

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

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- ① Direct Simulation Monte Carlo
- ② Existing Literature
- ③ 1D Fourier Flow using SPARTA
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① Direct Simulation Monte Carlo

General information

The algorithm

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General Information

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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 continuum methods 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

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- 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

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

The algorithm

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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

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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

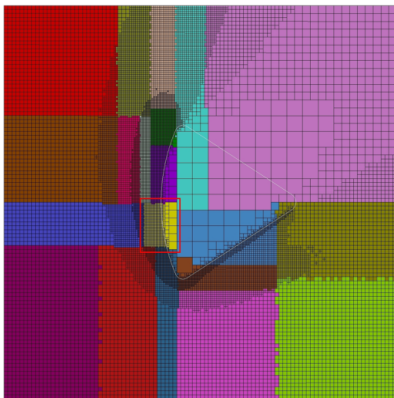


Fig. 1: Grid Hierarchy in SPARTA

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

SPARTA

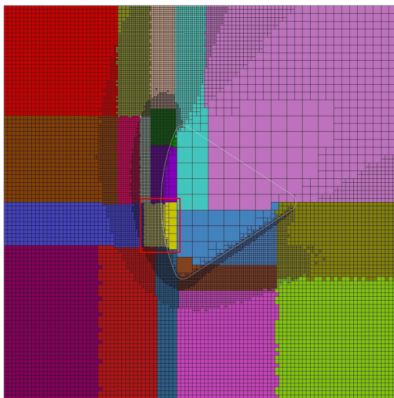


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- Grid cells are indexed hierarchically using bits. Cells store information about everything within them

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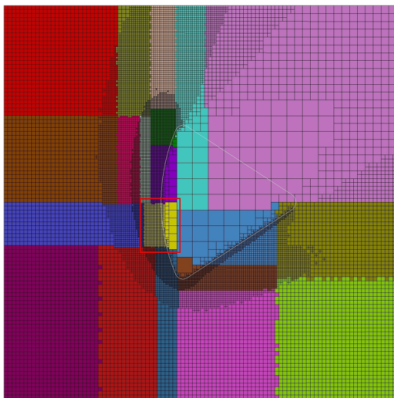
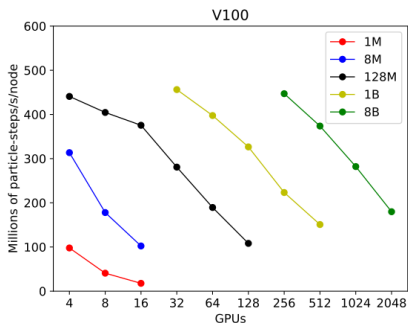


Fig. 1: Grid Hierarchy in SPARTA

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



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

Fig. 2: GPU Parallelisation in SPARTA

SPARTA

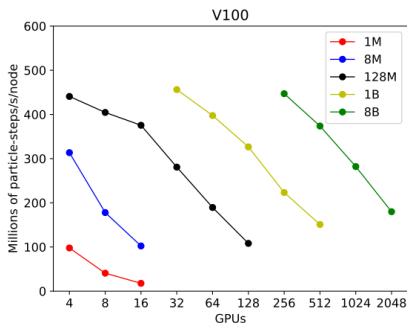


Fig. 2: GPU Parallelisation in SPARTA

- 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 2)

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Key Takeaways

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

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

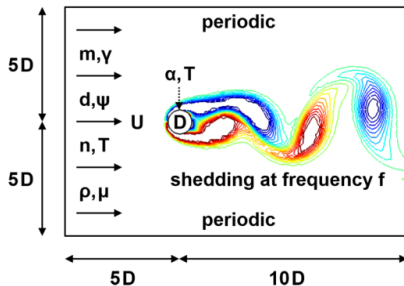


Fig. 3: Vortex Shedding Setup

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 3 was simulated using both DSMC and COMSOL Multiphysics

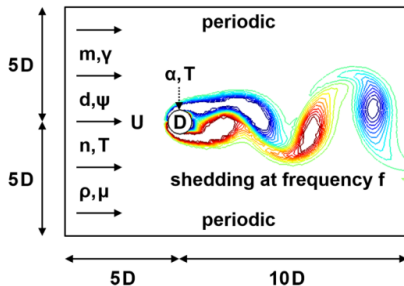


Fig. 3: Vortex Shedding Setup

Comparing Results from DSMC and CFD

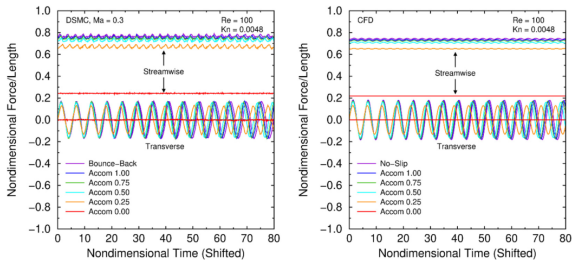


Fig. 4: Left : DSMC and Right : CFD

- Figure 4 illustrates the agreement between DSMC and CFD.

Comparing Results from DSMC and CFD

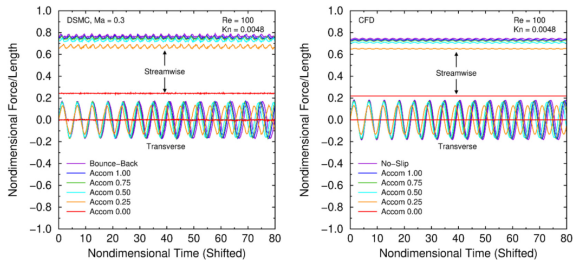


Fig. 4: Left : DSMC and Right : CFD

- Figure 4 illustrates the agreement between DSMC and CFD.
- As the Reynold's number decreases, the slip decreases.

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Knudsen number fixed at 0.1

The problem and the simulation details

- The setup of the simulation is given by Figure 5. The gas used is Argon

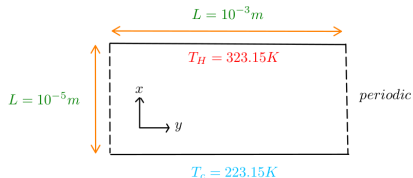


Fig. 5: Simulation Setup

The problem and the simulation details

- The setup of the simulation is given by Figure 5. The gas used is Argon
- The simulation parameters are given below [3]

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

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

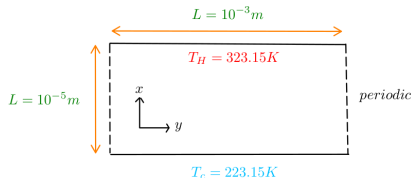


Fig. 5: Simulation Setup

Knudsen number fixed at 0.1

The results at 20 particles per grid cell

- The temperature profile in Figure 6 clearly resembling a linear profile

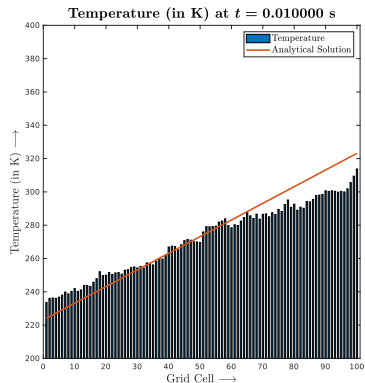


Fig. 6

Knudsen number fixed at 0.1

The results at 20 particles per grid cell

- The temperature profile in Figure 6 clearly resembling a linear profile
- A clear distinction can be seen from the expected continuum solution due to rarefaction effects

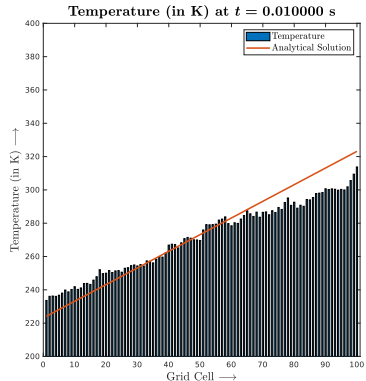


Fig. 6

Knudsen number fixed at 0.1

The results at 100 particles per grid cell

- The temperature profile in Figure 7 clearly resembling a linear profile

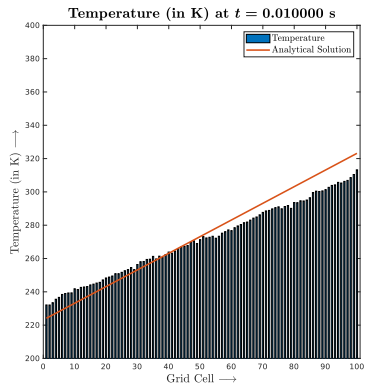


Fig. 7

Knudsen number fixed at 0.1

The results at 100 particles per grid cell

- The temperature profile in Figure 7 clearly resembling a linear profile
- A clear distinction can still be seen from the expected continuum solution due to rarefaction effects

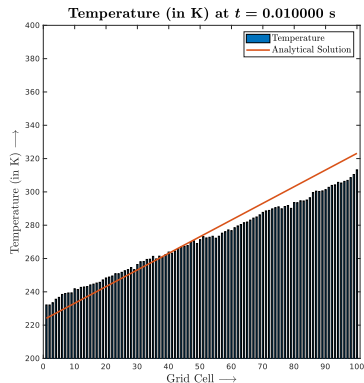


Fig. 7

Knudsen number fixed at 0.1

The results at 100 particles per grid cell

- The temperature profile in Figure 7 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

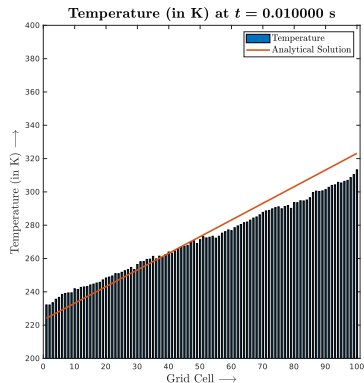


Fig. 7

Knudsen number fixed at 0.1

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

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

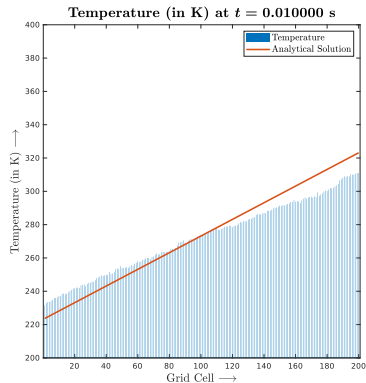


Fig. 8

Knudsen number fixed at 0.1

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

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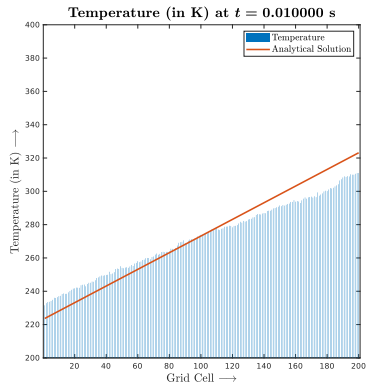


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The results at 100 particles per grid cell but with twice the resolution

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

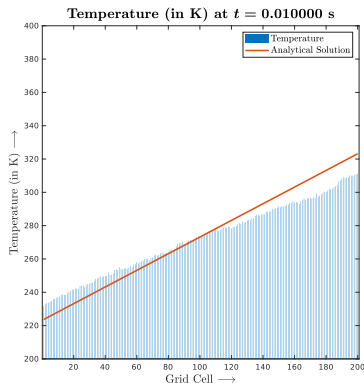


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- [1] Michail A Gallis and John R Torczynski.
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