Modeling of Micro-Fluidics by a Dissipative Particle Dynamics Method

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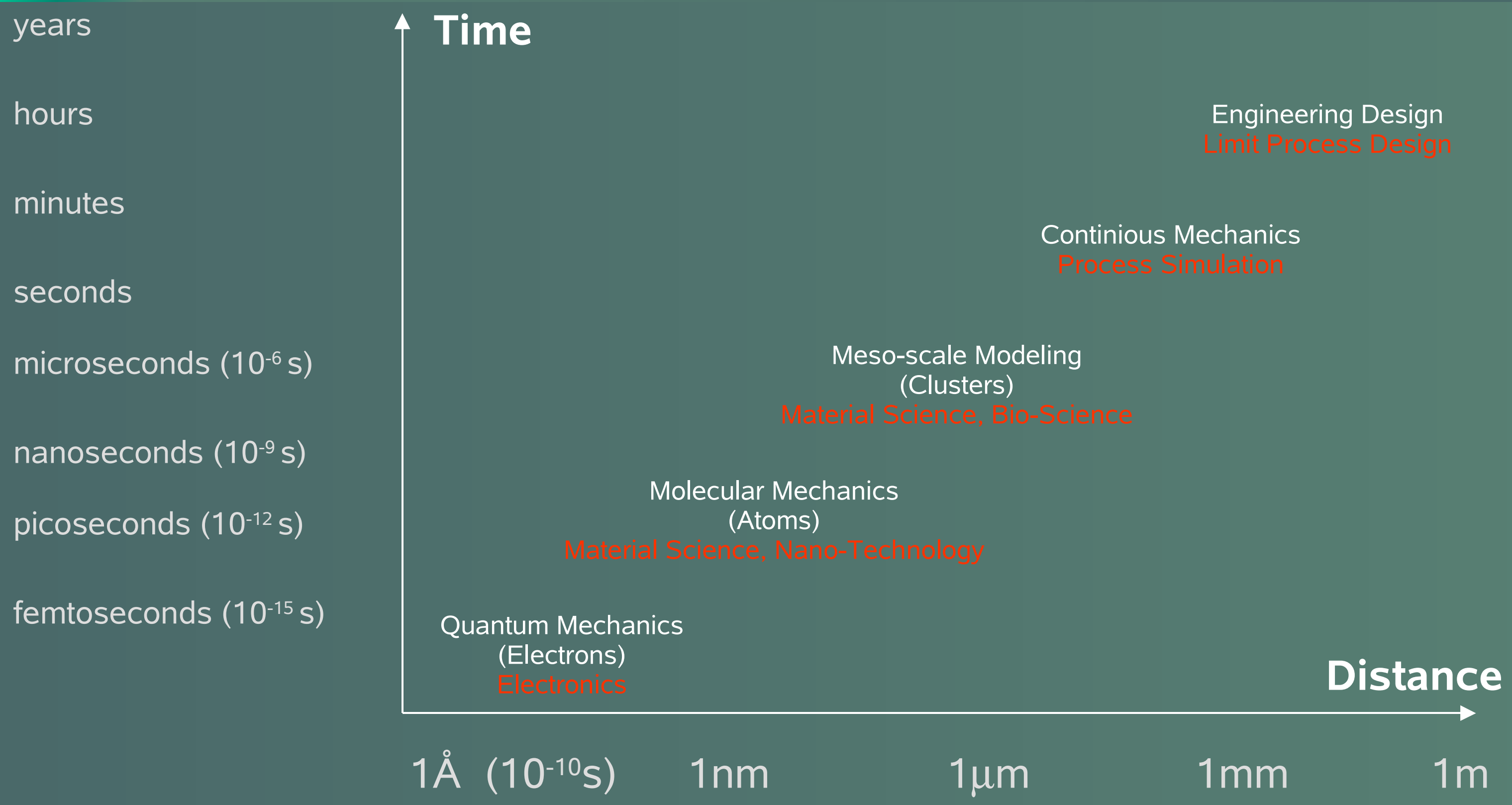
Scales and Physical Models



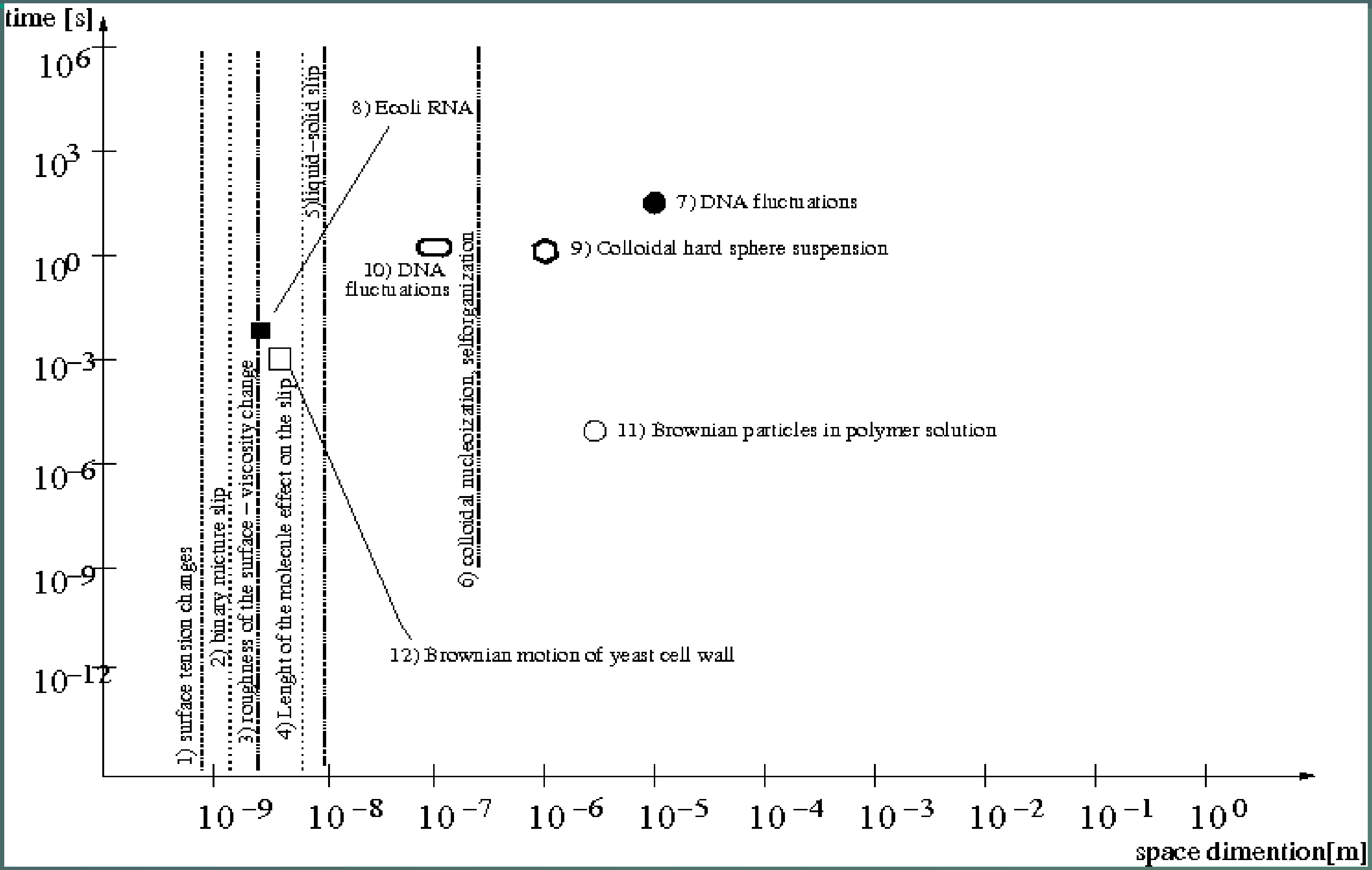
Micro- and Nanoscale effects

length	surface	volume
1m	$1m^2$	$1m^3$
1μm 10^{-6} m	$1μm^2$ 10^{-12} m	$1μm^3$ 10^{-18} m
S^1	S^2	S^3

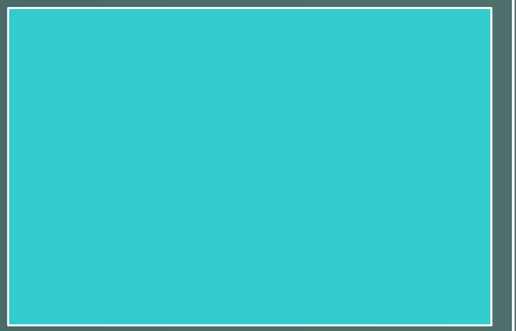
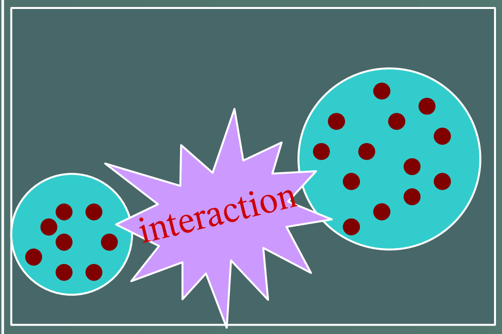
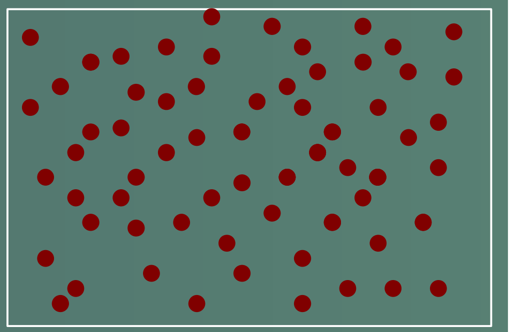
- increasing importance of surface to volume effects (surface tension important, gravity unimportant)
- slip, no-slip boundary conditions
- gas, liquid differences ($1\ \mu m^3$ -25 millions of air molecules, 34 billion water molecules)
- non-linear effects, thermodynamical nonequilibrium

1mm - MACRO - MICRO PHYSICS BARRIER

Nano- and Micro- Effects

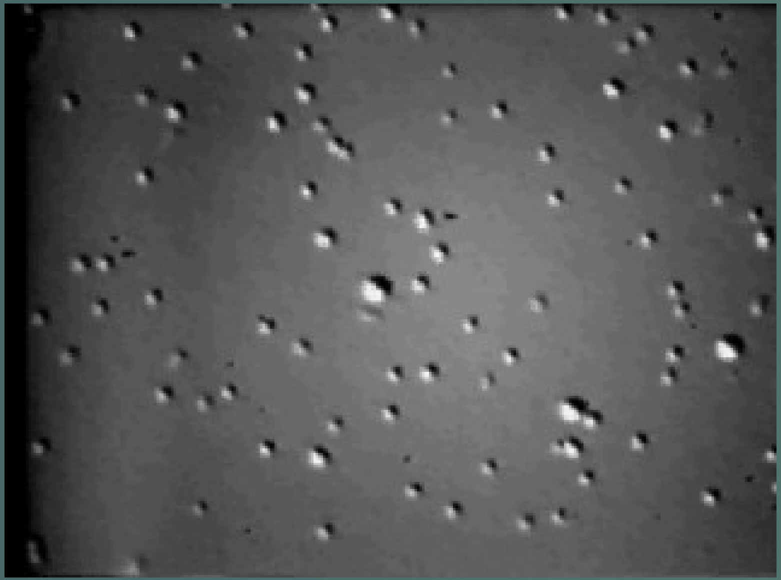


Models of fluids

Continuum	Meso-scale	Microscopic
■ Global parameters: density, velocity, energy, temperature	■ averaged properties, Brownian mechanics, stochastic equations of motion	■ local description, molecules kinetic energy and intermolecular interaction potential
		

Meso-scale physics

Brownian motion of coiled DNA

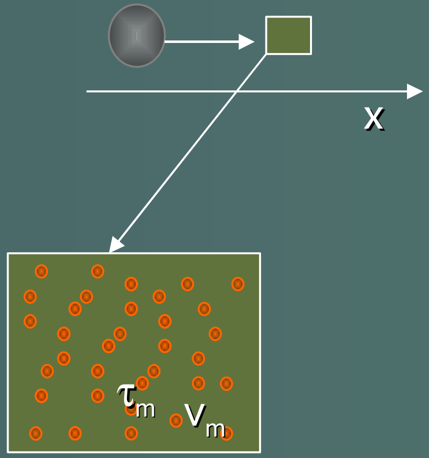


Micro-biological motor (1.50 μm/s)

Meso-scale physics

Langevin description of Brownian motion (1908)

$$M\frac{d\mathbf{V}}{dt} = -\xi M\,\mathbf{V} + F(\mathbf{R}) + \Theta(t)$$



- **V** – velocity
- **R** position; d**R**/dt = **V**
- ξ M **V** – systematic contribution of forces
- ξ M – friction coefficient
- F(**R**) – external forces
- Θ(t)- random forces
- 1/ξ – relaxation time, without random forces

Assumption: Typical time scale on which collisions take place is very small compared to the evolution of the average velocity

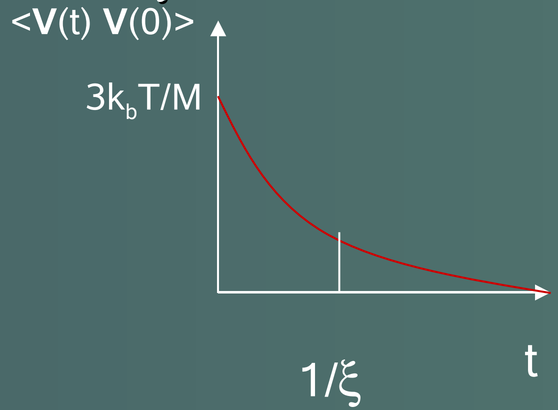
$$\langle \Theta_\alpha(t) \rangle = 0 \qquad \langle \Theta_\alpha(t)\,\Theta_\beta(t) \rangle = 2\Theta_0 \delta_{\alpha\beta}\delta(t-t')$$

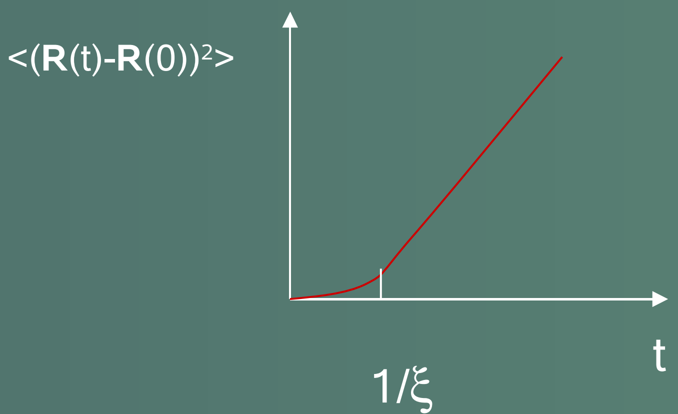
uncorrelated character of collisions

Meso-scale physics

Langevin description of Brownian motion (1908)

- Langevin equation as an evolution equation for PDF of velocity
- $1/\xi$ – relaxation time scale





Evolution from ballistic to the diffusive motion

Diffusion $D = k_bT/ M \xi$

Fokker-Plank equation; Kramers Smoluchowski: SDE -> PDE for PDF

$$\frac{\partial P(\mathbf{V},t)}{\partial t} = \frac{\partial}{\partial V}\left(\xi\, \mathbf{V}\, P(\mathbf{V},t) + \frac{\partial}{\partial \mathbf{V}}\left(\frac{\Theta_0}{M^2} P(\mathbf{V},t)\right)\right)$$

Fluctuation-Dissipation Theorem

General solution of the Langevin equation

$$V(t) = V(0)\exp(-\xi\, t) + \frac{1}{M}\int_0^t ds\,\exp(-\xi(t-s))\;\Theta(s)$$

$$\lim_{t\to\infty}\left\langle \mathbf{V}(t)^2 \right\rangle = \frac{3\Theta_0}{M^2\xi}$$

from equipartition theorem

$$\lim_{t\to\infty}\left\langle \mathbf{V}(t)^2 \right\rangle = \frac{3k_b T}{M}$$

Fluctuation-Dissipation theorem ensures for equilibrium that PDF is equal to Maxwell distribution

$$M\,\xi\,k_b\,T = \Theta_0$$

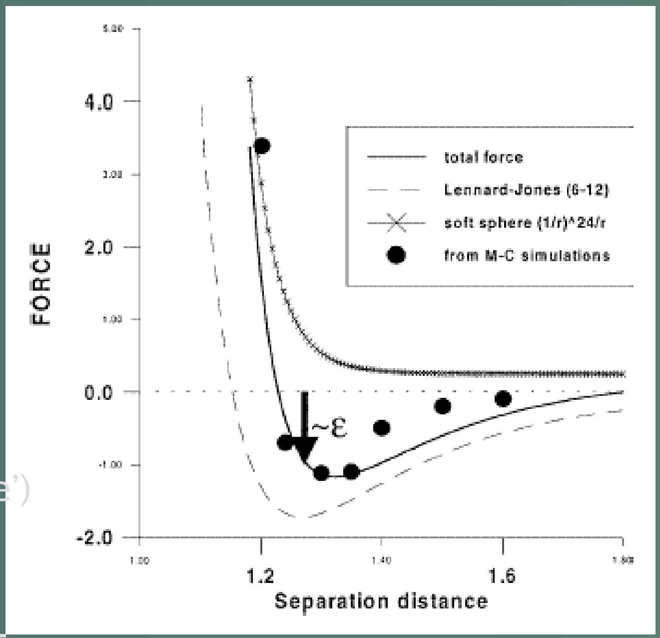
Numerical methods

Continuum fluid mechanics	Meso-scale mechanics	Microscopic mechanics
▪ Global parameters: density, velocity, energy, temperature	▪ lattice methods sacrifice detail in potential model, simpler interactions and motion rules; LBM ▪ particle methods particles as mesoscopic object; replace small particle with random forces; DPD, SPH	▪ Molecular Dynamics computation of forces, based on the interaction potential; particle move according to Newton’s equation of motion ▪ Monte Carlo methods Set a configuration, make a trial move; acceptance/rejection procedure, and accumulation of averages

Dissipative Particle Dynamics

Spherical formulation

two particle interaction



Three type of forces

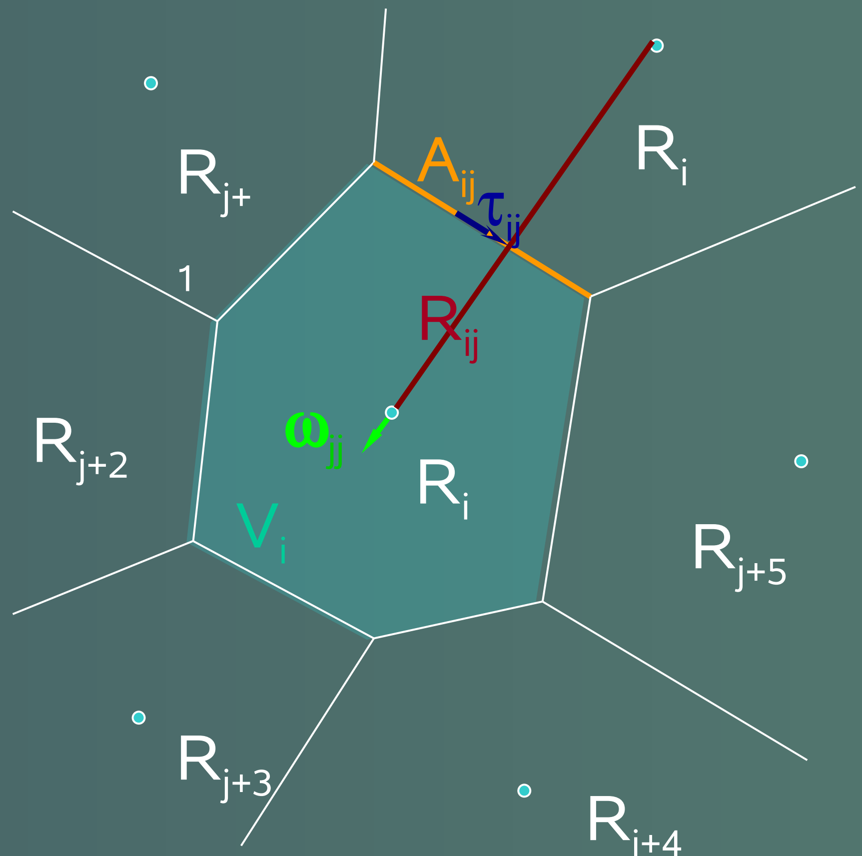
- **conservative** (purely repulsive, represents ‘pressure’)
- **dissipative** (reducing velocity difference between particles, ‘friction forces’)
- **stochastic** (‘degree of freedom’ removed by coarse-graining procedure)

$$F_C = \pi\ \omega(r_{ij})\ e_{ij};$$

$$F_D = \gamma M\, \omega(r_{ij})\, (e_{ij} \circ v_{ij})\ e_{ij};$$

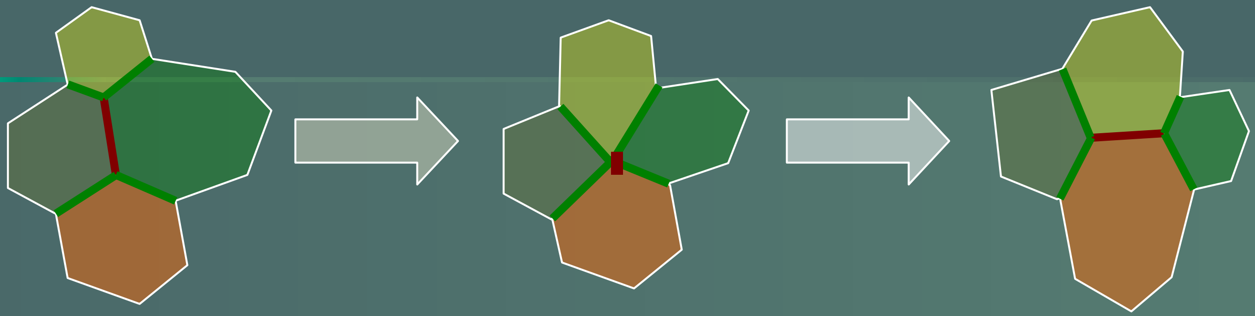
$$F_B = \frac{\delta\, \theta_{ij}}{\sqrt{\Delta t}}\ \omega(r_{ij})\ e_{ij};$$

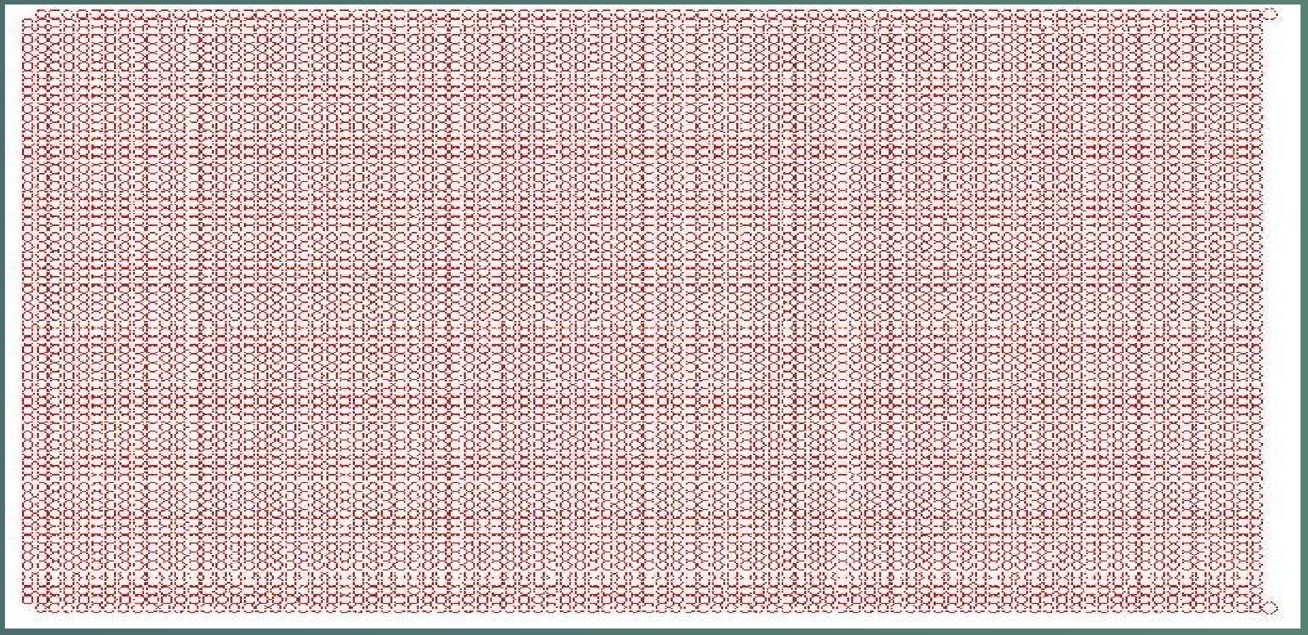
Dissipative Particle Dynamics



- R_{ij} – distance between centers of Voronois i and j;
- ϖ_{ij} – unit vector normal to the face ij, originated from the Voronoi center i;
- A_{ij} – area of the contact surface: length in 2D;
- r_{ij} – vector indicating the mass center of the contact surface ij originated from the center of the surface ij: edge in 2D ;
- V_i – is Voronoi volume: surface in 2D.

Topological Properties





Dissipative Particle Dynamics

Classical DPD

$$\frac{d\mathbf{r}_i}{dt} = \mathbf{v}_i(t) \qquad \frac{d\mathbf{p}_i}{dt} = f_i(t) \equiv \sum_{j \neq i} \left[\mathbf{F}_{ij}{}^{C}(\mathbf{r}_{ij}) + \mathbf{F}_{ij}{}^{D}(\mathbf{r}_{ij}, \mathbf{v}_{ij}) + \mathbf{F}_{ij}{}^{R}(\mathbf{r}_{ij}) \right]$$

DPDE – energy conservation

$$\frac{de_{ij}}{dt} = \sum_{j \neq i} \left[\frac{dq_{ij}}{dt} + \frac{dq_{ij}{}^{D}}{dt} + \frac{dq_{ij}{}^{R}}{dt} \right]$$

Voronoi DPD

reverssible part

$$\dot{\mathbf{R}}_{\mathrm{i}} = \mathbf{v}_{\mathrm{i}}$$

$$\dot{M}_i = \sum_j \frac{A_{ij}}{R_{ij}} \frac{\rho_i + \rho_j}{2} \boldsymbol{\tau}_{ij} \cdot (\mathbf{v}_i - \mathbf{v}_j)$$

$$\dot{\mathbf{P}}_{\mathrm{i}} = \sum_j A_{ij} \boldsymbol{\varpi}_{ij} (p_i - p_j)/2 + \sum_j \frac{A_{ij}}{\hat{R}_{ij}} \frac{\rho_i + \rho_j}{2} \frac{\mathbf{v}_i + \mathbf{v}_j}{2} \times \boldsymbol{\tau}_{ij} \cdot (\mathbf{v}_i - \mathbf{v}_j) +$$

$$+ \sum_j \frac{A_{ij}}{R_{ij}} \boldsymbol{\tau}_{ij} \left[(p_i - p_j) - \frac{\rho_i + \rho_j}{2} (\mu_i - \mu_j) + - \frac{s_i + s_j}{2} (T_i - T_j) \right]$$

$$\dot{S}_i = \sum_j \frac{A_{ij}}{R_{ij}} \frac{s_i + s_j}{2} \boldsymbol{\tau}_{ij} \cdot (\mathbf{v}_i - \mathbf{v}_j)$$

irreverssible part

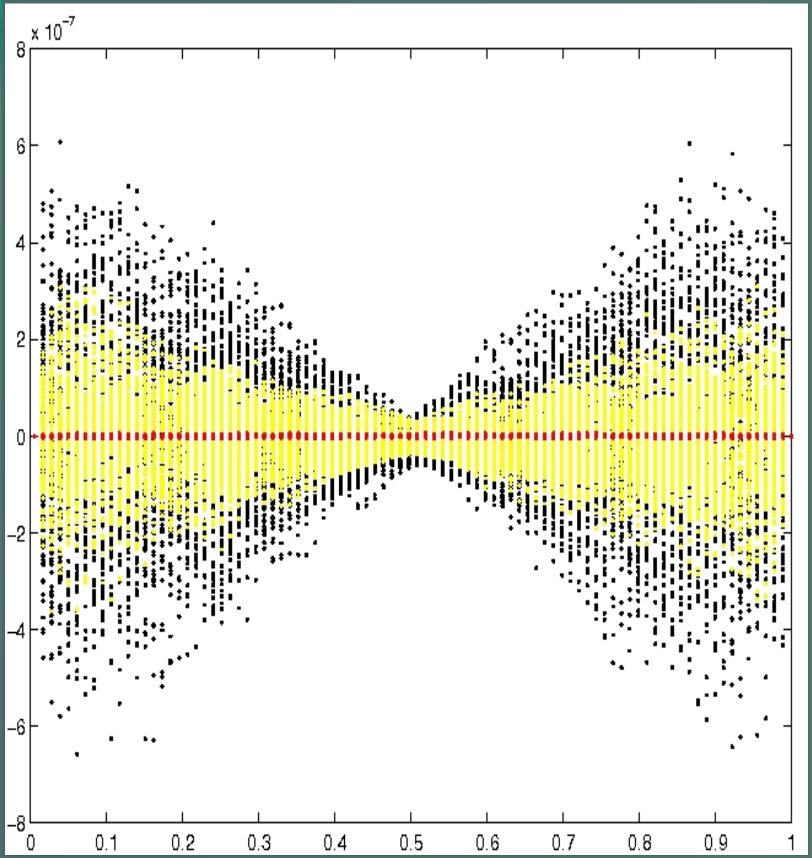
$$d\mathbf{P}_i^{irr} = \sum_j \boldsymbol{\sigma}_{ij} (\boldsymbol{\Pi}_j + \Pi_i \mathbf{1})\, dt + d\mathbf{P}_i$$

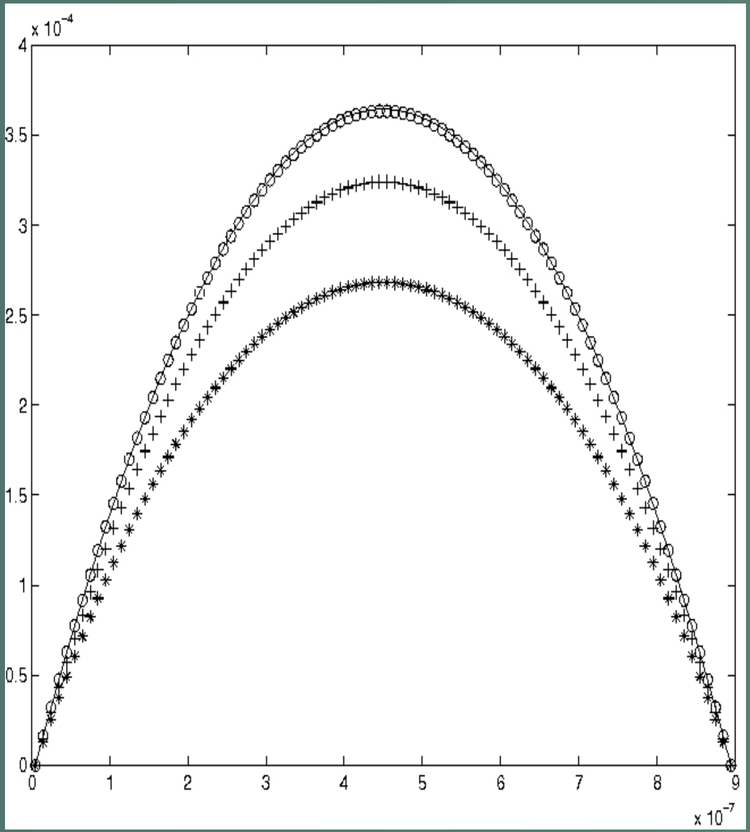
$$T_i dS_i^{irr} = \left(1 - \frac{k_B}{\hat{C}_i}\right) \left[\frac{2\eta_i}{\hat{V}_i} \overline{\boldsymbol{\Omega}}_i \otimes \overline{\boldsymbol{\Omega}}_i + \frac{\xi_i}{\hat{V}_i} \Psi_i^2 \right] d\hat{t} + \sum_j \boldsymbol{\sigma}_{ij} \boldsymbol{\Phi}_j dt$$

$$- \frac{k_B}{T_i C_i} \sum_j \boldsymbol{\sigma}_{ij}^2 \frac{\kappa_j}{V_j} T_j^2\, dt - T_i \left(\frac{2\eta_i}{\hat{V}_i} + \frac{\xi_i}{\hat{V}_i} \right) \sum_j \frac{\boldsymbol{\sigma}_{ij}}{M_j} dt + T_i d\breve{\hat{S}}_i$$

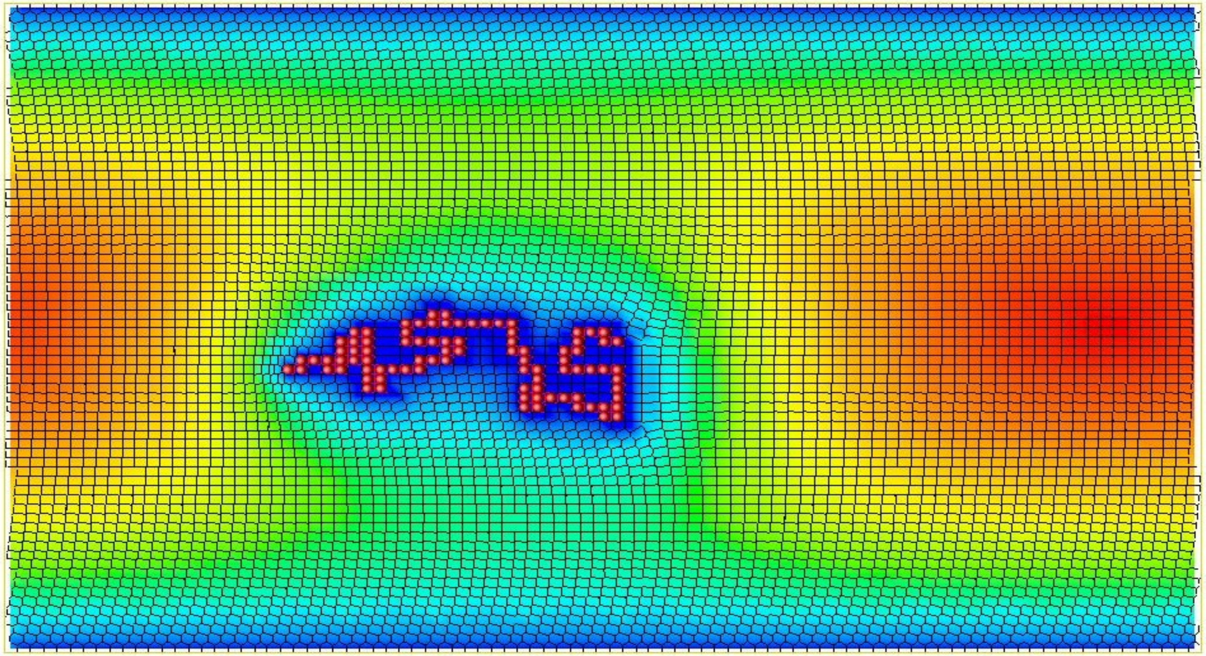
$$d\breve{S}_i = \frac{1}{T_i} \sum_j \boldsymbol{\sigma}_{ij} \cdot d\breve{\boldsymbol{\Phi}}_j - \frac{1}{T_i} d\breve{\boldsymbol{\theta}} \otimes \sum_j \boldsymbol{\sigma}_{ji} \mathbf{v}_j{}^{T}$$

Channel Flow

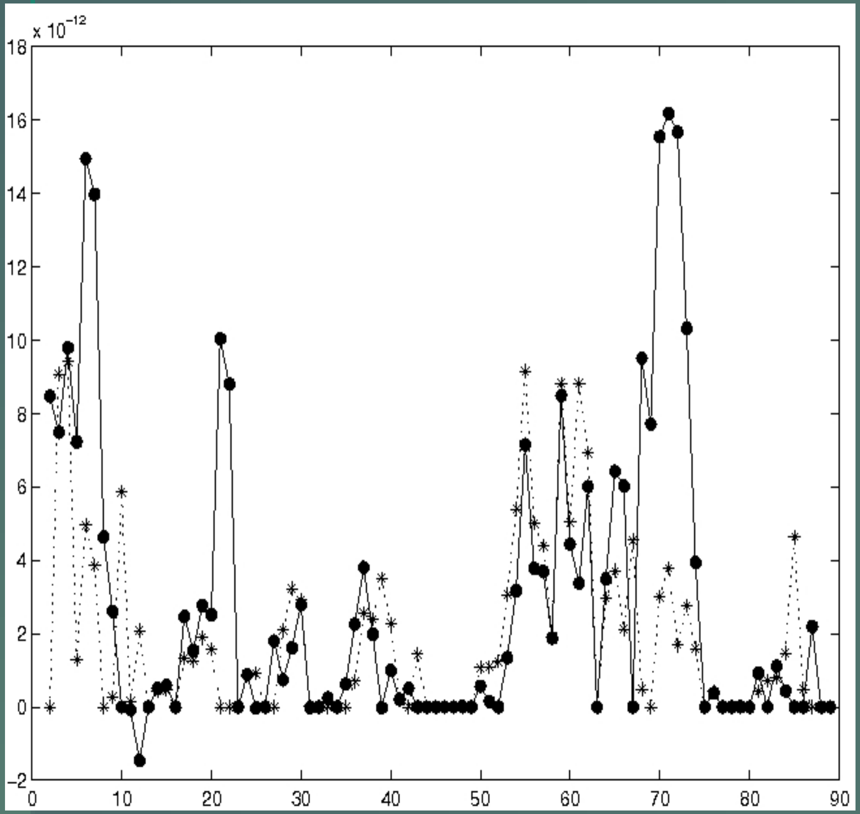


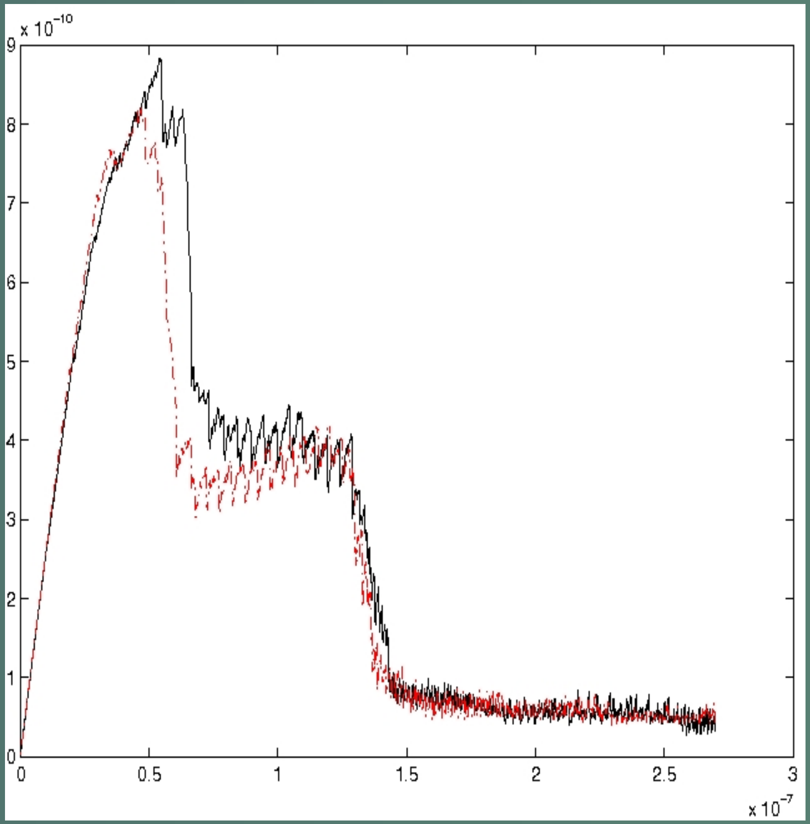


Channel Flow

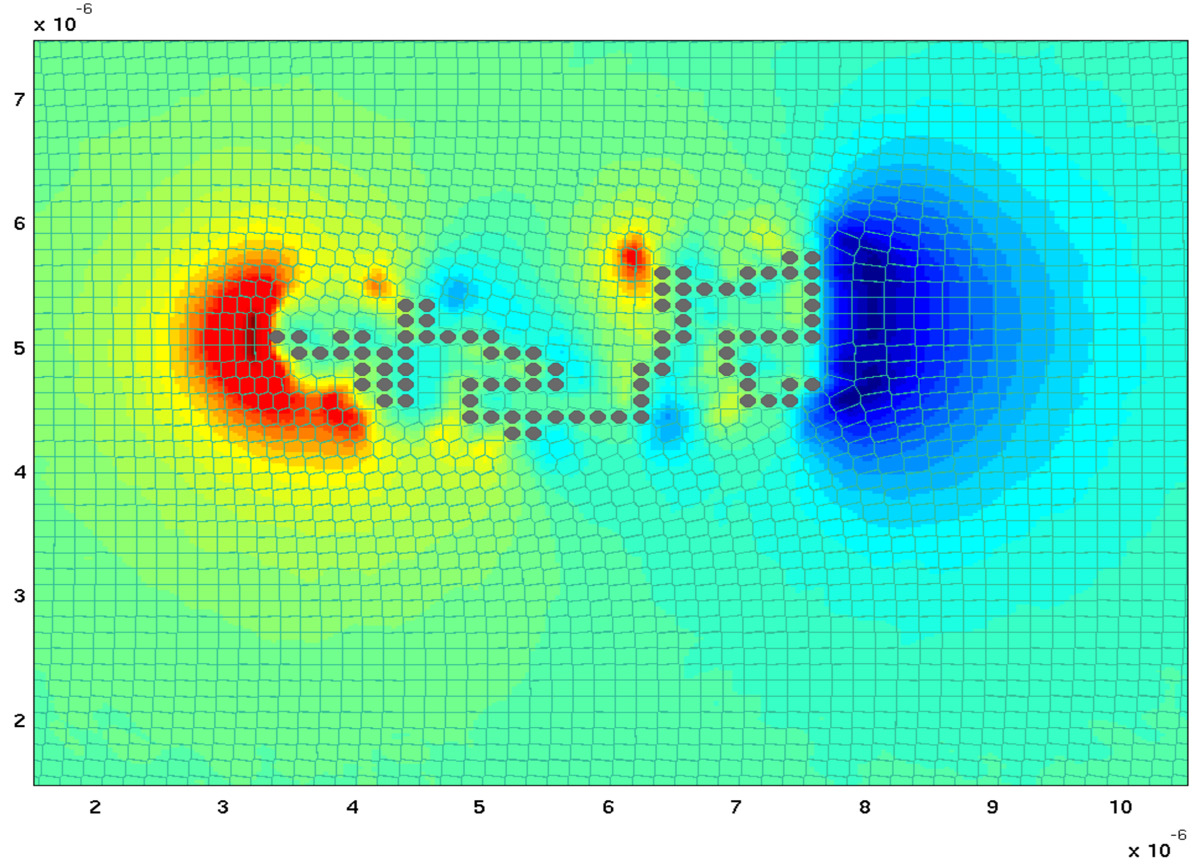


DNA in the Flow

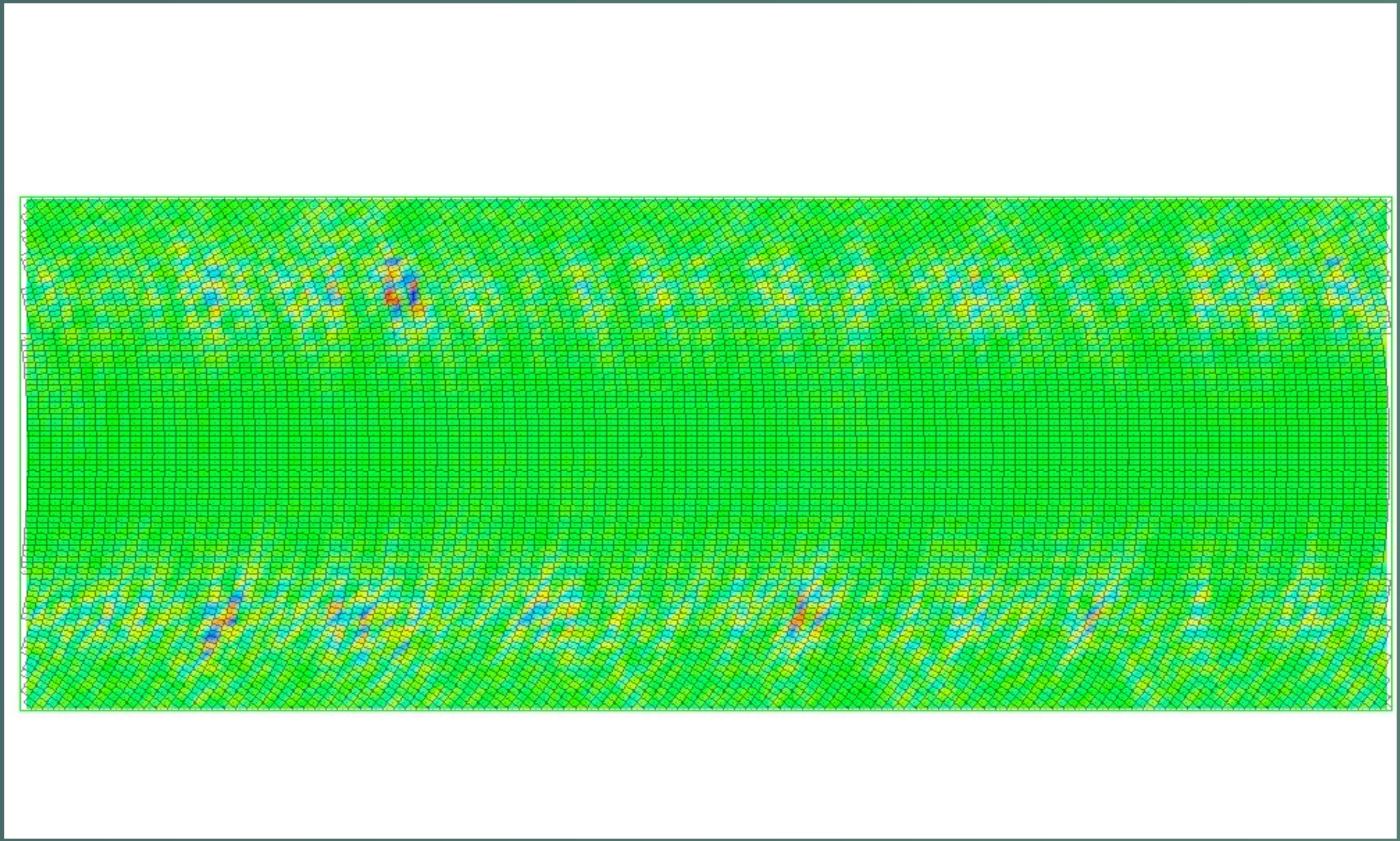




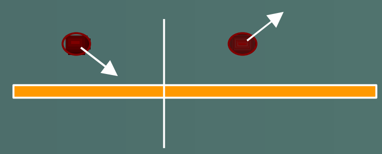
DNA in the Flow



Numerical Issues



Fluctuation-Relaxation Model



ideal reflecting wall

diffusively reflecting wall

Slip velocity
Maxwell

$$v_{gas}-v_{wall}=\frac{2-\sigma_v}{\sigma_v}\lambda\frac{\partial v}{\partial y}\Big|_{wall}$$

Slip flow and temperature jump
Smoluchowski

$$v_{gas}-v_{wall}=\frac{2-\sigma_v}{\sigma_v}\lambda\left|\frac{\partial v}{\partial y}\right|_{wall}+\frac{3}{4}\frac{\mu}{\rho T_{gas}}\left|\frac{\partial T}{\partial y}\right|_{wall}$$

$$T_{gas}-T_{wall}=\frac{2-\sigma_T}{\sigma_T}\left[\frac{2\gamma}{(\gamma+1)}\right]\frac{\lambda}{\Pr}\left|\frac{\partial T}{\partial y}\right|_{wall}$$

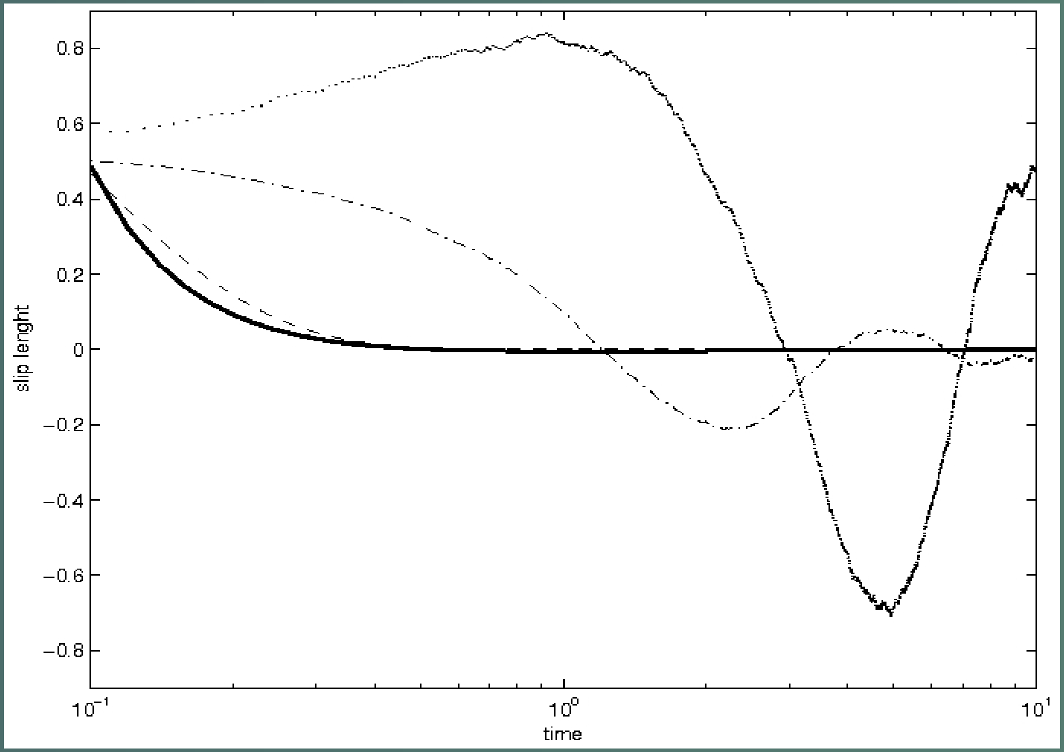
Fluctuation-Relaxation Model

- Relaxation time determines if velocity slip or thermal jump occurs; it defines scale for which meso-scopic (non-equilibrium) and continuum (equilibrium)boundary condition occurs
- Fluctuation Theorem (FDT) compensates molecular level interactions, which has been lost in coarse-grained procedure
- Gas-solid, liquid-solid interface need to be treated similarly; fluid-solid boundary interaction is represented as a non-equilibrium reological process, the difference between liquid and gas would be mainly in the relaxation time of this phenomena.

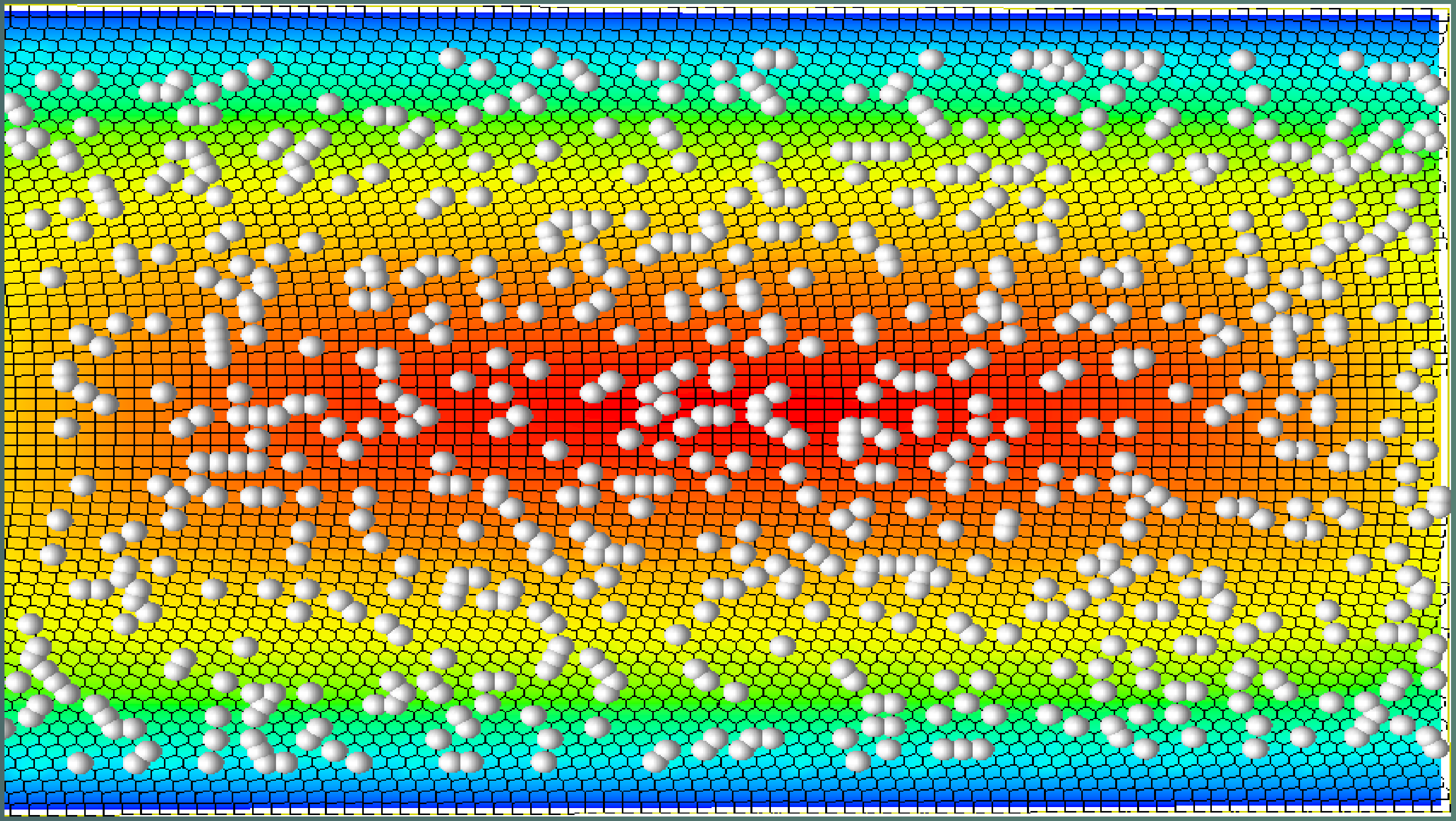
$$\dot{\sigma} = -\int_0^t \eta(t-\tau)\dot{\gamma}\, d\tau$$

$$\eta(t-\tau) = \Gamma e^{t/\tau} + \Omega$$

Slip : No-Slip Phenomena



Self-organization



Conclusion

- Mesoscopic description of fluid;
- Time scale and relaxation phenomena – slip, self-organization;
- Mesoscopic solid-fluid interaction – the most important scale for nano- and micro fluidics