Understanding DSMC, SPARTA and results from simulating 1D Fourier flow using SPARTA

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1. Direct Simulation Monte Carlo
   - General information
   - The algorithm
2. Existing Literature
3. 1D Fourier Flow using SPARTA
4. References

General Information

- The DSMC method is used whenever the Knudsen number is of the order of 1. For example, it is used in MEMS and Space Shuttle re-entry aerodynamics

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- It models fluid flows using probabilistic simulation molecules to solve the Boltzmann equation
- DSMC is better at describing the non-equilibrium behaviour of gases than most continuum models such as Navier-Stokes through higher fidelity[2]

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The algorithm

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- If a particle reaches a boundary, it's position and velocity are reset accordingly

The algorithm (boundary collisions)

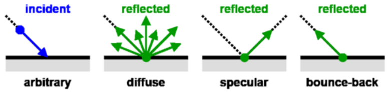

Fig. 1: Various types of boundary collisions

- The specular boundary collision is simply the preservance of the angle between the normal and the particle trajectory just before and after collision

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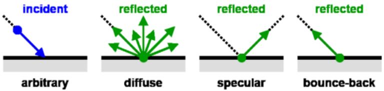

Fig. 1: Various types of boundary collisions

- The specular boundary collision is simply the preservance of the angle between the normal and the particle trajectory just before and after collision
- Diffuse boundary collisions are when there is a degree of randomness (α) in the specularity of the collision

The algorithm

- After all particles are moved, they are put into cells within which they randomly collide based on collision rates and probabilities obtained from the kinetic theory of gases

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- After all particles are moved, they are put into cells within which they randomly collide based on collision rates and probabilities obtained from the kinetic theory of gases
- The dimension of each collision cell is no longer than a mean free path. All particles in a cell are collision candidates, regardless of their actual trajectories
- For the **hard spheres** collision model, the collision probability for the pair of particles i and j is proportional to their relative speed,

$$P_{coll}[i,j] = \frac{|\vec{v}_i - \vec{v}_j|}{\sum_{m=1}^{N_c} \sum_{n=1}^{m-1} |\vec{v}_m - \vec{v}_n|}$$

N_c is the number of particles in the cell

The algorithm

- The double summation in the denominator can be computationally intensive, so a technique called **rejection sampling** is used to select collision pairs

$$v_r > v_{r_{max}} \cdot \mathcal{R} \text{ for } \mathcal{R} \in [0, 1]$$

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$$v_r > v_{r_{max}} \cdot \mathcal{R} \text{ for } \mathcal{R} \in [0, 1]$$

- The total number of hard sphere collisions given in a cell during a time 'τ' is given by

$$M_{coll} = \frac{1}{2}(N_c - 1)F_N f_{coll}\tau = \frac{N_c(N_c - 1)F_N \pi d^2 \langle v_r \rangle \tau}{2V_c}$$

where f_{coll} is the collision frequency given by KTG, d is the diameter of the cell and V_c is the volume of the cell

1. Direct Simulation Monte Carlo
2. Existing Literature
   - DSMC on petaflop supercomputers and beyond [2]
   - Effect of slip on vortex shedding from a circular cylinder in a gas flow [1]
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SPARTA

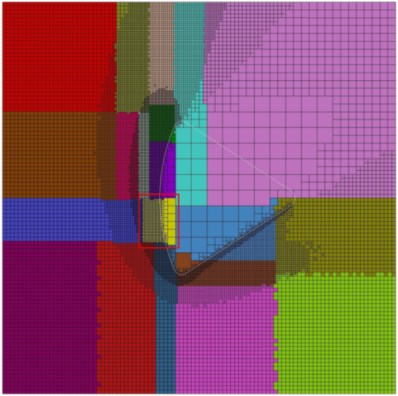
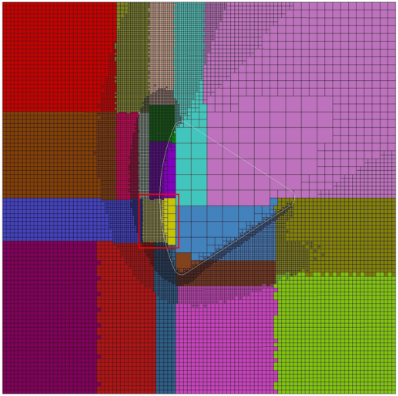


Fig. 2: Grid Hierarchy in SPARTA

- DSMC is inherently parallel. It has three kinds of elements : particles, grid cells and surfaces

SPARTA



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- Grid cells are indexed hierarchically using bits. Cells store information about everything within them

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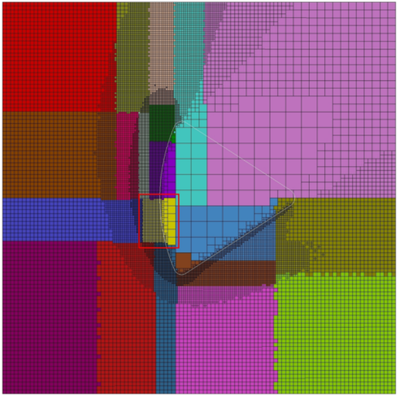

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- Grid cells are indexed hierarchically using bits. Cells store information about everything within them
- Each processor owns **ghost cells** that extend beyond its domain to minimize MPI calls during the run

SPARTA

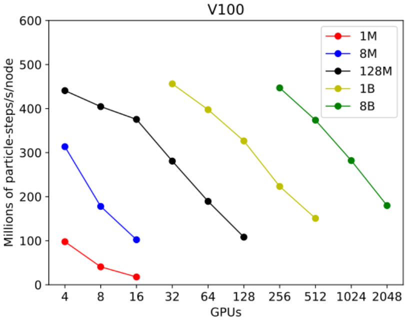
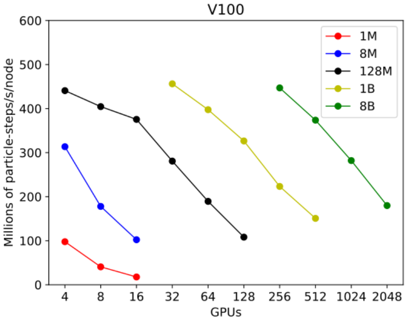


Fig. 3: GPU Parallelisation in SPARTA

- A typical simulation has about 20 particles per grid cell for adequate collision statistics

SPARTA



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- GPU parallelisation is seen to be more efficient for larger problems (Figure 3)

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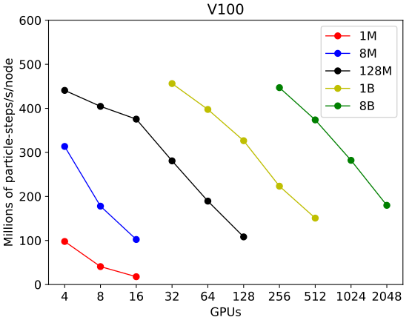


Fig. 3: GPU Parallelisation in SPARTA

- A typical simulation has about 20 particles per grid cell for adequate collision statistics
- GPU parallelisation is seen to be more efficient for larger problems (Figure 3)
- Performance per GPU decreases but the aggregate performance increases

Key Takeaways

- The relation between Knudsen number, Mach number and Reynold's number for gases is given by

$$Kn = \frac{Ma}{Re}\sqrt{\frac{\gamma\pi}{2}}$$

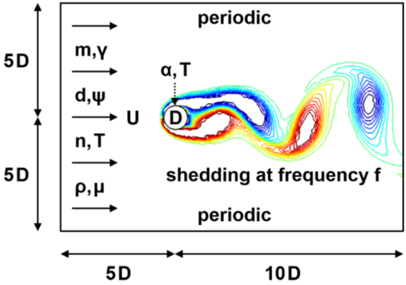


Fig. 4: Vortex Shedding Setup

Key Takeaways

- The relation between Knudsen number, Mach number and Reynold's number for gases is given by

$$Kn = \frac{Ma}{Re}\sqrt{\frac{\gamma\pi}{2}}$$

- The simulation given in Figure 4 was simulated using both DSMC and COMSOL Multiphysics

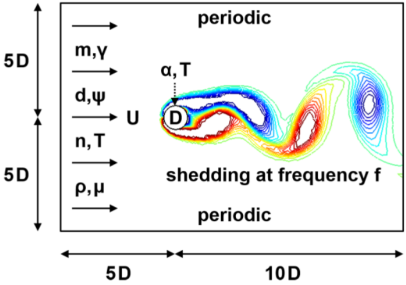


Fig. 4: Vortex Shedding Setup

Boundary Conditions

- The outlet boundary conditions by DSMC are the **inlet boundary condition** (Figure 5 img whereas CFD applies zero pressure and zero viscous stress

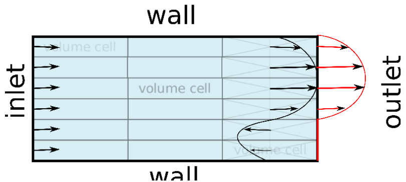


Fig. 5: Inlet boundary conditions at outlet

Boundary Conditions

- The outlet boundary conditions by DSMC are the **inlet boundary condition** (Figure 5 img whereas CFD applies zero pressure and zero viscous stress
- The inlet is at Ma = 0.3, Re = 100 and Kn = 0.0048

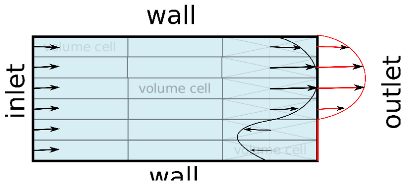


Fig. 5: Inlet boundary conditions at outlet

Comparing Results from DSMC and CFD

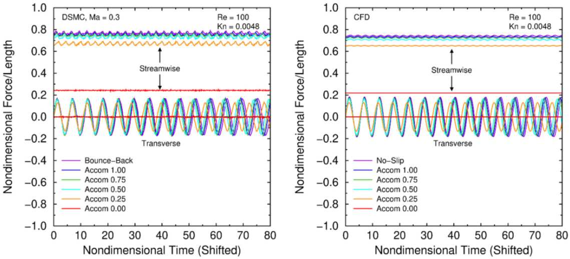


Fig. 6: Left : DSMC and Right : CFD

- Figure 6 illustrates the agreement between DSMC and CFD.

Comparing Results from DSMC and CFD

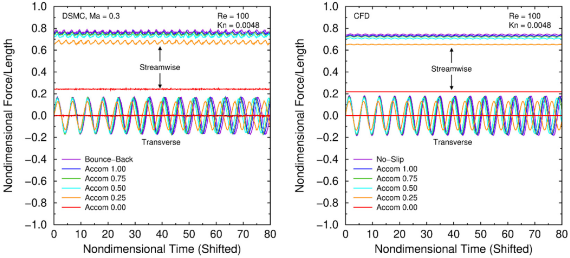


Fig. 6: Left : DSMC and Right : CFD

- Figure 6 illustrates the agreement between DSMC and CFD.
- As the Reynold's number decreases, the slip increases.

1. Direct Simulation Monte Carlo
2. Existing Literature
3. 1D Fourier Flow using SPARTA
    - Knudsen number fixed at 0.1
    - Knudsen number fixed at 0.02
    - Visualising the fluctuations in the solution
4. References

The problem and the simulation details

- The setup of the simulation is given by Figure 11. The gas used is Argon

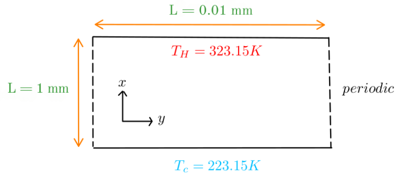


Fig. 7: Simulation Setup

The problem and the simulation details

- The setup of the simulation is given by Figure 11. The gas used is Argon
- The simulation parameters are given below [3]

$\lambda = 10^{-4} m \qquad \Delta t = 10^{-8} s$

$N = 1.682 \times 10^{14} \qquad t_o = 71 ns$

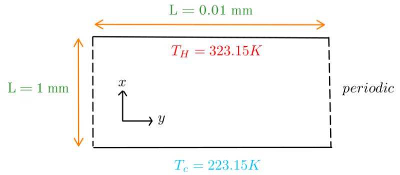


Fig. 7: Simulation Setup

The results at 20 particles per grid cell

- The temperature profile in Figure 8 clearly resembling a linear profile

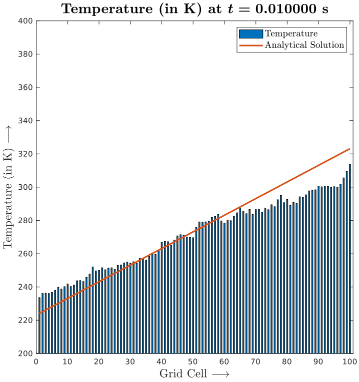


Fig. 8

The results at 20 particles per grid cell

- The temperature profile in Figure 8 clearly resembling a linear profile
- A clear distinction can be seen from the expected continuum solution due to rarefaction effects

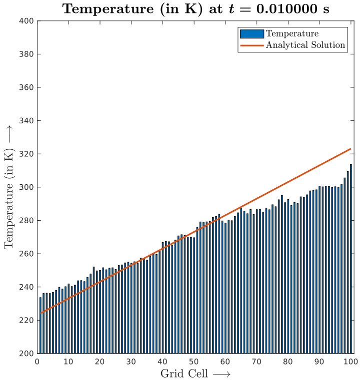


Fig. 8

The results at 100 particles per grid cell

- The temperature profile in Figure 9 clearly resembling a linear profile

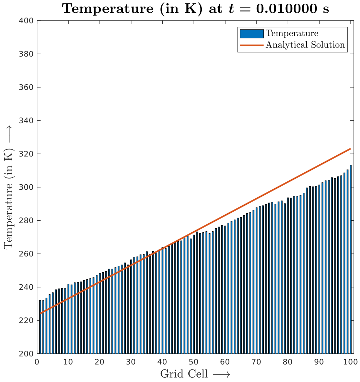
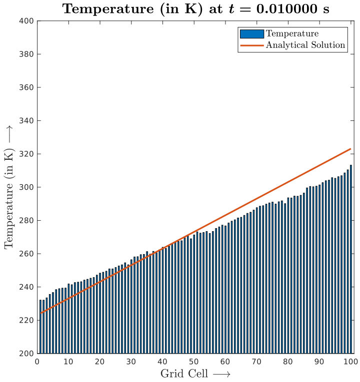


Fig. 9

The results at 100 particles per grid cell

- The temperature profile in Figure 9 clearly resembling a linear profile
- A clear distinction can still be seen from the expected continuum solution due to rarefraction effects



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The results at 100 particles per grid cell

- The temperature profile in Figure 9 clearly resembling a linear profile
- A clear distinction can still be seen from the expected continuum solution due to rarefaction effects
- However the statistical fluctuations are much less pronounced

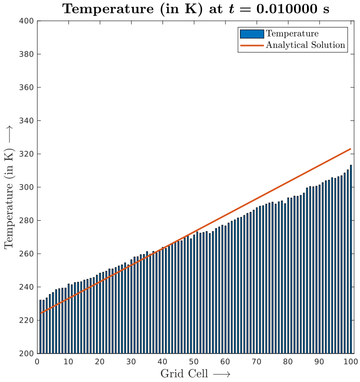
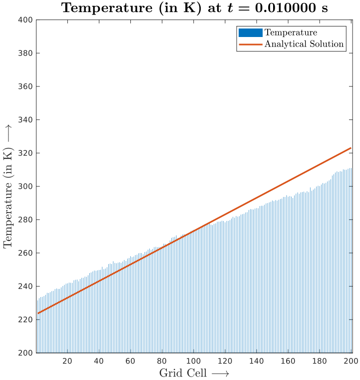


Fig. 9

The results at 100 particles per grid cell but with twice the resolution

- The temperature profile in Figure 10 clearly resembling a linear profile



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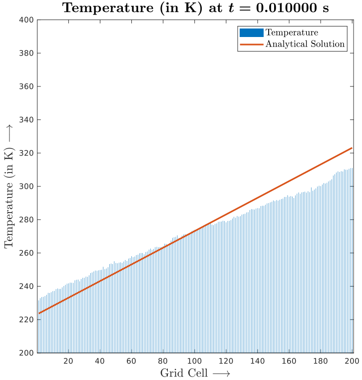

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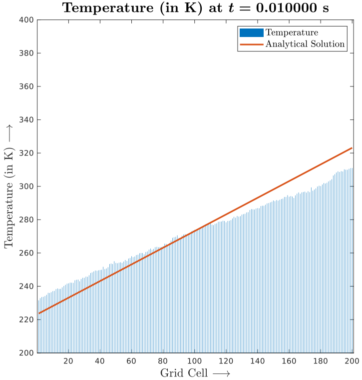
- The temperature profile in Figure 10 clearly resembling a linear profile
- A clear distinction can still be seen from the expected continuum solution due to rarefraction effects
- The deviation from the analytical solution doesn't reduce by resolving the grid. We can safely infer that the deviation is not a numerical error



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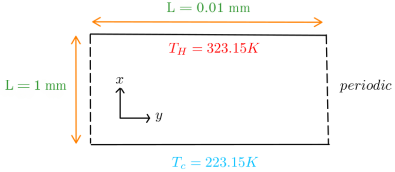

Fig. 11: Simulation Setup

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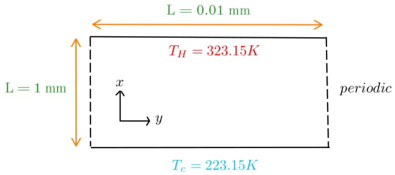

Fig. 11: Simulation Setup

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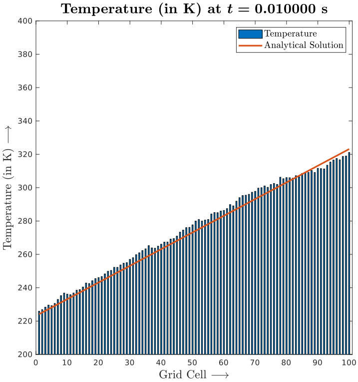
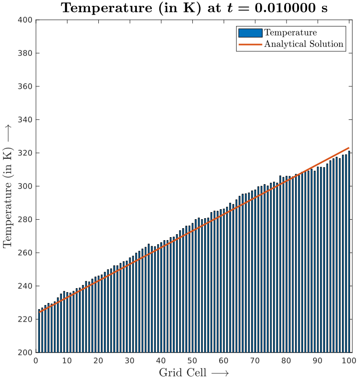


Fig. 12

- The temperature profile in Figure 12 clearly resembling a linear profile

The results at 100 particles per grid cell



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The results at 100 particles per grid cell

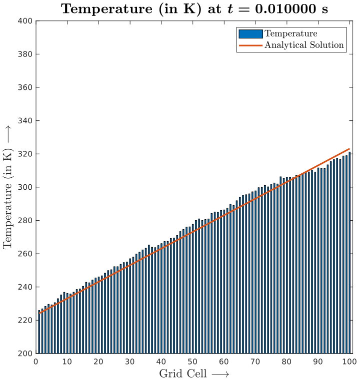

Fig. 12

- The temperature profile in Figure 12 clearly resembling a linear profile
- Here, the simulation closely resembles the analytical solution.
- We can conclude that the closer the Knudsen number is to zero, the simulation will agree more with the analytical solution

Fluctuations as a function of the number of particles per grid cell

- Let's visualize the fluctuations of the solution for different number of particles per grid cell using a few videos.

[1] Michail A Gallis and John R Torczynski.
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[2] Steve J Plimpton, SG Moore, A Borner, AK Stagg, TP Koehler, JR Torczynski, and MA Gallis.
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