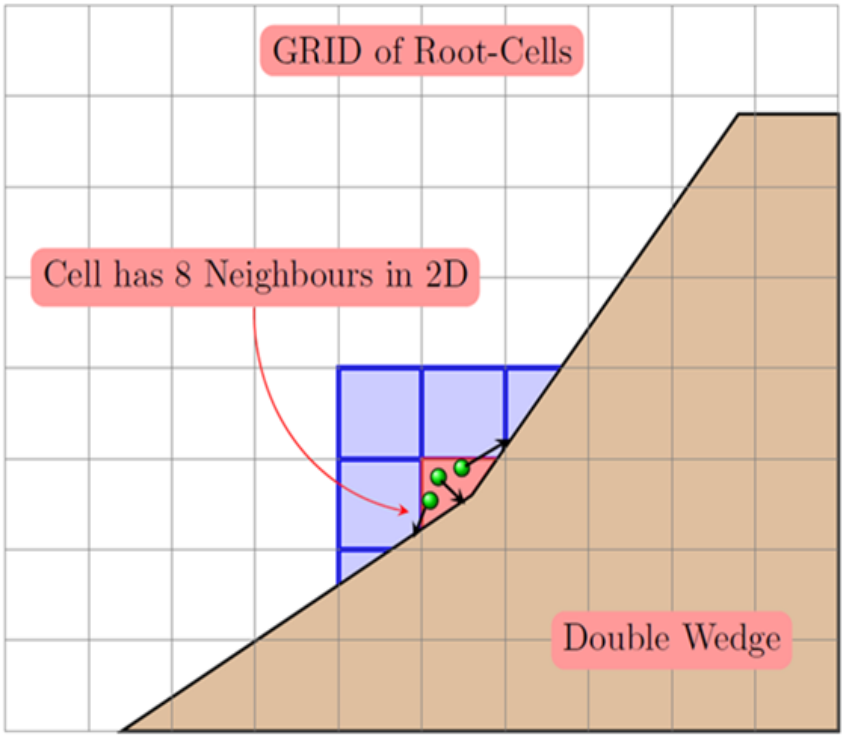
Gas-Surface Interaction (1/2)

- Particle does not keep track of the cells during the movement.
- Hence, each particle has to be checked for the possible collision with the surface. (Very inefficient)

- Efficient way:
  - Fact: Particle never crosses more than one cell in single time step.
  - Tagging the cut-cells and their neighbors. ("NearTheGeometry" ?= 1)
  - Cut-cell check performed earlier on root-cells comes in handy.



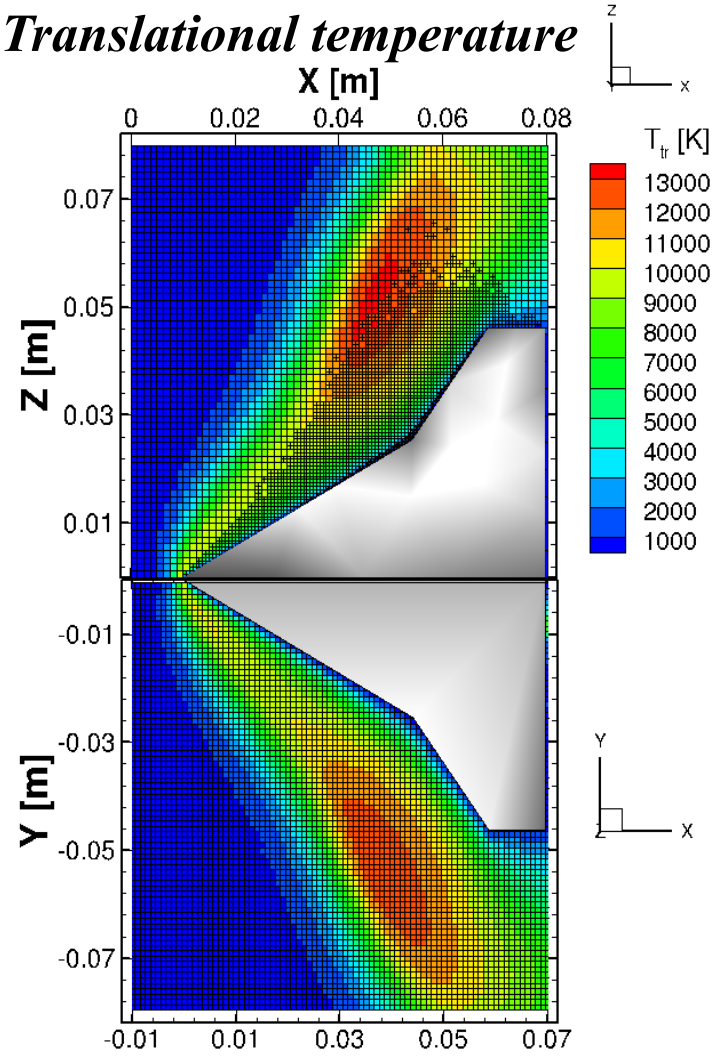
Gas-Surface Interaction (2/2)



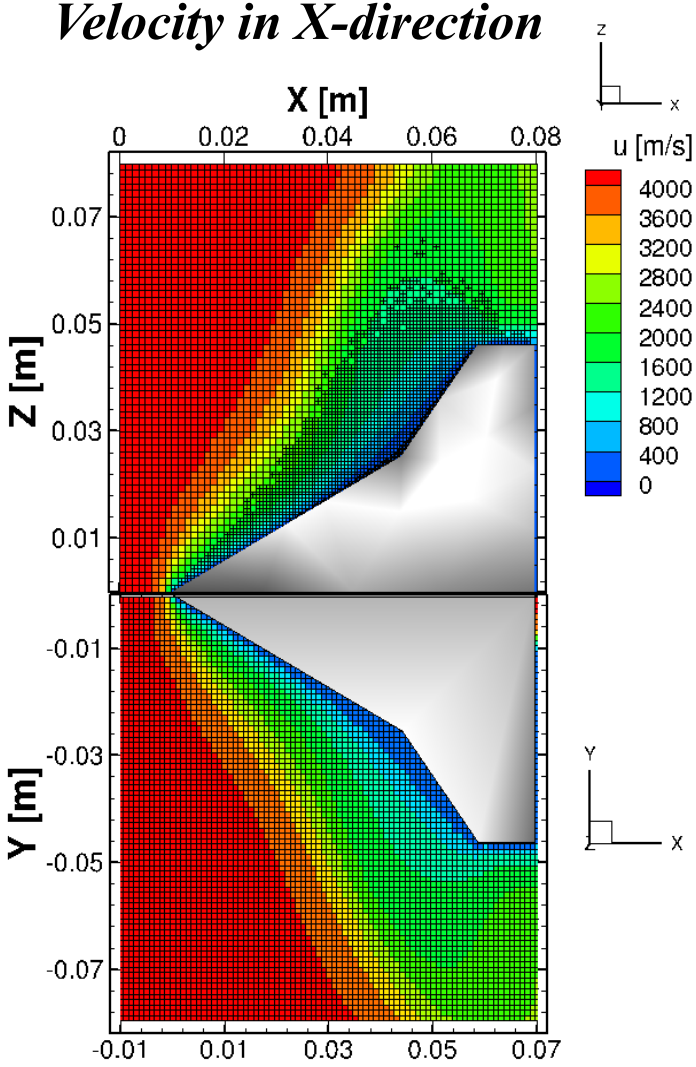
- Further improvement:
  - Instead of looping over all surface triangles, loop over the triangles in the lists of the root cut-cell and its neighboring cells.
  - 38% efficiency improvement for a hemisphere geometry composed of 1400 triangles.
  - Each particle loops over less than 20 triangles for possible intersection.
  - Procedure is trivially parallelizable.

Argon flow over a Double-wedge

Translational temperature



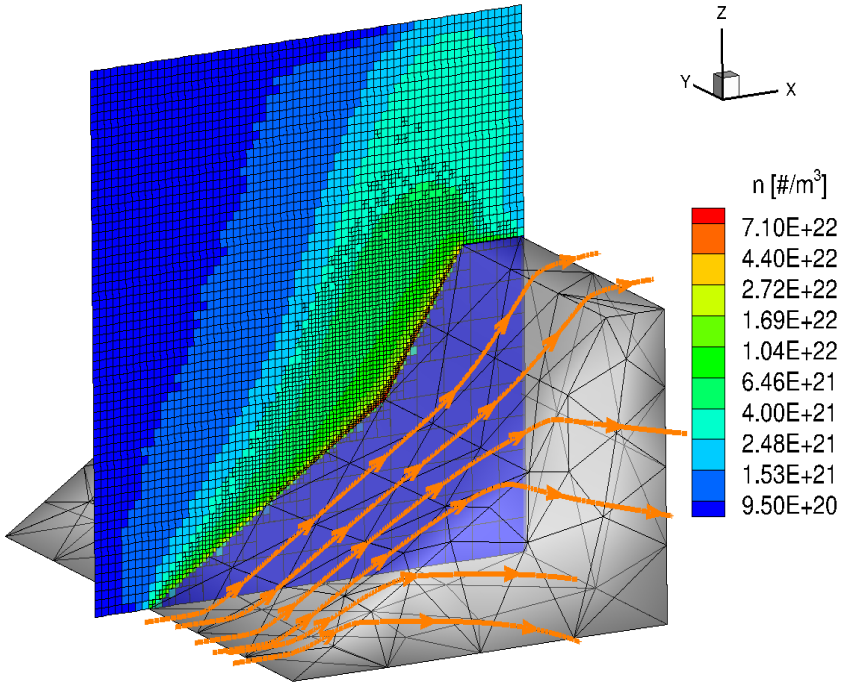
Velocity in X-direction



- Maximum temperature occurs after the bow shock.

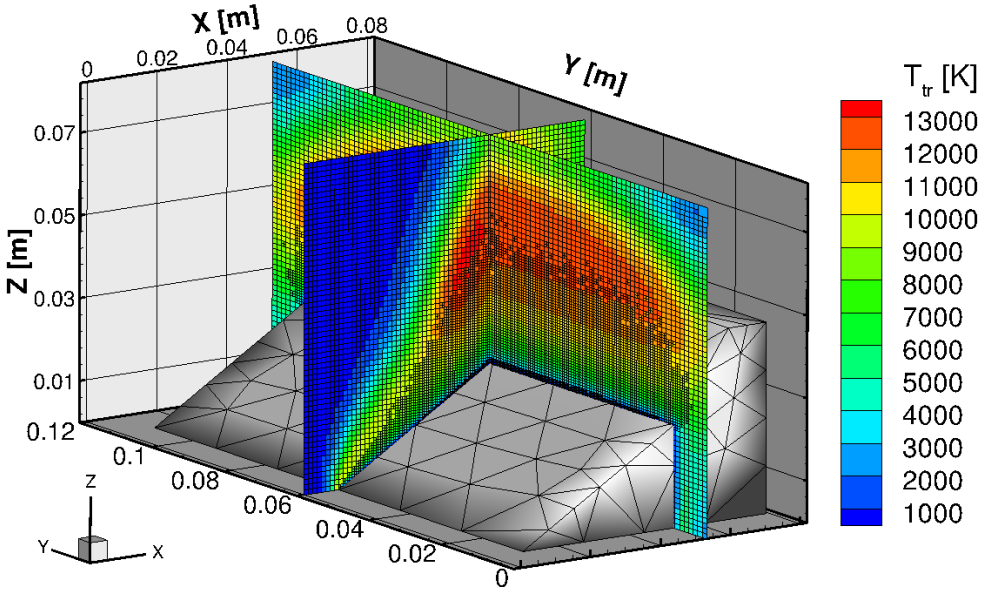
3-D Pressure Relief

Streamlines and Number Density Contour



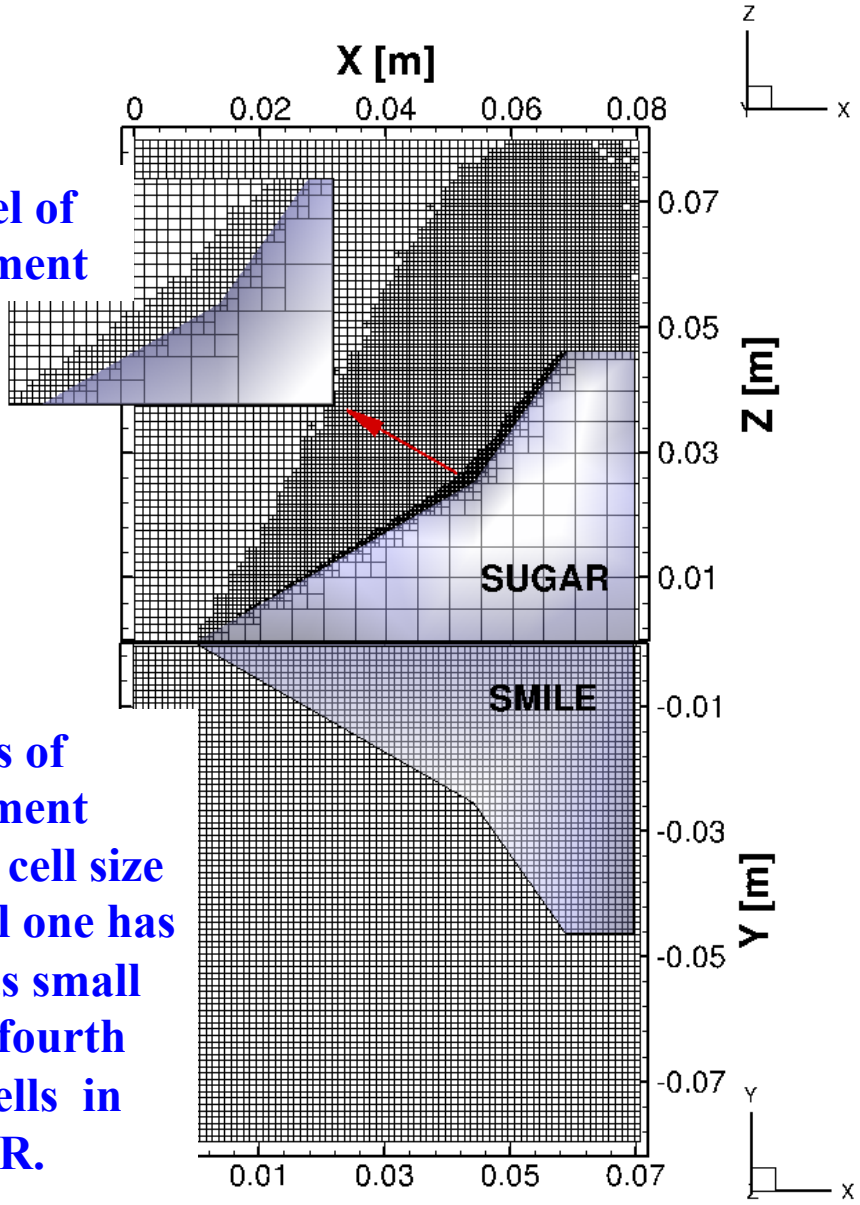
- Number density increases as the flow approaches the surface.
- Streamlines show that the 3-D effects are present.

3-D Effect on Temperature Contours



- Maximum temperature decreases along the span due to 3-D effects.

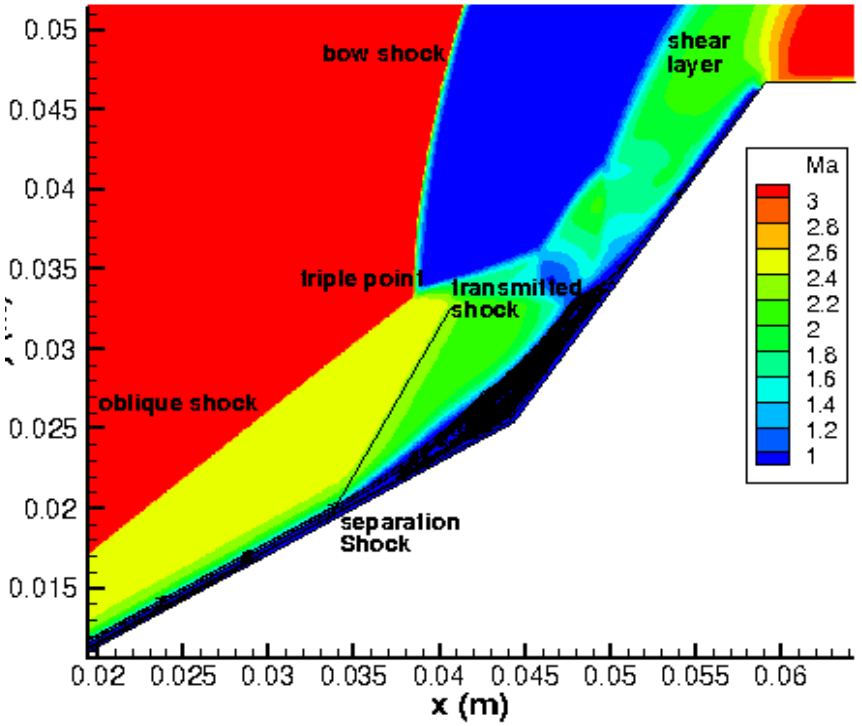
Collision Mesh Comparison



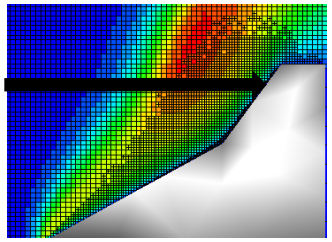
5th level of refinement

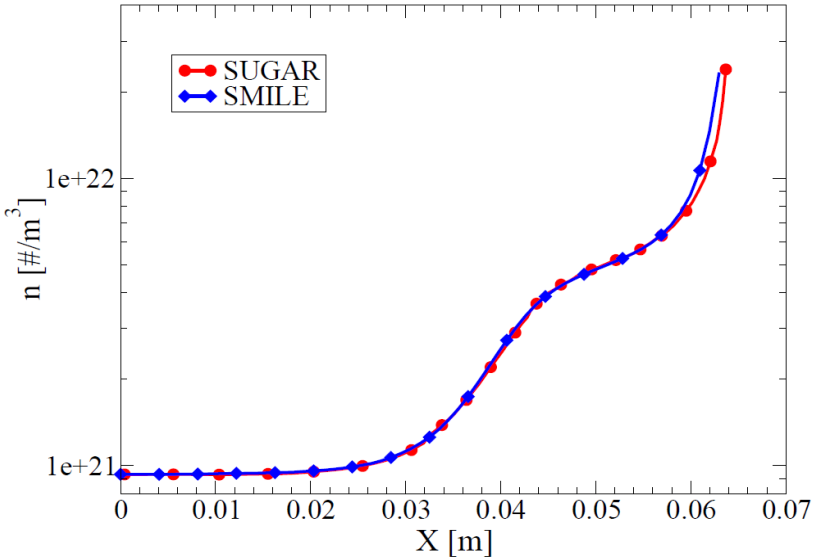
2 levels of refinement means cell size at level one has to be as small as the fourth level cells in SUGAR.

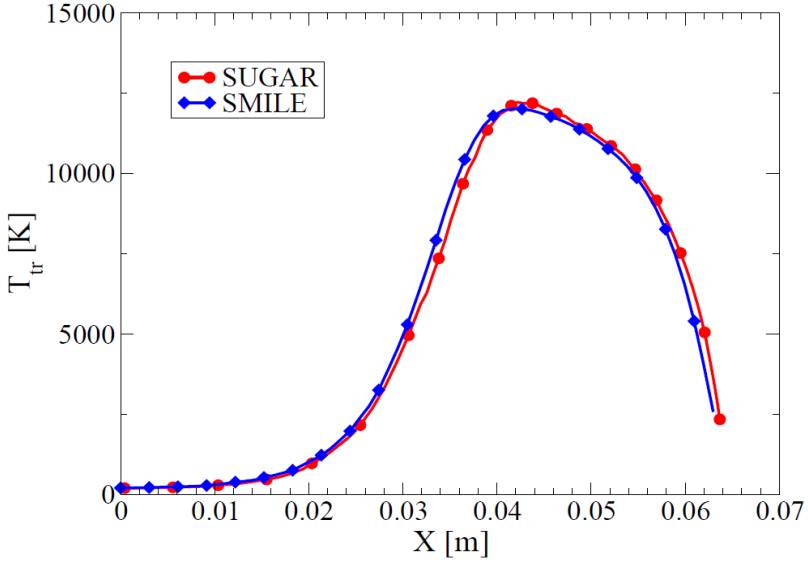
- A fifth level of refinement is observed in the vicinity of the surface.

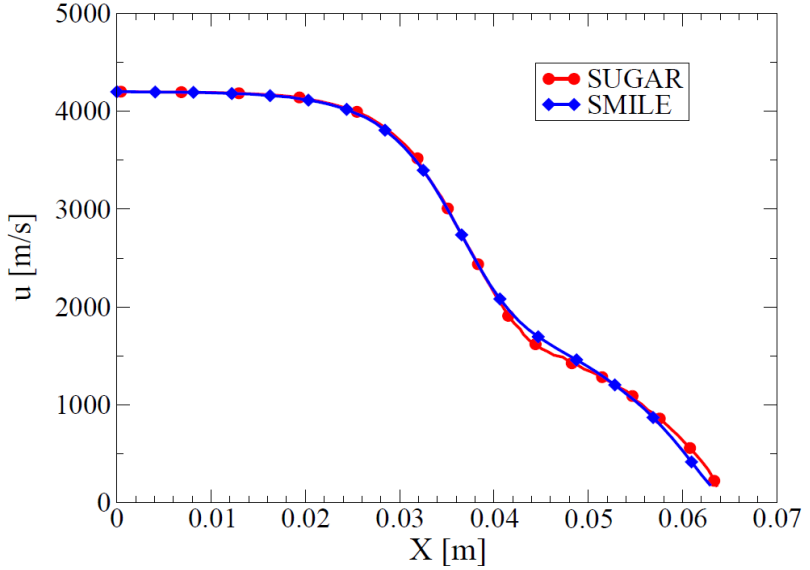


Quantitative Agreement with Physical Collision Models









Observations	SUGAR	SMILE
Smallest Cell Size	6.25E-04	8E-04
Number of Particles	51,990,000	59,850,000
Processors used	256	256
Sampling Time [min]	330	93

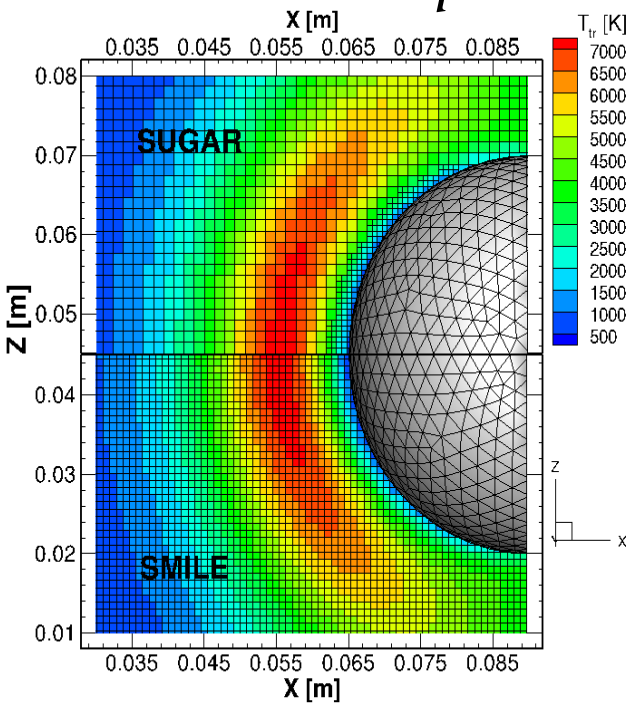
Nitrogen over a Hemisphere-Stronger Shock – Greater Non-equilibrium

Parameters	Value
Number Density	9.33E+19
FNUM	4.0E+09
Freestream Temperature [K]	200
Freestream Velocity	4200
Time step [s]	1.0E-07
Accommodation coeff., α_E	1
Surface Temperature [K]	200
Viscosity Index,	0.74
Rotational Number	15
Number of Samples	20,000

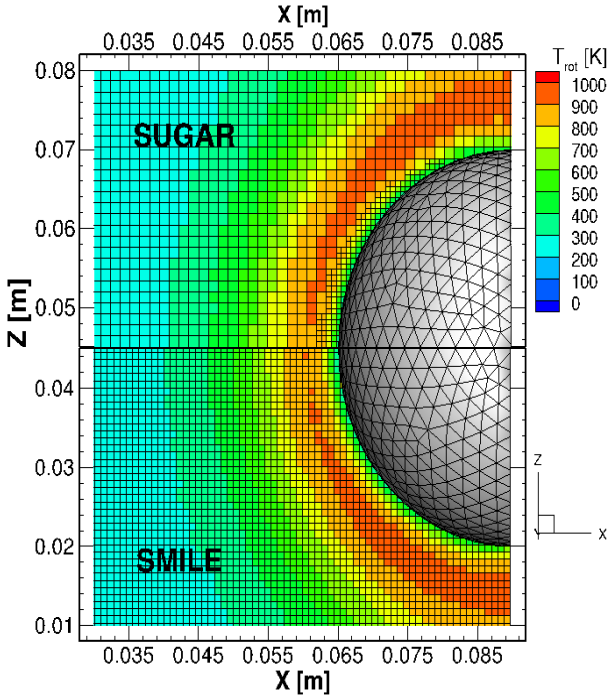
- Mach 14 flow encounters a strong bow shock.
- Knudsen number: 0.27
- High Kn imposes high non-equilibrium condition downstream of the shock.

Comparison of Sugar vs 2 Level Cartesian (SMILE)

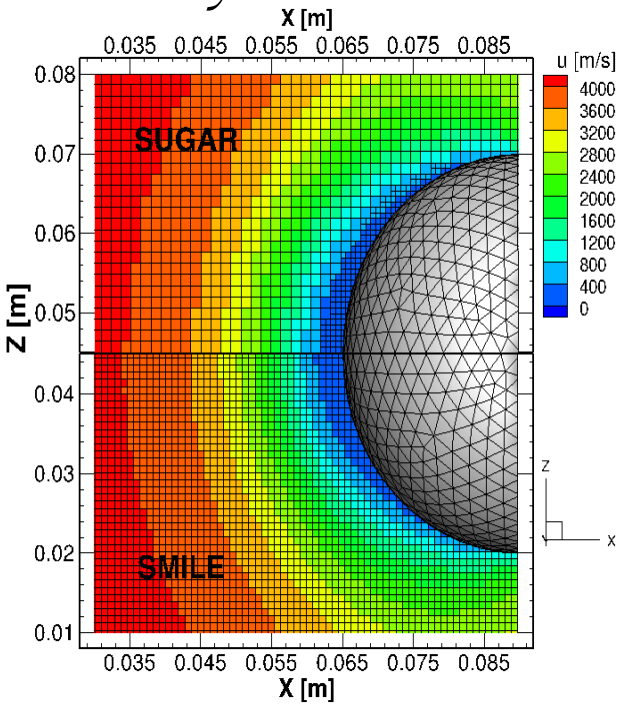
Translational temperature



Rotational temperature

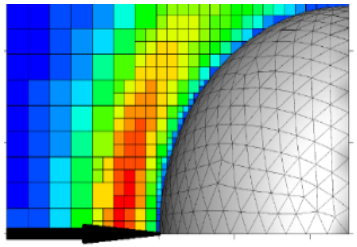


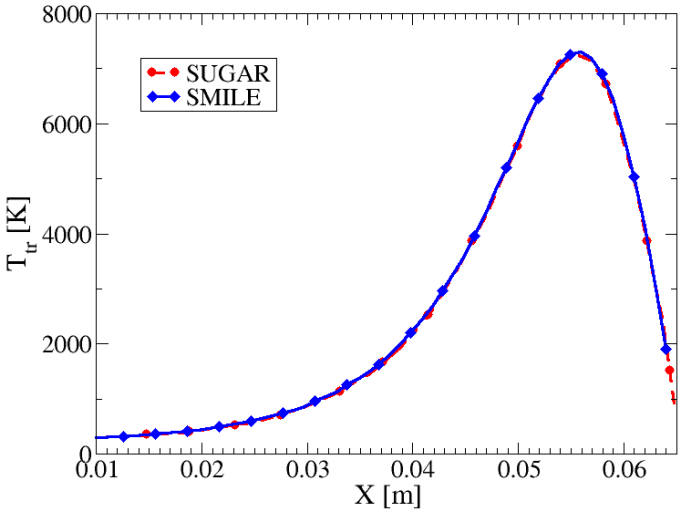
Velocity in X-direction

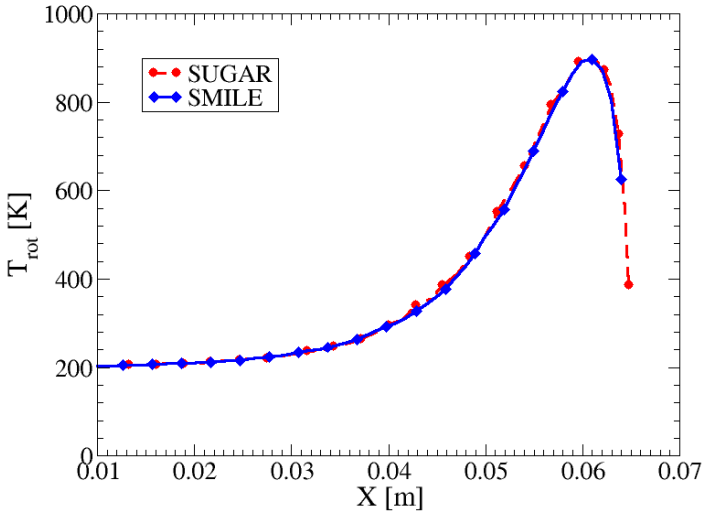


- **Reduced kinetic energy after the bow shock goes into translational and rotational modes.**
- **Particle-surface interaction dominate over particle-particle interaction.**

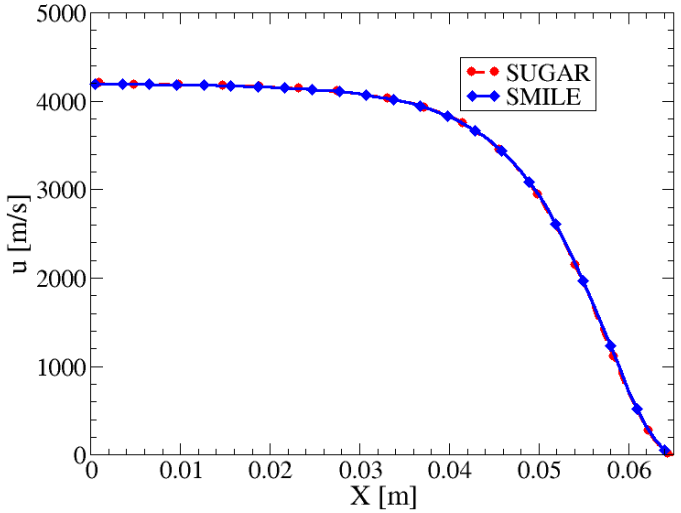
Quantitative Comparison and Numerical Comparisons







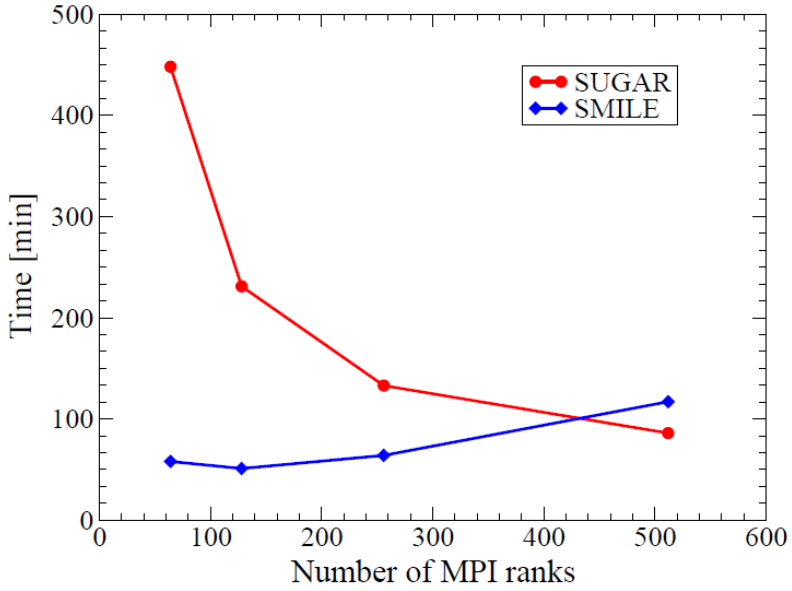
- Temperature slip is well predicted by the SUGAR code due to the finer level of refinement.



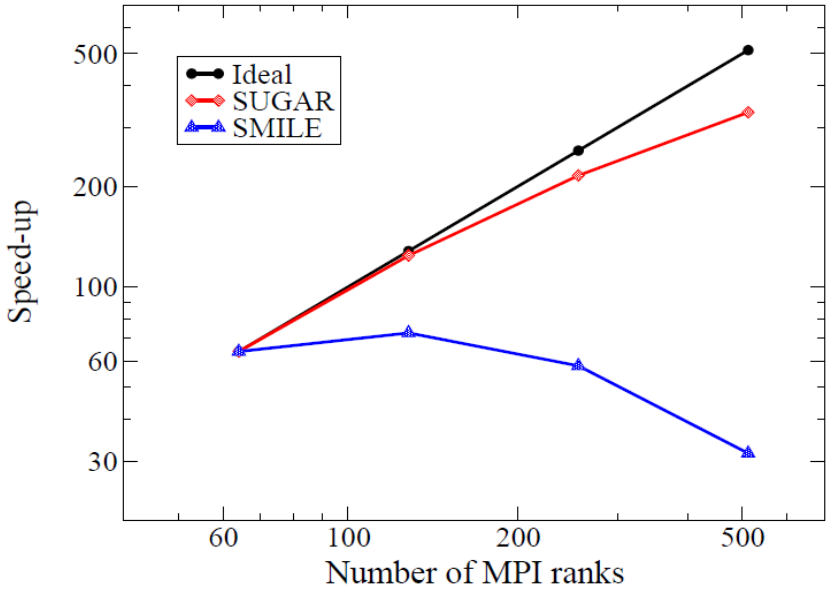
Observations	SUGAR	SMILE
Smallest Cell Size	6.25E-04	9E-04
Number of Particles	22,064,000	23,754,496
Processors used	512	256
Sampling Time [min]	298	56

Ar Flow over Double Wedge – Kn. = 0.02

Timing



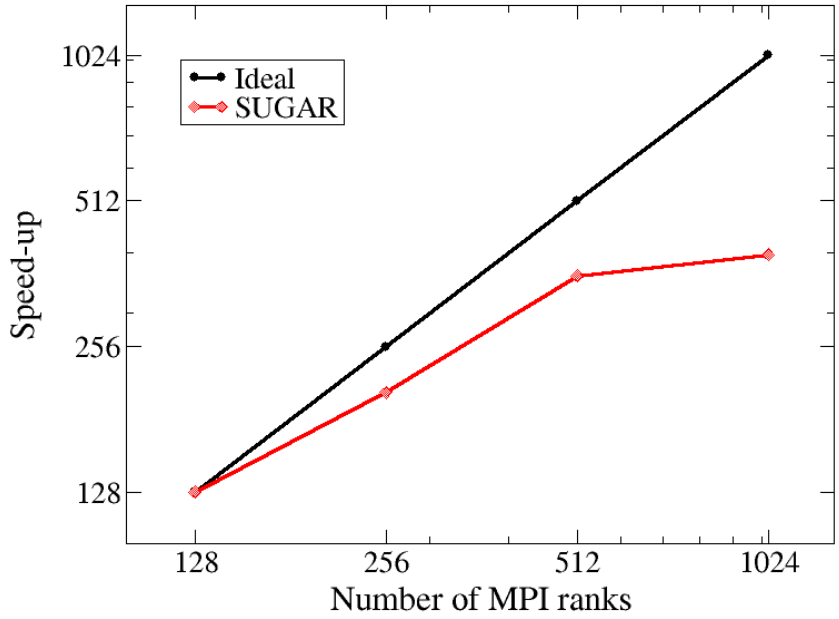
Scalability



- **The SUGAR code gives linear speed-up up to 128 processors and for 512 processors maximum speed-up of 335 - reduction in speed-up is observed for more than 128 processors.**
- **SMILE gives no speed-up beyond 64 processors.**
- **However, time taken by the SUGAR code is higher than that of SMILE for number of processors less than 512.**
- **The major reason for this is that in the SUGAR collision mesh near the surface is more refined.**

Preliminary Speed-up Study – Flow Over a Hemisphere – Strong Shock

Observations	SUGAR
Smallest Cell Size	6.25E-04
Number of Particles	22,064,000
Maximum level of refinement	3
Number of particles per (AMR level 3)	120 (in shock region, close to wall)
Number of particles per cell (AMR level 2)	80 (free stream) 150 (in shock region)



- For 512 processors maximum speed-up of 358 is observed, however, the profile flattens if the number are processors are increased.
- Speed-up decreases because of the load imbalance.
- Load imbalance is mainly caused by the processors that are located near the geometry where domain is much more refined, thus spending more time per step.
- Need to reduce communication time which could be a major bottleneck beyond 512 number of processors.

Acknowledgments

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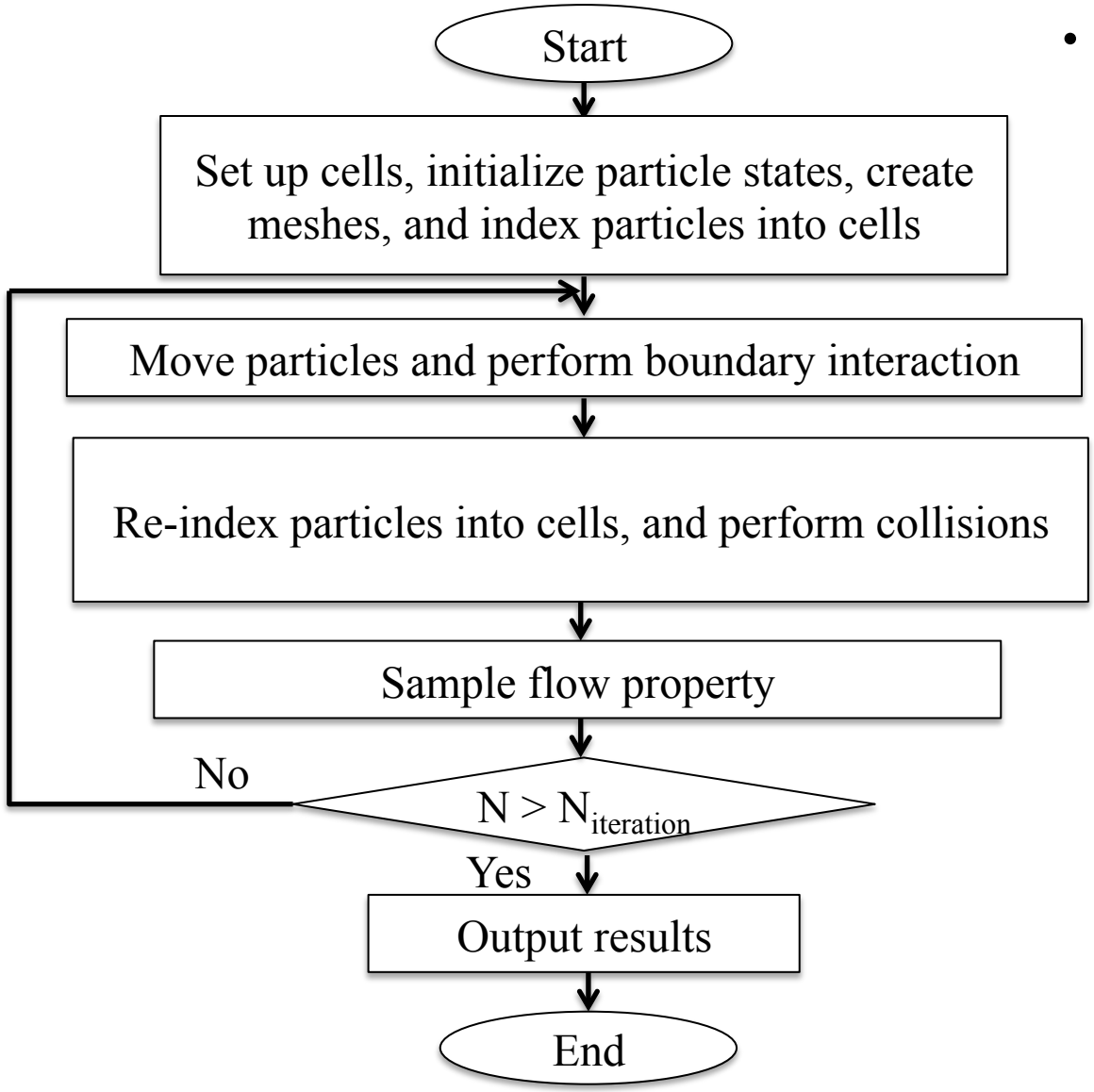
- We gratefully acknowledge the support provided by the Blue Waters sustained-petascale computing project, which is supported by the National Science Foundation (awards OCI-0725070 and ACI-1238993) and the state of Illinois.
- We gratefully acknowledge the support provided by DoD HPC, Drs. Ryan Gosse and Justin Koo.

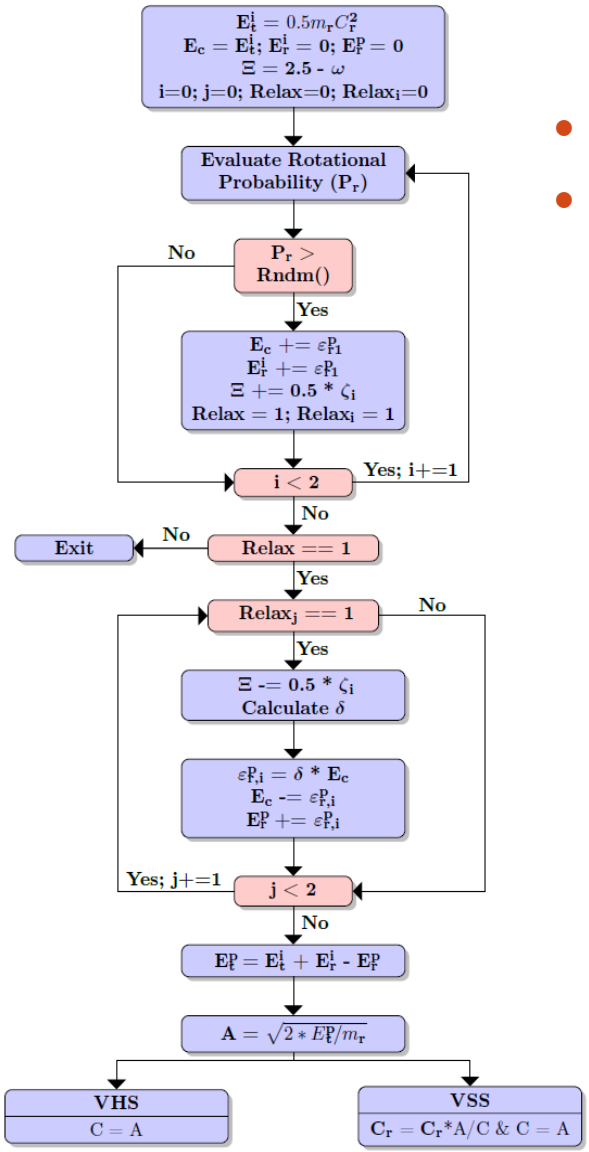
Scalability and Timing

Direct Simulation Monte Carlo (DSMC)



- Key Characteristics of DSMC:
  - Numerical method for rarefied gas flows
  - Particle based probabilistic approach
  - Numerical solution to Boltzmann's equation
  - Decoupling of the movement and collision phase
  - Each computational particle represents many real particles
    - FNUM: number of actual particles represented by a computational particle
  - Various Boundary Conditions

Rotational relaxation model



- Elastic collision models: VHS and VSS
- Inelastic collision model:
  - Borgnakke-Larsen continuous rotational relaxation model
  - Hierarchical implementation*
  - Model follows equipartition theorem.
  - Rotational number can be set as a constant or temperature dependent.
  - Temperature dependence is based on Parker's formula:

$$Z_r^C(T) = Z_{r,\infty} / \left[1 + \frac{\pi^{3/2}}{2} \left(\frac{T^*}{T}\right)^{1/2} + \left(\frac{\pi^2}{4} + \pi\right) \frac{T^*}{T_e}\right]$$

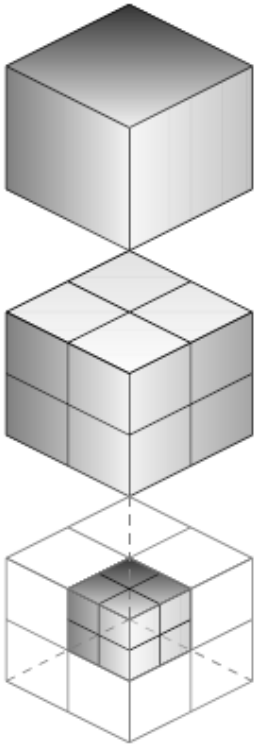
  - Lumpkin's correction is applied:

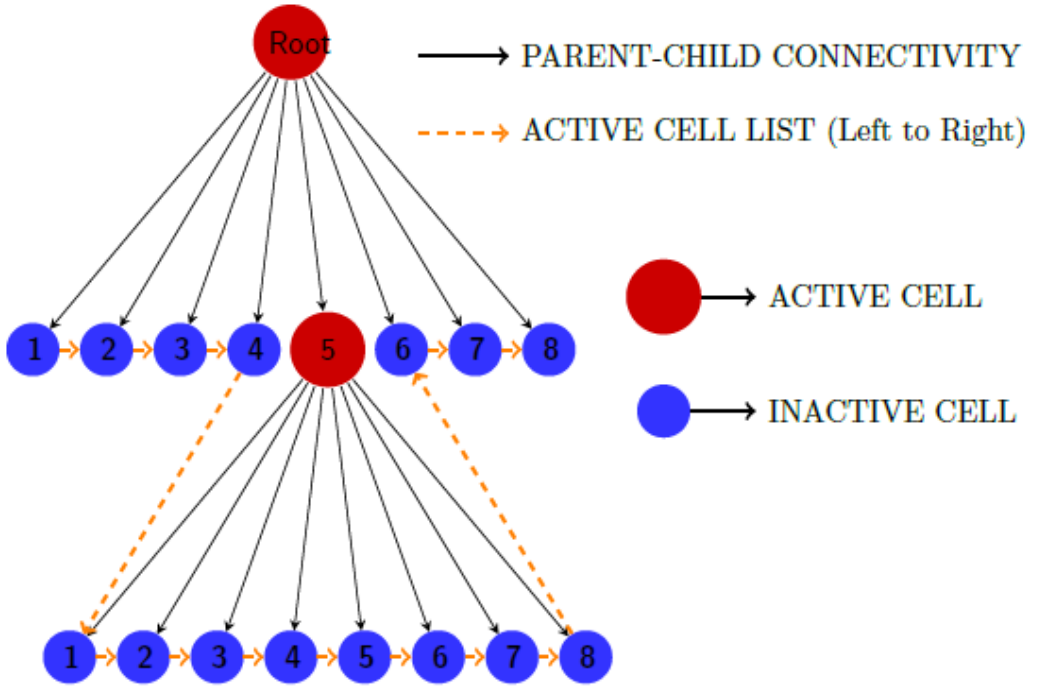
$$Z_r = \zeta_t / (\zeta_t + \zeta_R Z_r^C) \quad \text{and} \quad P_r = 1/Z_r$$

  - δ fraction of the available energy is given to the rotational and translational mode.

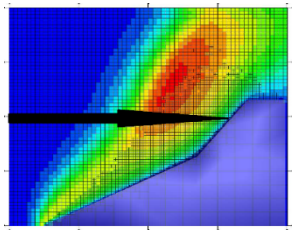
[*] Bird, G., *Molecular Gas Dynamics and the Direct Simulation of Gas Flows*, 1994.

AMR (2/2) – Description of Nodes





- A node is a computational cell.
- Once a cell is refined, a node is deactivated and 2^d (d=number of dimension) children nodes are created.
- Node without any child is a leaf; Node without any parent is a root.



Outline

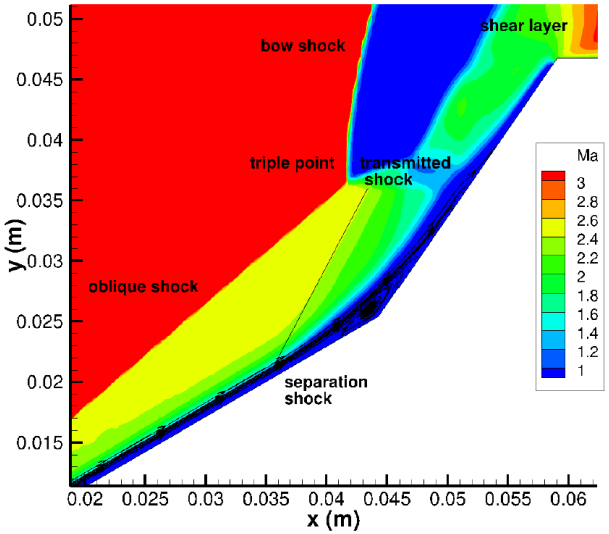
- Introduction
  - Numerical Approach
  - Adaptive Mesh Refinement
  - Parallelization Strategies
  - Cut-cell Approach
  - Reflection and Optimization in MPI-Parallelized Domain
  - Heat Flux Computation
- Results
  - Argon Flow over Hemisphere
  - Argon Flow over Double-Wedge
  - Heat Bath Study of a Simple Gas
  - Nitrogen Flow over Hemisphere
  - Scalability Study
- Conclusion
- Future Work

Previous Work

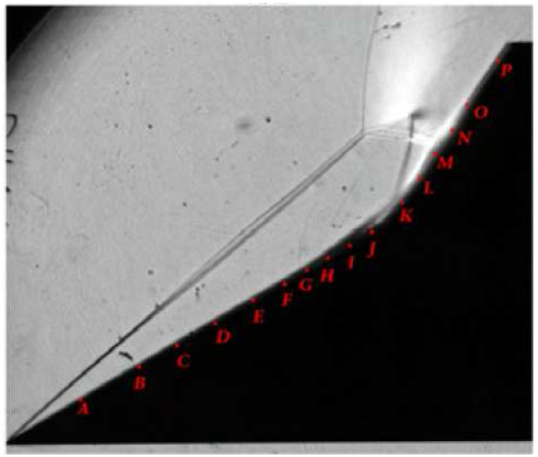
- Double-Wedge simulations using SMILE by Tumuklu et al.
- Experiments on a the double-wedge by Austin et al.
- Adaptive Mesh Refinement
  - Pioneer Work, Berger et al(1989)
  - Kolobov et al(2012), within DSMC context
- SUGAR Framework (DSMC & PIC) applied to expansion cases by Korkut *et al (2012).*
- Present work focuses on simultaneous implementation of the above.

Introduction

Shock interaction simulated by Tumuklu et al. using SMILE



Schlieren study performed by Swantek et al.



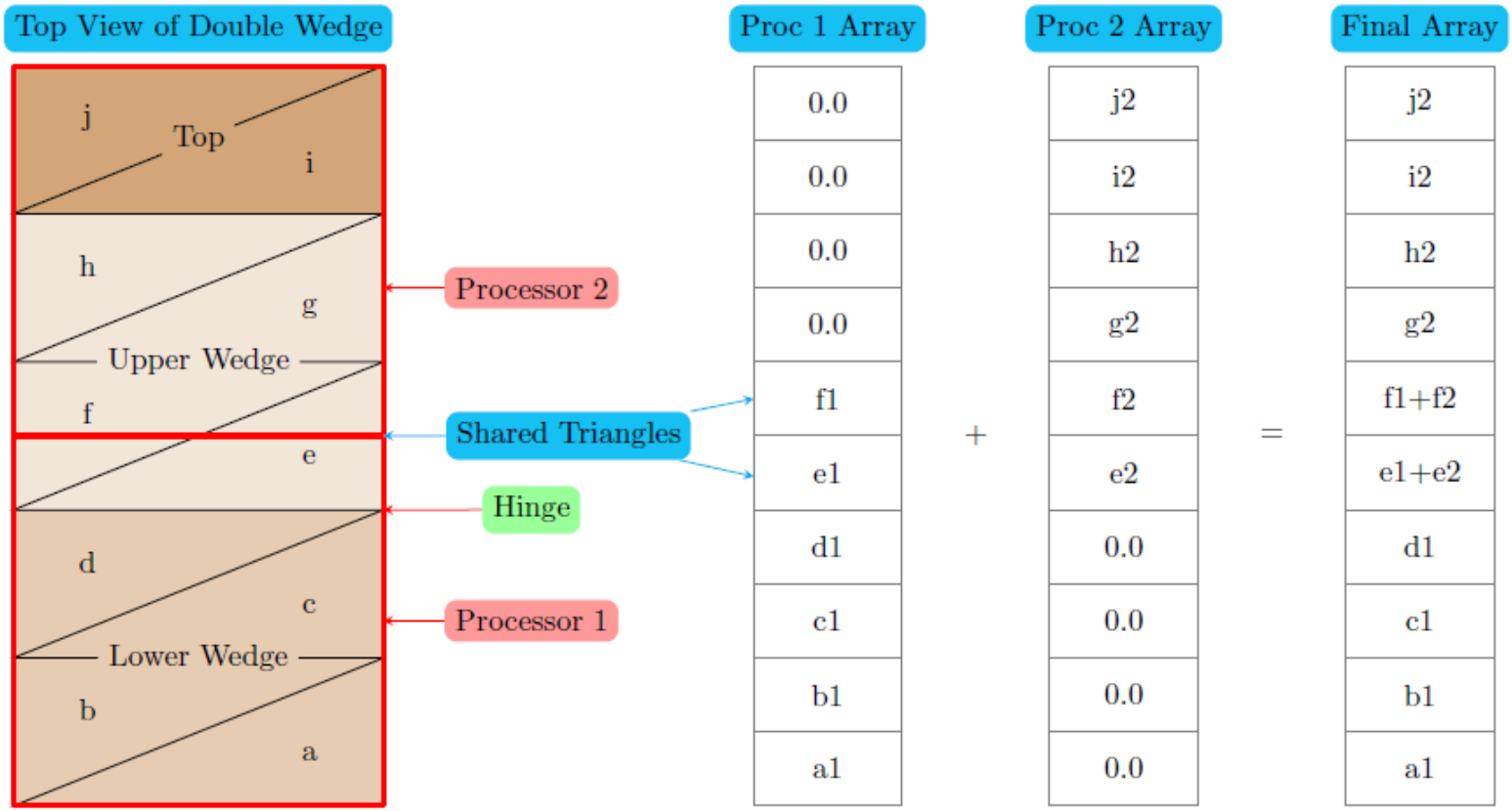
- Flow over a double-wedge is challenging because of:
  - Multiple shock-shock, shock-boundary layer interactions
  - Transition from laminar to turbulence
  - Three-dimensional effects
  - Sheer layer
  - Separation near the hinge
- These effects significantly impact aero-thermodynamics of the flow such as pressure loads, heat transfer rate, and skin friction.
- Accurate prediction of these effects has direct application in scramjet inlet design.
- These cases are computationally expensive because of the multi-scale phenomena.
- Experiments have been performed in continuum-like conditions.

Role of Grids in DSMC

- Two essential grids
  - Collision Mesh (C-Mesh)
    - Particle pairs are selected for potential collisions and momentum and energies are modified accordingly.
  - Visualization Mesh (V-Mesh)
    - Distributions are calculated to obtain macro parameters such as velocity, temperature and density.
- A flexible mesh that can capture the domain in an efficient and flexible way.
- Previous efforts:
  - SMILE System: two-level Cartesian grid.
  - NASA's DAC: two-level rectilinear grid; adaptation based on previous flow solution.
  - MGDS: adaptive mesh refinement up to three levels of Cartesian grid.
  - MONACO: unstructured body-fitted quadrilateral/tetrahedral meshes.
  - dsmcFOAM (open-source): unstructured polyhedral meshes.
- Adaptive Mesh Refinement with unlimited refinement along with an emphasis on octal trees is a great choice to capture multi-scale physics.

Heat Flux Computation

- How to compute heat flux of the triangles shared by processors?



Eg., a1= Coeff. of panel 'a' calculated by processor 1

Results

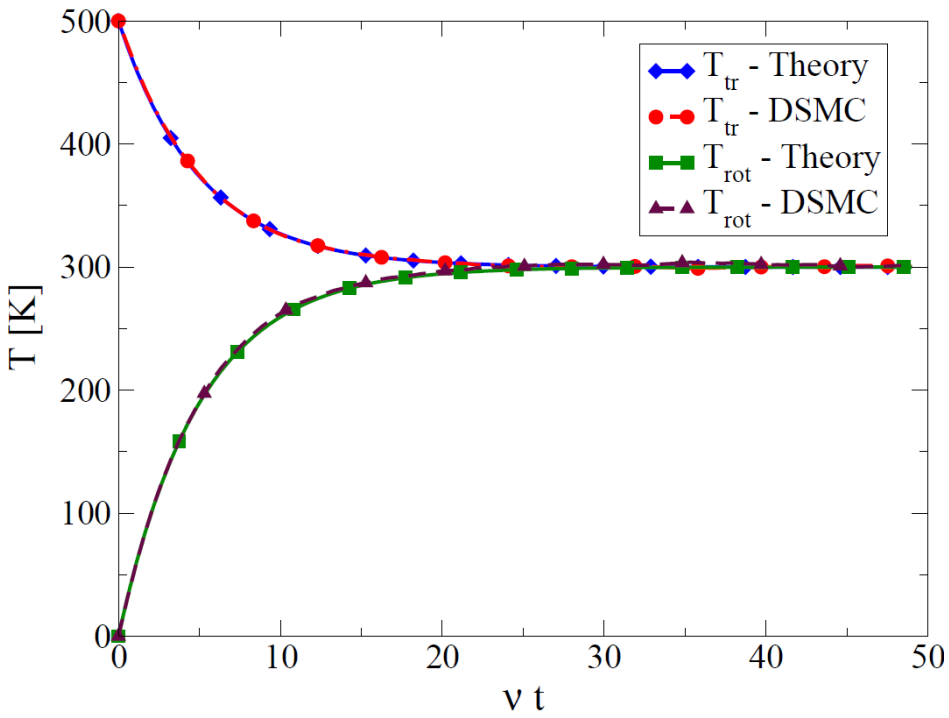
Case-III: Heat bath

- Serves the purpose of
  - validating the Borgnakke-Larsen continuous rotational relaxation model implemented in the SUGAR code.

Case-III – Heat Bath Study of a Diatomic Gas

Numerical Parameters	Value
Number Density	1.0E+20
FNUM	1.0E+11
Time step [s]	2.0E-05
Mass [Kg]	5.0E-26
S	3.5E-10
	1
Rotational Degrees of Freedom	2
Viscosity Index,	0.75
Rotational Number,	5
Timesteps for relaxation	100
Sampling Start	100
Number of Samples	900
Simulation Domain [m]	1 x 1 x 1

Temporal rotational relaxation



- Theoretical Expressions,
  - $T\downarrow tr = 300 + 200 e\uparrow - \nu t / Z\downarrow r$
  - $T\downarrow rot = 300\ \{1 - e\uparrow - \nu t / Z\downarrow r\ \}$

- **Boltzmann equation:**

$$\frac{\partial f_1}{\partial t} = -\dot{\vec{q}}_1 \cdot \frac{\partial f_1}{\partial \vec{r}} + \int d\vec{p}_2 \int d\Omega g \sigma(\theta, g)\left(f_{1'} f_{2'} - f_1 f_2\right)$$

= flux thru CV, ΔV1 + change due to collision in/out of CV

- **The DSMC is a numerical method for solving the Boltzmann equation, under the assumption of a dilute, binary "gas":**

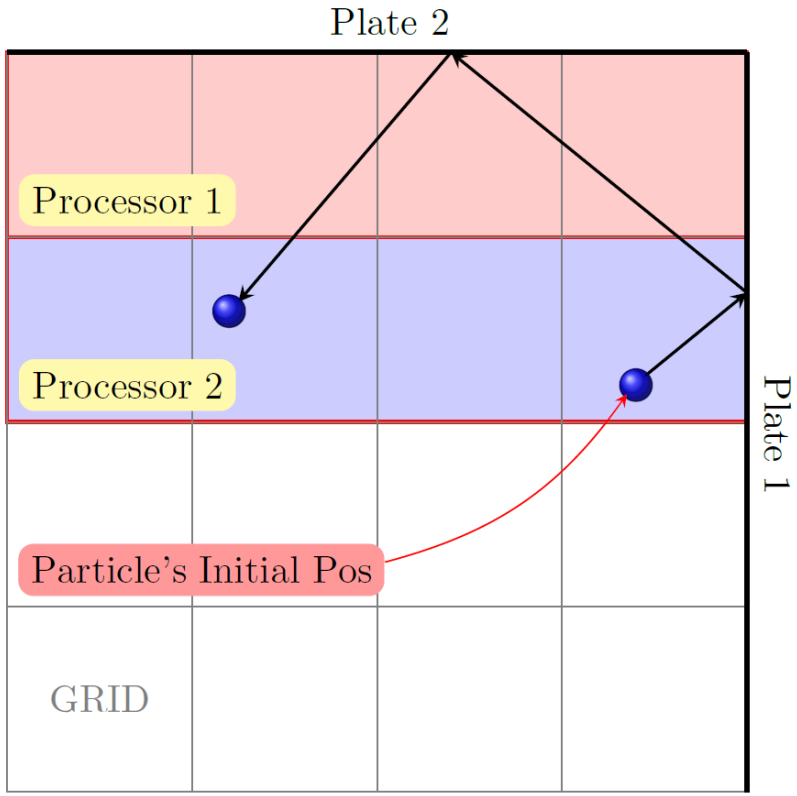
Robust Cut-Cell Approach (1/3)

- The code reads in a triangulated surface geometry
  - STL format
  - Normal of surface triangles should point outward.
- Two main functions:
  - Geometric Sorting: Organizing list of triangles in leaves of Octree.
    - Intersection of cell edges with the triangles using signed tetrahedral volume approach.
    - Crude way: Checking each triangle with each leave cost O(M*N).
    - Efficient way: using the inherent recursion in tracing the leaves.
  - Volume Computation of a cell cut by the geometry
    - Accurate Volume ➡ local number density ➡ local mean free path refinement criteria for the C-Mesh ➡ physics near the geometry.
    - Accurate Volume ➡ collision frequency for the cell ➡ gas-surface interaction.
    - Formation of the part of the cut-cell lying in the flow domain (polyhedron formation).
    - Algorithm is based on the implementation in DAC and MGDS code.*

[*] Zhang, C. and Schwartzentruber, T. E., "Robust Cut-cell Algorithms for DSMC Implementations Employing Multi-Level Cartesian Grids," Journal of Computers and Fluids, Vol. 69, October 2012, pp. 122-135.

Gas-Surface Interaction (3/3)

- Consideration during multiple reflections in a single timestep.
- Advantageous to broadcast the entire geometry to each processor at the start of the simulation.
- Saves communication efforts.
- In this case no communication is needed.



Verification and Validation

Case 1: Argon over a Hemisphere

- Serves the purpose of validating
  - the DSMC procedure
  - elastic collision model (VHS)
  - majorant frequency scheme
- All the results are compared with the 3-D version of the SMILE code written in Fortran.
- These cases are run at a Knudsen number much higher than the actual experimental conditions.

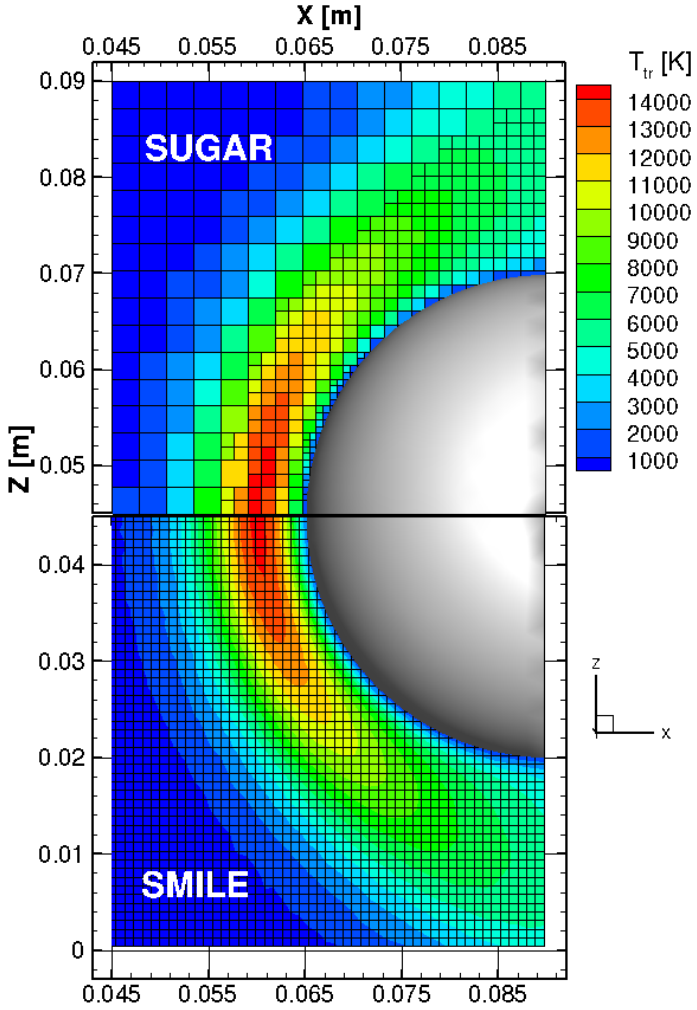
Case-I (1/3) – Input conditions

Parameters	Value
Number Density	9.33E+20
FNUM	0.25E+11
Freestream Temperature [K]	200
Freestream Velocity	4200
Time step [s]	5.0E-08
Accommodation coeff.	1
Surface Temperature [K]	200
Viscosity Index,	0.84
Number of Samples	12,000

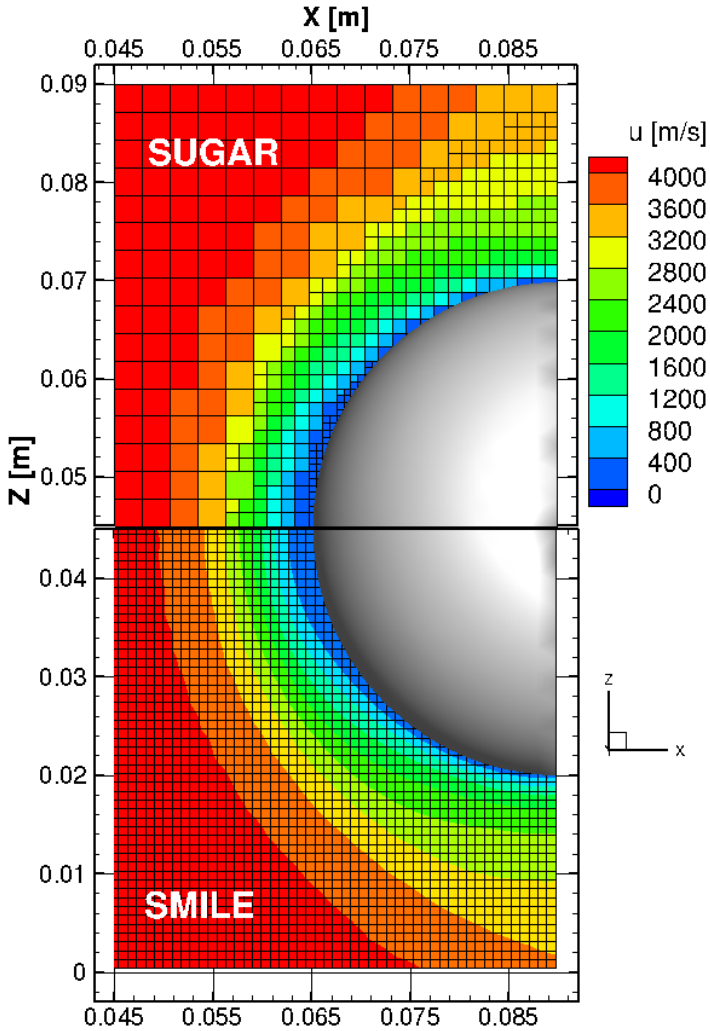
- Mach 14 flow encounters a strong bow shock
- Knudsen number: 0.02

Case-I (2/3) – Contour Plots

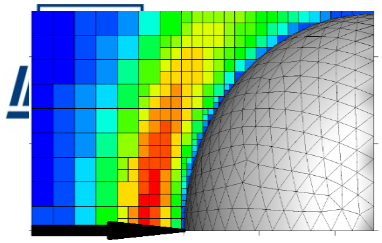
Translational temperature



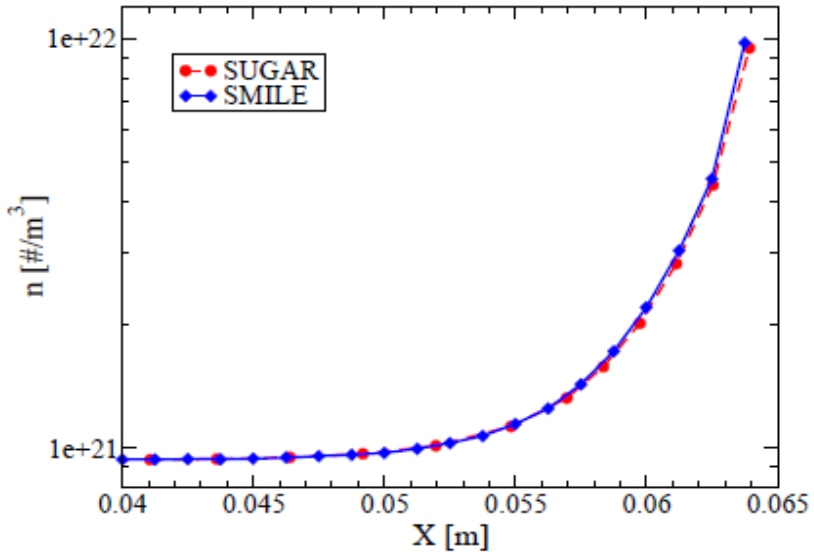
Velocity in X-direction

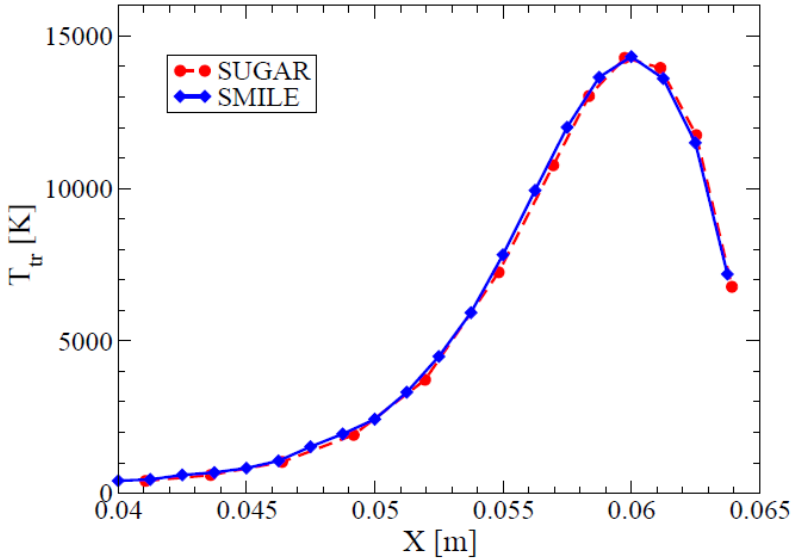


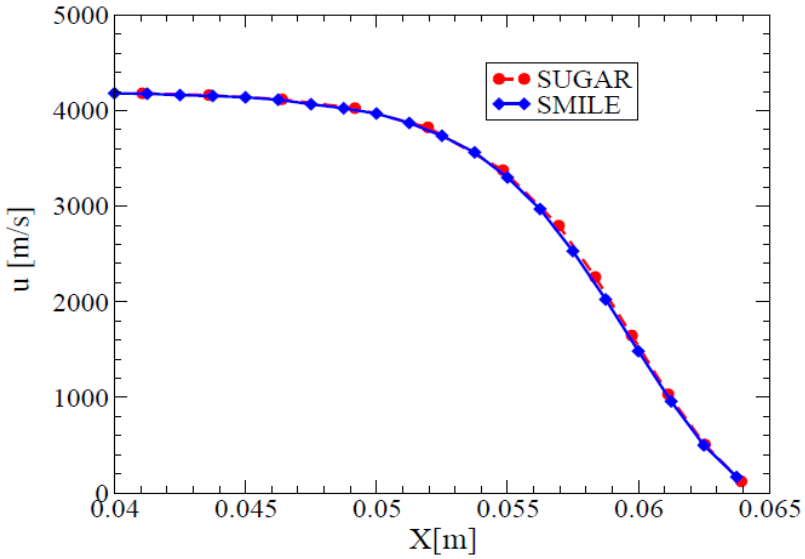
- Plots are shown on the V-Mesh.
- Shock stand-off distance is: 0.015 m
- SUGAR mesh refines only in the vicinity of the surface.
- Contour plots are in good agreement.
- SMILE results look smooth because of the interpolation done by the Tecplot on a uniform mesh.



Case-I (3/3) – Line Plots and Observations







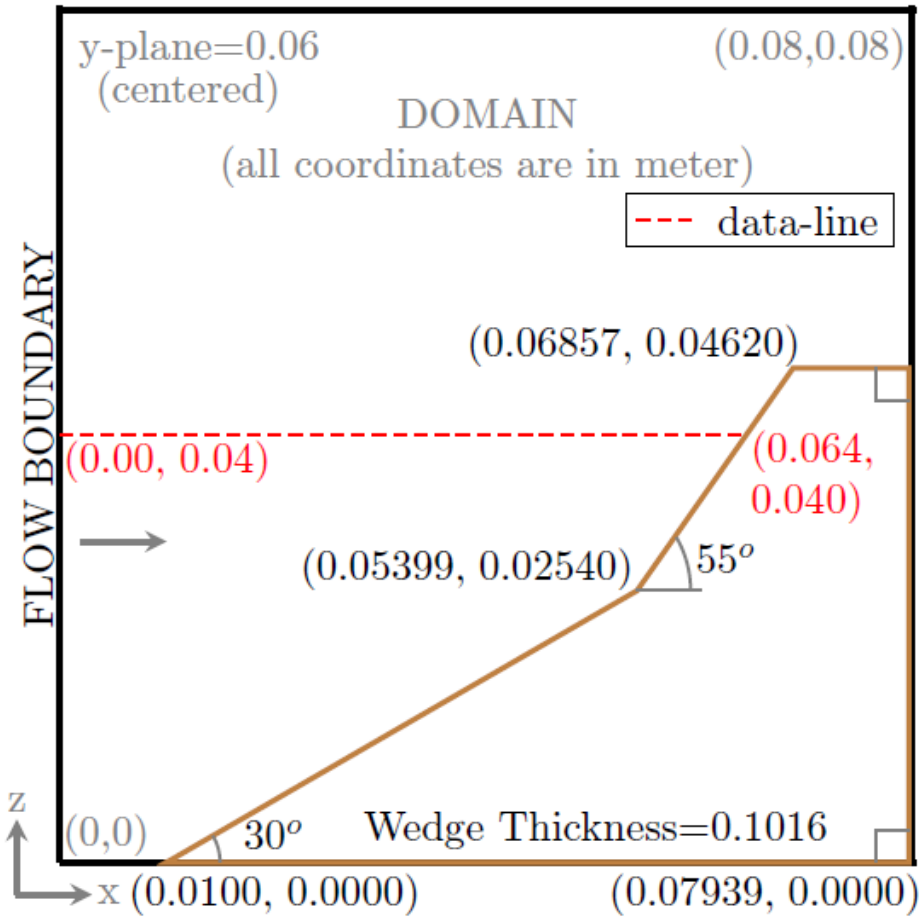
Observations	SUGAR	SMILE
Smallest Cell Size	7.0132E-04	9E-04
Number of Particles	12,709,000	17,608,704
Processors used	256	256
Sampling Time [min]	262	66

Case-I (1/3) – Input Conditions

Parameters	Value
Number Density	9.33E+19
FNUM	4.0E+09
Freestream Temperature [K]	200
Freestream Velocity	4200
Time step [s]	1.0E-07
Accommodation coeff.	1
Surface Temperature [K]	200
Viscosity Index,	0.74
Number of Samples	22000

- Mach 14 flow encounters a strong bow shock.
- Knudsen number: 0.2
- High Kn impose high non-equilibrium condition after the shock.

Case-II (1/5) – Problem Definition



Schematic of the Double-Wedge

- For encounters an oblique shock caused by the lower wedge and a bow shock formed by the upper wedge.
- Both the shocks meet at the triple point.
- Freestream conditions, Knudsen number and sampling period are the same as used for the case-I except for the FNUM, which is 0.25E+11.
- Knudsen number: 0.02

Conclusions

- Octree based DSMC approach proves to be advantageous for resolving small scales with relatively less computational efforts.
- The cut-cell approach gives the exact volume and even applicable where the split-cells are involved.
- The algorithm for improving particle-surface interactions gives efficiency of 38%.
- Broadcasting the geometry proves to be advantageous:
  - Saves communication in case of multiple reflections.
  - East in computation of surface coefficients in a MPI parallelized domain.
- The code is validated for accurate implementation of the DSMC method, majorant frequency, and elastic collision model by simulation the 14 Mach argon flow over a hemisphere.
- Preliminary results for the simulation of argon flow over a wedge successfully reproduced the flow characteristics such as an oblique and bow shock interaction.
- The code resolves the important regions near the surface of a double wedge.
- The code can accurately simulate diatomic gases using Borgnakke-Larsen continuous relaxation model.
- The code is slower than SMILE because of uneven load balancing caused mainly by the gas-surface interactions.
- The code is scalable.

Future Work

- Small spatial discrepancy in the nitrogen relaxation process in a flow over a hemisphere at Knudsen number 0.2 will be investigated in detail.
- The code will be applied to the cases involving continuum-like Knudsen number (0.0002) in a flow of nitrogen, argon, and air over a double-wedge configuration and compared with the SMILE and experimental results.
- Better relaxation models will be implemented.
- Better load balancing algorithm will be implemented that makes use of a graph-partitioner for domain decomposition.
  - Preliminary study done by Korkut et al. for an expansion case has shown promising results.
- Hybrid parallelization using OpenMP and GPUs is being explored for improving the performance and make use of new generation of computer architectures.