The Reflecting Particle Method (RPM)

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We want to study the Poiseuille fluid flow inside a microchannel. It is well known that this process, whether in steady state or not, is non-equilibrium in the sense of entropy: the work that drive the flow is continuously turned into heat by friction on the walls. The essential point here is how to set up the source, i.e., how to set up a pressure difference between the two ends of the channel such that it could drive a flow, and mimic the realistic situations as much as possible (we noticed that the straight-forward idea by adding body force terms such as "gravitation" can not ensure this — it alters the *form* of the corresponding Navier-Stokes equation of continuum mechanics). Other requirements for the new source are:

- conserve current: $\mathbf{J}_{in} = \mathbf{J}_{out}$, such that steady state solution is possible
- easy to implement
- algorithmly stable

Fortunately we are able to come up with a plan that satisfy all these requirements, and the early results are very encouraging. The idea lays in entropy. It is well known in history that if we could design the so called "Maxwell's daemons" then entropy can be reduced, contrary to nature's 2nd law of thermodynamics. It is also known that entropy is equivalent in many senses to "information content". Computers, on the other hand, are net producers of "information content". The specific version of "Maxwell's daemons" for our problem are on Fig.**??**. Suppose the intention is to drive flow in positive x-direction. We apply periodical boundary conditions on x but put a bunch of "Maxwell's genies", in actuality a membrane, at $x = 0$. The membrane is such that if a fluid atom cross $x = 0$ from left to right, it pass though without hindrance. But if it is to cross $x = 0$ from right to left, then it's elasticly reflected with probability prj (the so called "rejection ratio"), same as colliding onto a hard wall. The membrane is otherwise *transparent* in the sense that it allows particles on the two sides to interact.

It is intuitive that such a boundary condition would drive flow in the positive x-direction, because the fluid density on the right must be higher than the fluid density on the left, and so setting up pressure difference between two ends (if the fluid density on two sides are equal and there is no flow, then wall-hitting rate on the two sides should be equal — which must in turn induce net flow from left to right by our "*prj*" set-up). Because the particles on two sides are able to interact with each other across $x = 0$, these "Maxwell's daemons" also conserve energy: the atoms that cross through will automatically pick at spots that are energetically favorable, which is much much better than randomly inserting a particle on the other side. The latter plan is terrible because we have to re-scale the temperature feverishly all the time to get rid of the extra energy, which will unavoidably influence the particle dynamics. Our current plan, on the other hand, almost doesn't need any extra re-scaling. Our Berendson temperature coupling constant is the same as in the bulk liquid case!

Other details of the boundary set-up are as follows (see Fig.??): we use real walls that consist of layers of FCC units of particles interacting via LJ6-12 potential but with stronger interaction in between ($\varepsilon_{ww} = 5\varepsilon_{wf}$) and larger mass ($m_w = 5m_f$) such that at the same temperature of the fluid it lays in the solid region of the phase diagram. The layers are perpendicular to the crystal (001) direction. In order to prevent mechanical failure, we attach a fourth-power spring to each wall atom with its equilibrium position, such that it only shows effect under large deformations, but which won't influence the lattice dynamics of the wall under harmonic approximation. We then have PBC in both y- and z-direction. The first two units of the wall near $x = 0$ are fixed because pressure variations in region near the source are comparably big.

We have taken major efforts in the algorithm of our code, especially in memory allocations and link-lists, such that it is of $O(N)$ and can manage relatively large systems on a workstation. We achieved this by dividing the geometry into a collection of bins with bin-bin and bin-atom link-lists that makes the renewal of atom-atom link-lists on a local basis possible. The fact that we have wall and fluid atoms complicated the issue but in the end we made it. The largest system we have yet handled has 6426 fluid atoms and 2160 wall atoms, and the system approaches steady-flow state within reasonable DEC-alpha machine time.

In our reports, the figures should be mostly easy to understand. The front page gives the conditions of the run, which are:

- TR: reduced temperature
- DR: reduced density
- ALPHA: range of the 4th-power spring: $V(r) = \varepsilon_{ww}(r/\alpha\sigma)^4$
- TAUT1: Berendson temperature coupling constant before averaging initiates.
- TAUT2: Berendson temperature coupling constant after averaging initiates.
- RC: cutoff range of LJ6-12 interaction
- W: maximal re-displacement to cause a renewal of linklists for each atom.

- PMWALL: the ratio of wall atom mass to that of the fluid
- REJECTION RATIO: prj

Because the fluid density variates greatly near the wall, as shown on the second page of each report, it is of less meaning to plot the averaged fluid velocity. Rather, we plot the flow rate, which is the density multiplied by velocity. The "averaged flow rate" in the front page denotes on the average how many particles pass through a cross-section per unit time. If the flow is in a steady state, then the flow rate should be conserved along x-direction. We use this criteria to judge how good we are approaching steady state.

The local stresses are calculated by stipulating that for any pair interaction, we account their contribution to their center. The kinetic contributions are accounted for at the locality of each atom.

The major result of our simulation is that on the scale of 10σ in microchannel width and 200σ in x-direction, continuum mechanics gives a surprisingly good description of the problem, although density variations along the cross-section are far from small. For instance, by solving the Navier-Stokes equation for incompressible viscous fluid, the flow rate should be of parabolic profile in z, which is more or less the case for our simulation results (there are "bumps" though, due to layered fluid structure induced by the wall). So far we have not observed non-linearity in the mid-stream fluid pressure along x-direction. The P_{xx}, P_{yy}, P_{zz}, though different from each other, all drops linearly along x, and we can clearly see the desired pressure difference building up between the two ends. In one case where we have a $51.0 \times 5.1 \times 12.7$ geometry with rejection ratio 0.3, by taking the linear region of P_{xx} and the averaged flow rate obtained from simulation, and using the continuum model of Navier-Stokes equation, we get shear viscosity of 2.29, which is very close to the value 2.14 of corresponding bulk liquid.