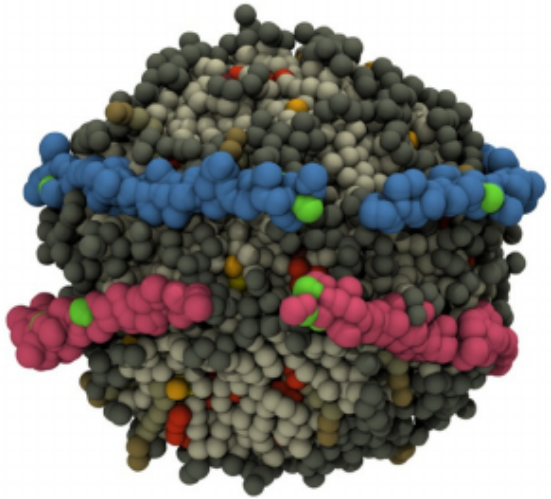
Western
UNIVERSITY · CANADA

Multiscale Modelling: Powerful Tool or Too Many Promises



Dr. Mikko Karttunen

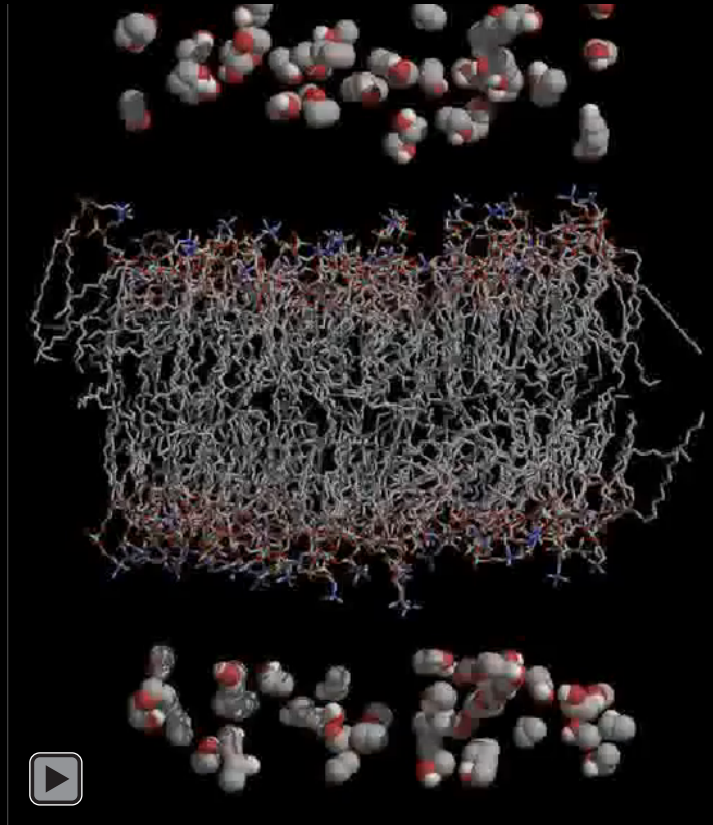
Department of Chemistry &
Department of Applied Mathematics
Western University, London, Ontario, Canada

Department of Mathematics & Computer Science,
Eindhoven University of Technology, the Netherlands


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Niagara Falls
Buffalo
Detroit
Chatham-Kent
Erie
Allegheny
National Forest
Cleveland
Sandusky
Akron
Youngstown
Canton
Pittsburgh
400
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407
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275
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480
76
80
71

Premise: Monoscale vs multiscale

Ethanol's + a cell membrane



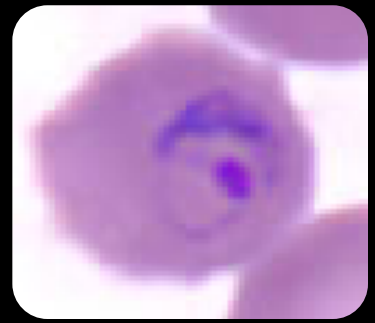
Electrokinetics: Many scales

High potential:

- Dielectrophoresis
- Electrorotation

Sub-micron range: no scale separation
Application: Malaria-infected cells





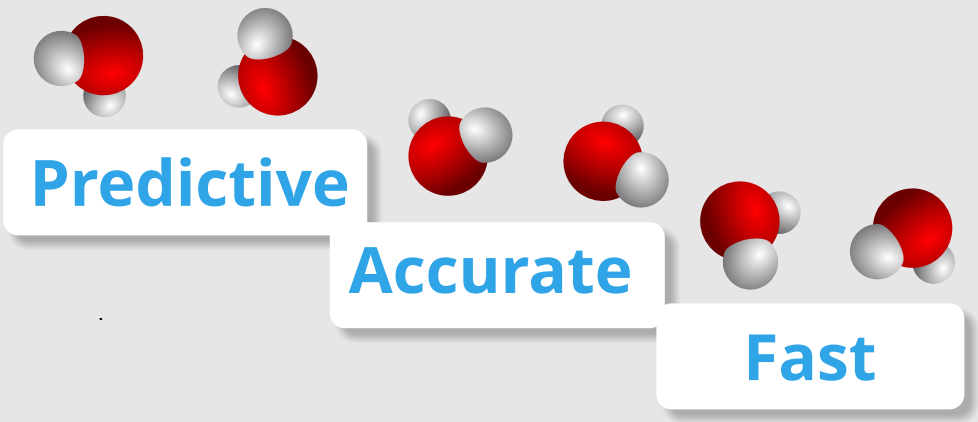
Under the influence of alcohol: The effect of ethanol and methanol on lipid bilayers, Biophys. J. 90, 1121-1135 (2006).

"By its nature, **multiscale modeling** is **highly interdisciplinary**, with developments occurring **independently across fields**. A broad range of scientific and engineering problems involve multiple scales. Traditional monoscale approaches have proven to be **inadequate, even with the largest supercomputers**, because of the range of scales and the prohibitively large number of variables involved. Thus, there is a growing need to develop **systematic modeling and simulation approaches** for multiscale problems."

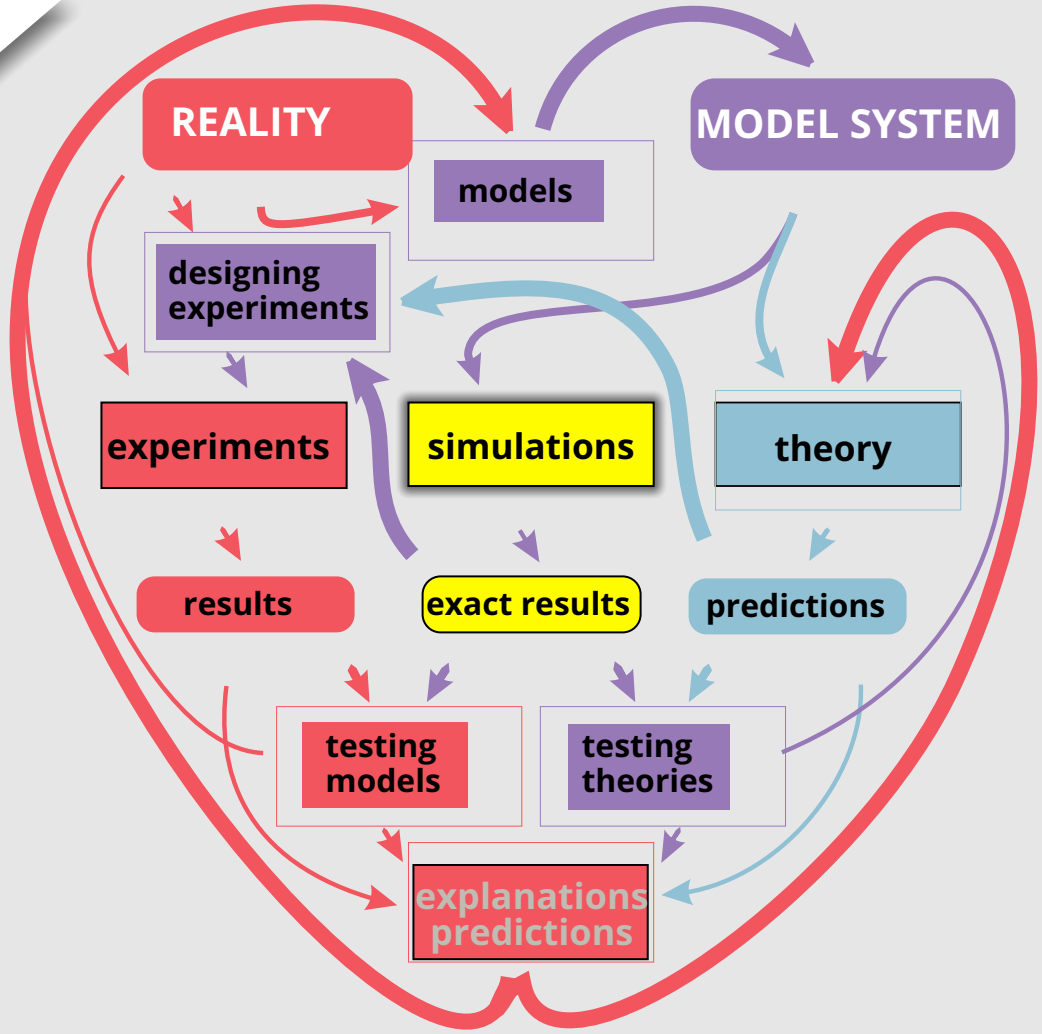
- Multiscale Modeling and Simulation: A SIAM Interdisciplinary Journal

- **In total:** over 14,000 papers with "multiscale" in the title (Web of Science).
- **Last year:** Over 1,400 papers with "multiscale" in title. **In year 2000:** 192. **In 1990:** 42
- **The first** paper with "multiscale" in title: "On selecting parameters of multscale measuring systems" in 1962 by Tetnev in Radio Engineering and Electronic Physics USSR.
- **Archetypal problem:** Modeling weather.

The Third Paradigm



- Simulations can be predictive and guide experiments.
- Can tell about perturbations experimental probes cause.
- Like other approaches: has problems



The good, the bad and the user in soft matter simulations, BBA Biomembranes, **1858**, 2529 (2016)

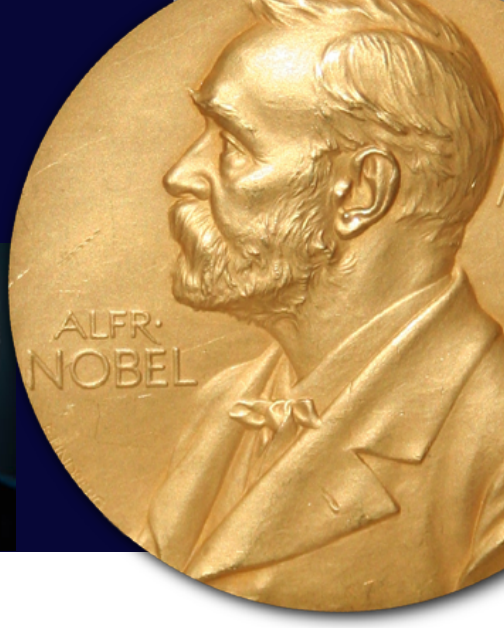
2013 NOBEL PRIZE IN CHEMISTRY

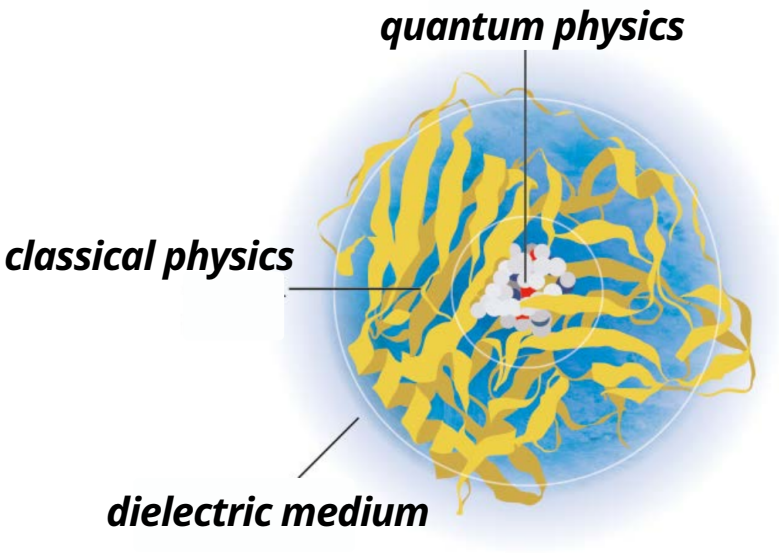
"for the development of multiscale models for complex chemical systems"



Martin Karplus - Harvard & Strasbourg
Arieh Warshel - Southern California
Michael Levitt - Stanford





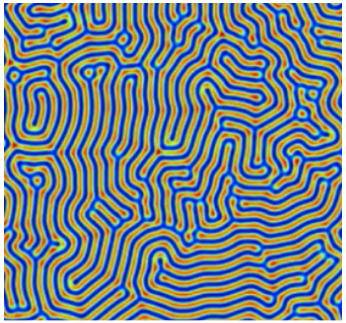


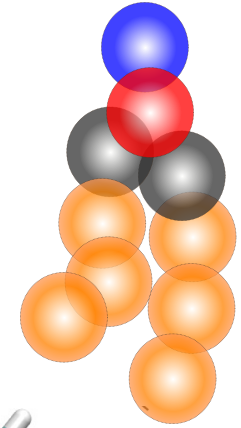
Pressmeddelande, Kungliga Vetenskapsakademien:

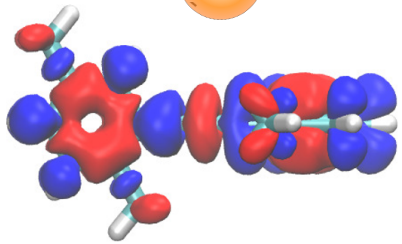
"Today the computer is just as important a tool for chemists as the test tube. Simulations are so realistic that they predict the outcome of traditional experiments."

Pictures: www.nobel.se

Multiscale modelling & coarse-graining







Macroscale
Times: 1 μs - 1ms
Lengths: >100 nm
Phase fields, FEM

Mesoscale
Times: 1 μs - 1ms
Lengths: >100 nm
Martini, PLUM, DPD

Atomistic scale
Times: 1 ns - 1 μs
Lengths: 10 nm
Classical MD, force fields

Subatomistic scale
Times: 10 ps
Lengths: 1 nm
Ab initio methods, DFT

Elastic properties
Coupling of slow variables

Henderson theorem
Ad hoc
Solubilities / experimental data
Adaptive Resolution (AdResS)
Neural networks

Henderson theorem
QM/MM
Parameters
Machine learning

Questions include:

- Sampling
- Algorithms
- Sequential vs concurrent
- Transerability
- Phase changes
- Entropy
- Conservation laws
- Response
- Charges
- pH changes

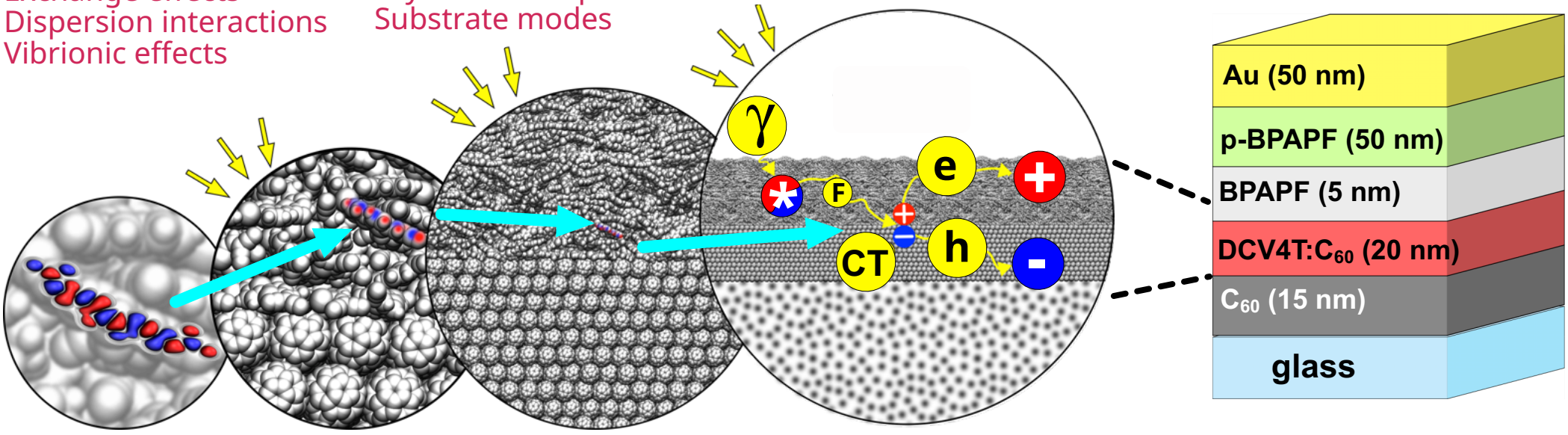
Multiscale Modeling of Emergent Materials..., Murtola, Bunker, Vattulainen, Deserno, Karttunen, PCCP 11, 1869 (2009)
Multiscale simulation of soft matter systems – from the atomistic to..., Peter & Kremer, Soft Matter (2009)

Example: Solar-cell materials

Charge flow
Exchange effects
Dispersion interactions
Vibrionic effects

Domains
Crystal vs amoprhous
Substrate modes

Electrodes
Thin film intefaces



0.1nm → 1nm → 10nm → 100 nm → device scale

0.1nm	1nm	10nm	100 nm
electronic structure	local morphology	meso-level morphology	global morphology

bi-molecular transport

microscopic transport

Impact of mesoscale order on thin-film interface electronic structure, Poelking et al., Nature Mat 14, 434 (2015)

Example: quantum-all atom

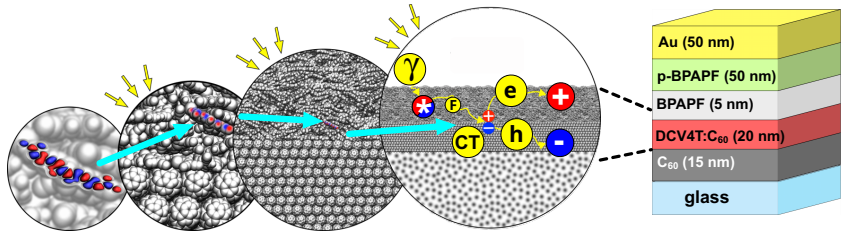
quantum
- force field

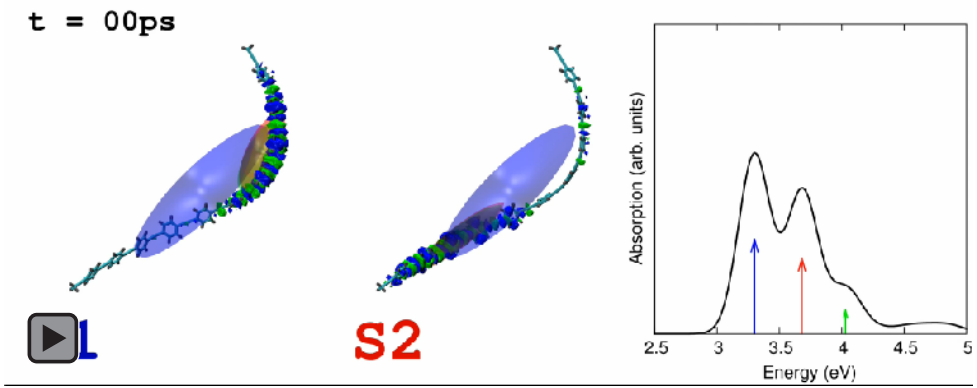
all-atom
- morphology

quantum
- excitation energies
- electronic coulings

(polarizable) force field
- site energies

Kinetic Monte Carlo
- dynamics

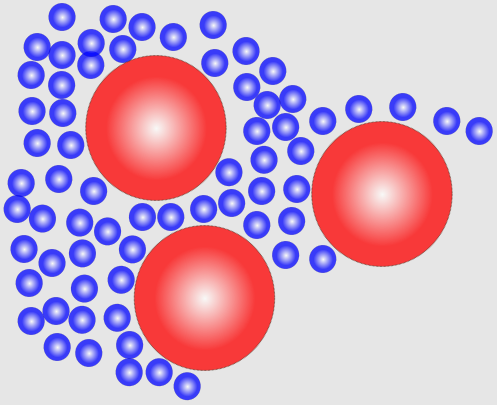




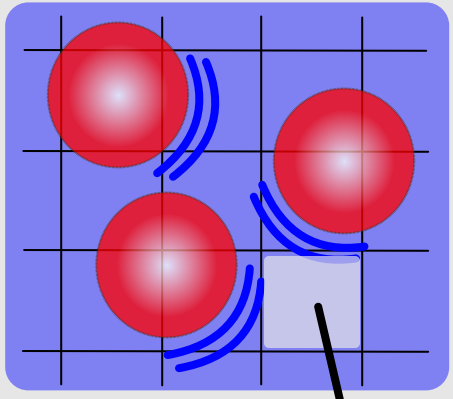
Getting excited: Challenges in quantum-classical studies of excitons in polymeric systems, PCCP 28, 30297 (2016).
Solvent effects on optical excitations studied by QM/MM simulations…, Eur. Phys. J. St. 225, 1743 (2016).

Alternative view

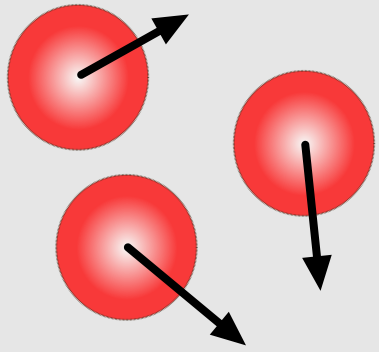
Classical mechanics



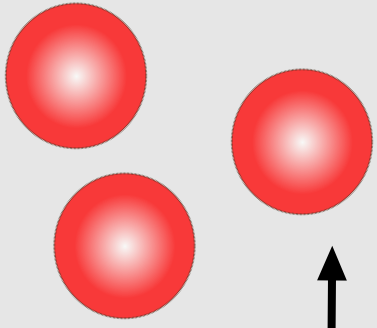
Hydrodynamics



Fokker-Planck



Thermodynamics



$$\begin{cases} \dot{\mathbf{p}}_i = -\dfrac{\partial H(z)}{\partial \mathbf{q}_i} \\ \dot{\mathbf{q}}_i = \dfrac{\partial H(z)}{\partial \mathbf{p}_i} \end{cases}$$

$$\begin{cases} \dot{\mathbf{P}}_i = -\dfrac{\partial H(z)}{\partial \mathbf{Q}_i} \\ \dot{\mathbf{Q}}_i = \dfrac{\partial H(z)}{\partial \mathbf{P}_i} \end{cases}$$

$$\begin{cases} \rho_{\mathbf{r}}(z) = \sum_i m\bar{\delta}(\mathbf{r}-\mathbf{q}_i) \\ \mathbf{g}_{\mathbf{r}}(z) = \sum_i \mathbf{p}_i\bar{\delta}(\mathbf{r}-\mathbf{q}_i) \\ e_{\mathbf{r}}(z) = \sum_i e_i\bar{\delta}(\mathbf{r}-\mathbf{q}_i) \end{cases}$$

$$\frac{\partial}{\partial t}P(x,t) = -\sum_i \left[\mathbf{V}_i \cdot \frac{\partial}{\partial \mathbf{Q}_i} + \mathbf{F}_i^{\mathrm{CC}} \cdot \frac{\partial}{\partial \mathbf{P}_i}\right] P(x,t)$$

$$+ k_{\mathrm{B}}T \sum_{ij} \frac{\partial}{\partial \mathbf{P}_i} \cdot \zeta_{ij}(Q) \cdot \left[\frac{\partial}{\partial \mathbf{P}_j} + \frac{\mathbf{P}_i}{M_i k_{\mathrm{B}}T}\right] P(x,t)$$

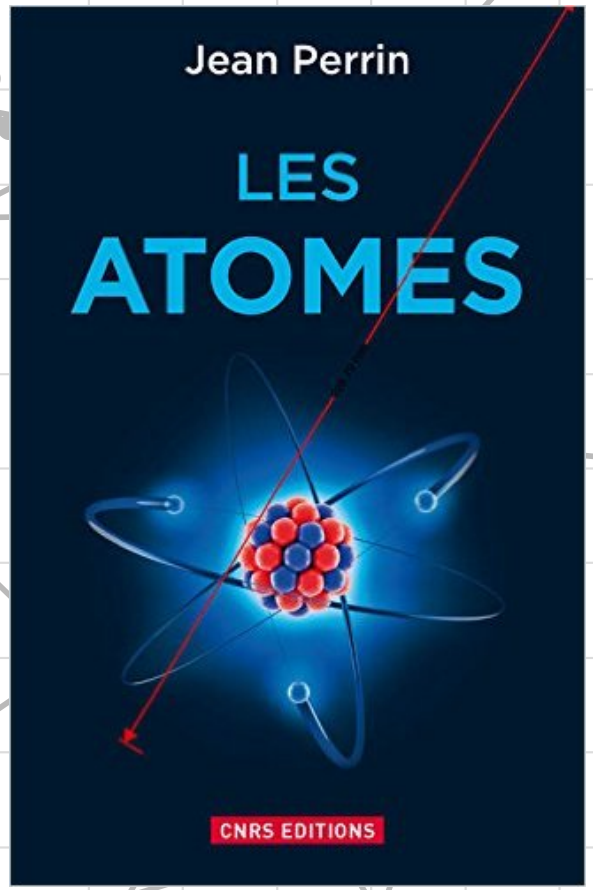
Smoluchowski → **Fick**

Q only — current

After: Español in *Novel Methods in Soft Matter Simulations* (Springer).

Brownian motion & fluctuations

- a concurrent multiscale problem



Background figure: Jean Perrin, Les Atomes, 1913

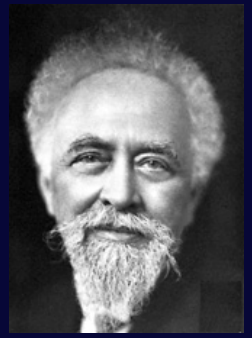
Particle size: 0.53 µm.

Recording interval : 30 seconds

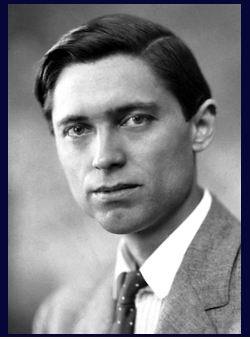
Mesh size: 3.2 µm

Brownian related Nobel Prizes and other notables

Jean Perrin



The Svedberg



Richard Zsigmondy



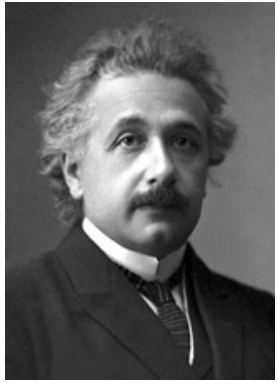




Leonard Ornstein



Sam Uhlenbeck



Albert Einstein



Marian Smoluchowski



Ludwig Boltzmann

Fluctuations in lattice-Boltzmann: Brief overview

Ladd. J. Fluid Mech. 271, 285 (1994):

- Noise to the stress tensor. Works close to equilibrium.
- **Problem:** Discretization → **ghost modes**. Noise leaks to ghosts.

Ahlrichs & Dünweg. JCP 111, 8225 (1999):

- Composite particles
- Ladd's approach + **noise onto the monomers**.
- Diffusion coefficient chosen *a priori.*

Adhikari et al. Europhys. Lett. 71, 473 (2005):

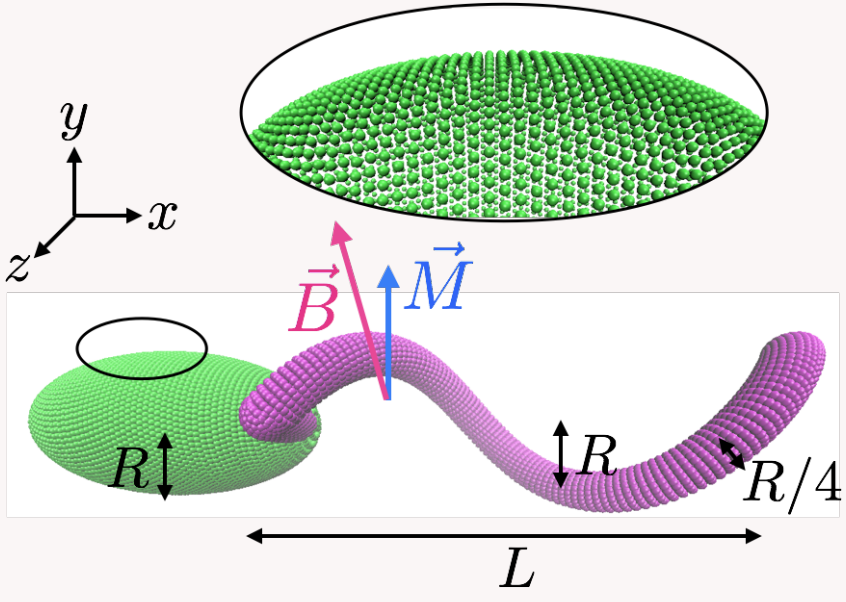
- Thermalization of **ghosts** → better temperature reproduction

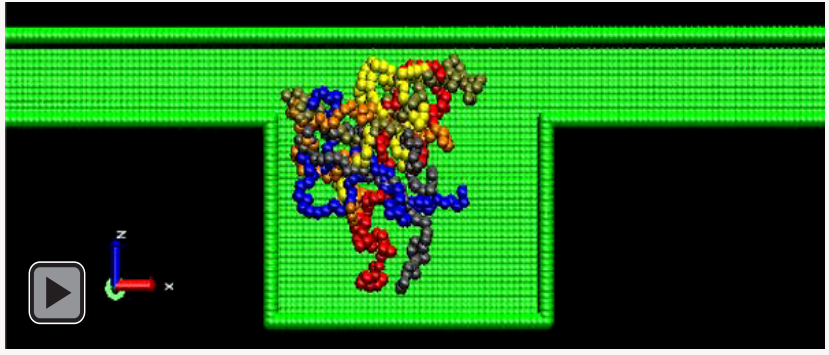
Dünweg et al. Phys Rev E 76, 036704 (2007):

- **Statistical mechanic framework** for LB fluids up to 2nd order in velocities when speed of sound is constrained to $1/\sqrt{3}$

Remaining problems include:

- Temperature preservation
- Coupling between the fluid and MD particles





How to include thermodynamically consistent fluctuations in lattice-Boltzmann?

Fluctuating lattice-Boltzmann model for complex fluids,
S.T.T. Ollila, C. Denniston, M. Karttunen, T. Ala-Nissila,
J. Chem. Phys. **134**, 064902 (2011).

Some formulas will follow....

> ***"Anyone who cannot cope with mathematics is not fully human. At best, he is a tolerable subhuman who has learned to wear his shoes, bathe, and not make messes in the house."***
>
> ***— Robert A. Heinlein***

Acknowledgements: Lattice-Boltzmann



Tapio Ala-Nissila
Aalto University



Colin Denniston
Western University



Michiko Alcanzare
Aalto University



Santtu Ollila
Aalto University



Vaibhav Thakore
Aalto University



Frances Mackay
Western / Yale

NSERC
CRSNG

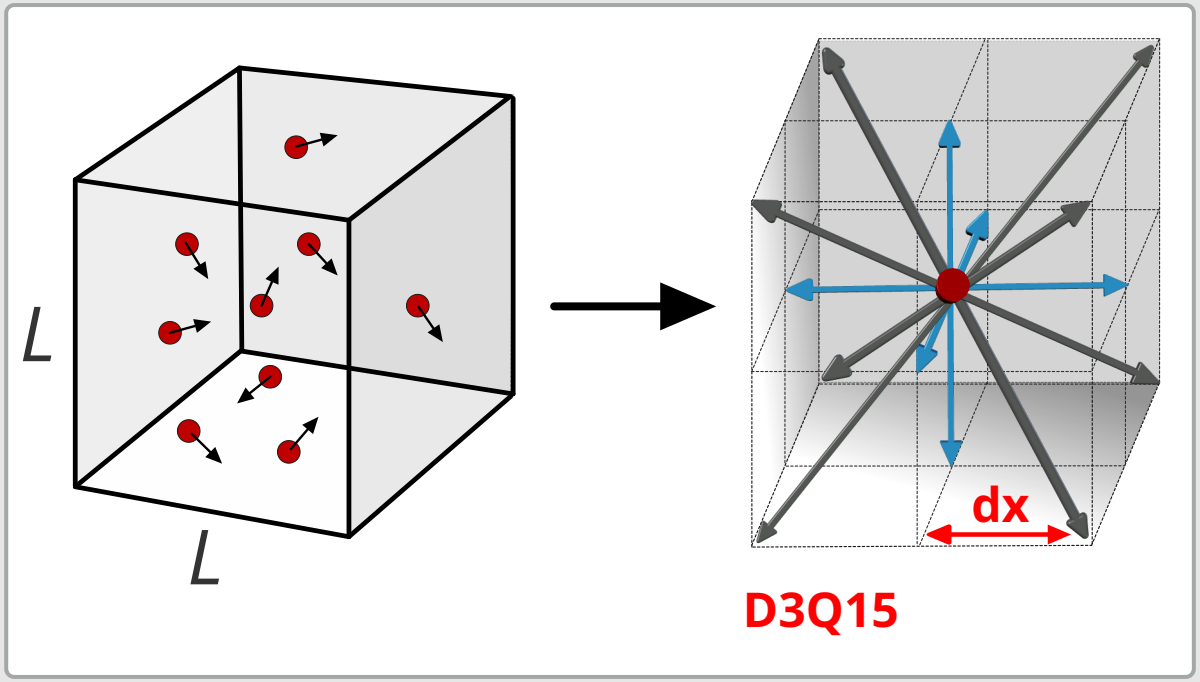
CSC

SHARCNET™

Highlights of the method

- **Thermal fluctuations** in a physically consistent way: **Temperature equal at *all* scales.**
- **Noise:** 1) In the stress tensor and 2) by shaking the whole system.
- **Speed of sound** no longer restricted (viscosity tensor).
- Allows for simulations of **compressible**, non-ideal fluids.
- Allows for simulations of **highly correlated** dense systems.
- Allows for simulations of fluids with **non-ideal equations of state.**
- **No noise is applied to the solute**! This is exactly what **Einstein suggested**.
- Rigorous test: Single chain diffusion agrees **quantitatively** with theory.
- The code is **implemented in LAMMPS**.

Lattice-Boltzmann in a nutshell



Pragmatic view:
LB solves the Navier-Stokes

Basic variable:
1-particle distribution

$$f_i(\vec{x}, t)$$

Discretized density at a node at time *t* moving with some velocity.

- Most common choice for a collision model: BGK – Bhtanagar-Gross-Krook
- Simulation has two steps: streaming and collision

Early review: Chen & Doolen, Ann. Rev. Fluid Mech. 30, 329 (1998).
Detailed discussion: Wagner: A Practical Introduction to the Lattice Boltzmann Method

Bhatnagar-Gross-Krook (BGK)

Lattice BGK:

partial density of material with $\vec{e}_i = (e_{ix}, e_{iy}, e_{iz})$

material derivative

$$D_i f_i \equiv (\partial_t + e_{i\alpha}\partial_\alpha) f_i = -\frac{1}{\tau}(f_i - f_i^{\mathrm{eq}}) + W_i$$

discrete velocities

relaxation time

forcing term

$$v_c = \frac{\Delta x}{\Delta t} = \frac{1}{\sqrt{3}}$$

$$W_i = p_i + \frac{1}{\tau}\xi_i$$

Instead of 3 momenta and 1 scalar density in 3-d continuum:

15 densities (D3Q15)
1 scalar density

Lattice structure: Accuracy of high-order moments

Bhatnagar, Gross, Krook, *Phys Rev* **94**, 511 (1954).

Navier-Stokes vs BGK

Premise for thermal noise: Must preserve mass & momentum.
Fluctuations in mass & momentum densities.
Difficult with Navier-Stokes.

Navier-Stokes:

$$\partial_t \rho + \partial_\beta(\rho u_\beta) = 0$$
$$\partial_t(\rho u_\alpha) + \partial_\beta(\rho u_\alpha u_\beta) = \partial_\beta \sigma_{\alpha\beta}$$

Tensors:

Stress:
$$\sigma_{\alpha\beta} = -P_{\alpha\beta} + \eta_{\alpha\beta\gamma\nu}\partial_\gamma u_\nu + s_{\alpha\beta}$$
fluctuating stress

Viscosity:
$$\eta_{\alpha\beta\gamma\nu} = \eta\left[\delta_{\alpha\gamma}\delta_{\beta\nu} + \delta_{\alpha\nu}\delta_{\beta\gamma} - \frac{2}{3}\delta_{\alpha\beta}\delta_{\gamma\nu}\right] + \Lambda\delta_{\alpha\beta}\delta_{\gamma\nu}$$
shear bulk

Connected by a fluctuation-dissipation relation:

$$\langle s_{\alpha\beta}(\mathbf{r},t)s_{\gamma\nu}(\mathbf{r}',t')\rangle = 2\eta_{\alpha\beta\gamma\nu}k_{\mathrm{B}}T\delta(\mathbf{r}-\mathbf{r}')\delta(t-t')$$

Eigenvectors of the moments

Distribution: $$f_i(\mathbf{x},t) = w_i \sum_a m_i^a M^a(\mathbf{x},t) N^a$$

BGK: $$D_i f_i \equiv (\partial_t + e_{i\alpha}\partial_\alpha) f_i = -\frac{1}{\tau}(f_i - f_i^{\mathrm{eq}}) + W_i$$

$$\Rightarrow \partial_t M^a + \partial_\alpha \Big(\sum_i m_i^a e_{i\alpha} f_i \Big) = -\frac{1}{\tau} \left(M^a - M^a_{\mathrm{eq}} \right) + \sum_i m_i^a W_i$$

Connect the moments with physical quantitites:

$$M^0(\mathbf{x},t) = \sum_i f_i(\mathbf{x},t) = \rho(\mathbf{x},t)$$

$$M^{1,2,3}(\mathbf{x},t) = \sum_i e_{i\alpha} f_i(\mathbf{x},t) = \rho(\mathbf{x},t) u_\alpha(\mathbf{x},t)$$

Apply Chapman-Enskog for the *0th* and *1st* moments & take the hydrodynamic limit

$$\partial_t \rho + \partial_\beta(\rho u_\beta) = 0 + \mathcal{O}(\partial^3)$$

$$\partial_t(\rho u_\alpha) + \partial_\beta(\sum_i f_i e_{i\alpha} e_{i\beta}) = 0 + \mathcal{O}(\partial^2)$$

Moments of equilibrium distribution & continuum noise

a	0	1	2	3	4	5	6	7	8	9	10 – 12	13	14
M^a_{eq}	ρ	ρu_x	ρu_y	ρu_z	$P_{xx}+\rho(u_x^2-\frac{v_c^2}{3})$	$P_{yy}+\rho(u_y^2-\frac{v_c^2}{3})$	$P_{zz}+\rho(u_z^2-\frac{v_c^2}{3})$	$P_{xy}+\rho u_x u_y$	$P_{xz}+\rho u_x u_z$	$P_{yz}+\rho u_y u_z$	0	$\rho u_x u_y u_z$	K^{eq}
$\bar{\zeta}^a$	0	0	0	0	s_{xx}	s_{yy}	s_{zz}	s_{xy}	s_{xz}	s_{yz}	$\bar{\zeta}^a$	$\bar{\zeta}^{13}$	$\bar{\zeta}^{14}$

Momentum densities: **Stress densities:** **Ghost densities:**

Connect the moments with physical quantitites:

$\neq 0$ when out of equilibrium

Leading-order stresses couple to ghosts (D3Q15):

$$\frac{2}{3}\nabla\cdot\begin{bmatrix}\rho(u_y^2+u_z^2)/2 & P_{xy}+\rho u_x u_y & P_{xz}+\rho u_x u_z\\ P_{xy}+\rho u_x u_y & \rho(u_x^2+u_z^2)/2 & P_{xy}+\rho u_y u_z\\ P_{xz}+\rho u_x u_z & P_{yz}+\rho u_y u_z & \rho(u_x^2+u_y^2)/2\end{bmatrix}+\frac{2}{9}\nabla\left(\mathrm{Tr}P-\rho+\frac{K^{\text{eq}}}{\sqrt{2}}\right)=-\frac{1}{\tau}\mathbf{J}^{(1)}$$

Terrible, isn't it.

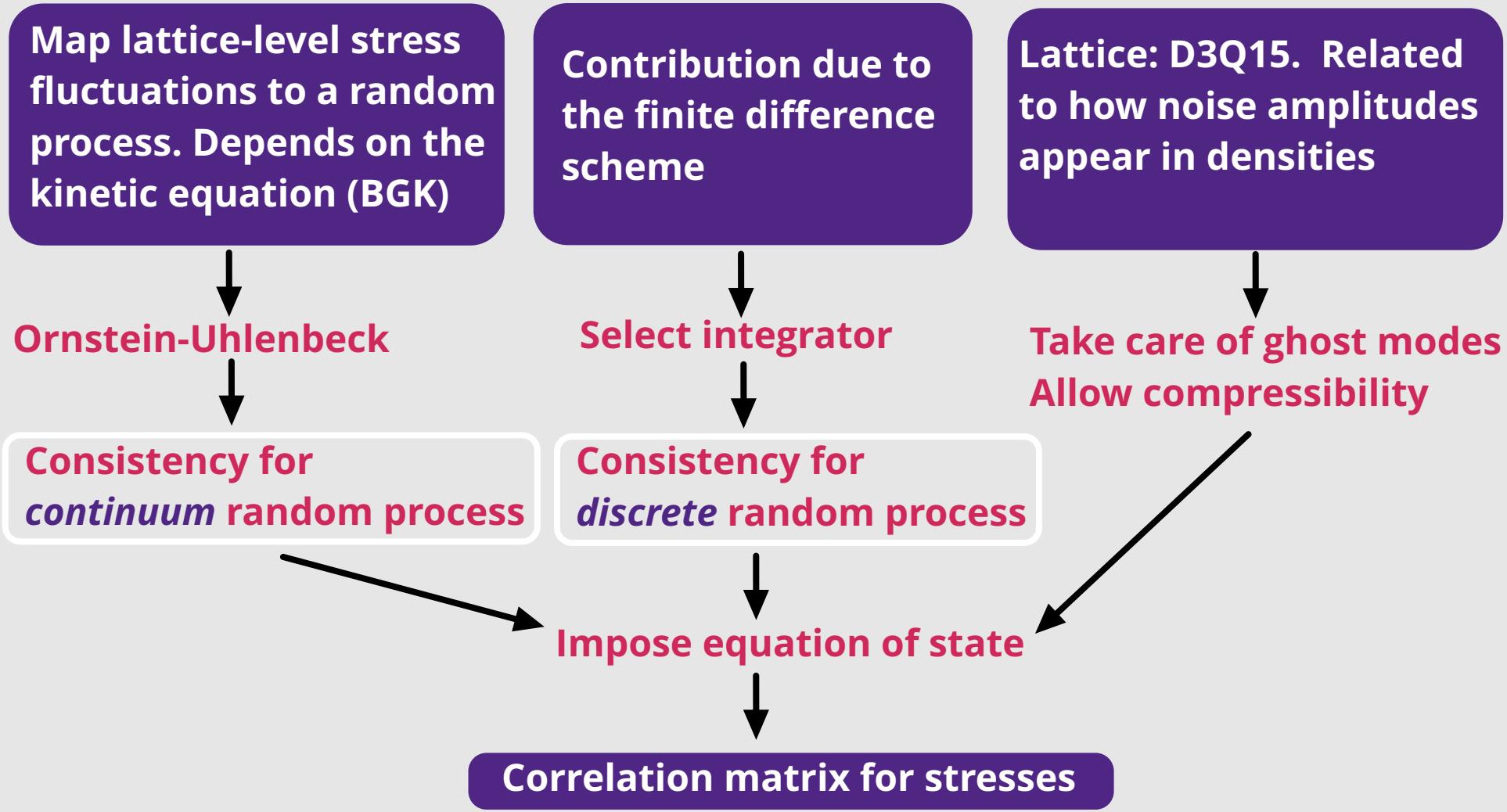
"A mathematical theory is not to be considered complete until you have made it so clear that you can explain it to the first man whom you meet on the street."
- David Hilbert

The good news: We can put this in practise.

The gory details:

Fluctuating lattice-Boltzmann model for complex fluids,
S.T.T. Ollila, C. Denniston, M. Karttunen, T. Ala-Nissila,
J. Chem. Phys. **134**, 064902 (2011).

Strategy: 3-steps to implement fluctuation



Step 1: Ornstein-Uhlenbeck process


Leonard Ornstein


Sam Uhlenbeck

Origin: Description of a Brownian particle in viscous medium.

Typical form:

$$d\,X_t = \theta(\mu + X_t)dt + \sigma dW_t$$

Map to:

$$\mathrm{d}X_t = [a(t) + b(t)X_t]\,\mathrm{d}t + [\alpha(t) + \beta(t)X_t]\,\mathrm{d}B_t$$

The only non-trivial stationary Gauss-Markov process.

Difference to plain Wiener process: Mean-reverting.

Uhlenbeck & Ornstein, "On the theory of Brownian Motion". Phys. Rev. 36: 823–841 (1930).

Step 1: Identification as an Ornstein-Uhlenbeck process

f_i ↓ τ^{-1} ↓ ↓ $\alpha(t)\mathrm{d}B_t = \frac{\xi}{\tau}dt$

Identify with the kinetic eqn (BGK)

$$\mathrm{d}X_t = [a(t) + b(t)X_t]\,\mathrm{d}t + [\alpha(t) + \beta(t)X_t]\,\mathrm{d}B_t$$

↑ $\frac{1}{\tau}(f_i^{\mathrm{eq}} + \tau p_i)$ ↑ $\beta(t) = 0$

General solution:

$$X_{t'} = U_{t'}\left[X_t + \int_t^{t'} \frac{a(s) - \beta(s)\alpha(s)}{U_s}\mathrm{d}s + \int_t^{t'} \frac{\alpha(s)}{U_s}\mathrm{d}B_s\right] \quad \text{where} \quad U_{t'} = \exp\left[\int_t^{t'} \beta(s)\mathrm{d}B_s + \int_t^{t'} (b(s) - \frac{1}{2}\beta^2(s))\mathrm{d}s\right]$$

Integrate over one time step to get variance:

$$\mathrm{Var}\left[e^{-\Delta t/\tau}\int_t^{t+\Delta t} \frac{1}{\tau}e^{(s-t)/\tau}\bar{\xi}_i\mathrm{d}t\right] = \langle\bar{\xi}_i^{\,2}\rangle\frac{(1 - \exp(-2\Delta t/\tau))}{2\tau} \equiv \langle\bar{\xi}_i^{\,2}\rangle q_{\mathrm{OU}}^2$$

Must be retained in discrete time and space variables!

Continuum process!

Step 2: Contribution from finite-differencing

$$
\begin{aligned}
& f_i(\mathbf{x} + \mathbf{e}_i \Delta t, t + \Delta t) \\
& \quad = e^{-\Delta t/\tau} f_i(\mathbf{x}, t) + (1 - e^{-\Delta t/\tau}) h_i^{\mathrm{eq}}(\mathbf{x}, t) \\
& \qquad + \Delta t \left(1 - \frac{\tau}{\Delta t}(1 - e^{-\Delta t/\tau})\right) D_t h_i^{\mathrm{eq}}(\mathbf{x}, t) \\
& \qquad + \Delta t^2 \left(\frac{\tau^2}{\Delta t^2}(1 - e^{-\Delta t/\tau}) - \frac{\tau}{\Delta t} + \frac{1}{2}\right) D_t^2 h_i^{\mathrm{eq}}(\mathbf{x}, t) \\
& \qquad + \mathcal{O}(\Delta t^4)
\end{aligned}
$$

Discrete noise.
Not the same as
on previous page!

$$h_i^{\mathrm{eq}} = g_i^{\mathrm{eq}} + \xi_i$$

$$f_i^{\mathrm{eq}} + \tau p_i$$

$$\langle \xi_i^2 \rangle = \langle \bar{\xi}_i^2 \rangle q_{\mathrm{OU}}^2 / q_{\mathrm{FD}}^2$$

Step 3: Effect of lattice. Noise amplitudes in densities

Discrete lattice-level fluctations: $$\xi_i(\mathbf{x}, t) = w_i \sum_a m_i^a \zeta^a(\mathbf{x}, t) N^a$$

Ideal case: $$\langle (\zeta^a)^2 \rangle = \frac{18}{N^a} A_\eta \equiv \frac{18}{N^a} \eta \, k_B T \frac{1}{\Delta x^3} \frac{1}{\Delta t} \frac{q_{\mathrm{OU}}^2}{q_{\mathrm{FD}}^2}$$

Non-ideal: Need the noise correlation matrix elements for lattice level noise

$$C = \frac{q_{\mathrm{OU}}^2}{q_{\mathrm{FD}}^2} \begin{bmatrix} \langle s_{xx}^2 \rangle & \langle s_{xx} s_{yy} \rangle & \langle s_{xx} s_{zz} \rangle \\ \langle s_{xx} s_{yy} \rangle & \langle s_{yy}^2 \rangle & \langle s_{yy} s_{zz} \rangle \\ \langle s_{xx} s_{zz} \rangle & \langle s_{yy} s_{zz} \rangle & \langle s_{zz}^2 \rangle \end{bmatrix}$$

Random variables with this correlation matrix: factorize the correlation matrix C for the diagonal components into Cholesky-decomposed form.

The explicit form requires equation of state. Positive-definitness of *C* must be imposed.

Eyes still open?

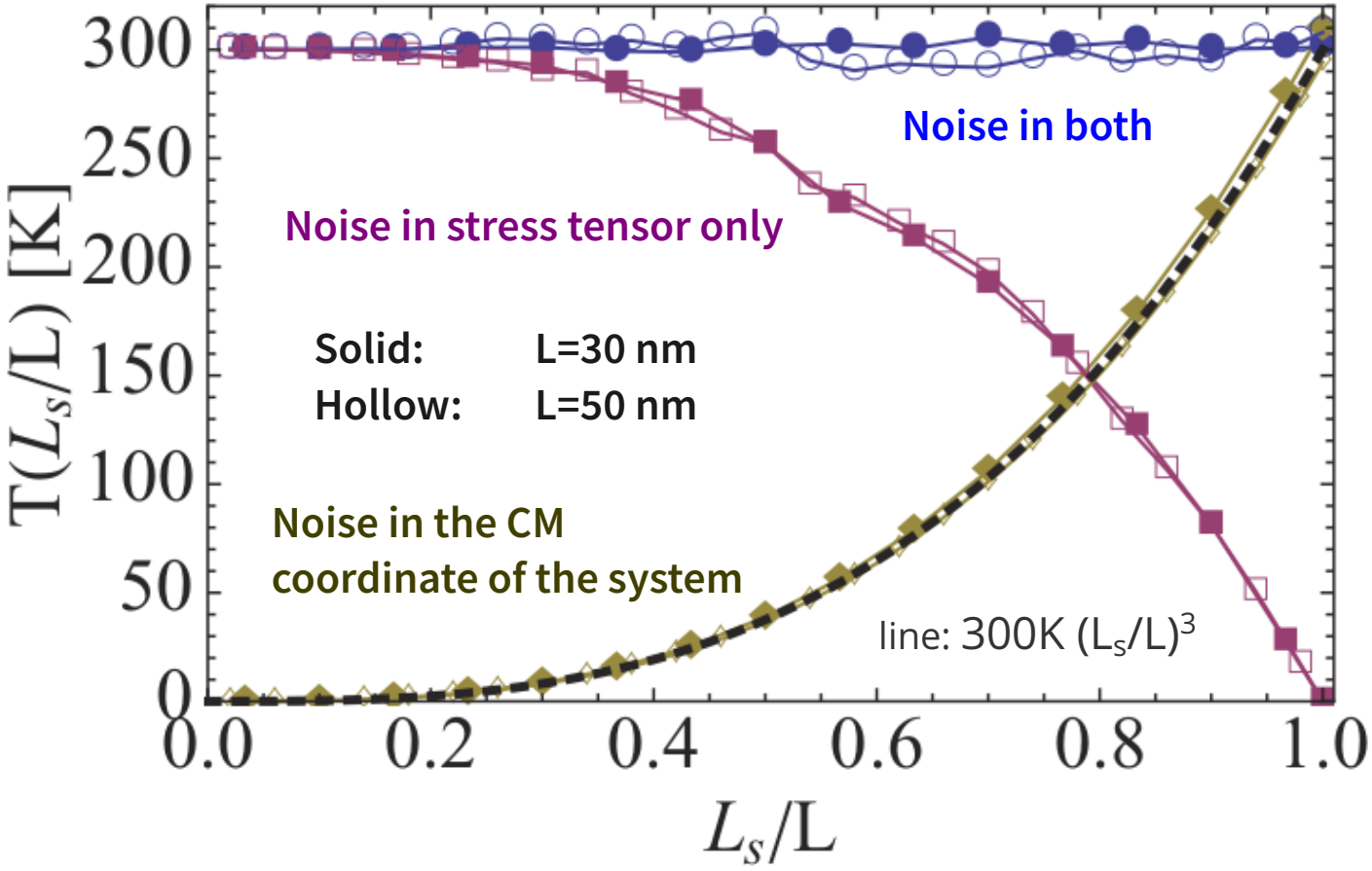
The good news: All this is now in LAMMPS.

Verification:

Tests of the LB fluid
Tests with embedded polymers

Fluctuating lattice-Boltzmann model for complex fluids,
S.T.T. Ollila, C. Denniston, M. Karttunen, T. Ala-Nissila,
J. Chem. Phys. **134**, 064902 (2011).

Temperature from block-averaged fluctuations



Fluctuating lattice-Boltzmann model for complex fluids,

Ollila, Denniston, Karttunen, Ala-Nissila, *J. Chem. Phys.* **134**, 064902 (2011).

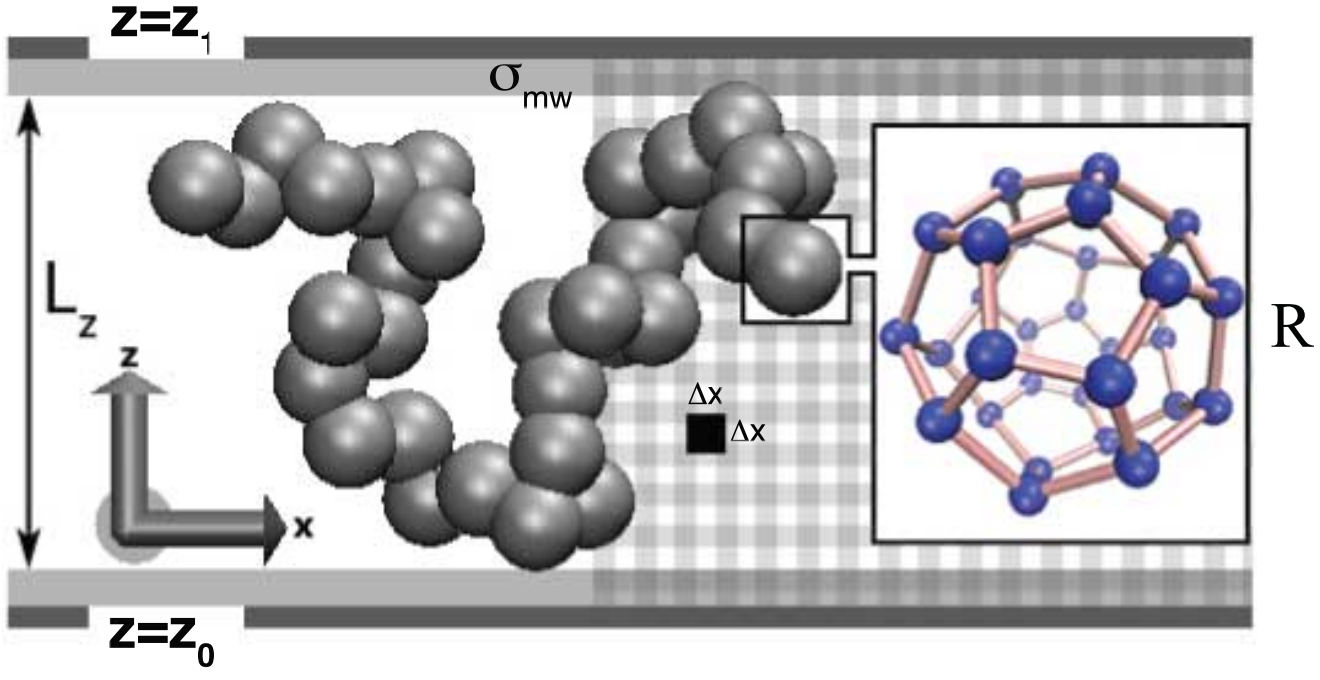
Quick look at polymers in flow

- separation & effect of boundaries

Biopolymer filtration in corrugated nanochannels,
S.T.T. Ollila, C. Denniston, M. Karttunen, T. Ala-Nissila,
Phys. Rev. Lett. **112**, 118301 (2014).

Hydrodynamic Effects on Confined Polymers,
S.T.T. Ollila, C. Denniston, M. Karttunen, T. Ala-Nissila,
Soft Matter **9**, 3478-3487 (2013)

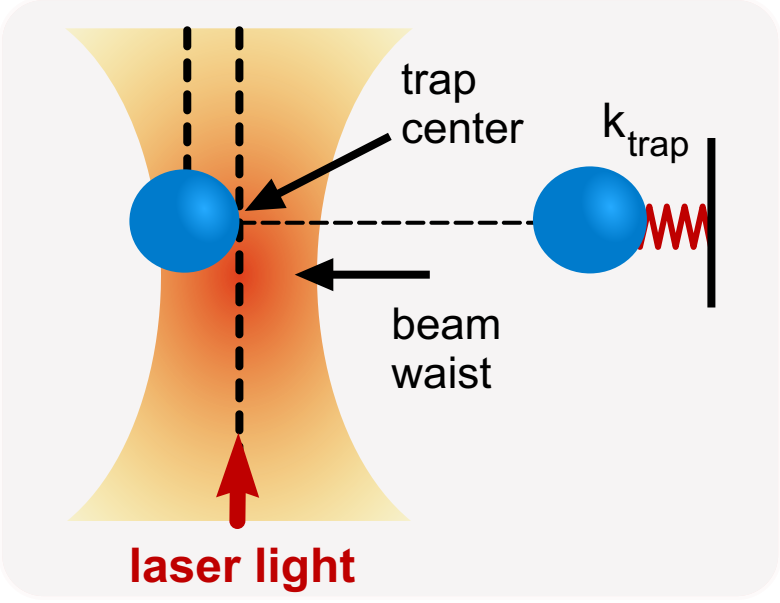
Coupling to Molecular Dynamics: Concurrent multiscaling



$$m\ddot{\vec{r}}_i = -\sum_{j\neq i} \nabla_i U(\vec{r}_i, \vec{r}_j) - \gamma[\vec{v}_i(\vec{r}_i, t) - \vec{u}_{\mathrm{ip}}(\vec{r}_i, t)]$$

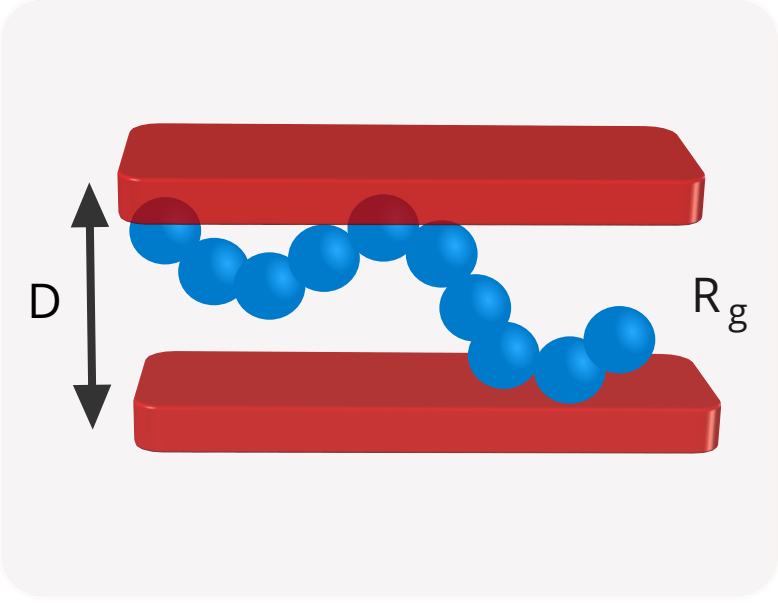
Interpolated fluid velocity at the particle.
Based on the flow field at nearby lattice sites.

Confinement: LB is very flexible with boundary conditions



Confinement using a potential:

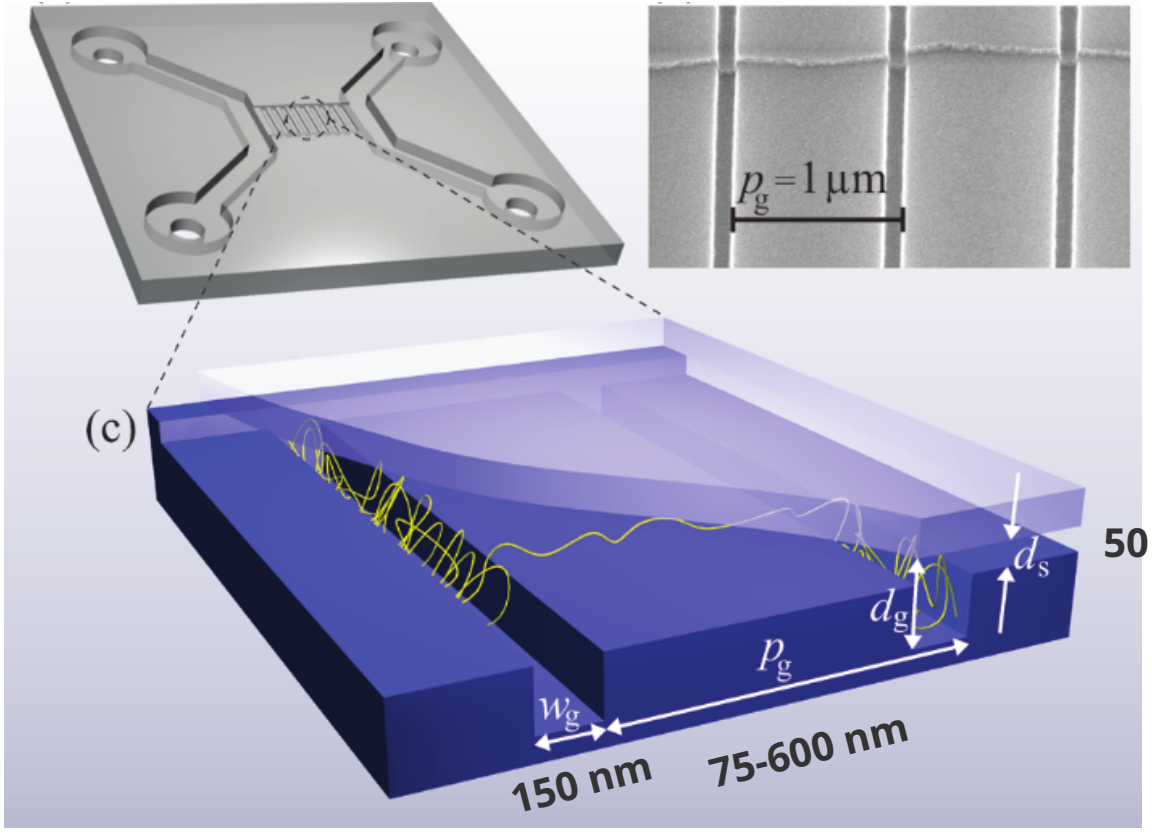
- Optical trapping
- No physical walls
- Periodic boundaries



Confinement using walls:

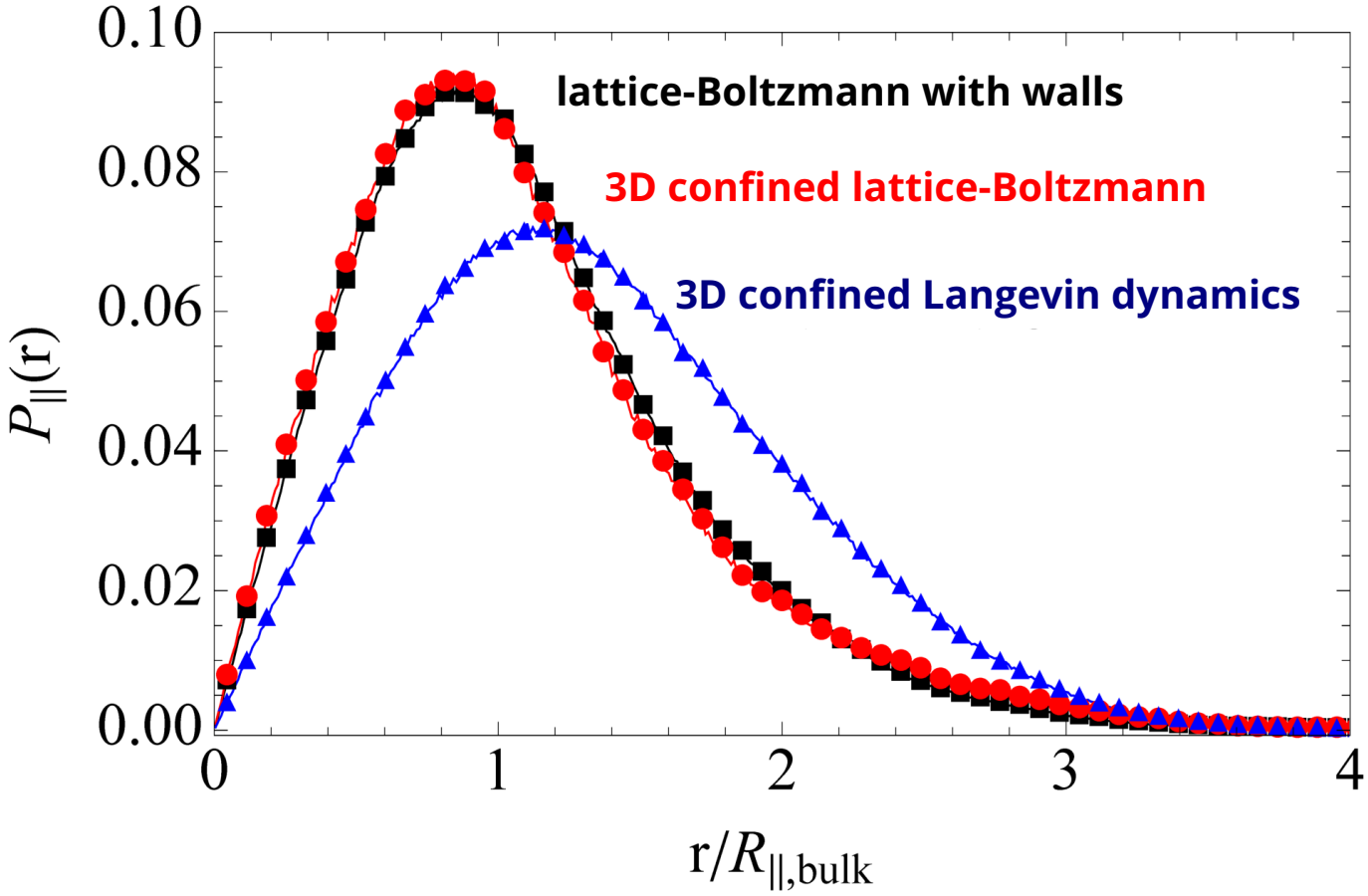
- Channels
- No-slip boundary conditions
- Breaks momentum conservation

Pressure driven DNA: Radius of gyration as a measure

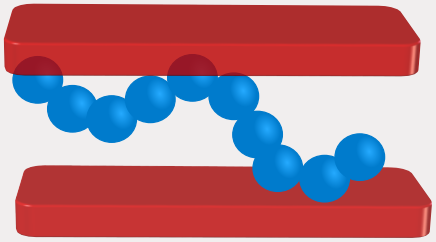


Pressure-driven DNA in Nanogroove Arrays: Complex Dynamics Leads to Length- and Topology-Dependent Separation, Mikkelsen, Reisner, Flyvbjerg, Kristensen, Nano Lett 11, 11598 (2011)

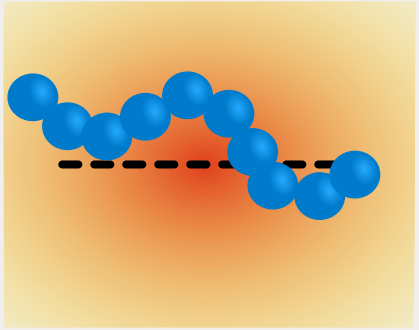
Confinement: Planar monomer center of mass distribution



Confinement: walls



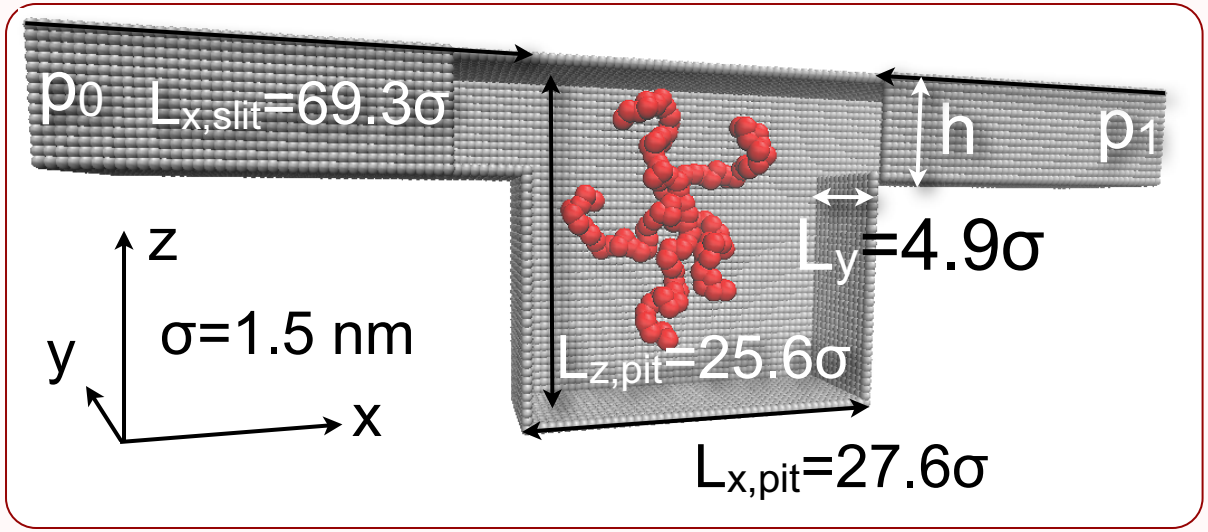
Confinement: potential



Hydrodynamic Effects on Confined Polymers,

S.T.T. Ollila, C. Denniston, M. Karttunen, T. Ala-Nissila, *Soft Matter* **9**, 3478-3487 (2013)

Polymers in confinement



Mobility: $\mu = \langle v_x \rangle / \Delta p$

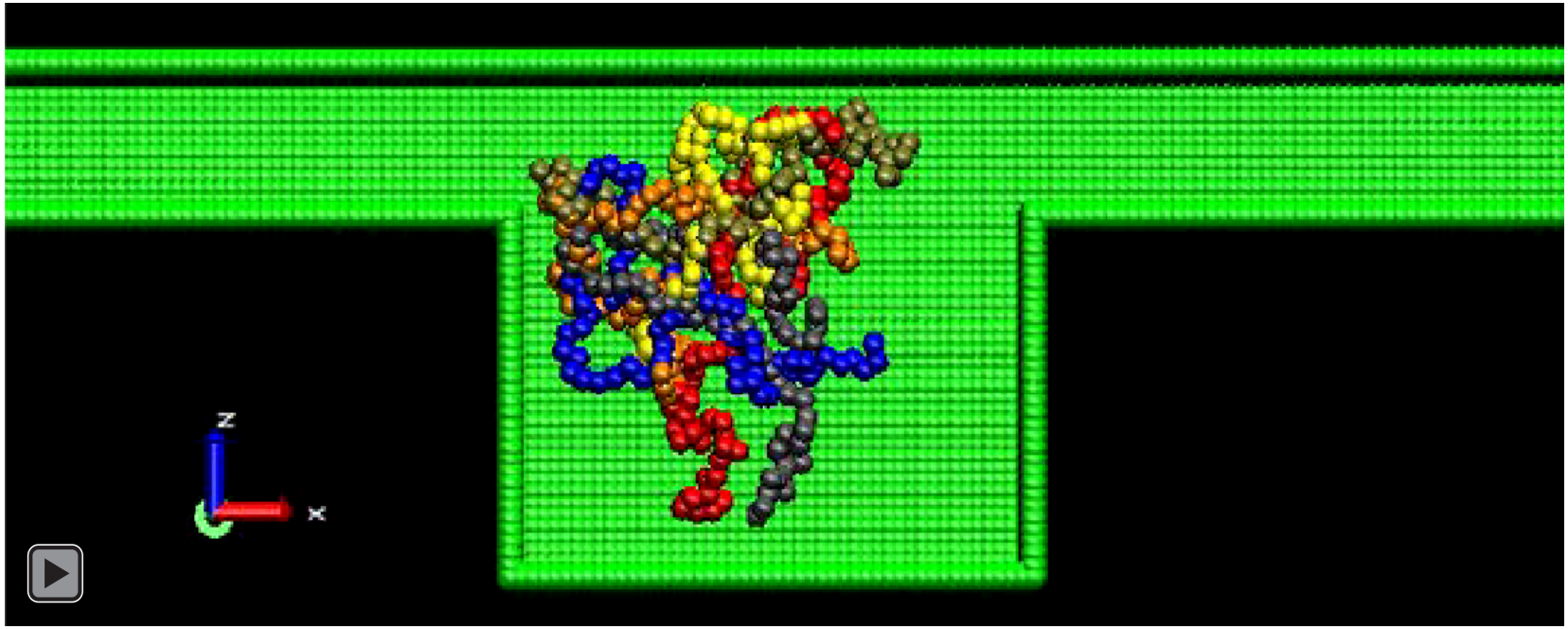
T = 300 K

- Linear, star, and circular polymers were simulated.
- Note: Pit geometry. Different from the grooves of Mikkelsen et al.
- Pressure driven flow, not body force

Biopolymer filtration in corrugated nanochannels,

S.T.T. Ollila, C. Denniston, M. Karttunen, T. Ala-Nissila, *Phys. Rev. Lett.* **112**, 118301 (2014).

Pressure driven separation & importance of fluctuations



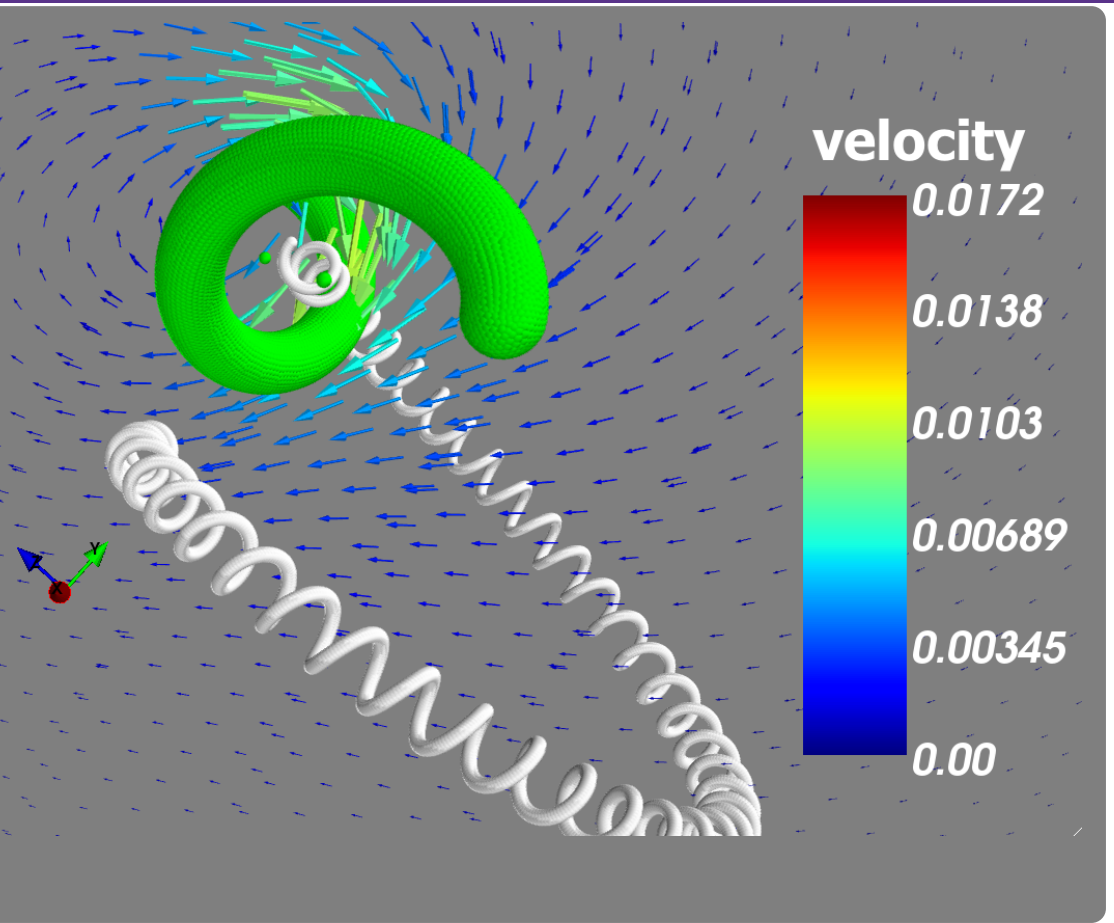
Mobility: Defined by the pressure difference and fluctuations

Fluctuations: Determine how quickly the polymer can move perpendicular to the flow streamlines

Biopolymer filtration in corrugated nanochannels,
Ollila, Denniston, Karttunen, Ala-Nissila, *Phys. Rev. Lett.* **112**, 118301 (2014).

Chiral particles & active transport

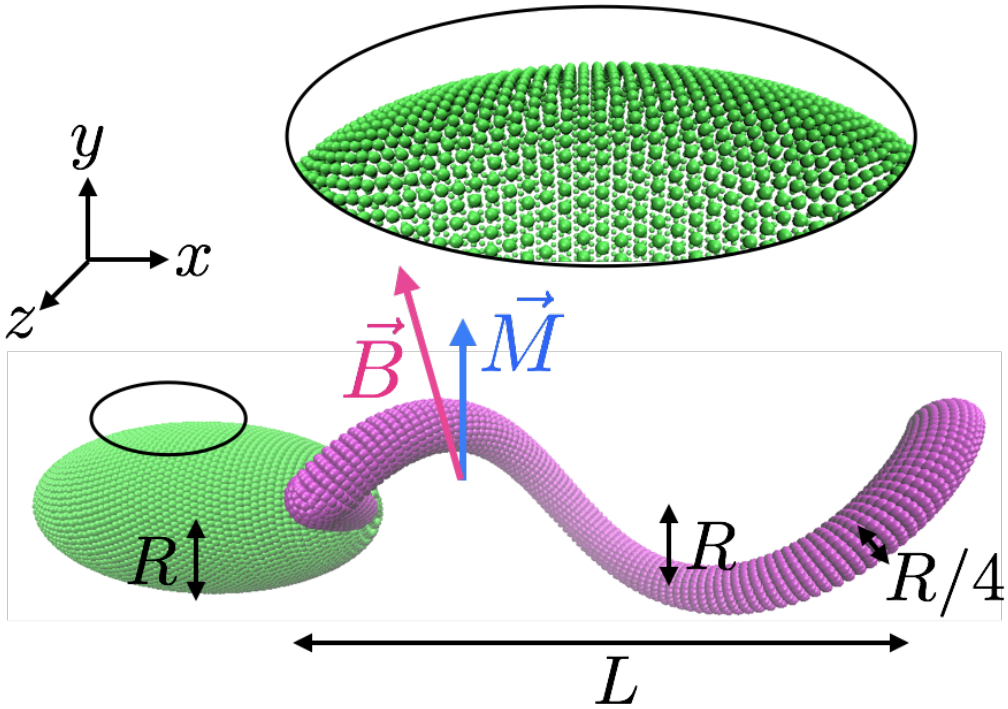
- beating fluctuations with magnetic fields



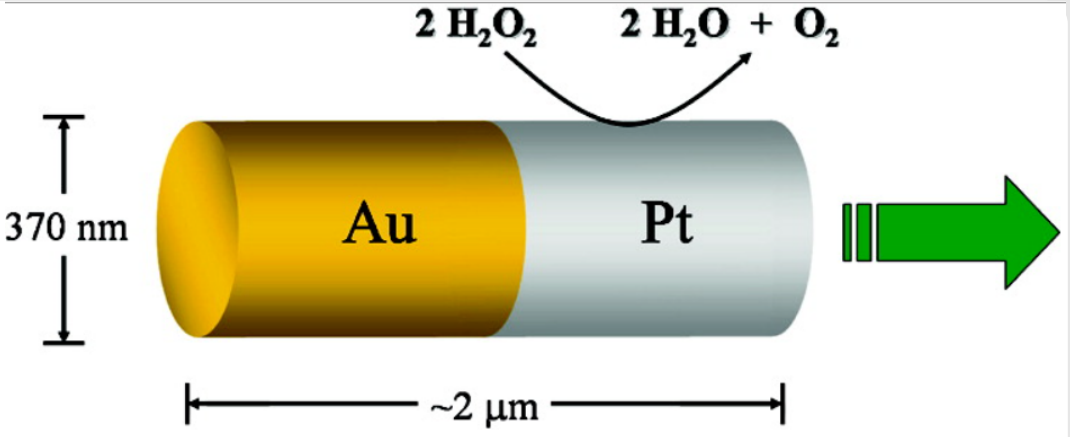
With and without cargo

Cargo: ~1000 nodes

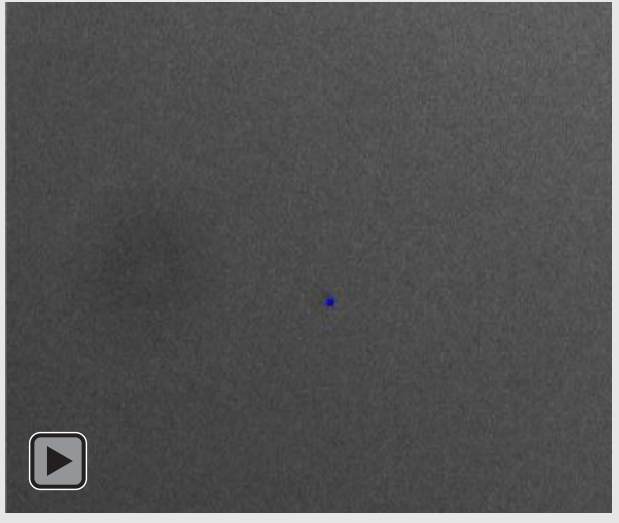
Helix: ~8000 nodes



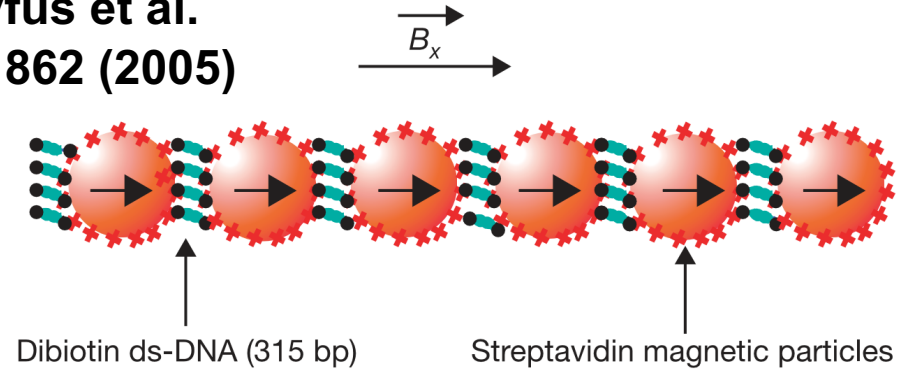
Background: Micro/nano transport using fields



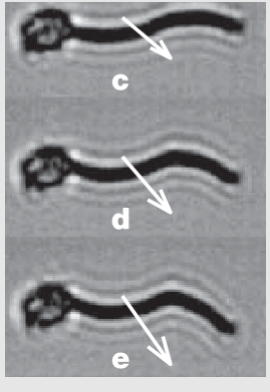
Paxton et al., JACS 126, 13424 (2004)



Dreyfus et al. 437, 862 (2005)



Ma, Han, Sanchez, JACS 137, 4976 (2015)

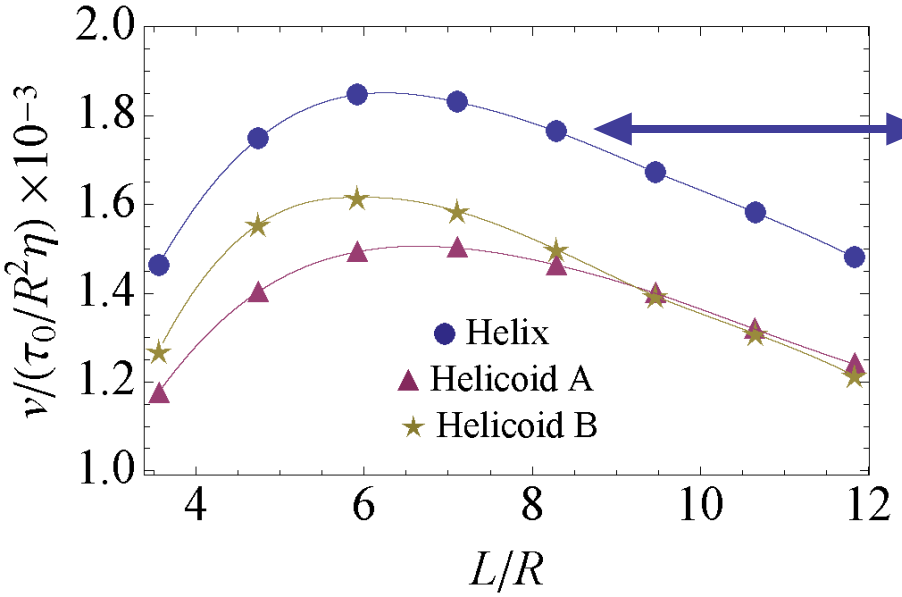


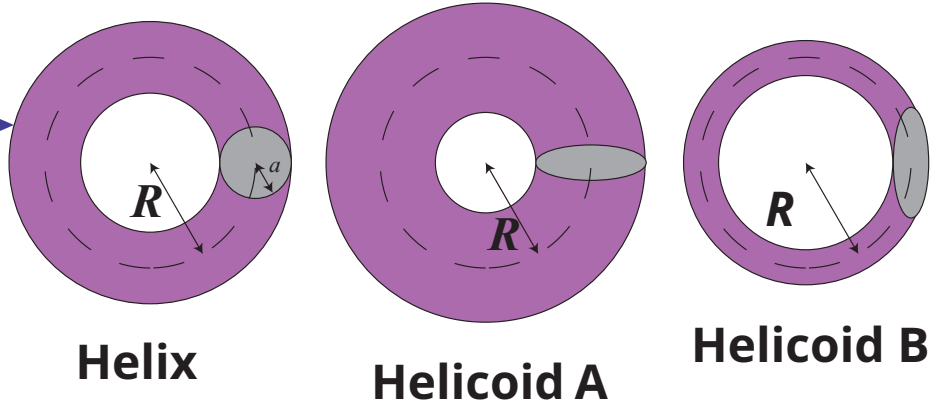
Helical particles: Optimize shape & velocity

Motion of chiral objects: Anisotropy gives translational-rotational coupling

$$\begin{pmatrix} F \\ \tau \end{pmatrix} = \begin{pmatrix} \xi^{\mathrm{TT}} & \xi^{\mathrm{TR}} \\ \xi^{\mathrm{RT}} & \xi^{\mathrm{RR}} \end{pmatrix} \begin{pmatrix} v \\ \omega \end{pmatrix}$$

This is how micro-organism propel.



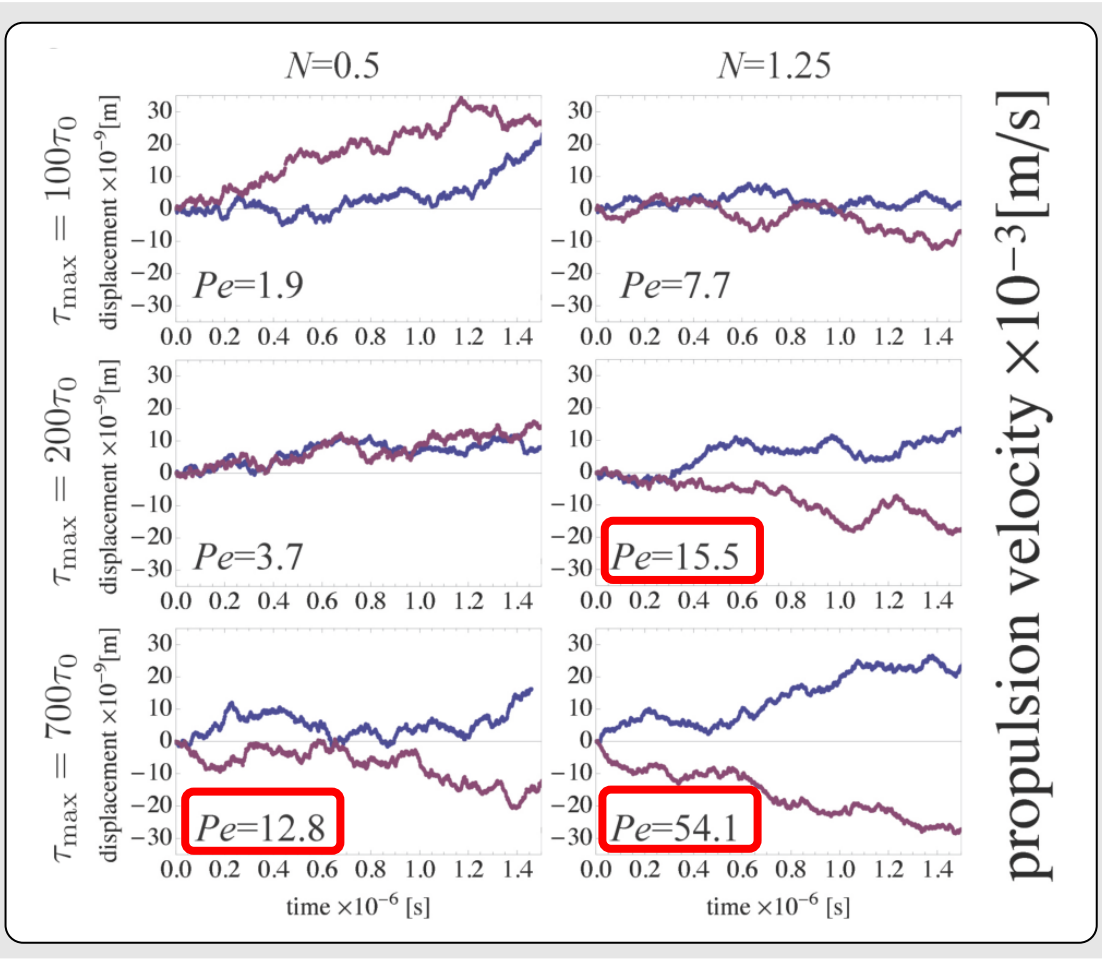


Circular cross-section: optimal propulsion

Medina-Sanchez et al., Toward assisted fertilization by sperm-carrying micromotors. Nano Lett. 16, 555 (2016).

Alcanzare, Thakore, Karttunen, Ala-Nissila, *Controlled propulsion and separation of helical*…, Soft Matter

Helical particles: Selection by chirality



Peclet number:

$$\mathrm{Pe} \equiv \frac{vL}{D_T} \quad \leftrightarrow \quad \frac{\text{propulsion}}{\text{fluctuations}}$$

Can also be written as

$$\mathrm{Pe} = \frac{6\pi\eta R_H}{k_B T}\varepsilon\omega RL$$

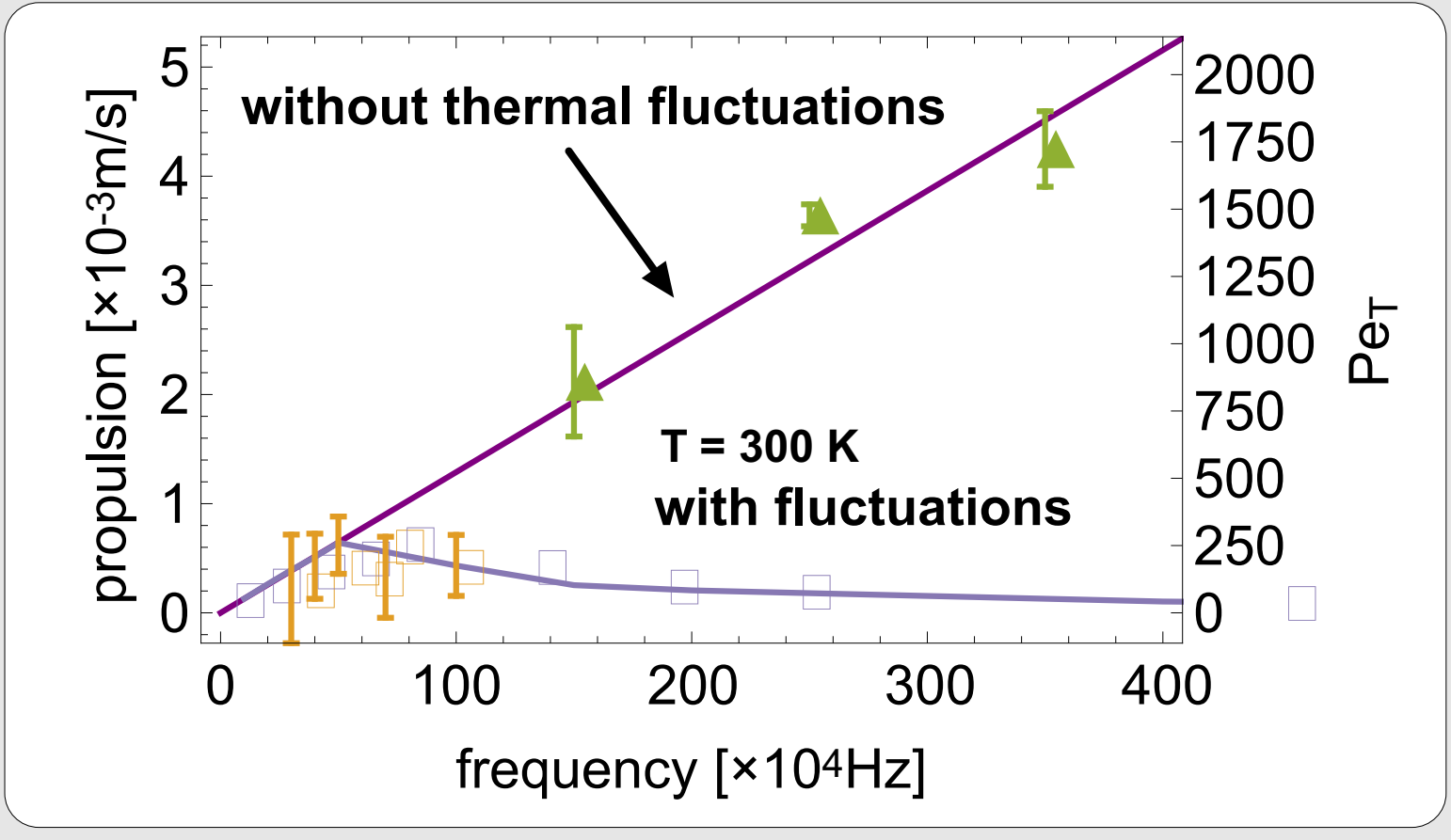
Efficiency: $\varepsilon \equiv \dfrac{v}{\omega R}$

For separation: Pe > 10

Separation (Pe>10): Consistent with Fu et al., Phys. Rev. Lett 102, 158103 (2009)

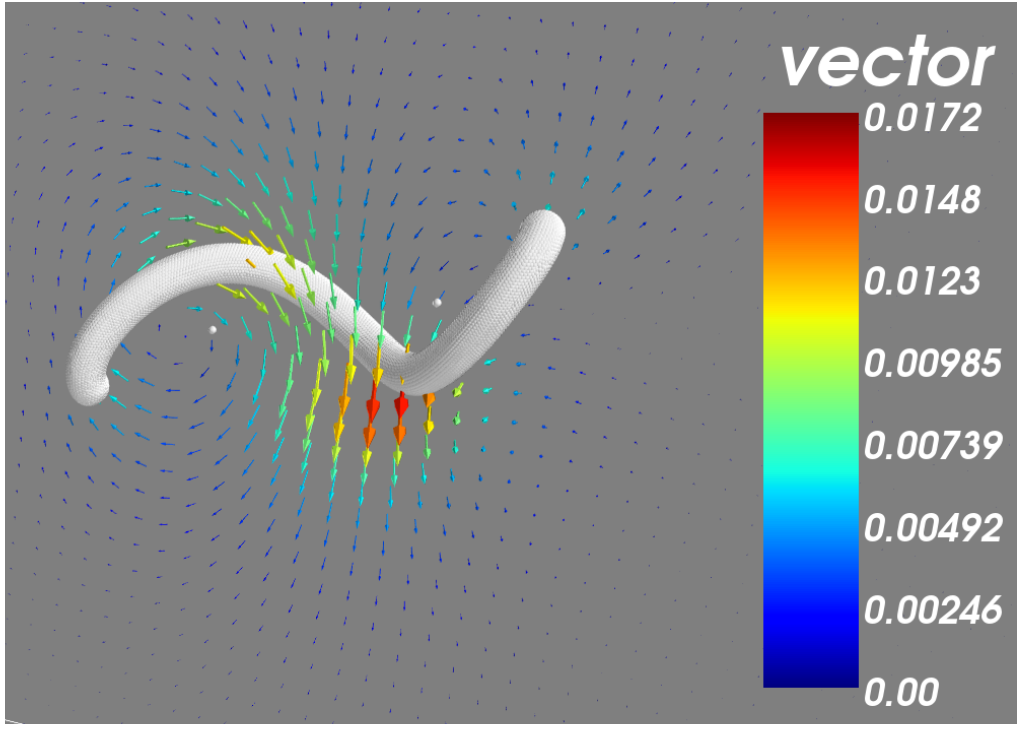
Alcanzare, Thakore, Karttunen, Ala-Nissila, *Controlled propulsion & separation of helical…*, Soft Matter

Effect of thermal fluctuations without cargo



Alcanzare, Karttunen, Ala-Nissila, *Propulsion and controlled steering of magnetic nanohelices*, submitted

Control using a magnetic field







Alcanzare, Karttunen, Ala-Nissila, *Propulsion and controlled steering of magnetic nanohelices*, submitted

Conclusions

Developed a lattice-Boltzmann technique with consistent fluctuations across length scales.

Showed the importance of fluctuations in polymer separation using nanopits.

Chiral particles: Established optimal and shape.

Achieved by balancing the competing requirements for maintaining the stability of the rotational motion and minimizing viscous drag.

Control by magnetic field: Established nanoparticle steering and control using magnetic field to overcome fluctuations.

How about the original question? What is the status of multiscale modeling?