KITP Conference "Modeling Soft Matter"
(June 4-8, 2012, KITP, UCSB)

Multiscale Simulations for Polymeric Flow: Particle-CFD Coupling Model

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Multiscale Simulations for Softmatters

http://multiscale.jp

MSS Project (2006/10 – 2012/03)

http://multiscale.jp

1. Particle-CFD Coupling Model for Colloidal Dispersions
   -> SP method [KAPSEL]

2. Particle-CFD Coupling Model for Polymeric Flow
   -> Local sampling method

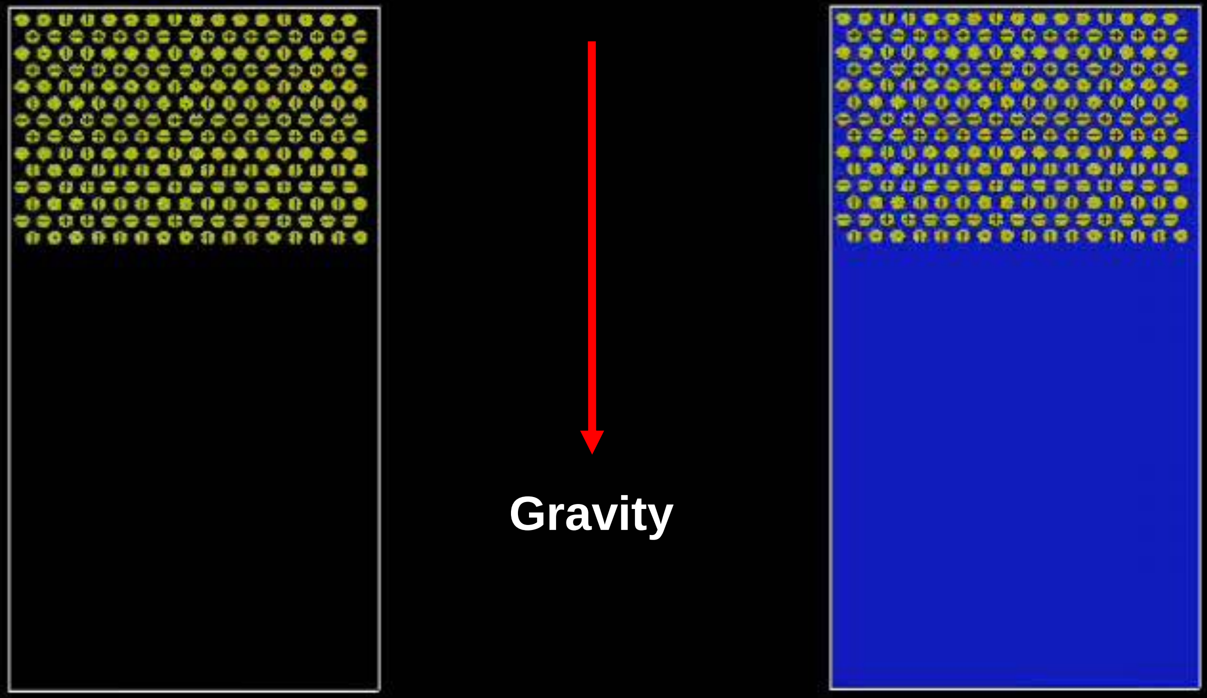
3. Meso-scopic Model for Entangled Polymer
   -> Primitive chain network (PCN) [NAPLES]
   -> Slip-link (SL) model [FRISCA]

4. HPC for general MD with Columbic Interaction
   -> GPU [CUDA library]
   -> MD-Grape
   -> Play station

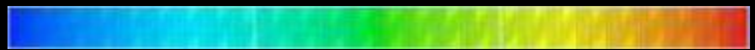
Importance of Hydrodynamics in Sedimentation Process

1) Without HI

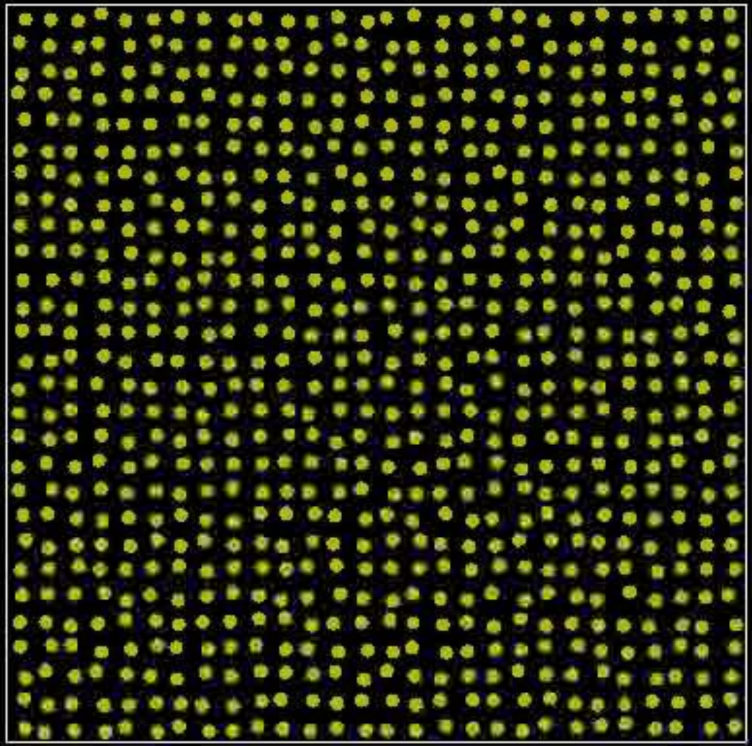
2) With HI



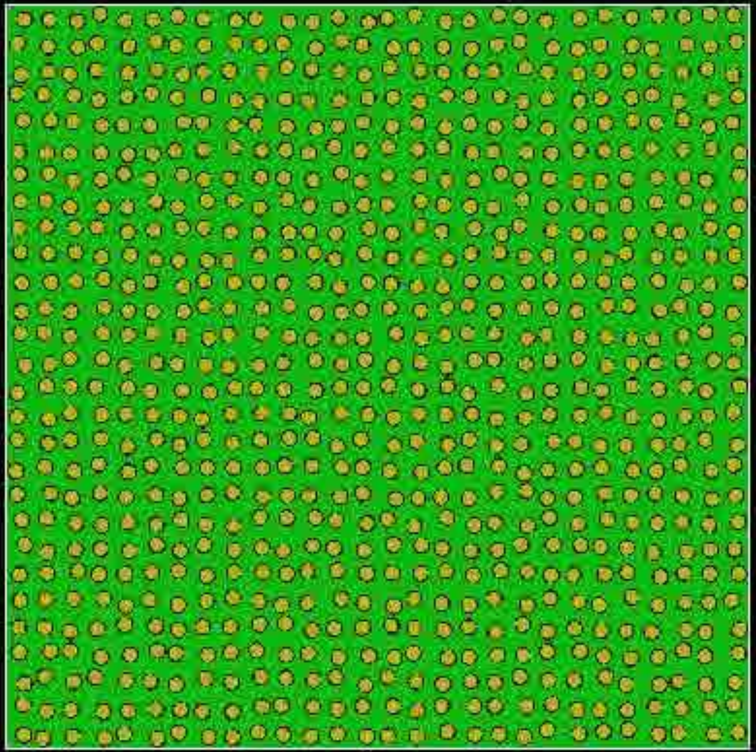
Importance of Hydrodynamics in Coagulation Process



1) Without HI



2) With HI



MSS Project (2006/10 – 2012/03)

http://multiscale.jp

1. Particle-CFD Coupling Model for Colloidal Dispersions
   -> SP method [KAPSEL]

2. Particle-CFD Coupling Model for Polymeric Flow
   -> Local sampling method (yet in primitive stage…)

3. Meso-scopic Model for Entangled Polymer
   -> Primitive chain network (PCN) [NAPLES]
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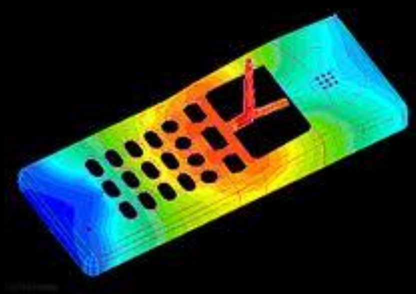
Our target: General flow problems of polymeric liquids

ex. injection molding (as a very distant goal…)



Highly non-equilibrium,
non-uniform flow problem over
wide length- ant time-scales

atom << polymer << flow scale < container

(nm) (μm) (mm) (m)

thermal fluctuation
maybe negligible

Models for polymeric systems

- Particle-based model (MD, CGMD, Network, etc…)
  - Good: intuitive modeling, high resolution
  - Bad: expensive computation

- Continuum model (CFD, TDGL, DFT, SCF, etc…)
  - Good: cheaper computation
  - Bad: need statistical model, low resolution

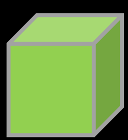
Models for polymeric systems

- Particle-based model (MD, CGMD, Network, etc…)
  - Good intuitive modeling, high resolution
  - Bad expensive computation
- Continuum model (CFD, TDGL, DFT, SCF, etc…)
  - Good cheaper computation
  - Bad need statistical model, low resolution
- Particle-Continuum coupling model
  - Good intuitive modeling, high resolution
  - Good cheaper computation

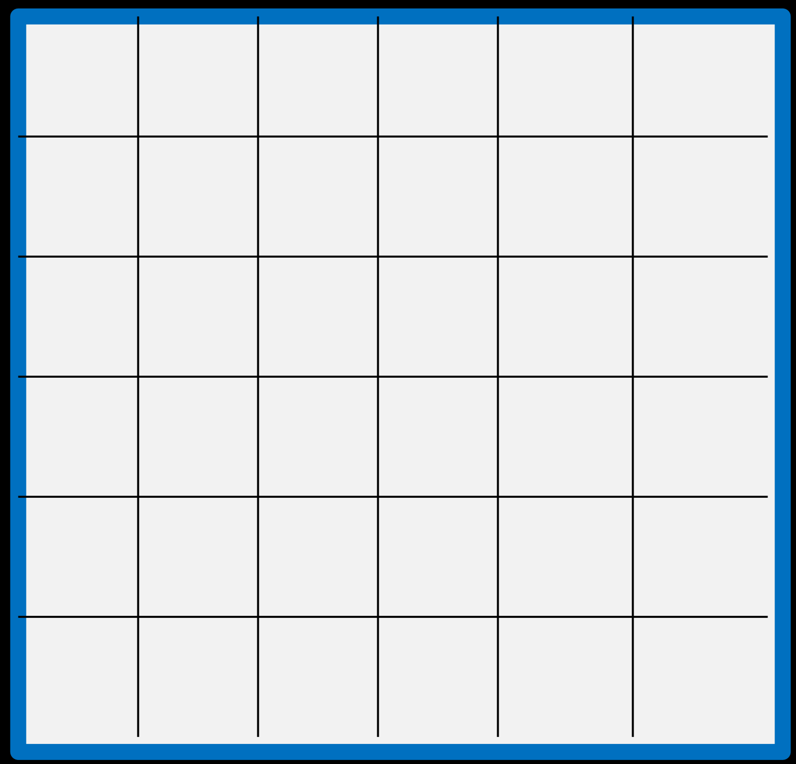
Basic ideas of coupling models

1. re-modeling (pre-computation, homogeneous)

Particle
(force field)



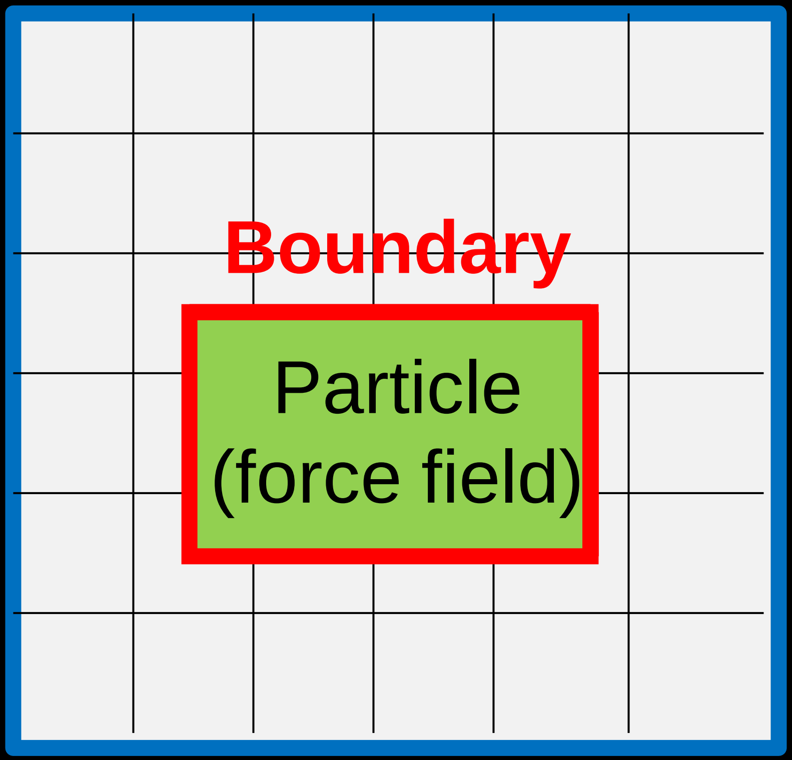
stress/strain
relation
(constitutive
model)



CFD

Basic ideas of coupling models

2. locally embedded (on-the-fly, heterogeneous)

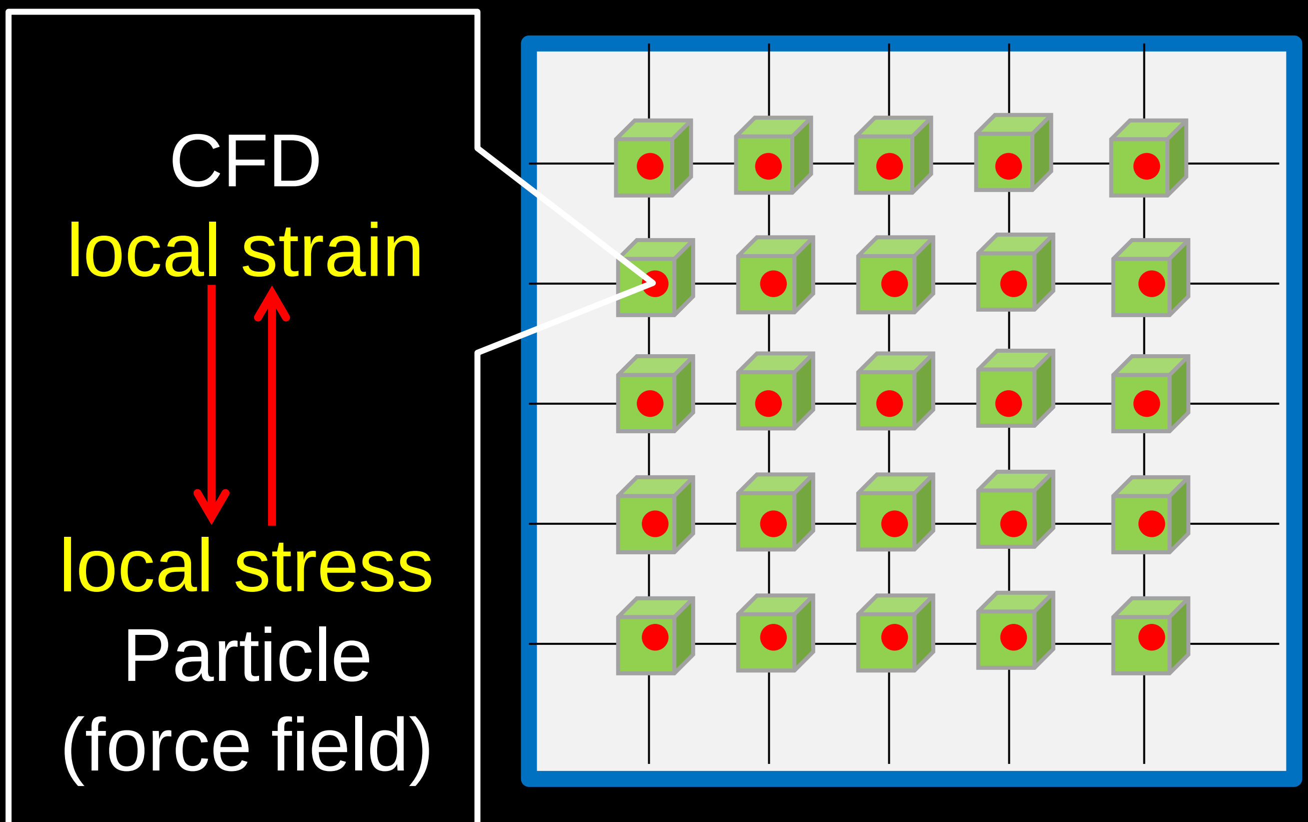


CFD (constitutive model)

ex. Koumoutsakos,
Praprotnik, Miller

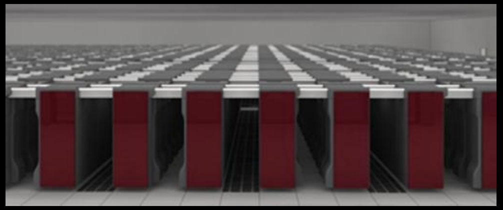
Basic ideas of coupling models

3. Local sampling (on-the-fly, homogeneous)



CFD (no model needed)

ideal for many -core computers



K computer
$6x10^5$ cores

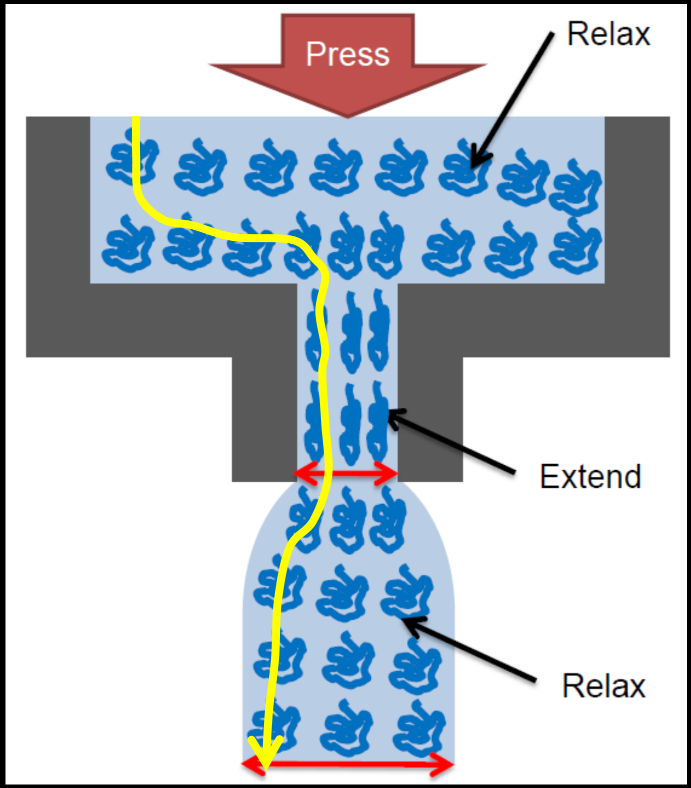
Related studies

- scale bridging algorithms
  - Equation-free: Kevrekidis, et al. (2003)
  - HMM: E & Engquist (2003)
  - …
- polymer flow
  - CONNFFESSIT: Laso & Öttinger (1993)
  - SPH+dumbbell: Ellero, et al. (2002)
  - GENERIC: Öttinger (2005)
  - HMM: Ren & E (2005)
  - Scale-bridging: De, Kumar, et al. (2006)
  - …

Unsolved problems

- General non-equilibrium non-uniform flow of polymers
  -> present work
- Non-linear polymers (star etc…)
- Boundary conditions
- Heat production / dissipation
- Thermal fluctuations, etc…

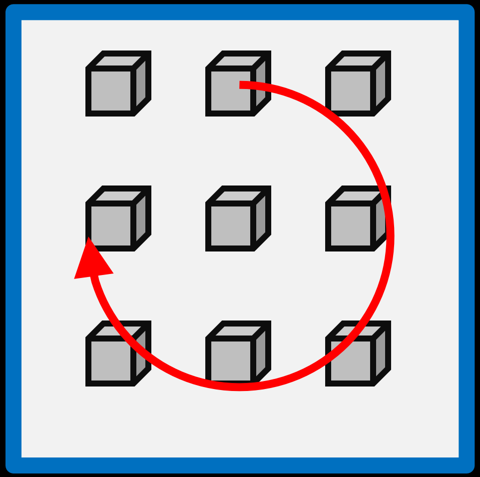
Ex. Die swell



Stream line

Multi-scale Modeling for Polymeric Flow

1. Simple Liquid (General)

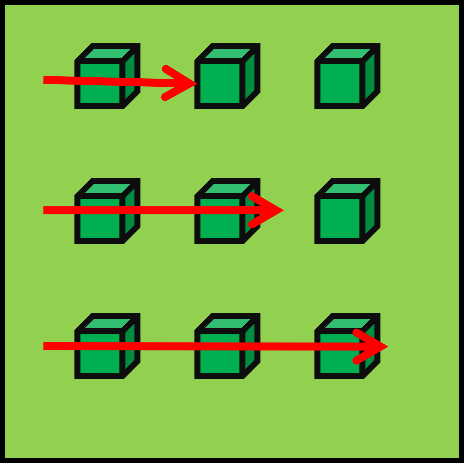


$$\sigma(t, \vec{x}) = f[\dot{\gamma}(t, \vec{x})]$$

Yasuda-RY

POF (2008)

2. Polymeric Liquid (Parallel)

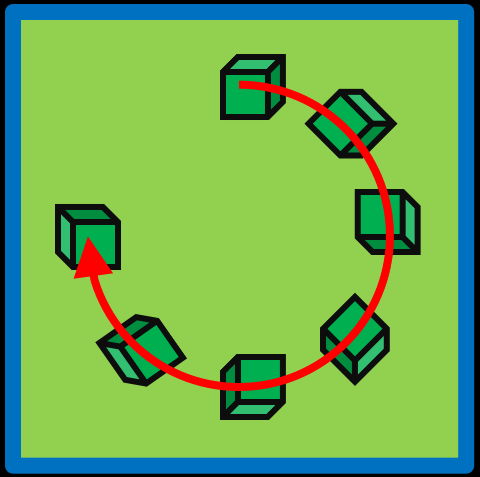


$$\sigma(t, y) = f[\dot{\gamma}(t', y)] \quad (0 \leq t' \leq t)$$

Yasuda-RY

EPL (2009)
PRE (2010)
PRE (2011)

3. Polymeric Liquid (General)



$$\sigma(t, \vec{x}) = f[\dot{\gamma}(t', \vec{x}(t'))] \quad (0 \leq t' \leq t)$$

Murashima-Taniguchi

PSJ (2010)
EPL (2011)

Multi-scale Modeling for Polymeric Flow

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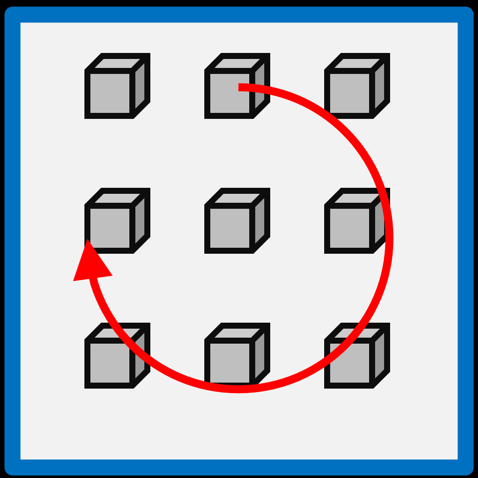

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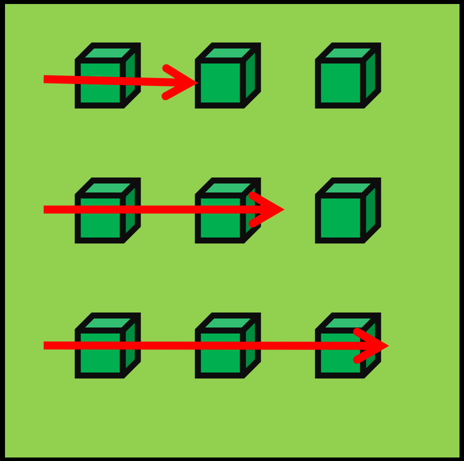

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Yasuda-RY

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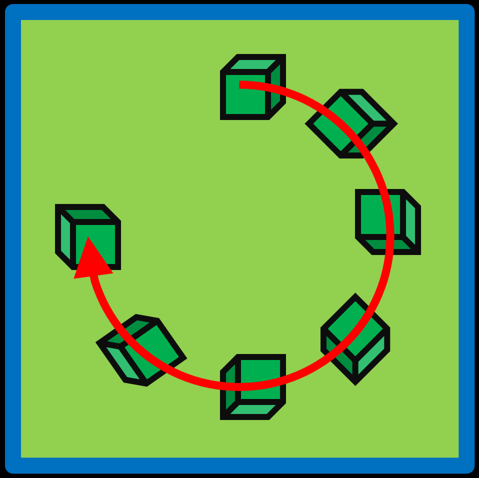

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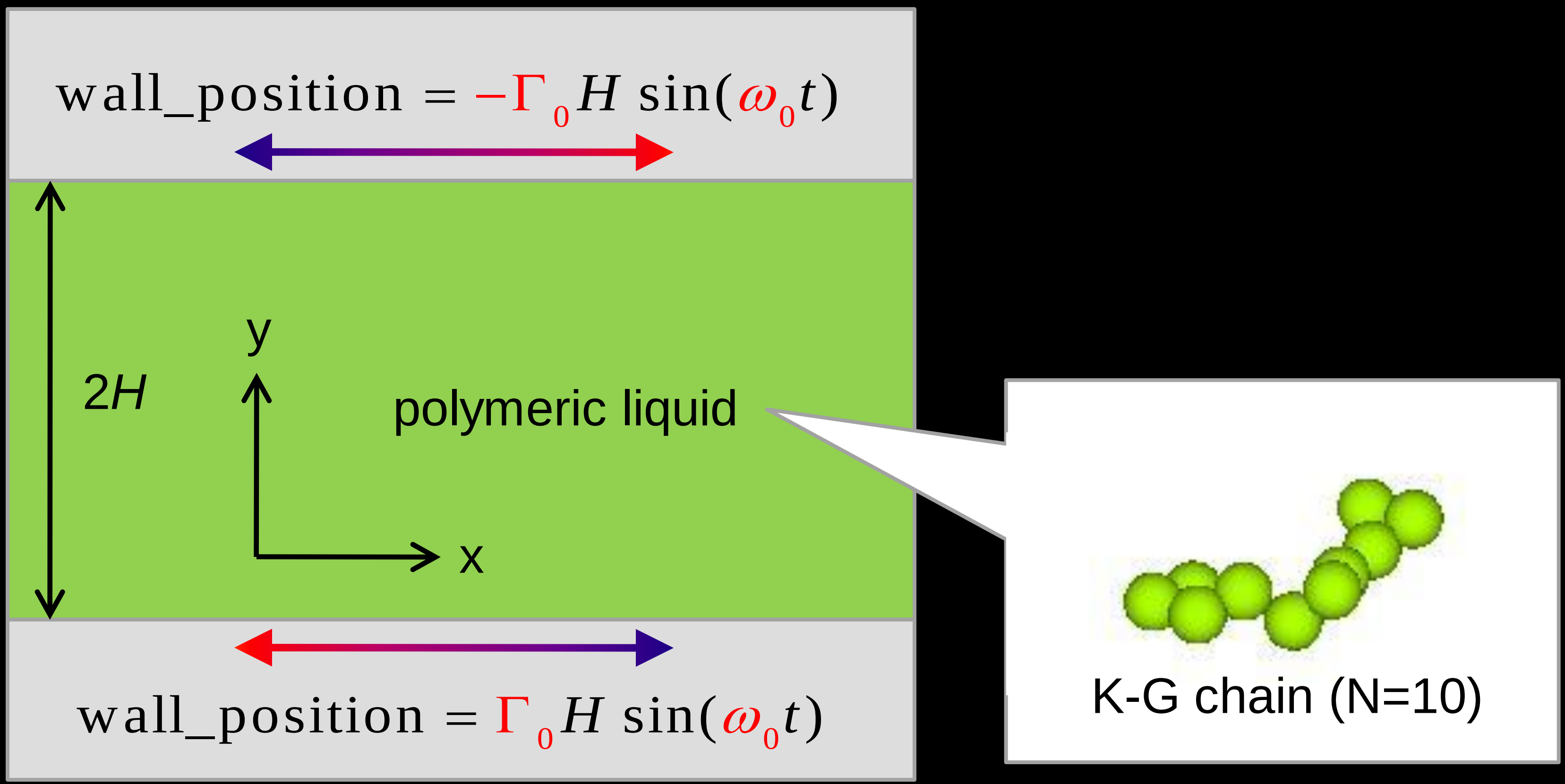
Murashima-Taniguchi

PSJ (2010)
EPL (2011)

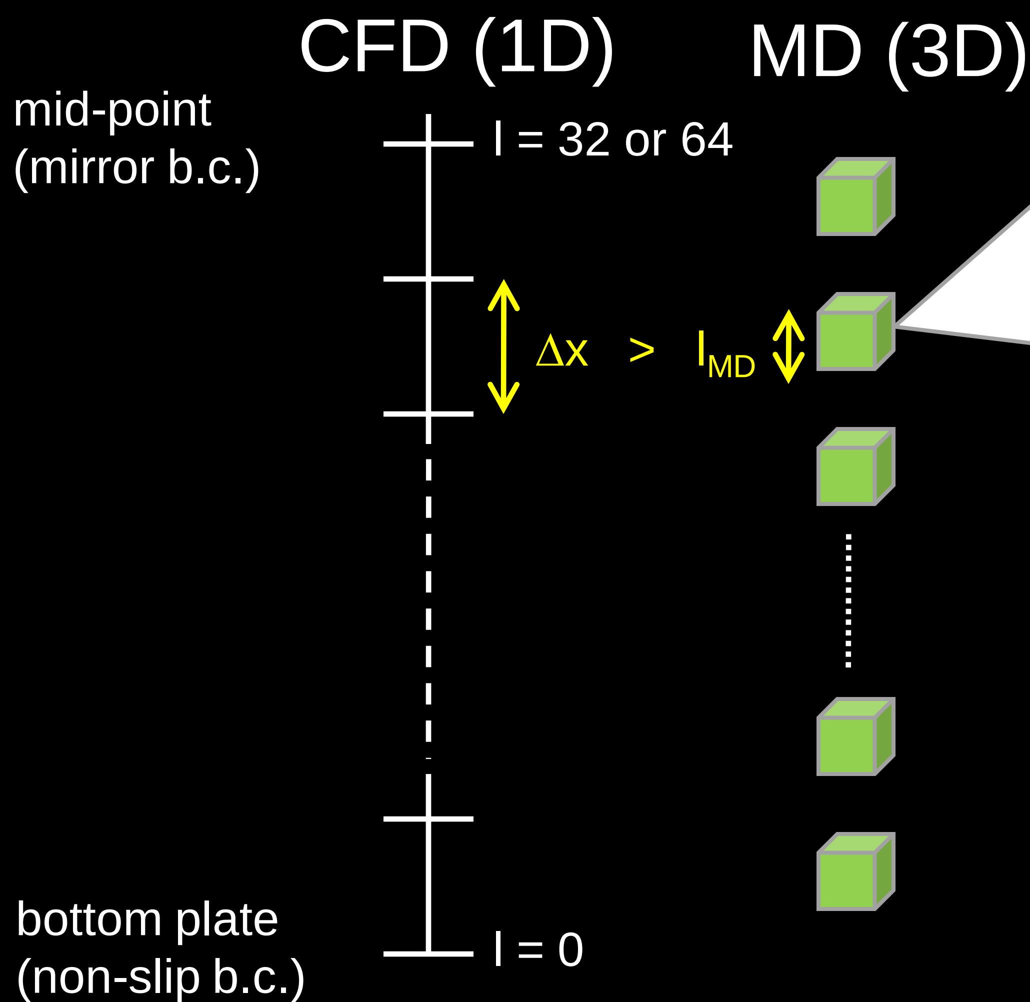
Yasuda & RY, EPL (2009)

System under consideration

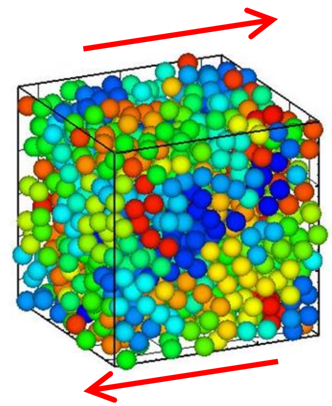
polymer melt between rapidly oscillating plates
-> shear wave appears at high frequency



Our multi-scale method



NEMD (SLLOD):



1000 beads in a box
(N=10 x 100 chains)

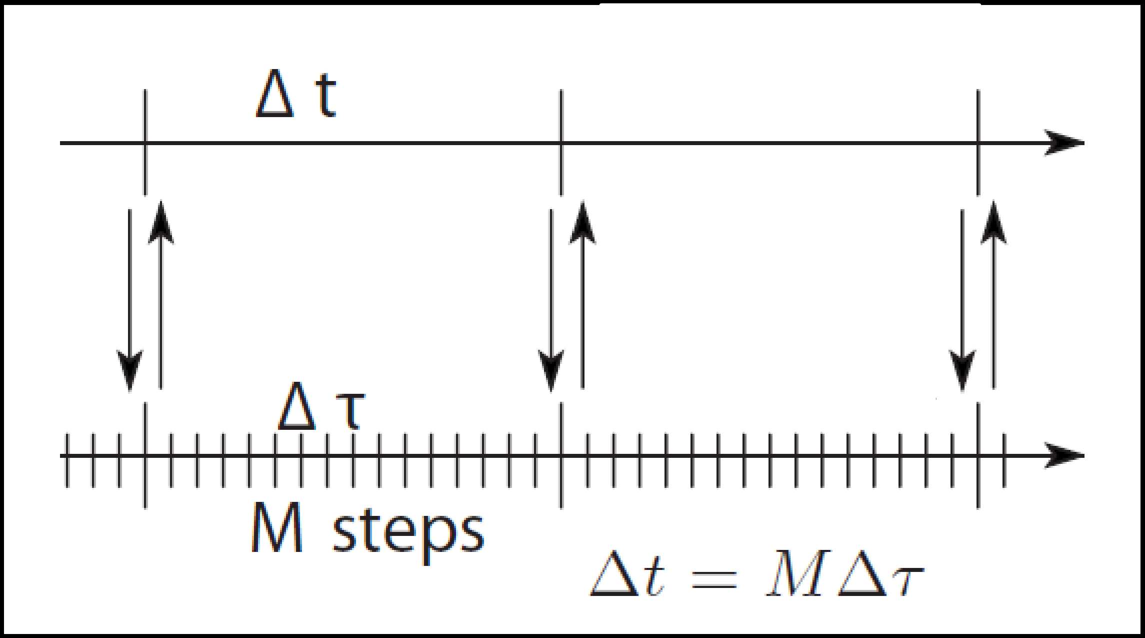
$$\sigma(t, \vec{x}) = f[\dot{\gamma}(t', \vec{x})]$$
$$(0 \leq t' \leq t)$$

saving factor
$= (\Delta x / l_{MD})^d$

Time-evolution scheme

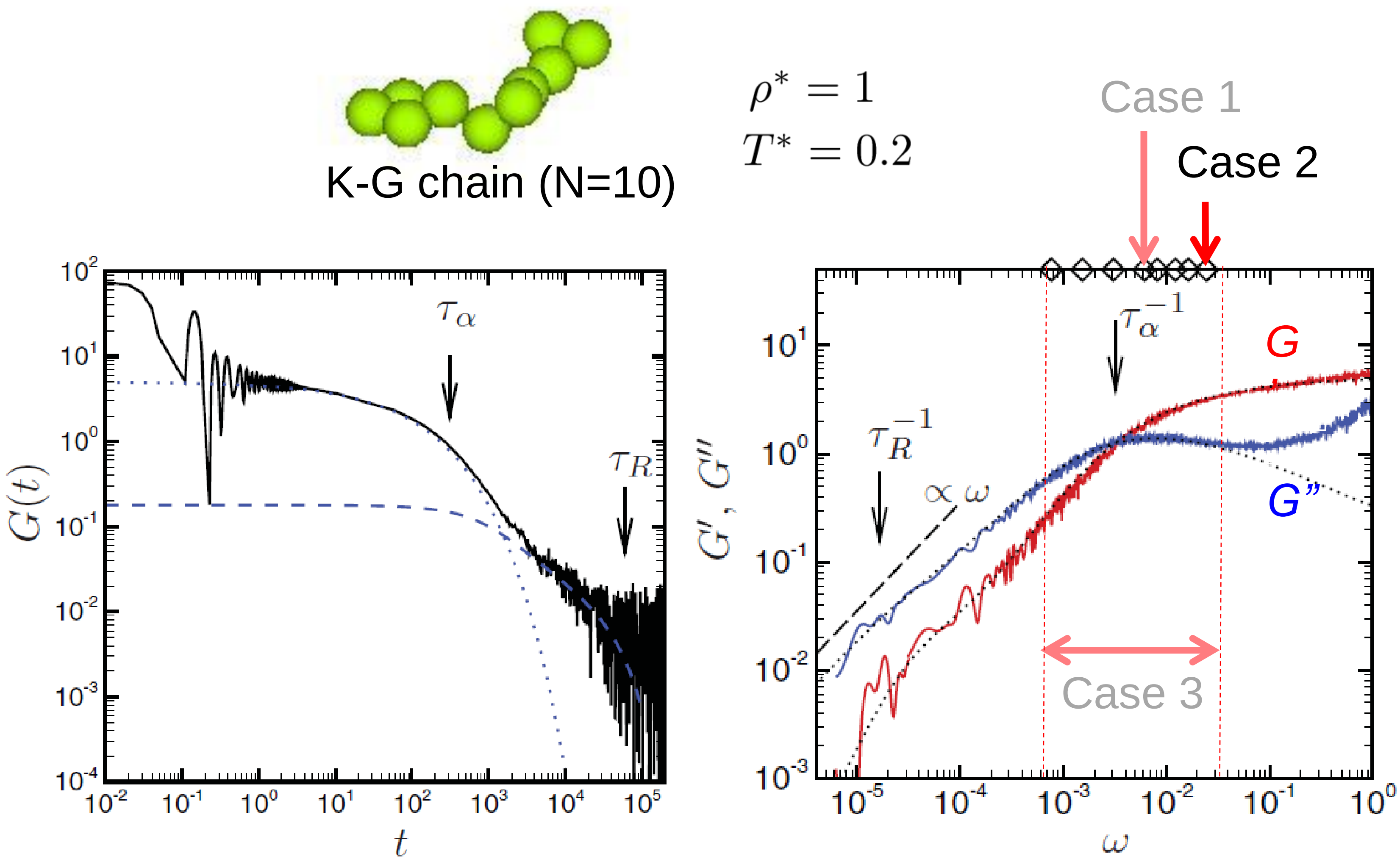
CFD

MD



communicate every $M(=1000)$ steps

Microscopic polymer model



Polymer (Case 2) vs. Newtonian

$H^* = 800$

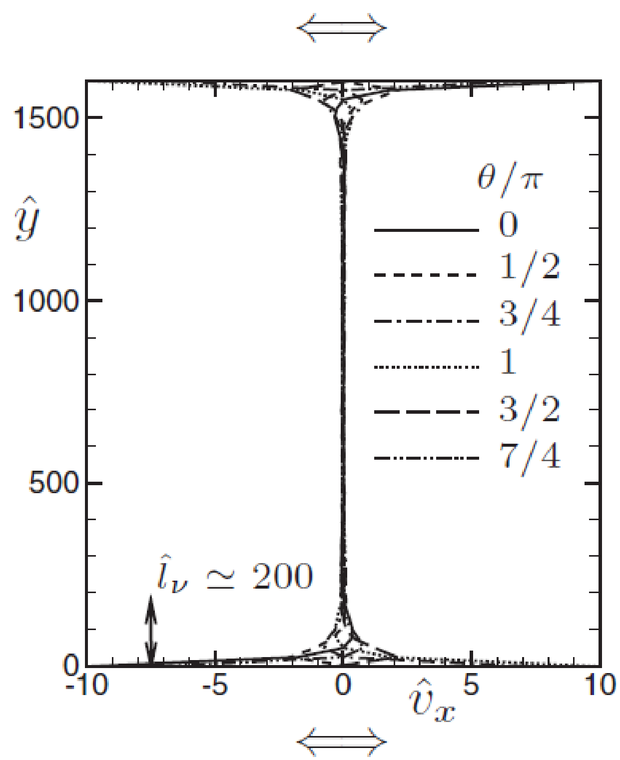
$\Gamma_0 = 0.5$

$\omega_0^* = 2\pi/256$

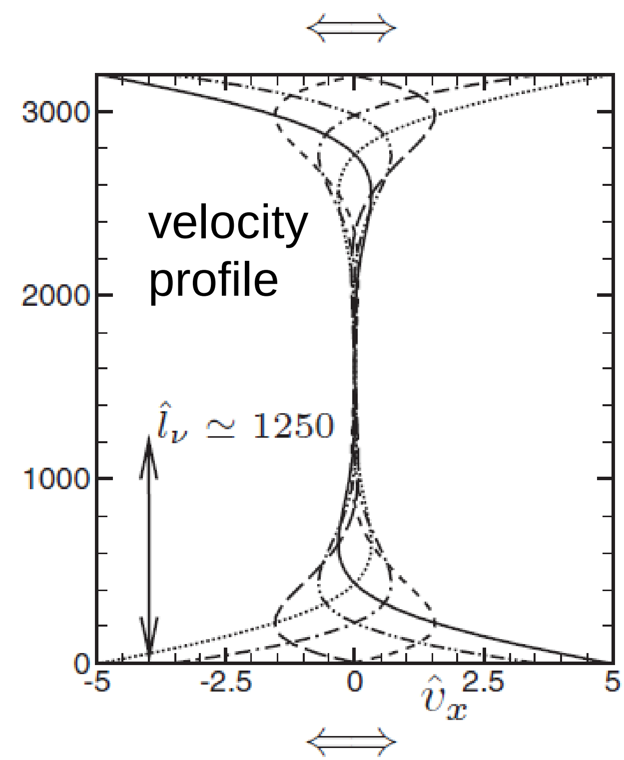
saving factor = 5

$\Delta x / l_{MD} = 5$

$\Delta t_{CFD} / t_{Sample} = 1$



Polymeric liquid



Newtonian

corresponds roughly to
H = 10μm and ω = 1MHz
for typical non-entangled polymer

$l_\nu \propto \sqrt{\nu/\omega_0}$

Yasuda & RY, EPL (2009)

local complex modulus

$$\dot{\gamma}(y,t) = \frac{dv_x(y,t)}{dy}, \quad \gamma(y,t) = \int_0^t \dot{\gamma}(y,t')dt'$$

strain amplitude — phase retardation

$$\begin{aligned} \gamma(y,t) &= \gamma_0(y)\cos(\omega_0 t + \delta(y)) \\ \sigma_{xy}(y,t) &= \sigma_1(y)\cos(\omega_0 t + \delta(y)) - \sigma_2(y)\sin(\omega_0 t + \delta(y)) \end{aligned}$$

elastic stress — viscous stress

storage modulus (elastic response)

$$G'(y) = \sigma_1(y)/\gamma_0(y)$$

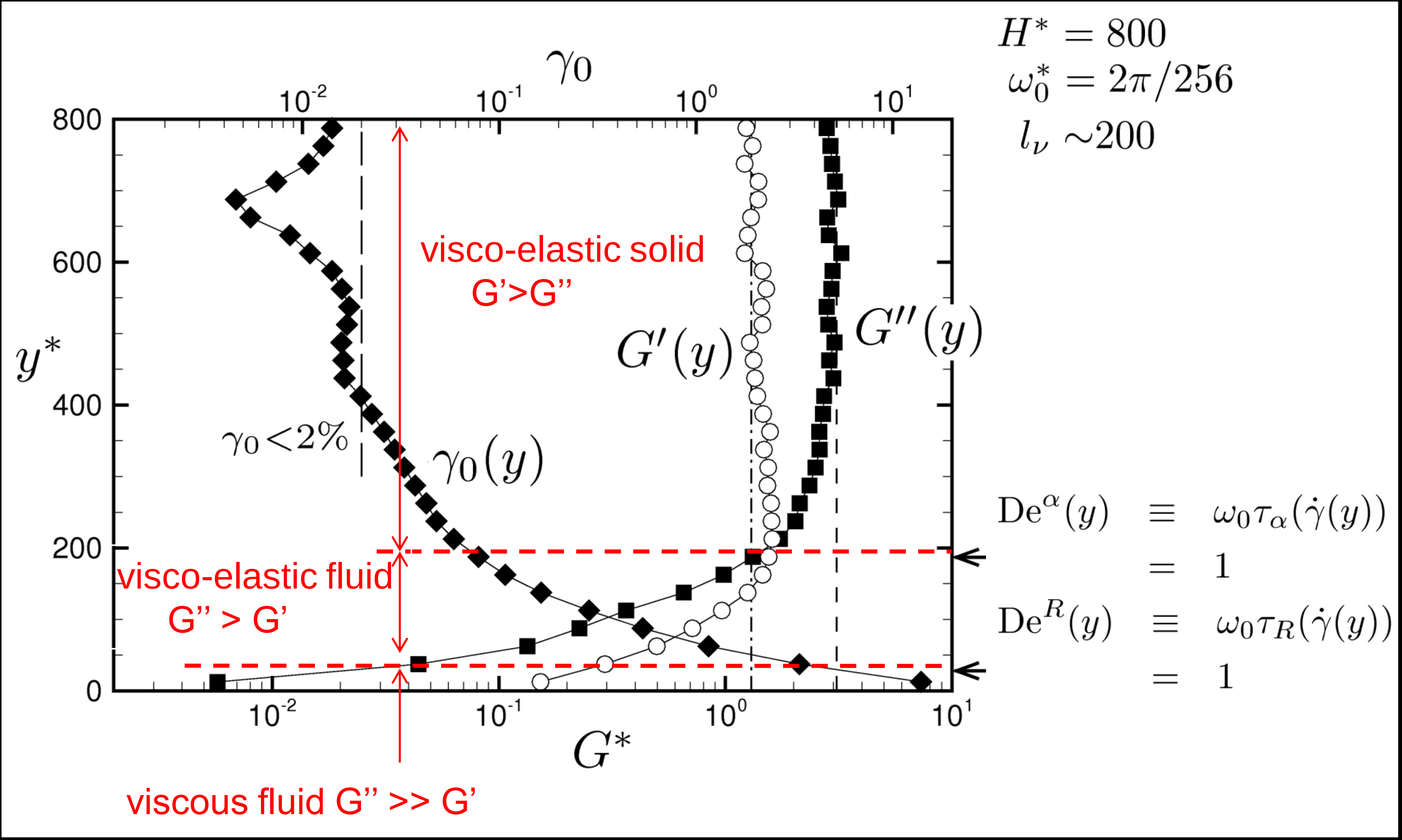
loss modulus (viscous response)

$$G''(y) = \sigma_2(y)/\gamma_0(y)$$

“local” complex modulus

Yasuda & RY, EPL (2009)

local complex modulus (Case 2)



Multi-scale Modeling for Polymeric Flow

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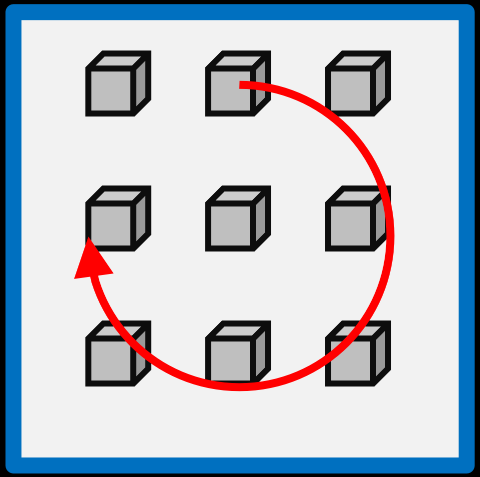

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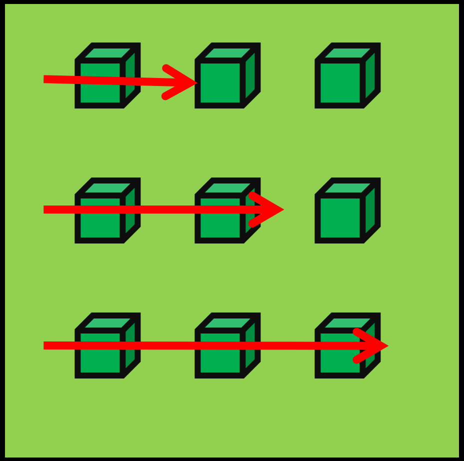
Yasuda-RY

POF (2008)

2. Polymeric Liquid (Parallel)

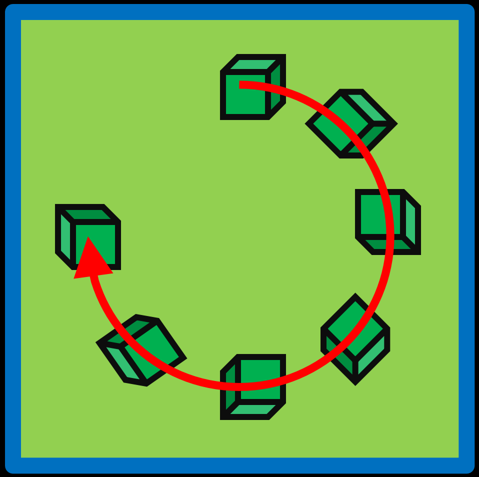


$$\sigma(t, y) = f[\dot{\gamma}(t', y)] \quad (0 \le t' \le t)$$

Yasuda-RY

EPL (2009)
PRE (2010)
PRE (2011)

3. Polymeric Liquid (General)



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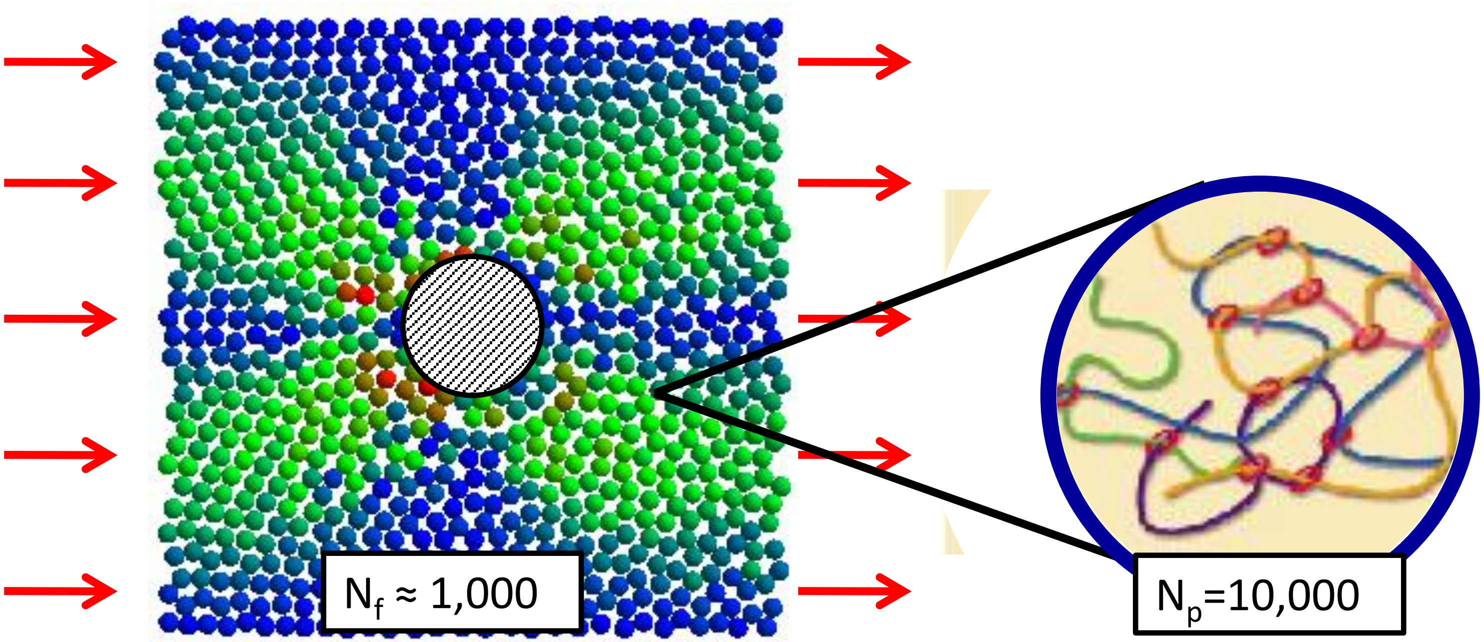
Murashima-Taniguchi

PSJ (2010)
EPL (2011)

Murashima & Taniguchi, EPL (2011)

Polymeric flow around a cylinder

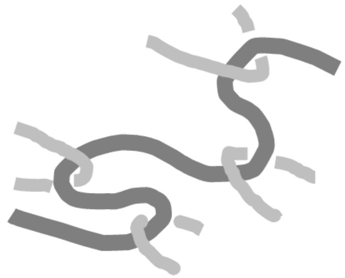


Modified SPH:
Mesh-free, particle based CFD

PASTA:
CG chain with slip-links

$$\mathbf{v}_i \dashrightarrow \nabla \mathbf{v}_i \dashrightarrow \sigma_i \dashrightarrow \mathbf{v}_i$$

Simulation methods at <u>particle level</u>



Entangled polymers

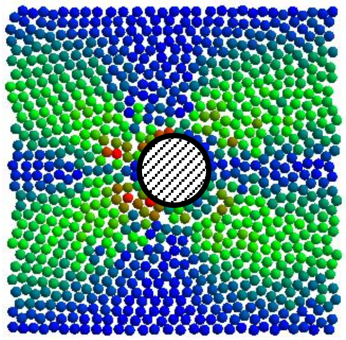
heavy

• All atom MD		Cost= 10^8
• Coarse grained MD		10^6
• Primitive Chain Network	(Naples)	10^2
• Slip-link model	(Pasta)	1
• Slip-link + GPU-CUDA	(Frisca)	

less heavy

PCN: Masubuchi, et al (2001)
SL: Doi-Takimoto (2003)
SL+Cuda: Uneyama (2011)

Simulation methods at CFD level



$$\rho \frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} = \boldsymbol{\nabla} \cdot \boldsymbol{\sigma} - \boldsymbol{\nabla} p + \mathbf{F}^b$$
$$\frac{\mathrm{d}\mathbf{r}}{\mathrm{d}t} = \mathbf{v}$$

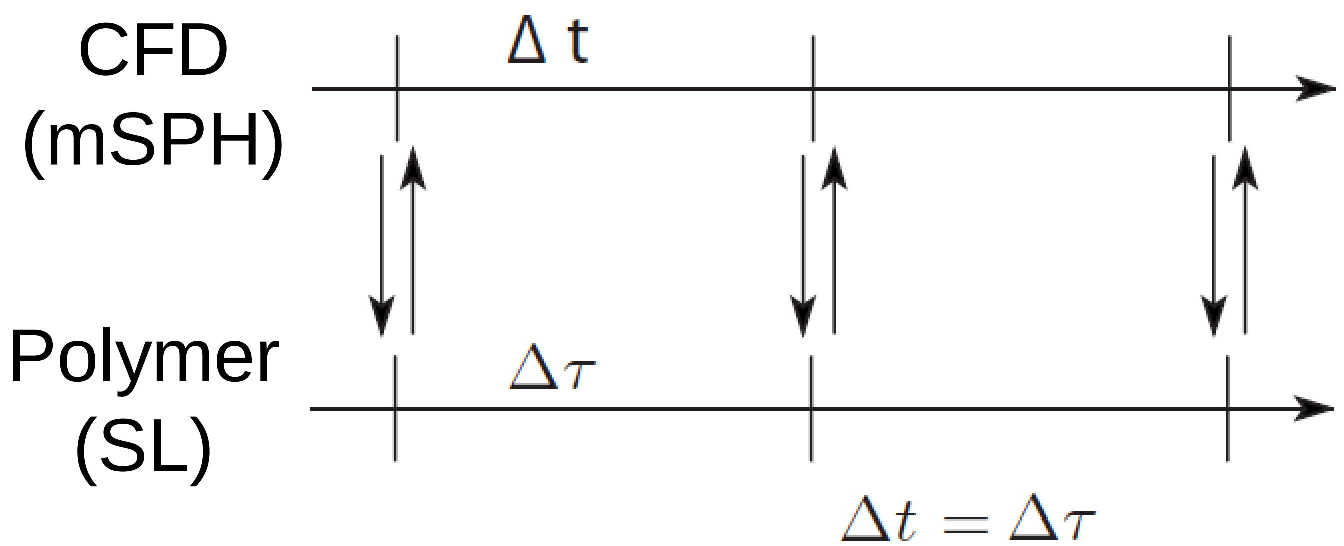
Lagrange solver for incompressible fluids

- Smoothed Particle Hydrodynamics (SPH)
- Modified SPH (mSPH)
- Moving Particle Semi-implicit (MPS)
- many other derivatives of SPH…

SPH: Lucy (1977), Gingold-Monaghan(1977)
mSPH: Zhang-Batra (2004)
MPS: Koshizuka-Oka (1996)

Murashima & Taniguchi, EPL (2011)

time-evolution scheme

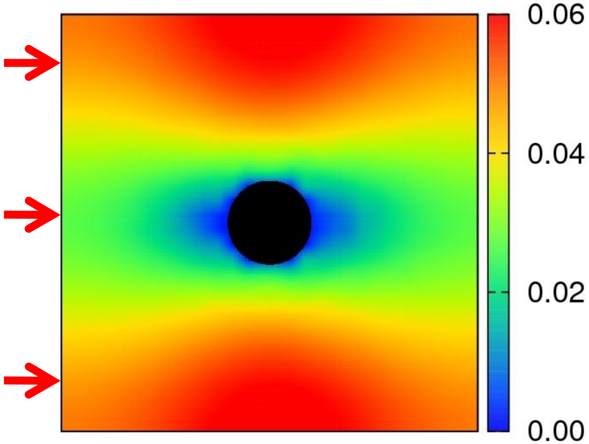


communicate every step

Newtonian fluid at Re << 1

velocity

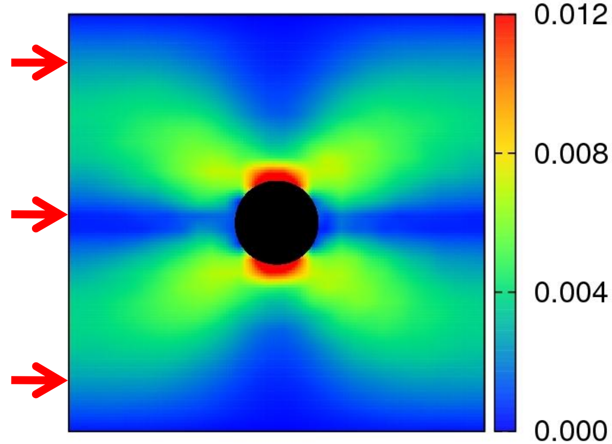
$|\mathbf{v}|$



symmetric

shear strain rate

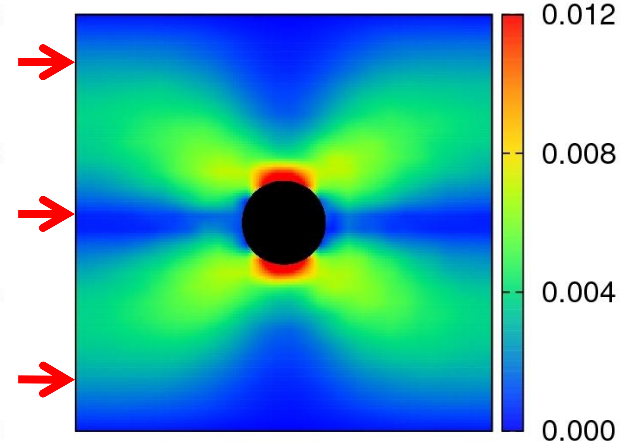
D_{xy}



symmetric

shear stress

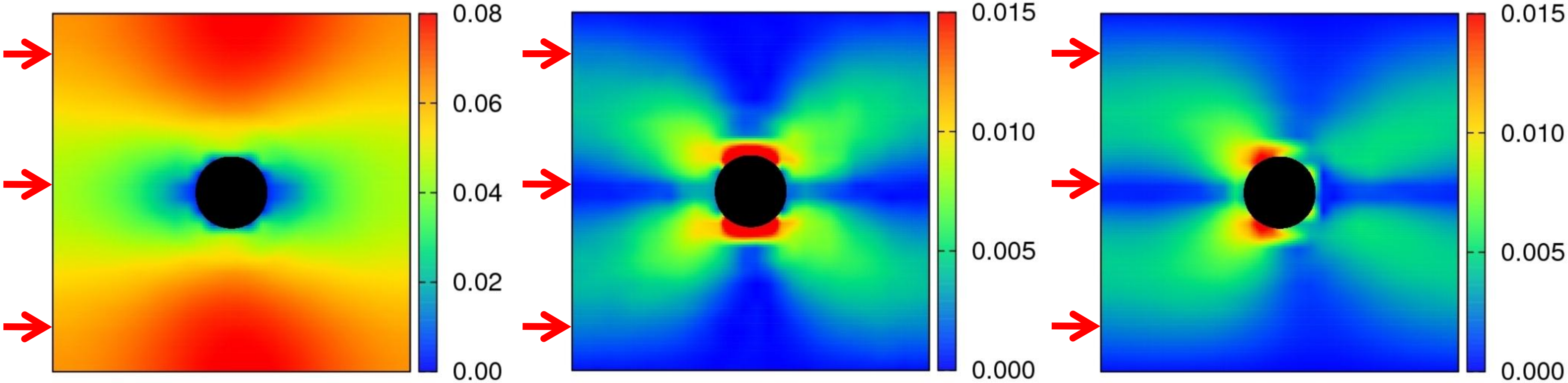
σ_{xy}/η



symmetric

Entangled polymer ($\langle Z \rangle_{eq}$=7) at Re << 1

velocity $|\mathbf{v}|$ | shear strain rate D_{xy} | shear stress σ_{xy}/η



almost symmetric | almost symmetric | highly asymmetric due to flow history

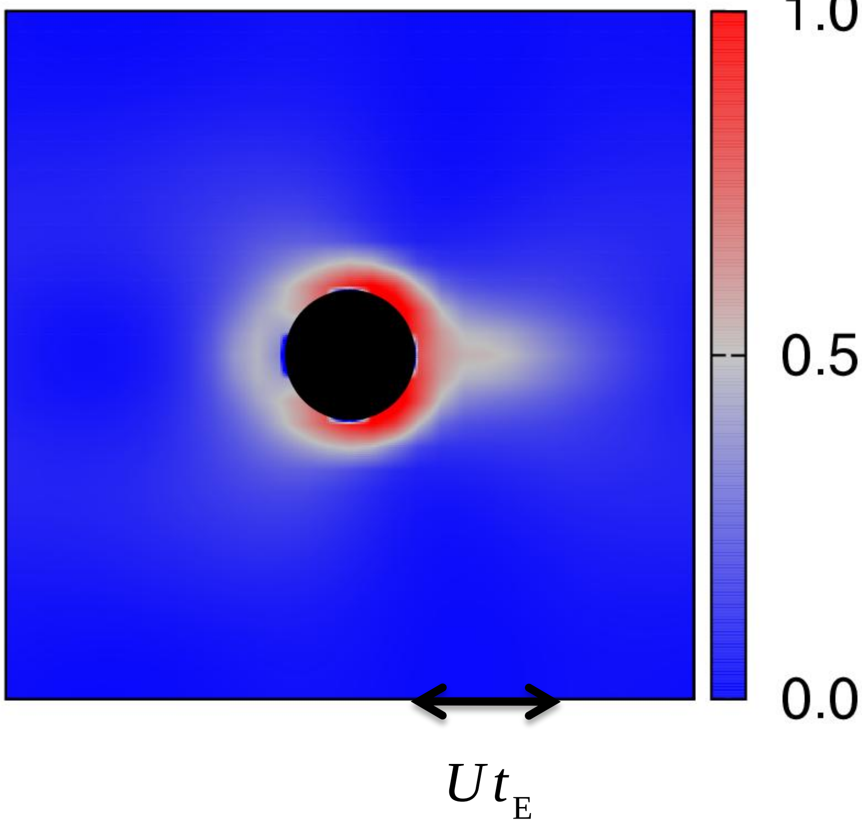
$$\mathrm{Re} = \frac{\rho U l}{\eta} \ll 1 \qquad \mathrm{De} = \frac{U}{l}\tau > 1 \qquad \mathrm{Wi} = \dot{\gamma}\tau > 1$$

(near cylinder)

Macroscopic distribution of Microscopic information

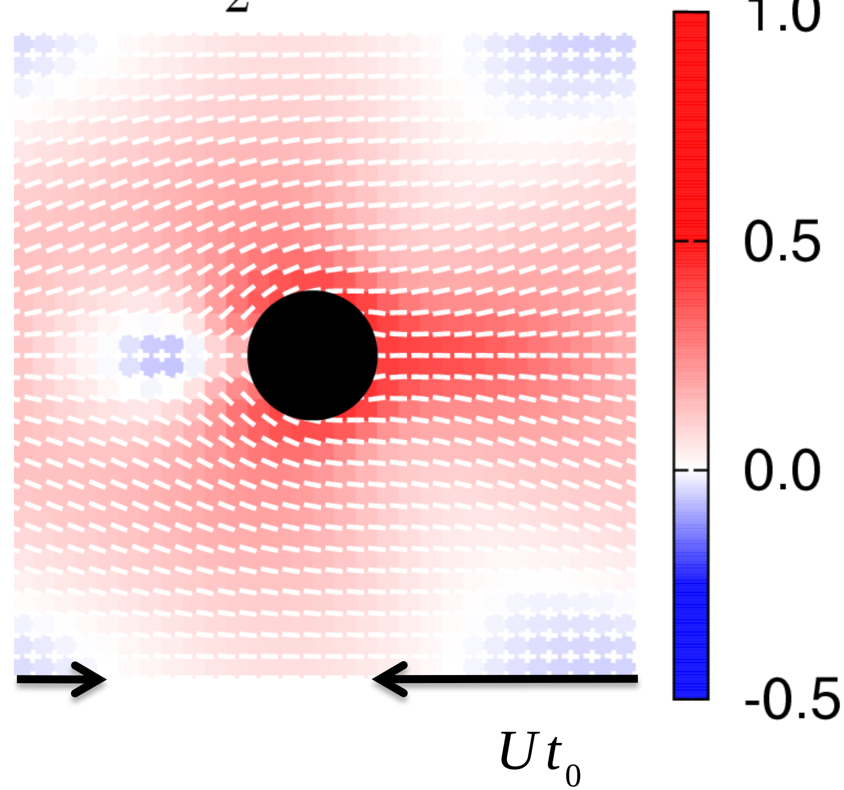
Elongation (color)

$$\Delta l = \langle l \rangle - \langle l \rangle_{\rm eq}$$



Orientation (white bar) and Orientational order (color)

$$S = \frac{1}{2}\langle 3\cos^2\theta - 1 \rangle$$



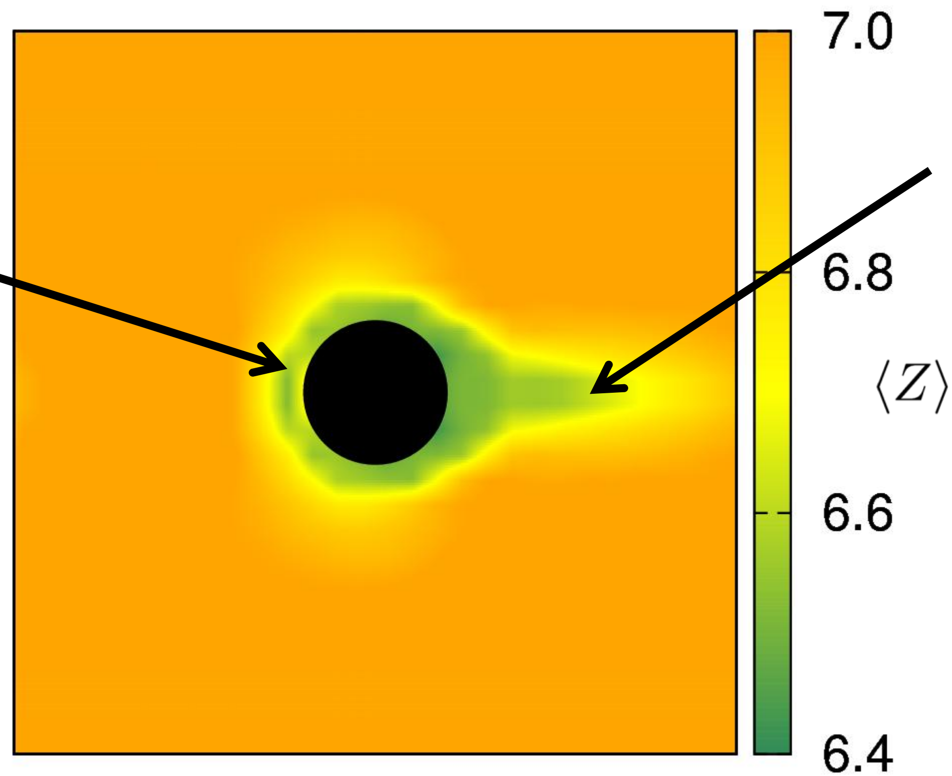
slower relaxation

Murashima & Taniguchi, EPL (2011)

The spatial distribution of <Z>

(entanglement number per a chain)

Less entangled
due to
shear thinning
at high shear rate



Less entangled
due to
flow history

Direct molecular level visualization of polymer
in non-equilibrium non-uniform flow!!

Future works

- 3D simulations of realistic flow geometry

-> larger system N_f =	50^3	1 day / 10^3 core,	2 TB Ram
	100^3	1 day / 10^4 core,	20 TB Ram
	200^3	1 day / 10^5 core,	200 TB Ram

- More complicated polymers

  -> branched, blend, polydisperse, etc…

- Boundary conditions

  -> consistent determination of slip on boundary

- Heat production/dissipation

  -> need thermodynamic consistency