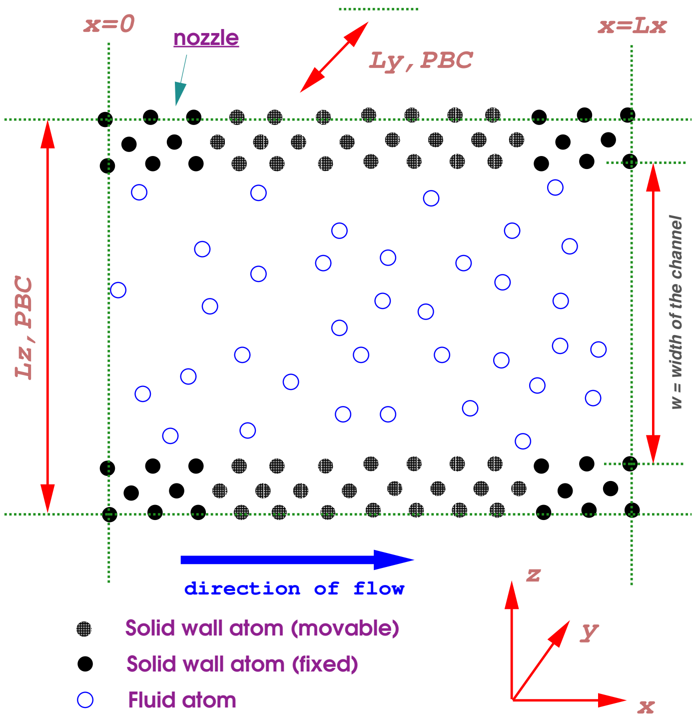
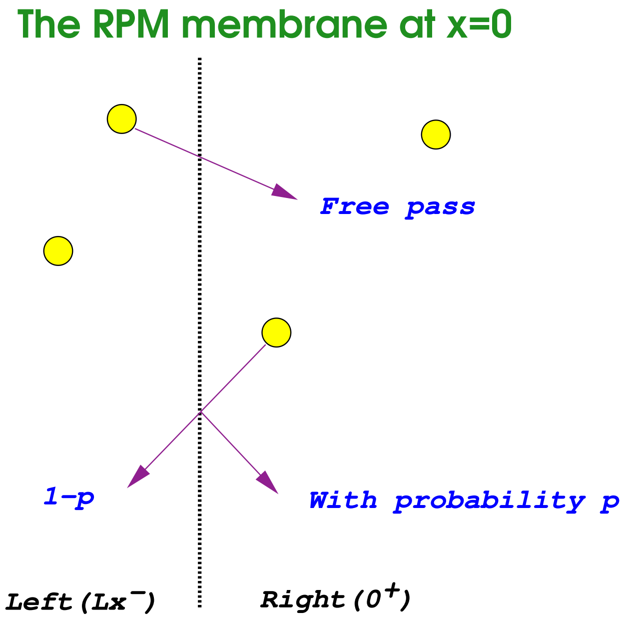
Pipe flow problem: fluid comes in with pressure $P_{\text{in}}$ and exits with pressure $P_{\text{out}}$. $P_{\text{in}} - P_{\text{out}}$ is what drives the fluid flow.




**How does one set up the pressure head $P_{\text{in}} - P_{\text{out}}$ in MD?**

**Reflecting Particle Method to Generate Pipe Flow:**




- Conserve **number of particles** (efficient PBC setup)
- Conserve **total energy** (no need for temperature rescaling)
- Faithful to Navier-Stokes eqn; reach steady-state gracefully, etc.

- **Demon vs Heat – Facts:**

– Demons don't do work; system energy stays constant.

– Heat *is* generated by viscous shearing inside fluid. Continuum solution predicts a dissipation rate of

$$\frac{dQ}{dt} = \int \tau_{ij} v_{i,j} d\Omega = \frac{L_X L_Y w^3}{12\mu} \left(\frac{\Delta P}{\Delta x}\right)^2 .$$

– Steady-state is observed to be reached; system does not heat up.

- **Then, where does the heat go?**

$\Delta Q = T\Delta S$. The demons reduce system entropy by selectively reflecting atoms at $x = 0$.

- **How to estimate $\Delta S$?**

Let $f_1/f_2$ be the rate of atoms hitting $x = 0$ from left/right when the system reaches steady-state. In unit time, the number of ways of crossing are

$$\Omega_1 = \frac{(f_1 + f_2)!}{f_1! f_2!} \qquad \longrightarrow \qquad \Omega_2 = \frac{(f_1 + f_2)!}{(f_1 + p f_2)!((1-p) f_2)!}$$

And,

$$\Delta S = k_{\mathrm{B}} \log \Omega_1 - k_{\mathrm{B}} \log \Omega_2 \ ,$$

therefore, there should be (?),

$$\frac{dQ}{dt} = \frac{L_X L_Y w^3}{12\mu} \left(\frac{\Delta P}{\Delta x}\right)^2 \qquad =^?$$

$$k_{\mathrm{B}} T \log \frac{\Omega_1}{\Omega_2} \approx k_{\mathrm{B}} T \left\{ f_1 \log(1 + \frac{p f_2}{f_1}) + p f_2 \log( + \frac{f_1}{f_2}) + f_2 (1-p) \log(1-p) \right\} .$$