Molecular Dynamics Simulations of Polymers in Micro-environments.

Martin Kenward, F. Tessier, Y. Tatek, Y. Gratton, S. Guillouzic and G. W. Slater

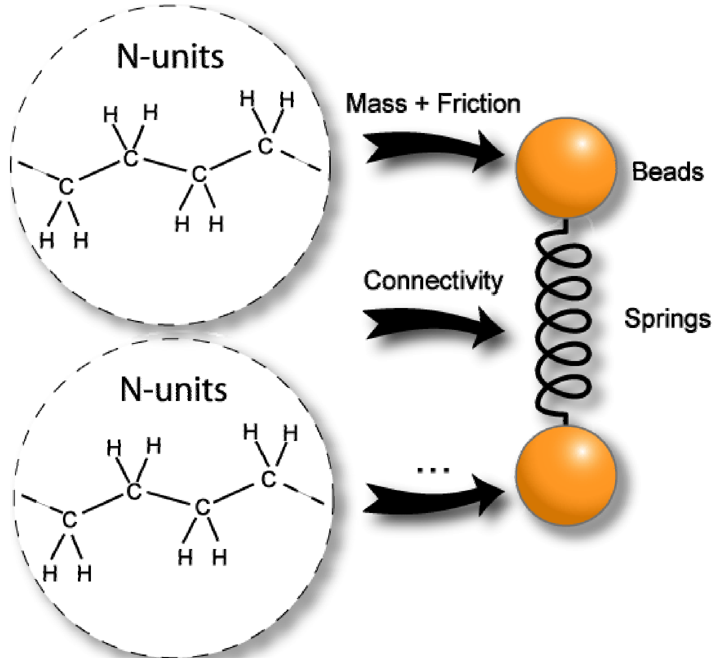
Department of Physics
University of Ottawa

Ottawa, Ontario,
Canada

mkenward@science.uottawa.ca

Molecular Dynamics (MD): A Brief Overview

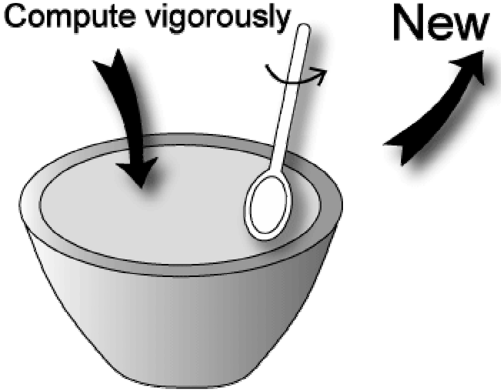
- Solve N-body classical eqs. of motion.
- Coarse grained MD.
- Parallelism via OpenMP.
- Reduced units.



Recipe for MD:
1 supervisor + graduate students
pinch of Physics + Math + Comp Sci.
1 dollop Computational Resources
Brainfull of New Ideas + Coffee

Instructions:
Compute vigorously

New Physics?



$$V_{\mathrm{LJ}}(r) = 4\epsilon\left(\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right) + \epsilon, \quad r \le r_c$$

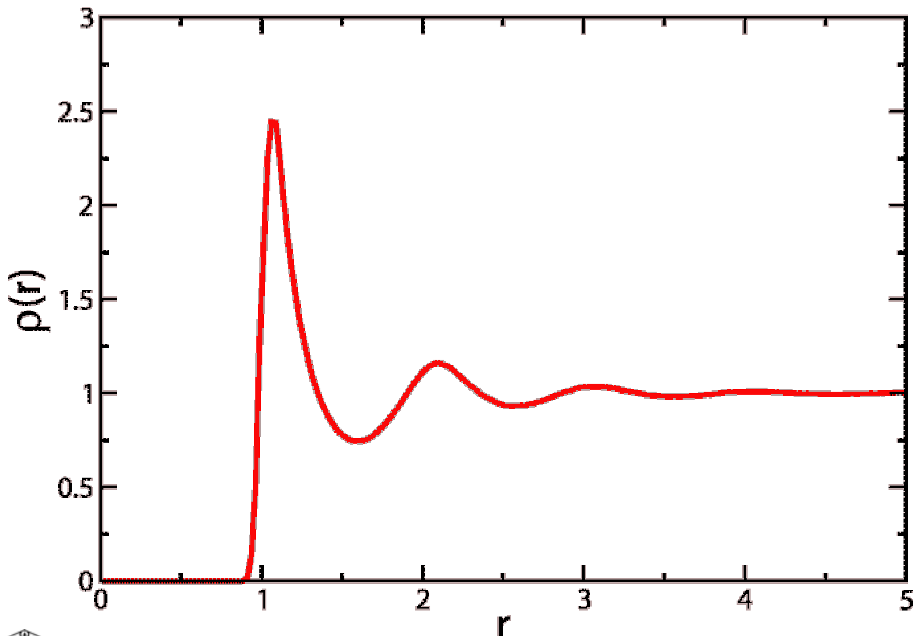
$$V_{\mathrm{F}}(r) = -\frac{k}{2}R_0^2 \ln\left(1 - \frac{r}{R_0^2}\right)^2$$

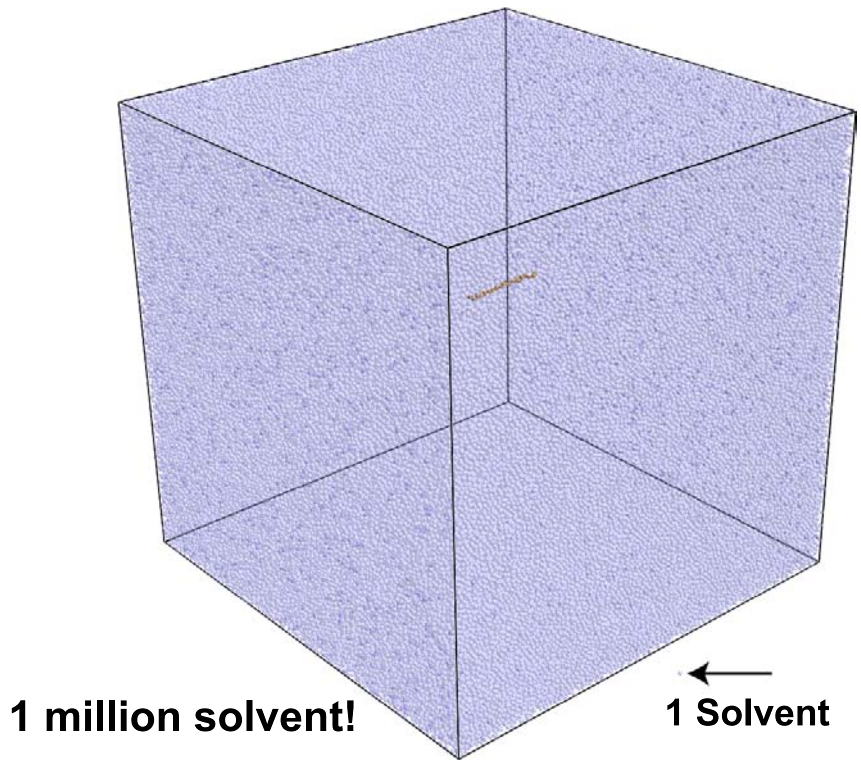
Molecular Dynamics (MD): A Brief Overview
continued…

- 2nd order integrator, Velocity Verlet.
- Constant reduced temperature T*=1 (thermostat).
- Reduced density $\rho \approx 0.85$.

Polymers, Hydrodynamics
and the micro-macro divide

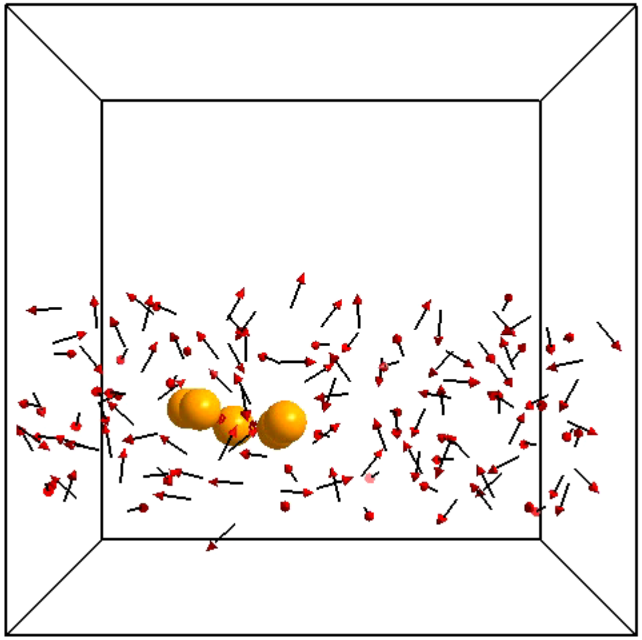
- Explicit solvent ⇒ Explicit Hydrodynamics.
- Hydrodynamics at the <100 atom length scale.
- Bridge gap between micro-macro (or meso-scale)?



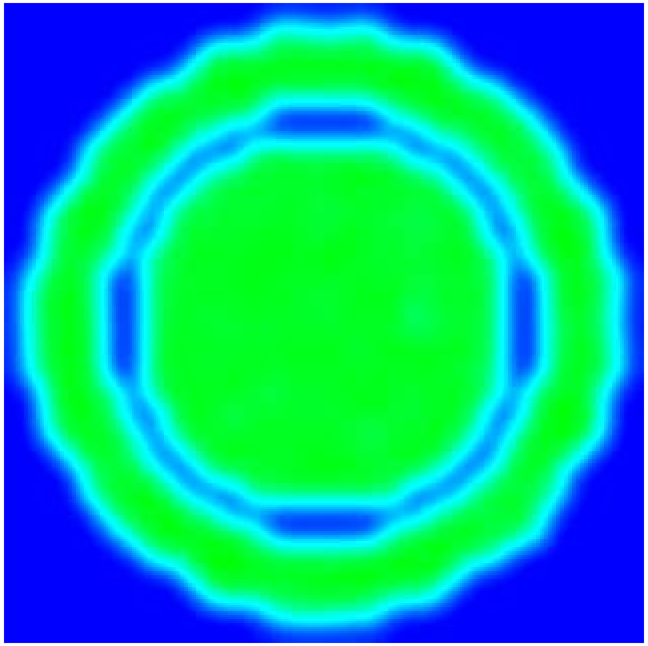


Visualization and Data Analysis

- Developed versatile viewer in OpenGL©.
- Debugging tool and intuitive way to examine systems.



Polymer and fluid vector field.



Temperature in cross-section of capillary.

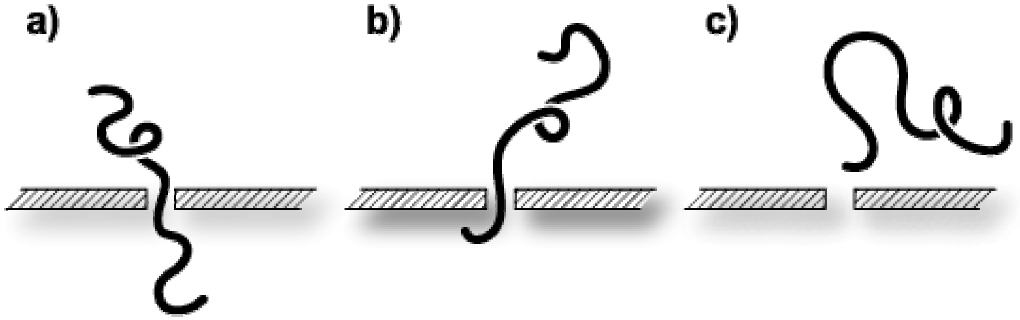
MD: Several Examples and Applications

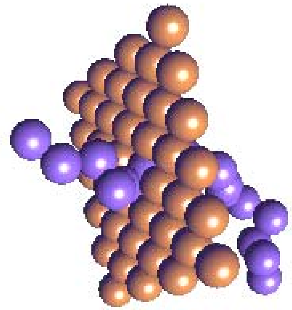
- Current research, fundamental and practical.
- Ex: Micro (nano)-fluidics and separation science.
- New physics may emerge!
- Computing Resources: HPCVL and various C3.ca sites.

- MD $\Rightarrow$ test fundamental theories?
- MD $\Rightarrow$ practical applications?

Polymer Translocation in Nanopores

- Nanopore technologies = ultimate sequencing tool?
- DNA diffuses through a narrow constriction (chemical structure ideally) can be 'read'.





$$\langle \Delta s^2 \rangle \propto t^{0.918 \pm 0.016}$$

$$\tau_{\text{trans}} \propto N^{\beta} \quad \text{with} \quad \beta \geq 2.27 \pm 0.04$$

Polymer- Obstacle Collisions

- Arrays of microscopic obstacles can sieve polymers.
- What role does hydrodynamics play?
- Can we optimize these systems?
- External force **vs.** Velocity field.

External Force regime:

$$\xi_{\cap}^{\mathrm{HI}} = \frac{2\pi\eta L}{\ln(L/b) + \gamma^{||}} \cong \frac{1}{3\ln(N)} \times \xi_{\cap}^{\mathrm{R}}$$

$$\frac{dl(t)}{dt} = -\frac{f_0}{\xi} \times \frac{L - 2l(t)}{b}$$

$$\tau_{\mathrm{esc}} = \ln\left(\frac{L}{L - 2l(0)}\right)\frac{\xi b}{f_0}$$

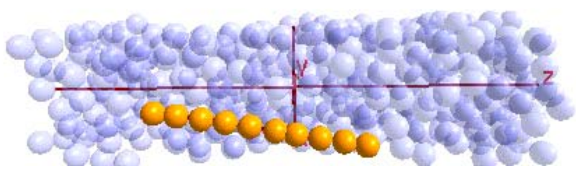
Velocity Field Regime:

$$\frac{dl(t)}{dt} = -v_s\frac{\xi(L - 2l(t))}{\xi(L)}$$

$$\tau_{\mathrm{esc}} = \ln\left(\frac{L}{L - 2l(0)}\right)\frac{\xi L}{2\pi\eta v_s}$$

Microscopic friction coefficients

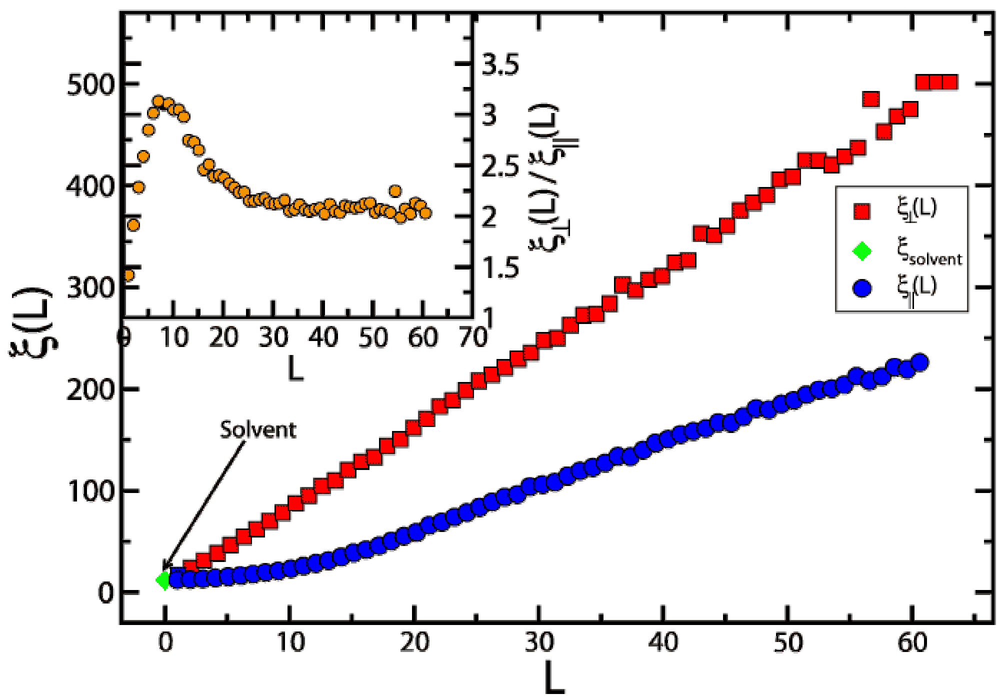
- Test well known? results at the microscopic level.
- Ex: Slender body theory of hydrodynamics.
- Typically one solves Navier-Stokes.



$$\xi_{||}(L) = \frac{C\pi\eta L}{\ln(L/2b) + \gamma_{||}}$$

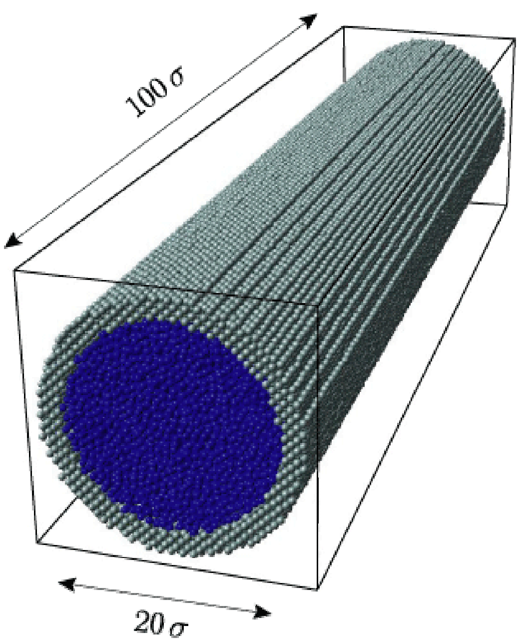
$$\xi_{\perp}(L) = \frac{2C\pi\eta L}{\ln(L/2b) + \gamma_{\perp}}$$

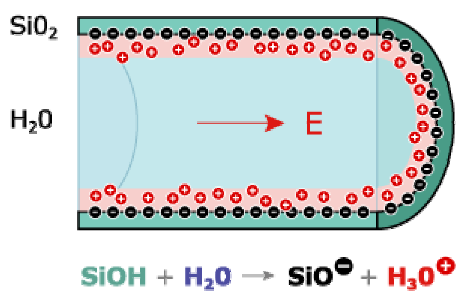
$$\frac{\xi_{\perp}(L)}{\xi_{||}(L)} \approx 2$$

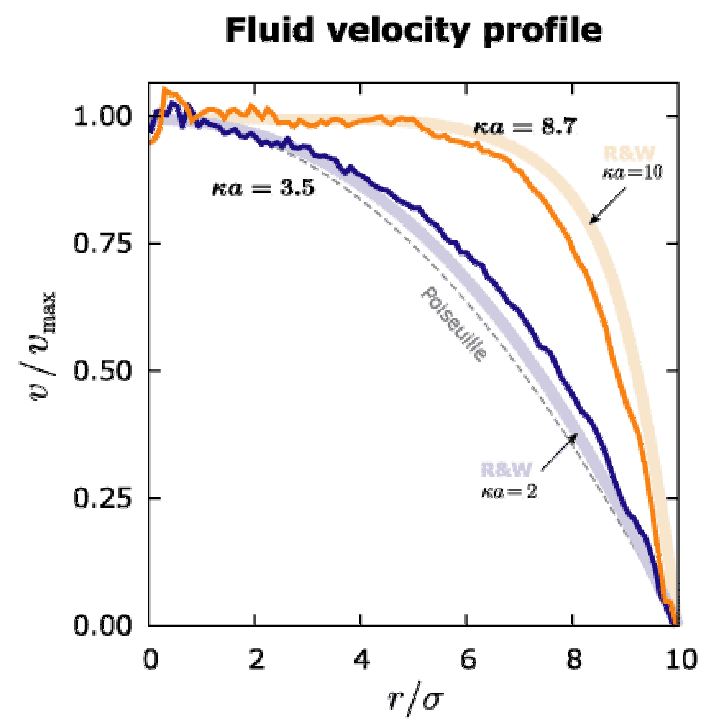


Electroosmotic Flow

- Explicit electrostatics.
- Velocity profile and counter-ion distributions.
- Compare with Poisson-Boltzmann.
- Important in micro-fluidics.

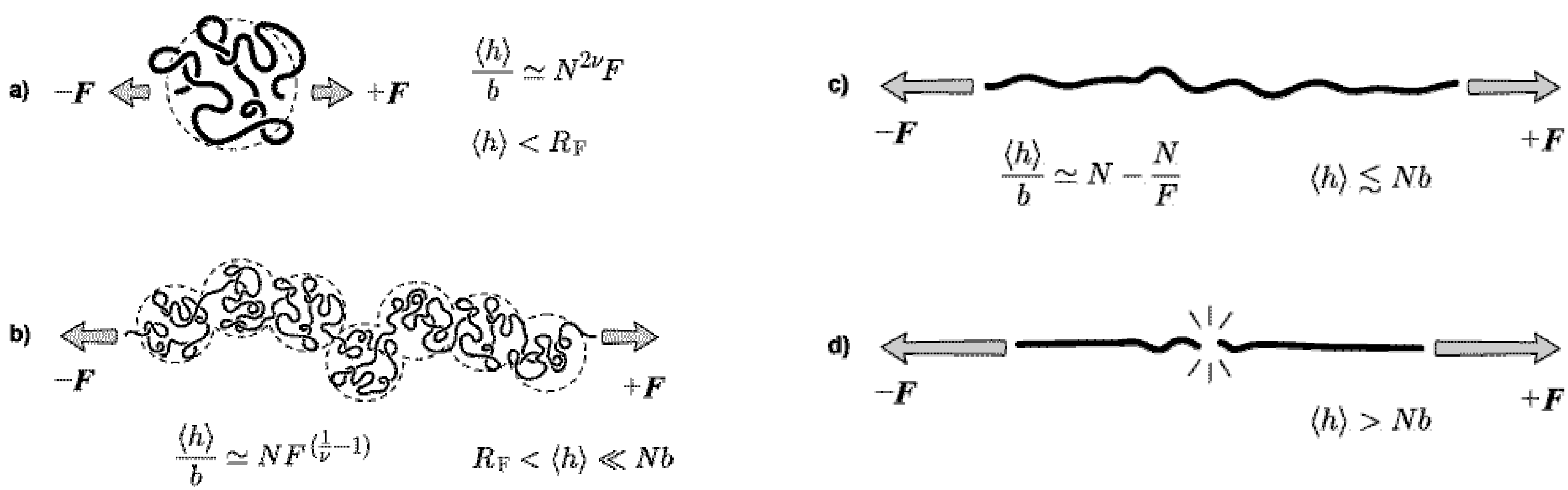






Polymer stretching

- Optical tweezers and fluorescence microscopy.
- Dynamics, correlation functions etc...
- Test theories and fundamental physics.

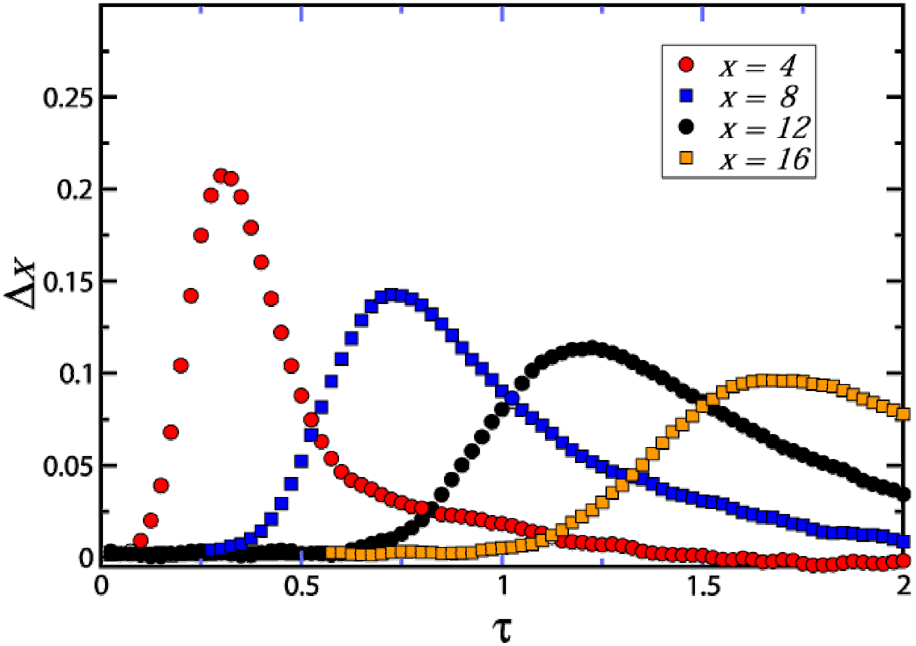


Planar perturbations in a simple liquid

- Sound propagation at the molecular scale.
- Perturbations can wreak havoc in micro-fluidic devices.
- Model sound, density fluctuations and diffusion, viscosity?
- Can we use this as a analytical tool?

$$\langle \Delta x(D, x, v, t) \rangle \sim \frac{1}{\sqrt{Dt}} \exp\left(-\frac{(x - vt)^2}{4Dt} \right)$$

$$t_{\max}(x) = \frac{D}{2v^2} \left[2\sqrt{\frac{1}{4} + x^2 \frac{v^2}{D^2}} - 1 \right]$$



Conclusions

- MD is versatile, easily applied to a host of problems.
- HPC allows us to examine ~+1 million atoms.
- We can examine smaller dimensions.
- Many opportunities for new and interesting science!

Acknowledgements

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- Computational Resources:
  HPCVL (www.hpcvl.org), various C3 sites across the country.