DSMC code for pressure-driven orifice flow

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1 Overview

This is a brief description of my 2-D DSMC code for pressure-driven flow of dilute, monoatomic gas through an orifice. On linux machines, the code can be built by running 'make'. For details on the optional command-line arguments, see README.TXT or run 'dsmc -h'. The implementation roughly follows Alexander's exposition [1].

Initially, the inlet and outlet cell columns are filled with the required number of particles corresponding to the given pressures. The remaining cell columns are then initialized to the particle numbers that interpolate linearly between the inlet and outlet values. The main time loop of the DSMC procedure consists of the following stages:

- Advection of particles (streaming) with the corresponding boundary treatment. The particles experience specular and diffuse reflections at the partition and walls, respectively. Simple analytical geometry is used to determine the intersection points of particle trajectories and the boundaries.

- The particles are sorted into collision cells (several auxiliary sorting arrays are created and maintained for this purpose).

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- The particle numbers in inlet and outlet boundary cells are adjusted so as to maintain the given pressure gradient. I tested the particle control method outlined in [2], but observed spurious velocity bias at the boundaries. The current implementation uses reservoir boundaries maintained at desired pressures.
- The particles are re-sorted into collision cells.
- The stochastic binary collisions are simulated between hard spheres. Acceptance-rejection criterion is used to accelerate the procedure.
- Sampling of density, velocity and temperature fields is conducted, with sampling cells being identical to the collision cells for convenience.

Most of the arrays are implemented as C++ STL classes. As the pressure depends on the axial position, so does the effective weight (ratio of the number of atoms and number of simulated particles), mean free path and Knudsen number.

2 Results

The results for a trial run were obtained with the following parameters: argon gas at room temperature, inlet pressure $p_1 = 8 \times 10^{-3}$ Torr, outlet pressure $p_1 = 2 \times 10^{-3}$ Torr, orifice diameter $h = 0.5 \times 10^{-3}$ m, length and height of computational domain $L = 20h$ and $H = L/2$, respectively. Initial number of particles $N_0 = 100000$, with the average number of atoms represented by each particle being approx. 1.6×10^{10}. The collision grid consists of 20×10 cells, with the length of collision cells at inlet and outlet being 3.86 and 0.02 mean free paths. The number of time steps is 1000, with the time step and simulation time set to $dt = 0.2$ and $t = 200$ cell advection times, respectively.

Fig. 1 shows the pressure and temperature distribution with the orifice located near the bottom wall. Fig. 2 shows the velocity field.

References

[1] Francis J Alexander and Alejandro L Garcia, *The direct simulation Monte Carlo method*, Computers in Physics **11** (1997), no. 6, 588.

[2] Mao Xiaohai, *Direct simulation Monte Carlo (DSMC) in micro flows*, 2004.

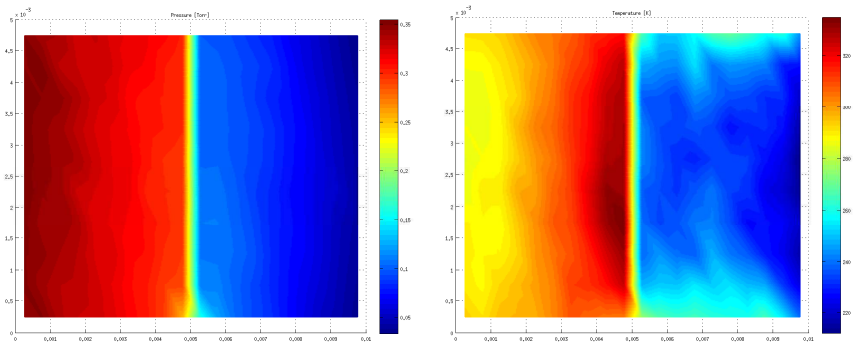

Fig. 1: Left: Pressure [Torr]. Right: Temperature [K]

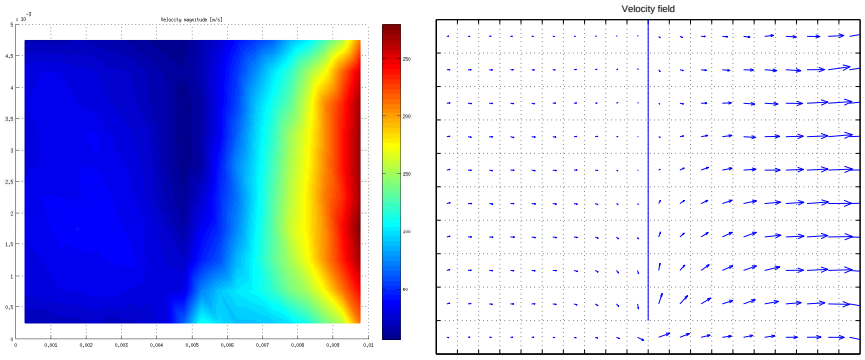

Fig. 2: Velocity field. Left: Magnitude [m/s]. Right: Averaged velocity field with sampling cells depicted