2015 DPD Workshop

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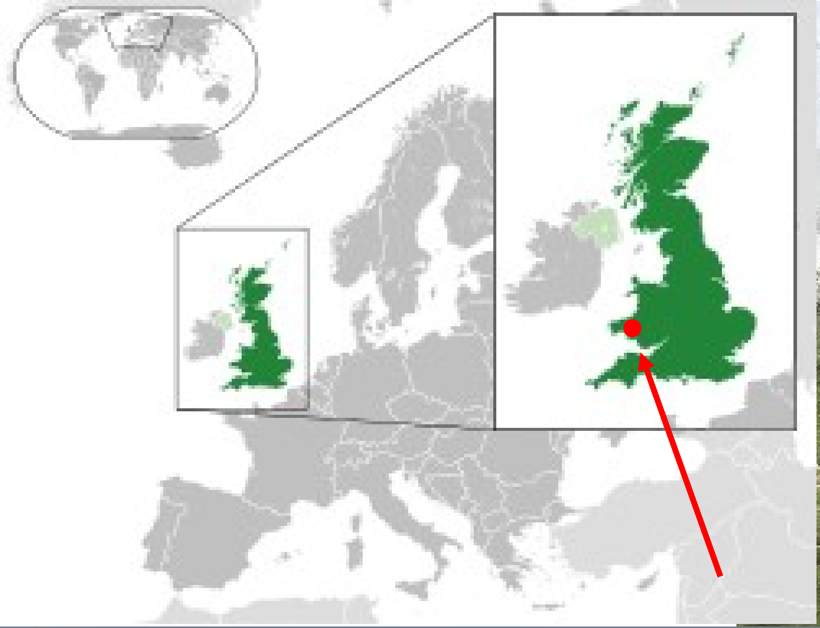
Smoothed Dissipative Particle Dynamics:

theory and applications to complex fluids

Marco Ellero

Zienkiewicz Centre for Computational Engineering (ZCCE)
College of Engineering, Swansea University Bay Campus
Swansea SA1 8EN, United Kingdom

Swansea - Wales - Bay Campus



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* Xin Bian (Brown U.)
* Sergey Litvinov (ETH)

Outline:

Smoothed Particle Hydrodynamics (continuum)

Smoothed Dissipative Particle Dynamics

Dissipative Particle Dynamics (mesoscopic)

Part I: theory

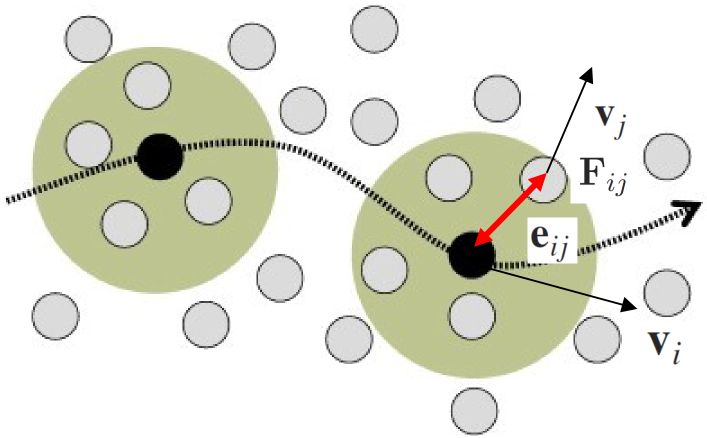
I. What is S-DPD?

Smoothed Dissipative Particle Dynamics

Smoothed Dissipative Particle Dynamics (**SDPD**)
Español, Revenga, Phys. Rev E, *E* **67**: 026705 (2003)

$$\dot{\mathbf{r}}_i = \mathbf{v}_i$$

$$m\dot{\mathbf{v}}_i = -\sum_j \underbrace{\left(\frac{P_i}{d_i^2}+\frac{P_j}{d_j^2}\right) W'_{ij}\mathbf{e}_{ij}}_{\mathbf{F}_{ij}^C} + \frac{5\eta}{3}\sum_j \underbrace{\frac{W'_{ij}}{d_i d_j r_{ij}}\left[\mathbf{v}_{ij} + (\mathbf{e}_{ij}\cdot\mathbf{v}_{ij})\,\mathbf{e}_{ij}\right]}_{\mathbf{F}_{ij}^D} + \sum_j \underbrace{A_{ij}\frac{d\bar{\boldsymbol{\xi}}_{ij}}{dt}\cdot\mathbf{e}_{ij}}_{\mathbf{F}_{ij}^R}$$



Smoothed Dissipative Particle Dynamics

Smoothed Dissipative Particle Dynamics (**SDPD**)
Español, Revenga, Phys. Rev E, *E* **67**: 026705 (2003)

$$
\begin{aligned}
\dot{\mathbf{r}}_i &= \mathbf{v}_i \\
m\dot{\mathbf{v}}_i &= -\sum_j \left(\frac{P_i}{d_i^2} + \frac{P_j}{d_j^2}\right) W'_{ij}\mathbf{e}_{ij} + \frac{5\eta}{3}\sum_j \frac{W'_{ij}}{d_i d_j r_{ij}}\left[\mathbf{v}_{ij} + (\mathbf{e}_{ij}\cdot\mathbf{v}_{ij})\,\mathbf{e}_{ij}\right] + \sum_j A_{ij}\frac{d\bar{\boldsymbol{\xi}}_{ij}}{dt}\cdot\mathbf{e}_{ij}
\end{aligned}
$$

General Equation for Non-Equilibrium Reversible-Irreversible Coupling (**GENERIC**)
Öttinger,Grmela Phys. Rev E, *E* **56**: 6620–6632 (1997)

$$
d\mathbf{x} = \mathbf{L}\cdot\frac{\partial E}{\partial \mathbf{x}}\,dt
$$

- **Total energy *E* conserved (1st Law Thermodynamics)**

Smoothed Dissipative Particle Dynamics

Smoothed Dissipative Particle Dynamics (**SDPD**)
Español, Revenga, Phys. Rev E, *E* **67**: 026705 (2003)

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General Equation for Non-Equilibrium Reversible-Irreversible Coupling (**GENERIC**)
Öttinger,Grmela Phys. Rev E, *E* **56**: 6620–6632 (1997)

$$d\mathbf{x} = \mathbf{L} \cdot \frac{\partial E}{\partial \mathbf{x}} dt + \mathbf{M} \cdot \frac{\partial S}{\partial \mathbf{x}} dt$$

- **Total energy *E* conserved (1st Law Thermodynamics)**
- **Monotonic entropy increase *S* (2nd Law Thermodynamics**

Smoothed Dissipative Particle Dynamics

Smoothed Dissipative Particle Dynamics (**SDPD**)
Español, Revenga, Phys. Rev E, *E* **67**: 026705 (2003)

$$\dot{\mathbf{r}}_i = \mathbf{v}_i$$

$$m\dot{\mathbf{v}}_i = -\sum_j \left(\frac{P_i}{d_i^2} + \frac{P_j}{d_j^2}\right) W'_{ij}\mathbf{e}_{ij} + \frac{5\eta}{3}\sum_j \frac{W'_{ij}}{d_i d_j r_{ij}} \left[\mathbf{v}_{ij} + (\mathbf{e}_{ij}\cdot\mathbf{v}_{ij})\,\mathbf{e}_{ij}\right] + \sum_j A_{ij}\frac{d\bar{\boldsymbol{\xi}}_{ij}}{dt}\cdot\mathbf{e}_{ij}$$

General Equation for Non-Equilibrium Reversible-Irreversible Coupling (**GENERIC**)
Öttinger,Grmela Phys. Rev E, *E* **56**: 6620–6632 (1997)

$$d\mathbf{x} = \mathbf{L}\cdot\frac{\partial E}{\partial \mathbf{x}}dt + \mathbf{M}\cdot\frac{\partial S}{\partial \mathbf{x}}dt + d\tilde{\mathbf{x}}$$

- ❑ **Total energy *E* conserved (1st Law Thermodynamics)**
- ❑ **Monotonic entropy increase *S* (2nd Law Thermodynamics)**
- ❑ **Fluctuation Dissipation Theorem (FDT)**

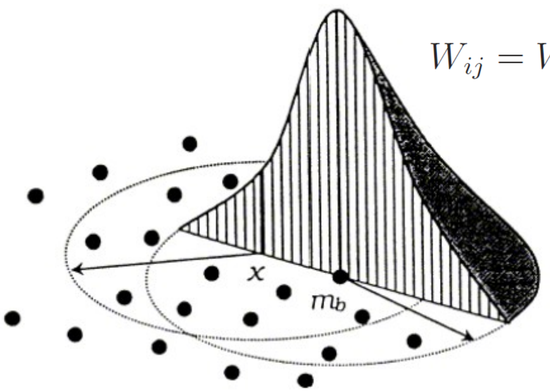
$$d\tilde{\mathbf{x}}d\tilde{\mathbf{x}}^T = 2k_B\mathbf{M}dt$$

Conservative (pressure) forces

$$\underbrace{\left(\frac{P_i}{d_i^2} + \frac{P_j}{d_j^2}\right) W'_{ij} \mathbf{e}_{ij}}_{\mathbf{F}_{ij}^C}$$

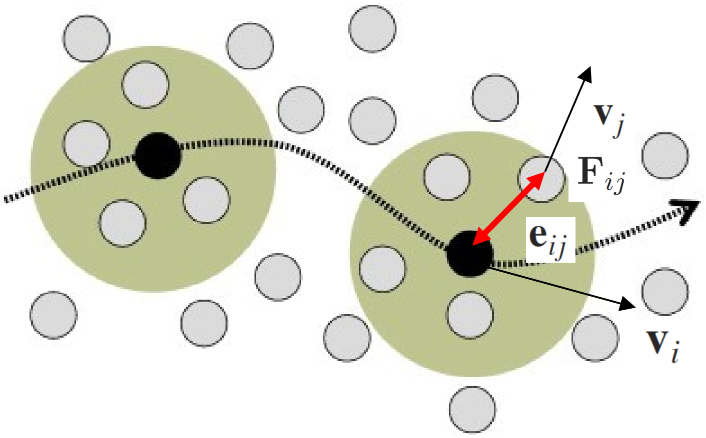
Fluid particle density/volume

$$d_i = \frac{1}{\mathcal{V}_i} = \frac{\rho_i}{m_i} = \sum_j W_{ij} \longrightarrow P(\rho)$$



$$W_{ij} = W\left(\left|\mathbf{x}_i - \mathbf{x}_j\right|, h\right)$$

Non-local repulsive forces



Conservative (pressure) forces

$$\left(\frac{P_i}{d_i^2}+\frac{P_j}{d_j^2}\right)W'_{ij}\mathbf{e}_{ij}$$

Discrete representation **pressure gradient** (Euler equations):
Smoothed Particle Hydrodynamics

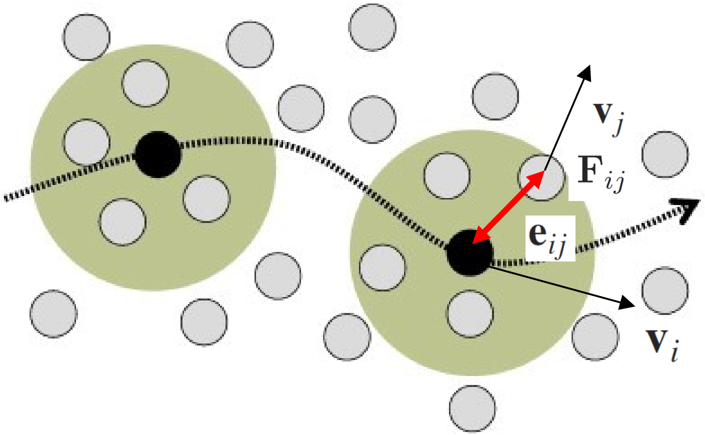
$$f_i=\sum_j \mathcal{V}_j f_j W_{ij} \longrightarrow \nabla f_i=\sum_j \mathcal{V}_j f_j \underbrace{\nabla_i W_{ij}}_{W'_{ij}\mathbf{e}_{ij}}$$

$$\frac{\nabla p}{\rho}=\nabla\left(\frac{p}{\rho}\right)-\frac{p}{\rho^2}\nabla\rho$$

L.B. Lucy, Astron. J. 82 (12) (1977) 1013–1924.
R.A. Gingold, J.J. Monaghan,, Monthly Notices Roy. Astron. Soc. 181 (1977) 375–389.

Dissipative (viscous) forces

$$\underbrace{\frac{W'_{ij}}{d_i d_j r_{ij}}\left[\mathbf{v}_{ij} + (\mathbf{e}_{ij}\cdot\mathbf{v}_{ij})\,\mathbf{e}_{ij}\right]}_{\mathbf{F}^D_{ij}}$$



Smoothed Dissipative Particle Dynamics (**SDPD**)
Español, Revenga, Phys. Rev E, *E* **67**: 026705 (2003)

Dissipative (viscous) forces

$$\frac{5\eta}{3}\sum_j \frac{W'_{ij}}{d_i d_j r_{ij}}\left[\mathbf{v}_{ij} + \left(\mathbf{e}_{ij}\cdot\mathbf{v}_{ij}\right)\mathbf{e}_{ij}\right]$$

Discrete representation **viscous dissipation** (Navier-Stokes equations):
Smoothed Particle Hydrodynamcs

Smoothed Dissipative Particle Dynamics (**SDPD**)
Español, Revenga, Phys. Rev E, *E* **67**: 026705 (2003)

Random forces

$$\underbrace{A_{ij}\frac{d\bar{\boldsymbol{\xi}}_{ij}}{dt}\cdot\mathbf{e}_{ij}}_{\mathbf{F}_{ij}^{R}}$$

Matrix independent Wiener process

$$d\bar{\boldsymbol{\xi}}_{ij} = \frac{1}{2}\left(d\boldsymbol{\xi}_{ij} + d\boldsymbol{\xi}_{ij}^{T}\right)$$

$$\begin{aligned}\langle d\xi_{ij}^{\alpha\beta}\rangle &= 0\\ \langle \xi_{ij}^{\alpha\alpha'}\xi_{i'j'}^{\beta\beta'}(t')\rangle &= \left(\delta_{ii'}\delta_{jj'} + \delta_{ij'}\delta_{ji'}\right)\delta^{\alpha\beta}\delta^{\alpha'\beta'}dt\end{aligned}$$

SDPD – Fluctuation Dissipation Theorem

$$d\tilde{\mathbf{x}}d\tilde{\mathbf{x}}^{T} = 2k_B\mathbf{M}dt$$

$$A_{ij} = \left[-\frac{20}{3}k_B T\eta\frac{W'_{ij}}{d_i d_j r_{ij}}\right]^{1/2}$$

Smoothed Dissipative Particle Dynamics

Similar to **Dissipative Particle Dynamics**

$$\begin{aligned}\dot{\mathbf{r}}_i &= \mathbf{v}_i \\ m\dot{\mathbf{v}}_i &= -\sum_j \underbrace{\left(\frac{P_i}{d_i^2}+\frac{P_j}{d_j^2}\right) W'_{ij}\mathbf{e}_{ij}}_{\mathbf{F}_{ij}^C} + \frac{5\eta}{3}\sum_j \underbrace{\frac{W'_{ij}}{d_i d_j r_{ij}}\left[\mathbf{v}_{ij}+\left(\mathbf{e}_{ij}\cdot\mathbf{v}_{ij}\right)\mathbf{e}_{ij}\right]}_{\mathbf{F}_{ij}^D} + \sum_j \underbrace{A_{ij}\frac{d\bar{\boldsymbol{\xi}}_{ij}}{dt}\cdot\mathbf{e}_{ij}}_{\mathbf{F}_{ij}^R}\end{aligned}$$

.. but connected to **Smoothed Particle Hydrodynamics**

$$\begin{aligned}\dot{\mathbf{r}}_i &= \mathbf{v}_i \\ m\dot{\mathbf{v}}_i &= \underbrace{-\sum_j \left(\frac{P_i}{d_i^2}+\frac{P_j}{d_j^2}\right) W'_{ij}\mathbf{e}_{ij}}_{(\nabla p/\rho)_i} + \underbrace{\frac{5\eta}{3}\sum_j \frac{W'_{ij}}{d_i d_j r_{ij}}\left[\mathbf{v}_{ij}+\left(\mathbf{e}_{ij}\cdot\mathbf{v}_{ij}\right)\mathbf{e}_{ij}\right]}_{\eta\nabla^2\mathbf{v}_i+(\eta/3)\ \nabla(\nabla\cdot\mathbf{v}_i)}\end{aligned}$$

II. SDPD: meso or macro method?

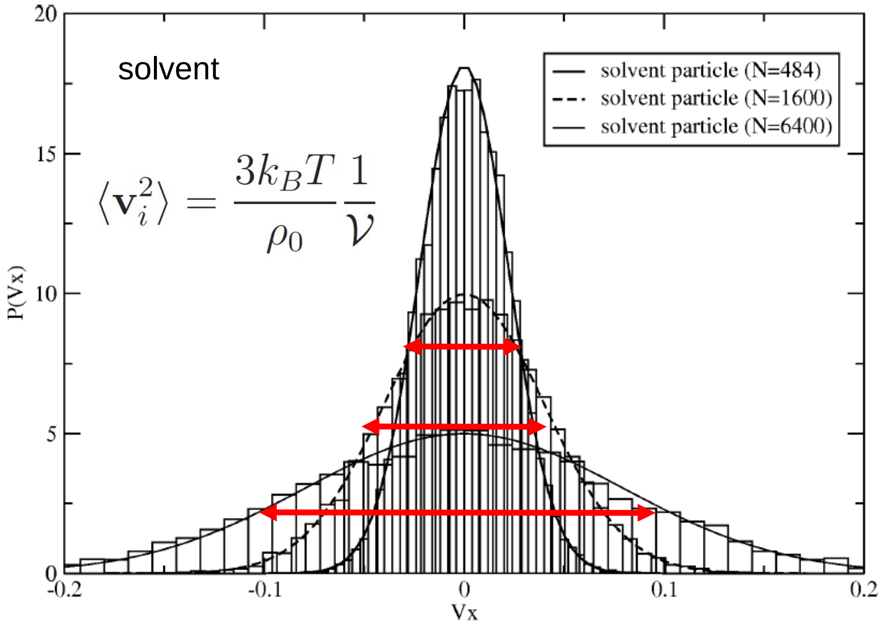
Consistent scaling SDPD thermal fluctuations

Vazquez, Ellero, Español, J. Chem. Phys. **130**: 034901 (2009)

Maxwell-Boltzmann velocity distribution variance

$$\langle \mathbf{v}_i^2 \rangle = \frac{3k_B T}{\rho_0} \frac{1}{\mathcal{V}}$$

$$\mathcal{V}_i = \left(\sum_j W_{ij} \right)^{-1}$$



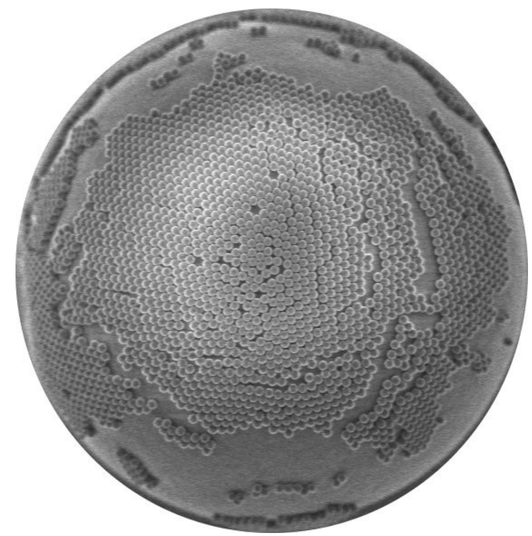
Consistent scaling SDPD thermal fluctuations

Vazquez, Ellero, Español, J. Chem. Phys. **130**: 034901 (2009)

$l = 3cm$

$L = 30cm$

$$\left\langle \mathrm{v}_i^2 \right\rangle = D \frac{k_B T}{\rho_0} \frac{1}{V} \approx 0$$



$l = 1\mu m$

$L = 10\mu m$

$$\left\langle \mathrm{v}_i^2 \right\rangle = D \frac{k_B T}{\rho_0} \frac{1}{V} \neq 0$$

Consistent scaling SDPD thermal fluctuations

Vazquez, Ellero, Español, J. Chem. Phys. **130**: 034901 (2009)

$$\begin{aligned} \dot{\mathbf{r}}_i &= \mathbf{v}_i \\ m\dot{\mathbf{v}}_i &= -\sum_j \left(\frac{P_i}{d_i^2} + \frac{P_j}{d_j^2}\right) W'_{ij}\mathbf{e}_{ij} + \frac{5\eta}{3}\sum_j \frac{W'_{ij}}{d_i d_j r_{ij}}\left[\mathbf{v}_{ij} + (\mathbf{e}_{ij}\cdot\mathbf{v}_{ij})\,\mathbf{e}_{ij}\right] + \sum_j \underbrace{A_{ij}\frac{d\bar{\boldsymbol{\xi}}_{ij}}{dt}\cdot\mathbf{e}_{ij}}_{\mathbf{F}^R_{ij}} \end{aligned}$$

$$\mathcal{V}_i = \left(\sum_j W_{ij}\right)^{-1} \longrightarrow \infty \qquad \rightarrow 0$$

Fluid particle volume

$\lim_{\mathcal{V}_i\to\infty}$ SDPD = SPH

IV. Advantages in using S-DPD?

Solvent properties specification

DPD

SDPD

Thermodynamic behaviour (Equation of State)

DPD:

$$P(\rho) = \rho k_B T + \alpha a \rho^2$$

Groot, Warren, J. Chem. Phys. **107**, 4423 (1997)

SDPD:

- $P(\rho) = c_s^2 \rho$
- $P(\rho) = P_o \left[\left(\frac{\rho}{\rho_0} \right)^{\gamma} + B \right]$
- $P(\rho) = \frac{\rho k_B T}{1 - A\rho} - B\rho^2$

Transport coefficients

DPD:

- $\nu = \frac{45 k_B T}{4\pi\gamma\rho r_c^3} + \frac{2\pi\gamma\rho r_c^5}{1575}$
- $c_s = \sqrt{k_B T + 2\alpha a \rho}$

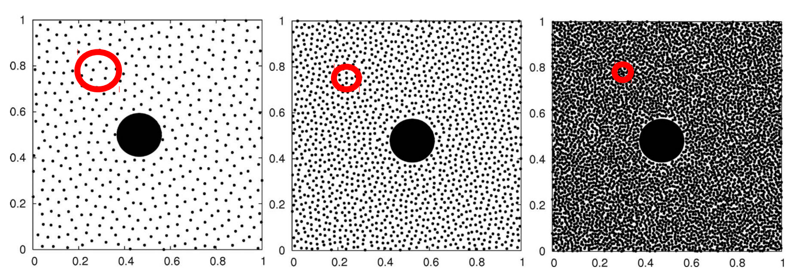
Groot, Warren, J. Chem. Phys. **107**, 4423 (1997)

SDPD:

- $\nu = \frac{\eta}{\rho_0}$
- c_s

Scaling particle volumes, resolution analysis

Difficult to preserve physical quantities :Ma, Re, Sc, …. (depend on particle size)



Specified once for all.

Independent fluid particle size

V. SDPD accuracy?

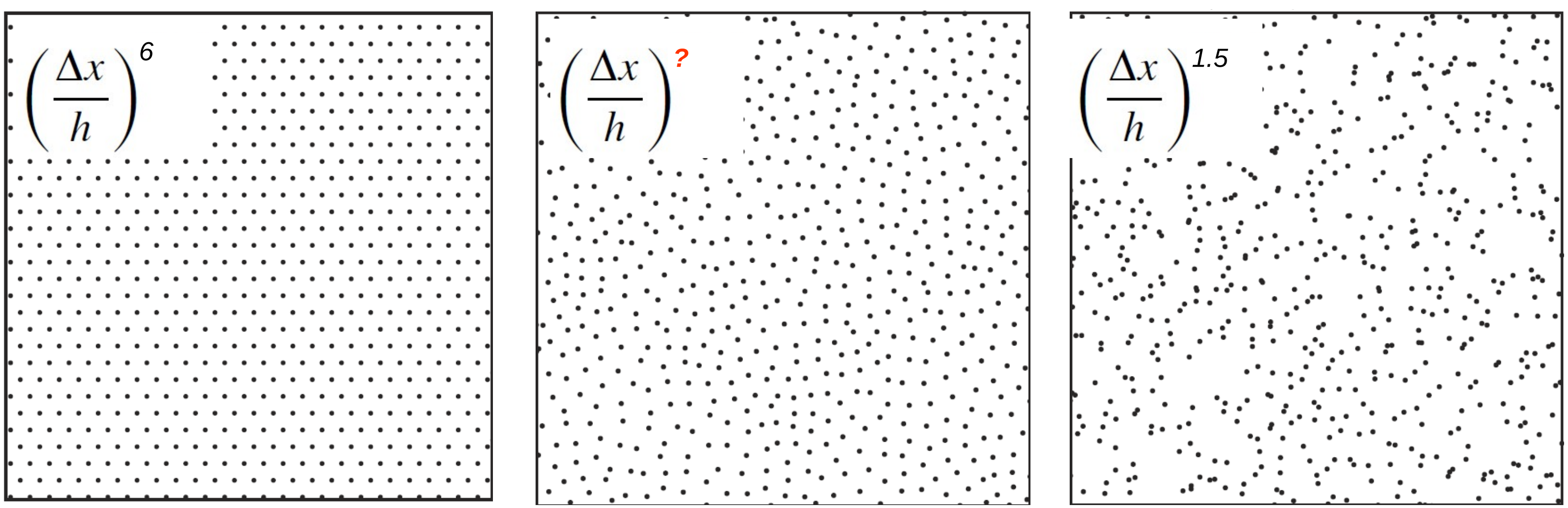
Approximation/convergence SDPD-SPH

$$f(\mathbf{r}) \longrightarrow \underbrace{\langle f(\mathbf{r})\rangle_h = \int f(\mathbf{r}')W(|\mathbf{r}-\mathbf{r}'|)d\mathbf{r}'}_{\text{Mollification: smoothing kernel}} \longrightarrow \underbrace{\langle f(\mathbf{r})\rangle_h^{\Delta} = \sum_{j=1}^{N} \mathcal{V}_j f(\mathbf{r}_j)W(|\mathbf{r}-\mathbf{r}_j|)}_{\text{Quadrature}}$$

Errors

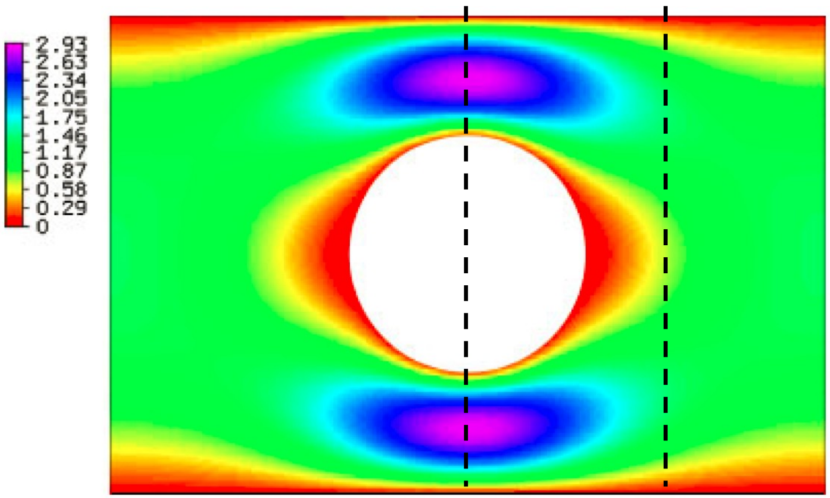
$$\|f(\mathbf{r}) - \langle f(\mathbf{r})\rangle_h^{\Delta}\| = \mathcal{O}\left(\left(\frac{h}{L}\right)^n\right) + \mathcal{O}\left(\left(\frac{\Delta}{h}\right)^m\right)$$

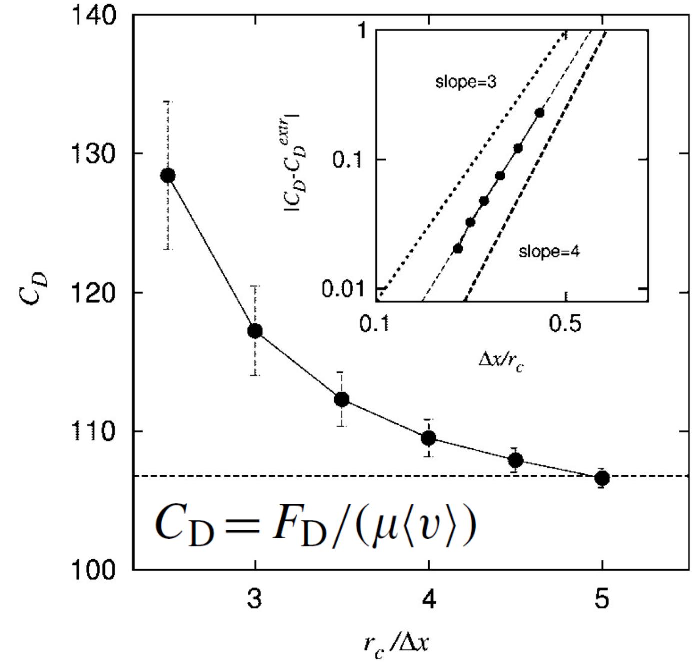
- ❑ $n = 2$ radially-symmteric kernel
- ❑ $m = \begin{cases} 3/2, & \textit{random} \\ \approx 3, & \textit{structured} \\ \beta + 4, & \textit{lattice} \end{cases}$

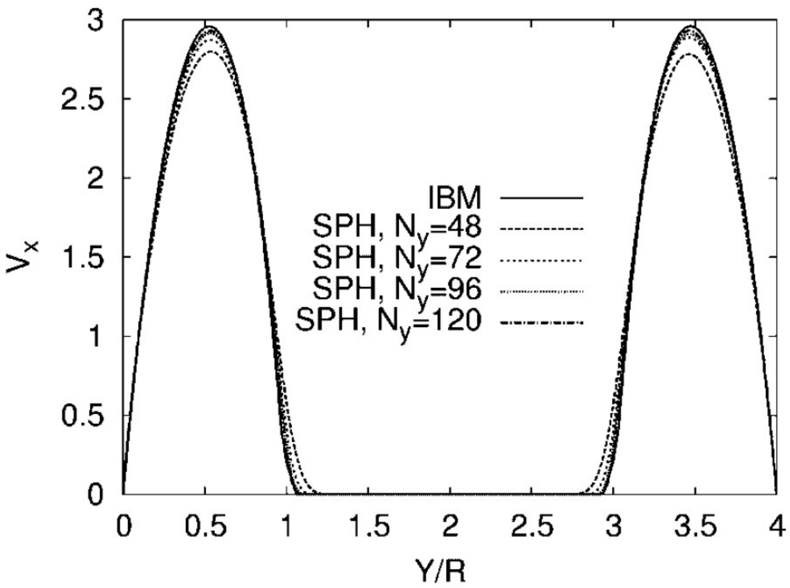


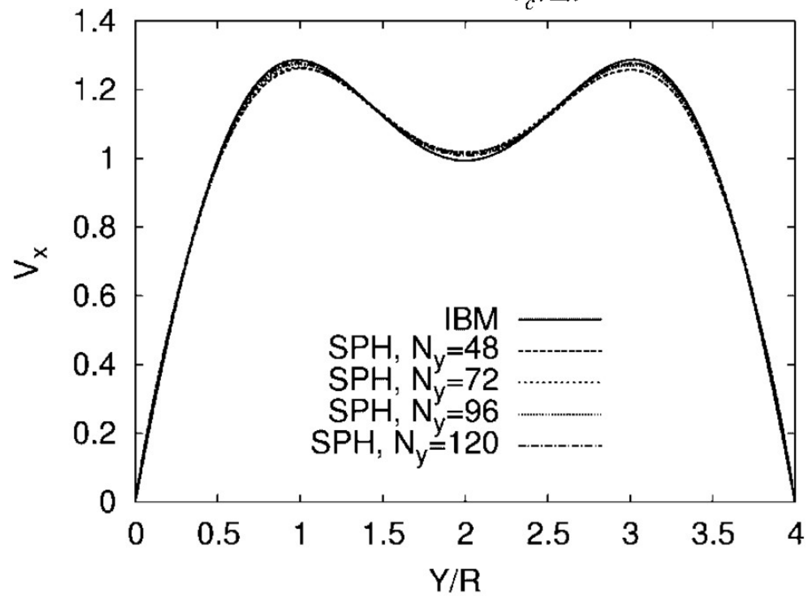
Approximation/convergence SDPD-SPH

Ellero, Adams, Int. J. Num. Meth. Engng. **86**, 1027 (2011)









VI. SDPD slower than DPD ?

SDPD vs DPD: algorithmic complexity

$$\begin{aligned}\dot{\mathbf{r}}_i &= \mathbf{v}_i \\ m\dot{\mathbf{v}}_i &= \sum_j \mathbf{F}_{ij}^C + \sum_j \mathbf{F}_{ij}^D + \sum_j \mathbf{F}_{ij}^R\end{aligned}$$

DPD

$$\begin{aligned}\mathbf{F}_{ij}^C &= a_{ij}\max\left(1 - r_{ij}/r_c, 0\right) \\ \mathbf{F}_{ij}^D &= \gamma\omega^D\left(r_{ij}\right)\left(\mathbf{e}_{ij}\cdot\mathbf{v}_{ij}\right)\mathbf{e}_{ij} \\ \mathbf{F}_{ij}^R &= \sigma\omega^R\left(r_{ij}\right)\xi_{ij}\mathbf{e}_{ij}\end{aligned}$$

SDPD

$$\begin{aligned}\mathbf{F}_{ij}^C &= \left(\frac{P_i}{d_i^2} + \frac{P_j}{d_j^2}\right) W'_{ij}\mathbf{e}_{ij} \\ \mathbf{F}_{ij}^D &= \frac{W'_{ij}}{d_i d_j r_{ij}}\left[\mathbf{v}_{ij} + \left(\mathbf{e}_{ij}\cdot\mathbf{v}_{ij}\right)\mathbf{e}_{ij}\right] \\ \mathbf{F}_{ij}^R &= A_{ij}\frac{d\bar{\boldsymbol{\xi}}_{ij}}{dt}\cdot\mathbf{e}_{ij}\end{aligned}$$

- ❑ $d_i = \dfrac{1}{\mathcal{V}_i} = \sum_j W_{ij}$ extra density evaluation
- ❑ $d\bar{\boldsymbol{\xi}}_{ij} = \dfrac{1}{2}\left(d\boldsymbol{\xi}_{ij} + d\boldsymbol{\xi}_{ij}^T\right)$ tensorial Wiener process

SDPD vs DPD: algorithmic complexity

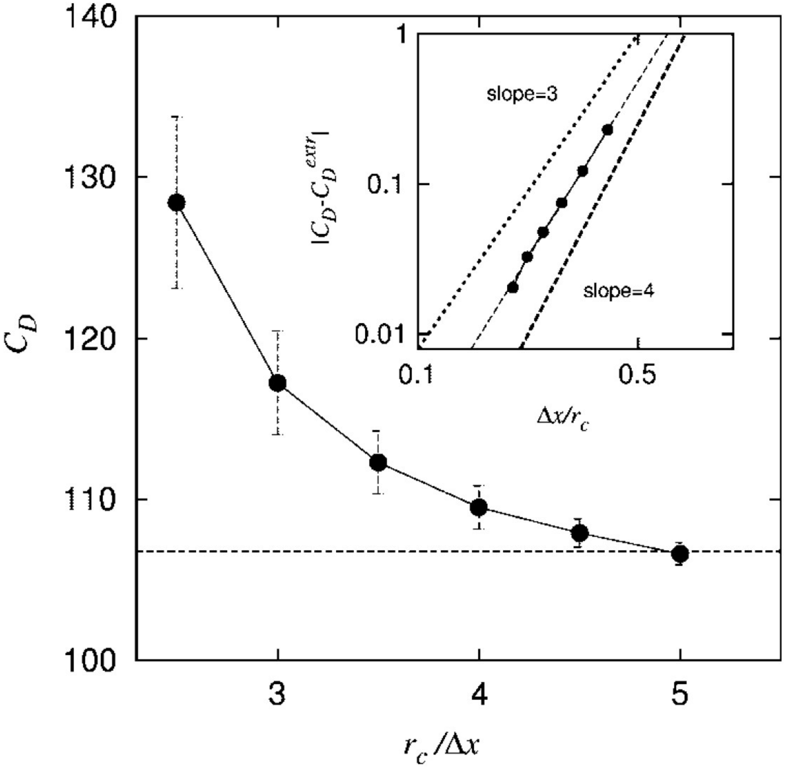
- Number of neighbours/particle (2D)

$$\frac{h}{\Delta} = 2 \longrightarrow N_{neigh} \approx 12$$

$$\frac{h}{\Delta} = 3 \longrightarrow N_{neigh} \approx 27$$

$$\frac{h}{\Delta} = 4 \longrightarrow N_{neigh} \approx 48$$

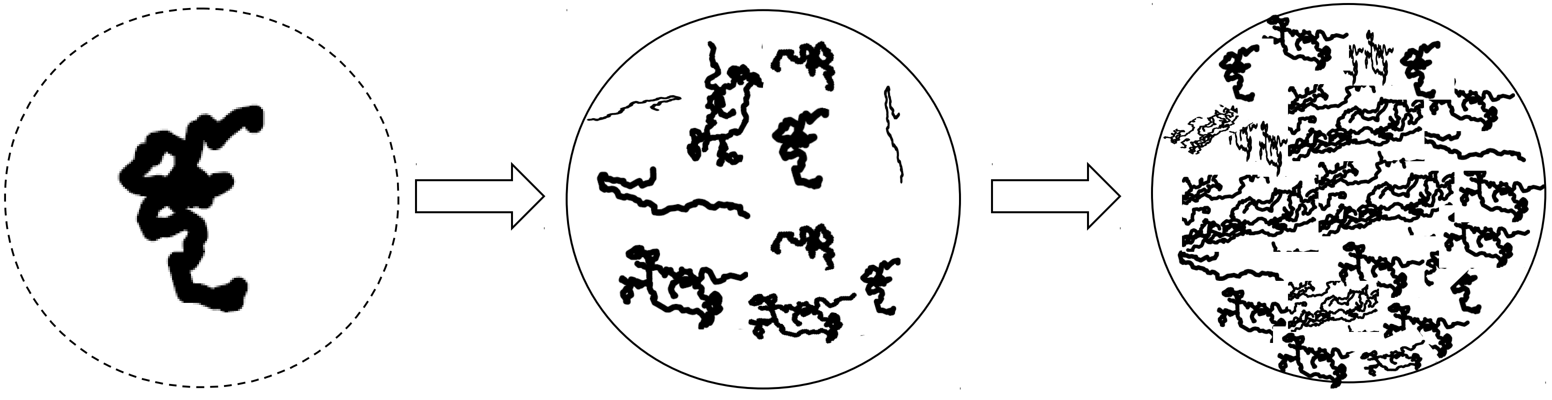
Ellero, Adams, Int. J. Num. Meth. Engng. **86**, 1027 (2011)



- Large # neighbours required only for exact specification transport coefficients
- If less accuracy is required, one can run with same # neighbors as DPD.

Part II: complex fluids

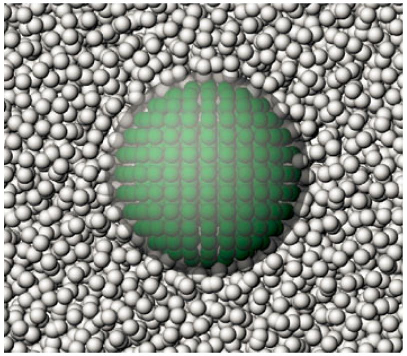
SDPD: **hierarchical modelling** of complex fluids

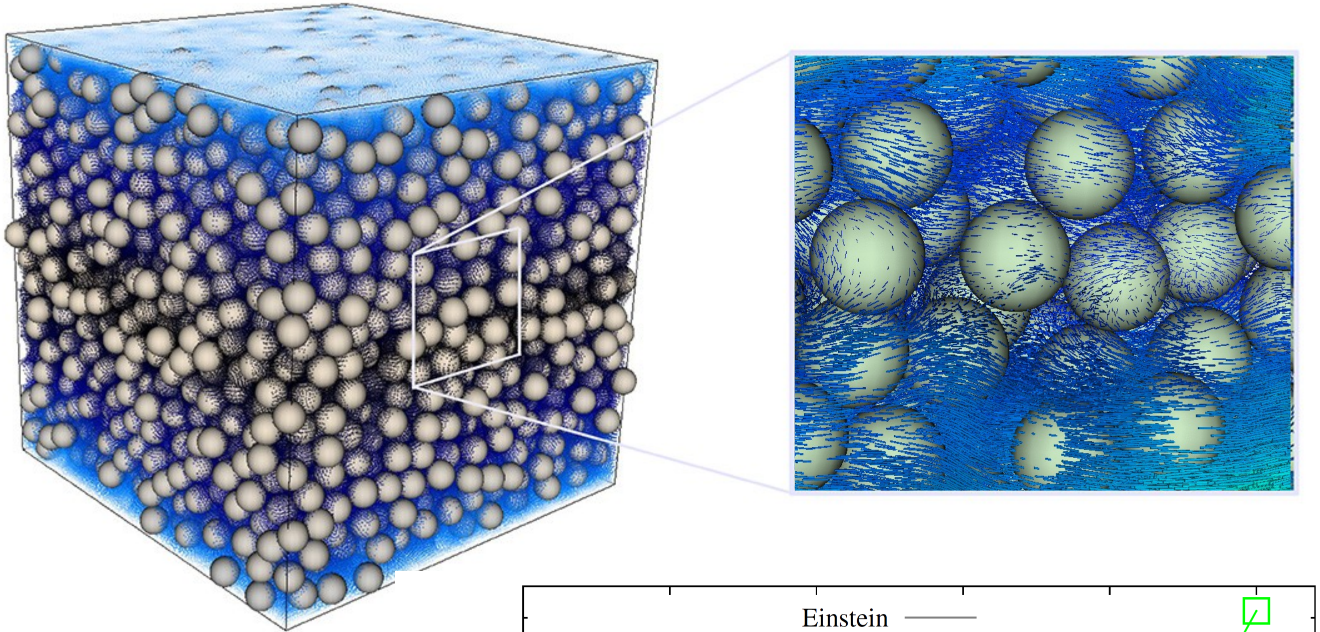


- **I:** ***Mesoscopic***
- **II.** ***Coarse-graining***
- **III.** ***Macroscopic***

I: Mesoscopic

Colloidal fluid: ***mesoscopic*** model

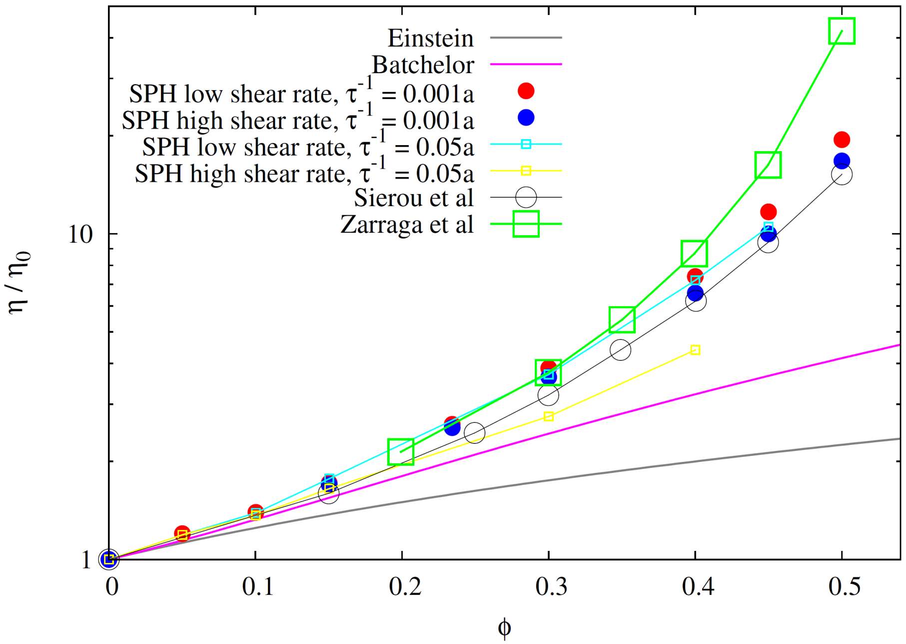




❑ Suspension rheology

- Frozen boundary particles: rigid structure
- Long range SDPD/SPH mediate hydro interactions
- Short range interparticle lubrication forces

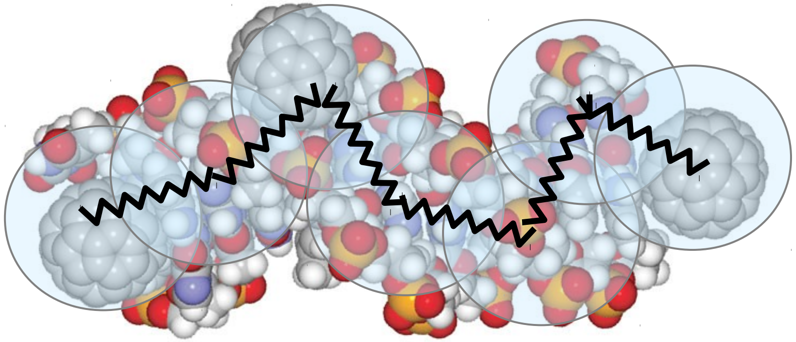
Bian et al., Phys. Fluids, **24** 012002 (2012)
Bian et al., Comp. Phys. Comm. **185**, 53-62 (2014).
Bian et al. J. Non-Newt- Fluid Mech. **213**, 39-49 (2014)
Vazquez-Quesada et al. J. Comp. Part. Mech. In press (2015)
Vazquez-Quesada et al.
J. Non-Newt- Fluid Mech. Submitted (2015)

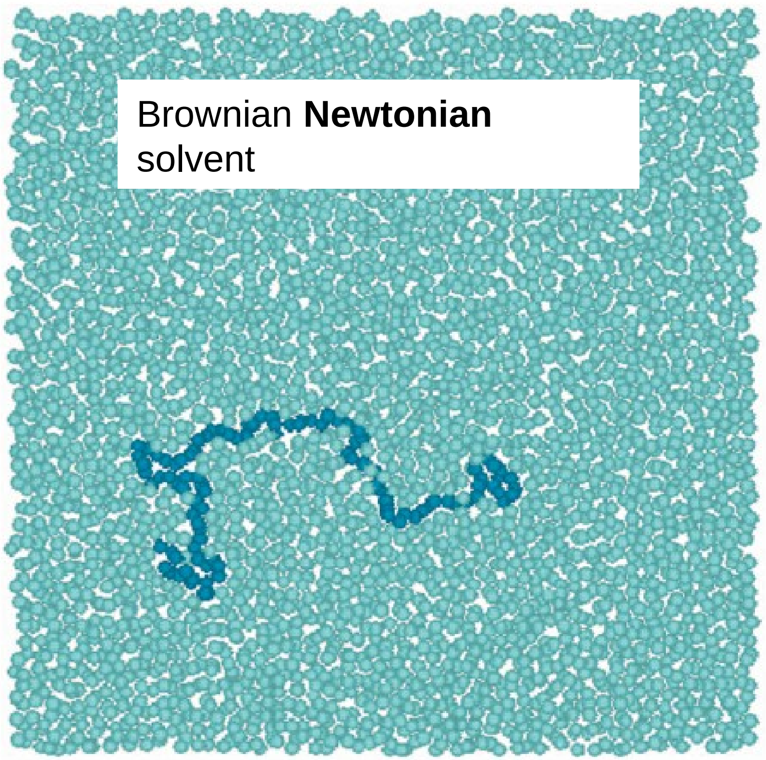


NO TUNING PARAMETERS

Polymeric fluid: ***mesoscopic*** model

Litvinov et al., Phys.Rev. E **77**, 66703 (2008)





$$m_i \frac{d\mathbf{v}_i}{dt} = \mathbf{F}_i^{\text{hydro}} + \mathbf{F}_{i,i_1}^{\text{FENE}} + \mathbf{F}_{i,i_2}^{\text{FENE}}$$

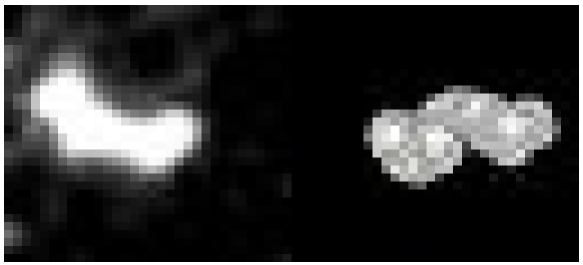
$$\mathbf{F}^{\text{FENE}}(\mathbf{r}_{ij}) = \frac{K\mathbf{r}_{ij}}{1-(r/R_0)^2}$$

- excluded volume effect: self-avoidance
- correcty hydrodynamics interactions
- preserved chain topology
- finite extensibility

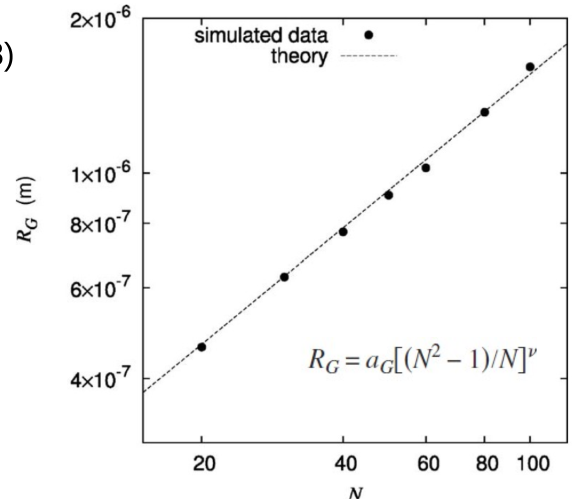
Polymeric fluid: ***mesoscopic*** model

- Equilibrium properties

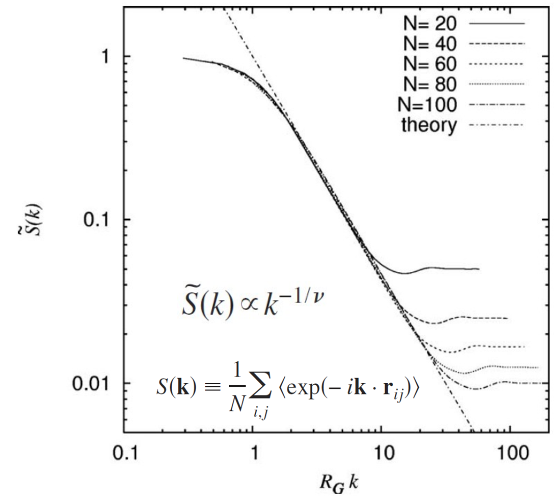
Litvinov et al., Phys.Rev. E **77**, 66703 (2008)



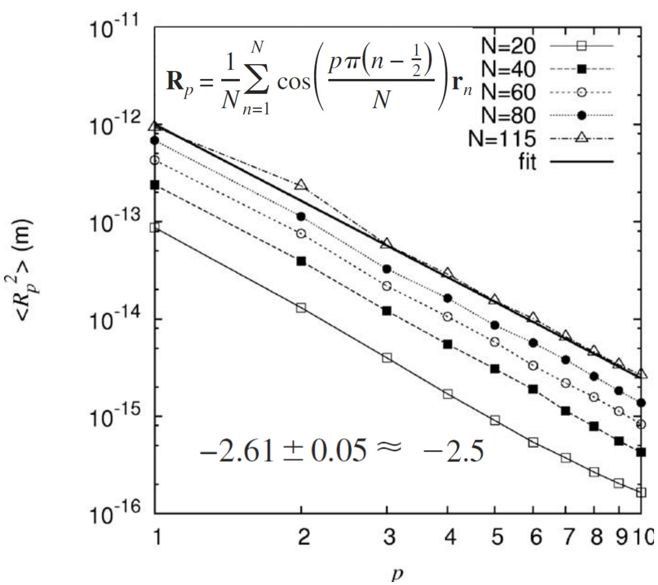
Gyration radius



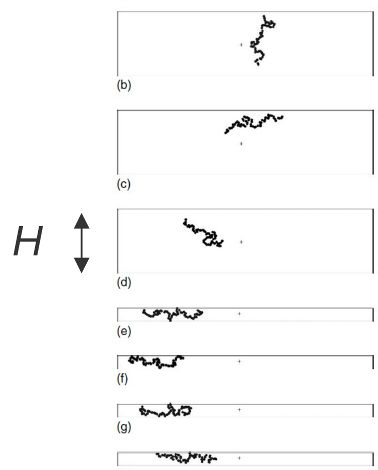
Structure factor

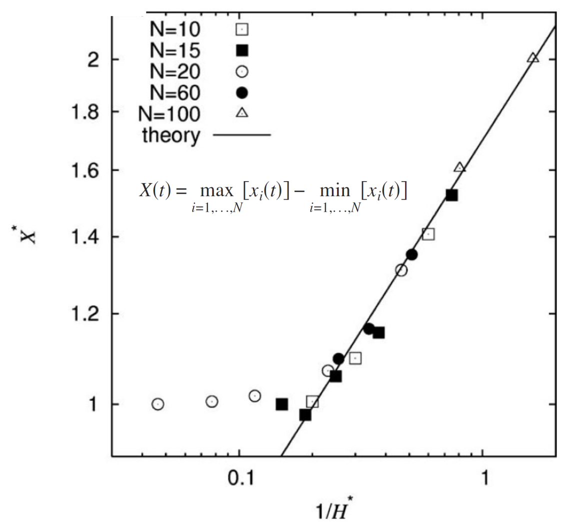


Internal Rouse modes



Confinement

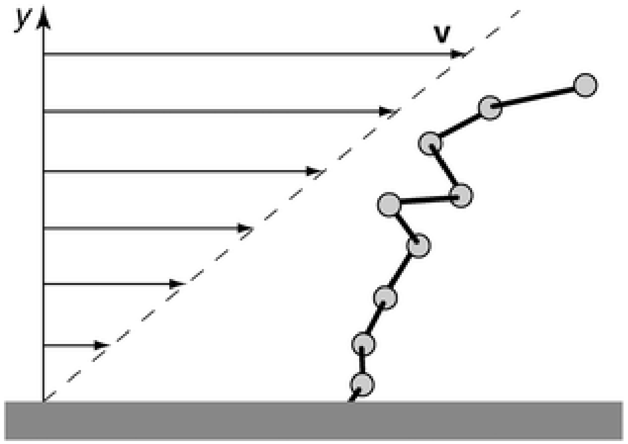


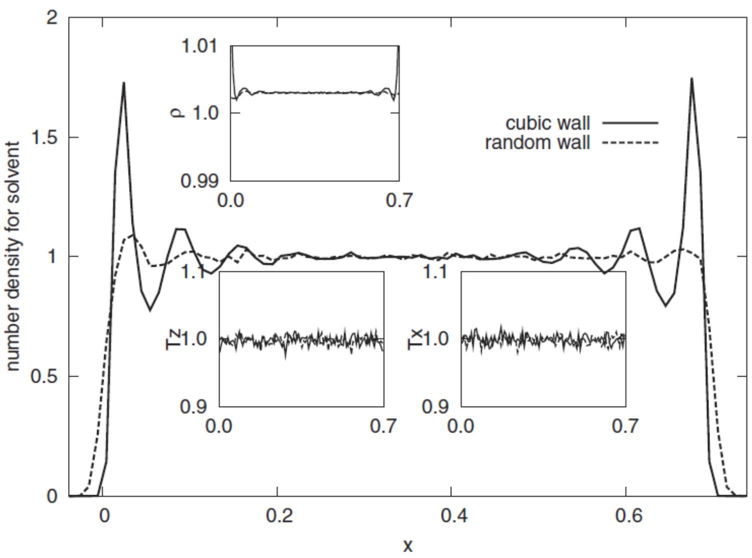


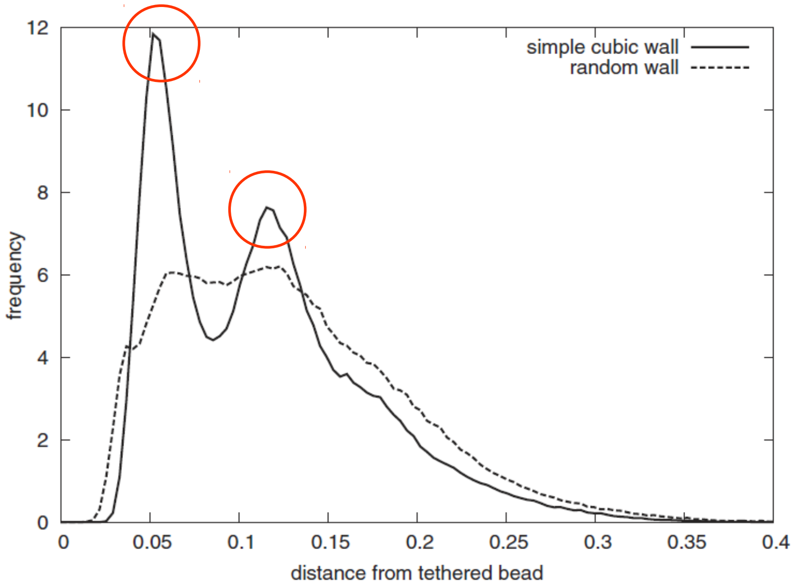
Polymeric fluid: ***mesoscopic*** model

- Tethered polymer under shear

Litvinov et al., Phys.Rev. E **82**, 066704 (2010)



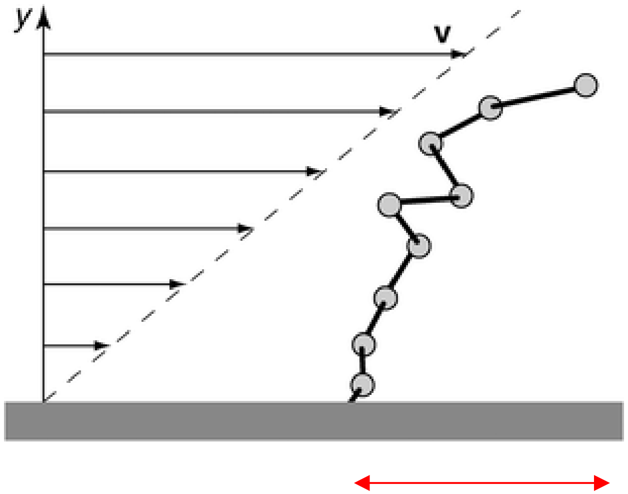


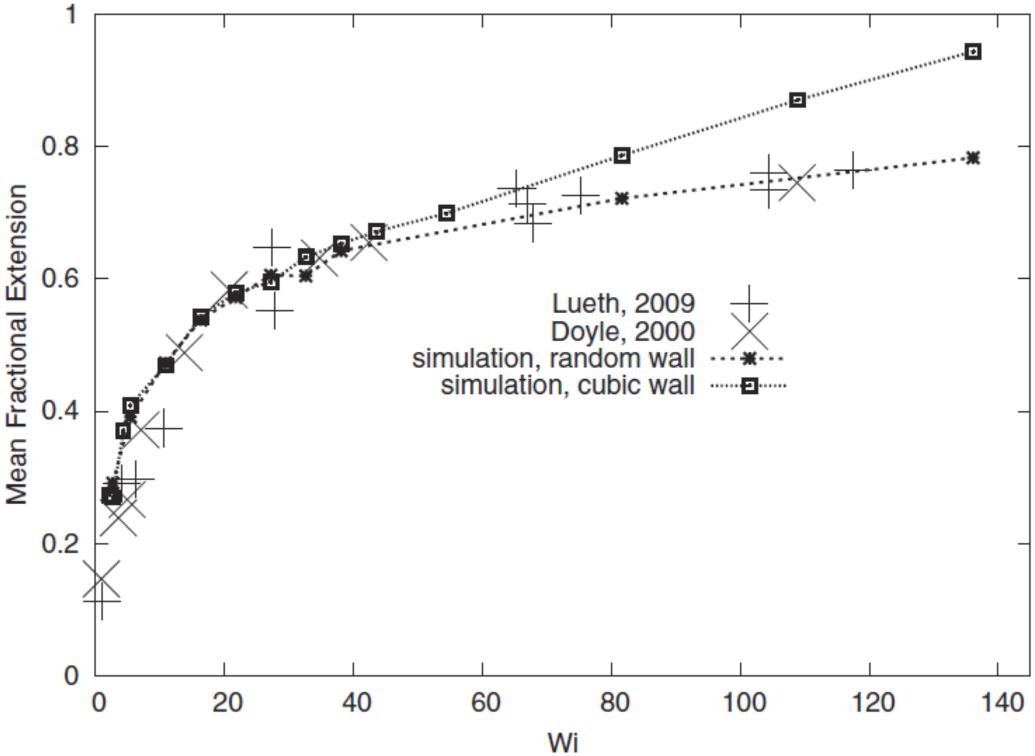


Polymeric fluid: ***mesoscopic*** model

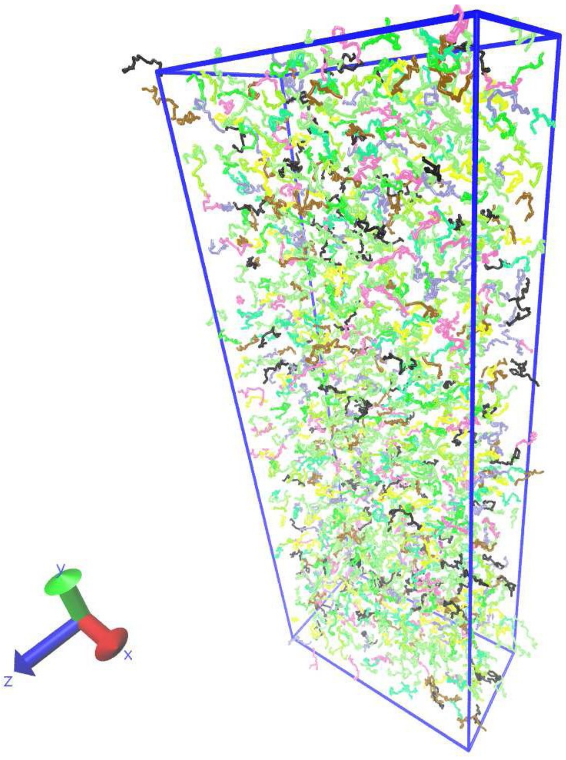
- ❑ Tethered polymer under shear

Litvinov et al., Phys.Rev. E **82**, 066704 (2010)

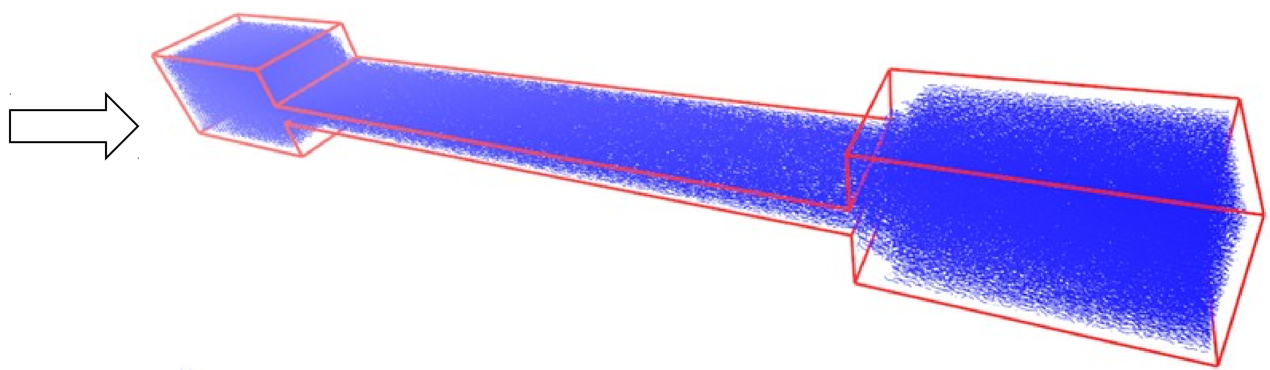




Polymeric ***mesoscopic*** model: applications



- Rheology/collective dynamics
  (DNS – no need of constituive equation)

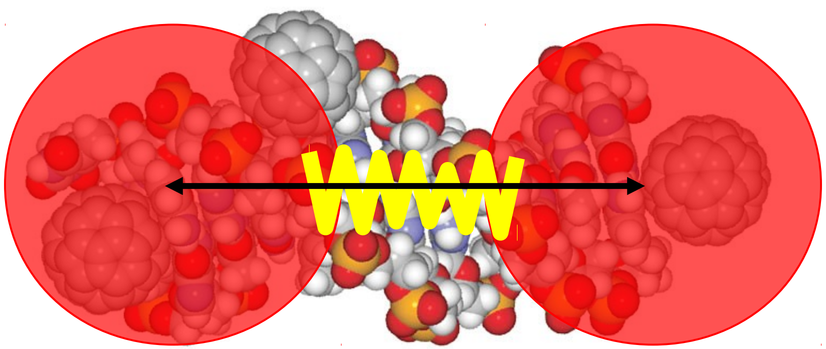


Litvinov et al., Microfluidics Nanofluidics **16**, 257-264 (2014)

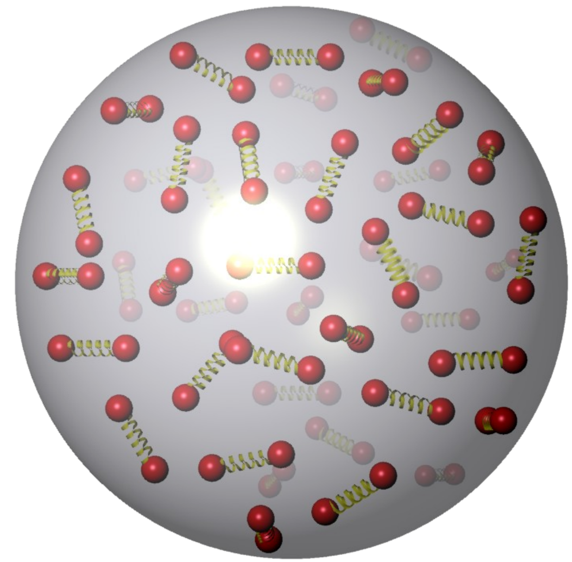
II: Coarse-graining

Polymeric fluid: ***coarse-graining*** model

Polymeric fluid: ***coarse-graining*** model



$\mathbf{q}_a$



Langevin equation (Brownian Dynamics)

$$d\mathbf{q}_a = \underbrace{(\nabla \mathbf{v})_i^T \cdot \mathbf{q}_a \, dt}_{\text{flow stretching}} + \underbrace{\frac{2\mathbf{F}(\mathbf{q}_a)}{\gamma} dt}_{\text{elastic recoil}} + \underbrace{d\tilde{\mathbf{q}}_a}_{\text{thermal noise}}$$

$$d\tilde{\mathbf{q}}_a d\tilde{\mathbf{q}}_b = \delta_{ab} 4 D_0 \mathbf{1} dt$$

Coarse-grained variable: **conformation tensor**

$$\mathbf{c}_i = \frac{1}{N_p q_0^2} \sum_{a=1}^{N_p} \mathbf{q}_a \mathbf{q}_a$$

$$\boxed{d\mathbf{c}_i \;=\; ?}$$

Polymeric fluid: ***coarse-graining*** model

Vazquez, Ellero, Espanol, Phys.Rev. E **79**, 056707 (2009)

$$d\mathbf{q}_a = \underbrace{(\nabla \mathbf{v})_i^T \cdot \mathbf{q}_a \, dt + \frac{2\mathbf{F}(\mathbf{q}_a)}{\gamma} \, dt}_{} + d\tilde{\mathbf{q}}_a \qquad d\tilde{\mathbf{q}}_a d\tilde{\mathbf{q}}_b = \delta_{ab} 4 D_0 \mathbf{1} dt$$

Hookean spring

$$d\mathbf{c}_i = -\mathbf{c}_i \cdot \underbrace{\left(\sum_j \mathcal{V}_j W'_{ij} \mathbf{v}_{ij} \mathbf{e}_{ij} \right)}_{\nabla \mathbf{v}_i} dt - \left(\sum_j \mathcal{V}_j W'_{ij} \mathbf{v}_{ij} \mathbf{e}_{ij} \right)^T \cdot \mathbf{c}_i \, dt + \frac{1}{\tau} \left[\mathbf{1} - \mathbf{c}_i \right] dt$$

Polymeric fluid: ***coarse-graining*** model

Vazquez, Ellero, Espanol, Phys.Rev. E **79**, 056707 (2009)

$$d\mathbf{q}_a = (\nabla \mathbf{v})_i^T \cdot \mathbf{q}_a \, dt + \frac{2\mathbf{F}(\mathbf{q}_a)}{\gamma} \, dt + \underbrace{d\tilde{\mathbf{q}}_a}$$

$$d\tilde{\mathbf{q}}_a d\tilde{\mathbf{q}}_b = \delta_{ab} 4 D_0 \mathbf{1} dt$$

$$d\mathbf{c}_i = -\mathbf{c}_i \cdot \underbrace{\left(\sum_j \mathcal{V}_j W'_{ij} \mathbf{v}_{ij} \mathbf{e}_{ij} \right)}_{\nabla \mathbf{v}_i} dt - \left(\sum_j \mathcal{V}_j W'_{ij} \mathbf{v}_{ij} \mathbf{e}_{ij} \right)^T \cdot \mathbf{c}_i \, dt + \frac{1}{\tau} \left[\mathbf{1} - \mathbf{c}_i \right] dt + d\tilde{\mathbf{c}}_i$$

Tensorial Wiener process

$$\langle d\tilde{c}^{\alpha\beta} d\tilde{c}^{\alpha'\beta'} \rangle = \frac{dt}{N_p \tau} \left[c^{\alpha\alpha'} \delta^{\beta\beta'} + c^{\alpha'\beta} \delta^{\alpha\beta'} + c^{\alpha\beta'} \delta^{\beta\alpha'} + c^{\beta'\beta} \delta^{\alpha\alpha'} \right]$$

Polymeric fluid: ***coarse-graining*** model

Vazquez, Ellero, Espanol, Phys.Rev. E **79**, 056707 (2009)

$$\begin{aligned}
\dot{\mathbf{r}}_i &= \mathbf{v}_i \\
m\dot{\mathbf{v}}_i &= \sum_j \left(\frac{\mathbf{\Pi}_i}{d_i^2} + \frac{\mathbf{\Pi}_j}{d_j^2}\right) W'_{ij}\mathbf{e}_{ij} + \frac{5\eta}{3}\sum_j \frac{W'_{ij}}{d_i d_j r_{ij}}\left[\mathbf{v}_{ij} + (\mathbf{e}_{ij}\cdot\mathbf{v}_{ij})\,\mathbf{e}_{ij}\right] + \sum_j A_{ij}\frac{d\bar{\boldsymbol{\xi}}_{ij}}{dt}\cdot\mathbf{e}_{ij} \\
d\mathbf{c}_i &= -\mathbf{c}_i\cdot\left(\sum_j \mathcal{V}_j W'_{ij}\mathbf{v}_{ij}\mathbf{e}_{ij}\right) dt - \left(\sum_j \mathcal{V}_j W'_{ij}\mathbf{v}_{ij}\mathbf{e}_{ij}\right)^T \cdot \mathbf{c}_i\, dt + \frac{1}{\tau}\left[\mathbf{1} - \mathbf{c}_i\right] dt + d\tilde{\mathbf{c}}_i
\end{aligned}$$

$$\mathbf{\Pi}_i = -P_i\,\mathbf{1} + n_p k_B T\,\mathbf{c}_i$$

Polymeric fluid: ***coarse-graining*** model

Vazquez, Ellero, Espanol, Phys.Rev. E **79**, 056707 (2009)

$$\dot{\mathbf{r}}_i = \mathbf{v}_i$$

$$m\dot{\mathbf{v}}_i = \sum_j \left(\frac{\mathbf{\Pi}_i}{d_i^2} + \frac{\mathbf{\Pi}_j}{d_j^2}\right) W'_{ij}\mathbf{e}_{ij} + \frac{5\eta}{3}\sum_j \frac{W'_{ij}}{d_i d_j r_{ij}}\left[\mathbf{v}_{ij} + (\mathbf{e}_{ij}\cdot\mathbf{v}_{ij})\,\mathbf{e}_{ij}\right] + \sum_j A_{ij}\frac{d\bar{\boldsymbol{\xi}}_{ij}}{dt}\cdot\mathbf{e}_{ij}$$

$$d\mathbf{c}_i = -\mathbf{c}_i\cdot\left(\sum_j \mathcal{V}_j W'_{ij}\mathbf{v}_{ij}\mathbf{e}_{ij}\right)dt - \left(\sum_j \mathcal{V}_j W'_{ij}\mathbf{v}_{ij}\mathbf{e}_{ij}\right)^T\cdot\mathbf{c}_i\,dt + \frac{1}{\tau}\left[\mathbf{1}-\mathbf{c}_i\right]dt + d\tilde{\mathbf{c}}_i$$

$$\mathbf{\Pi}_i = -P_i\,\mathbf{1} + n_p k_B T\,\mathbf{c}_i$$

$$d\mathbf{x} = \mathbf{L}\cdot\frac{\partial E}{\partial\mathbf{x}}\,dt$$

Thermodynamic consistent (GENERIC)

Polymeric fluid: ***coarse-graining*** model

Vazquez, Ellero, Espanol, Phys.Rev. E **79**, 056707 (2009)

$$\begin{aligned}
\dot{\mathbf{r}}_i &= \mathbf{v}_i \\
m\dot{\mathbf{v}}_i &= \sum_j \left(\frac{\mathbf{\Pi}_i}{d_i^2} + \frac{\mathbf{\Pi}_j}{d_j^2} \right) W'_{ij} \mathbf{e}_{ij} + \frac{5\eta}{3} \sum_j \frac{W'_{ij}}{d_i d_j r_{ij}} \left[\mathbf{v}_{ij} + (\mathbf{e}_{ij} \cdot \mathbf{v}_{ij}) \mathbf{e}_{ij} \right] + \sum_j A_{ij} \frac{d\bar{\boldsymbol{\xi}}_{ij}}{dt} \cdot \mathbf{e}_{ij} \\
d\mathbf{c}_i &= -\mathbf{c}_i \cdot \left(\sum_j \mathcal{V}_j W'_{ij} \mathbf{v}_{ij} \mathbf{e}_{ij} \right) dt - \left(\sum_j \mathcal{V}_j W'_{ij} \mathbf{v}_{ij} \mathbf{e}_{ij} \right)^T \cdot \mathbf{c}_i \, dt + \frac{1}{\tau} \left[\mathbf{1} - \mathbf{c}_i \right] dt + d\tilde{\mathbf{c}}_i
\end{aligned}$$

$$\mathbf{\Pi}_i = -P_i \, \mathbf{1} + n_p k_B T \, \mathbf{c}_i$$

$$d\mathbf{x} = \mathbf{L} \cdot \frac{\partial E}{\partial \mathbf{x}} dt + \mathbf{M} \cdot \frac{\partial S}{\partial \mathbf{x}} dt$$

Thermodynamic consistent (GENERIC)

Polymeric fluid: ***coarse-graining*** model

Vazquez, Ellero, Espanol, Phys.Rev. E **79**, 056707 (2009)

$$\dot{\mathbf{r}}_i = \mathbf{v}_i$$

$$m\dot{\mathbf{v}}_i = \sum_j \left(\frac{\mathbf{\Pi}_i}{d_i^2} + \frac{\mathbf{\Pi}_j}{d_j^2} \right) W'_{ij}\mathbf{e}_{ij} + \frac{5\eta}{3} \sum_j \frac{W'_{ij}}{d_i d_j r_{ij}} \left[\mathbf{v}_{ij} + (\mathbf{e}_{ij} \cdot \mathbf{v}_{ij})\, \mathbf{e}_{ij} \right] + \sum_j A_{ij} \frac{d\bar{\boldsymbol{\xi}}_{ij}}{dt} \cdot \mathbf{e}_{ij}$$

$$d\mathbf{c}_i = -\mathbf{c}_i \cdot \left(\sum_j \mathcal{V}_j W'_{ij} \mathbf{v}_{ij} \mathbf{e}_{ij} \right) dt - \left(\sum_j \mathcal{V}_j W'_{ij} \mathbf{v}_{ij} \mathbf{e}_{ij} \right)^T \cdot \mathbf{c}_i \, dt + \frac{1}{\tau} \left[\mathbf{1} - \mathbf{c}_i \right] dt + d\tilde{\mathbf{c}}_i$$

$$\mathbf{\Pi}_i = -P_i \, \mathbf{1} + n_p k_B T \, \mathbf{c}_i$$

$$d\mathbf{x} = \mathbf{L} \cdot \frac{\partial E}{\partial \mathbf{x}} dt + \mathbf{M} \cdot \frac{\partial S}{\partial \mathbf{x}} dt + d\tilde{\mathbf{x}}$$

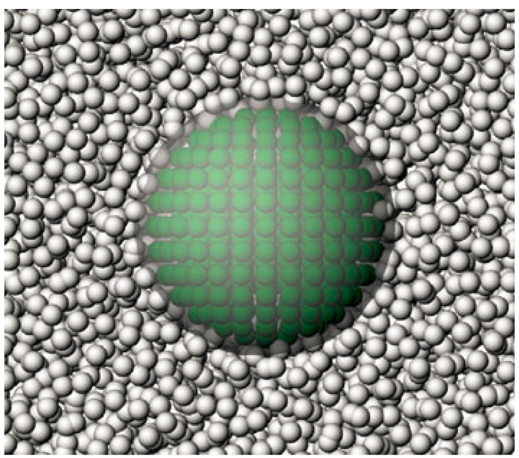
Thermodynamic consistent (GENERIC)

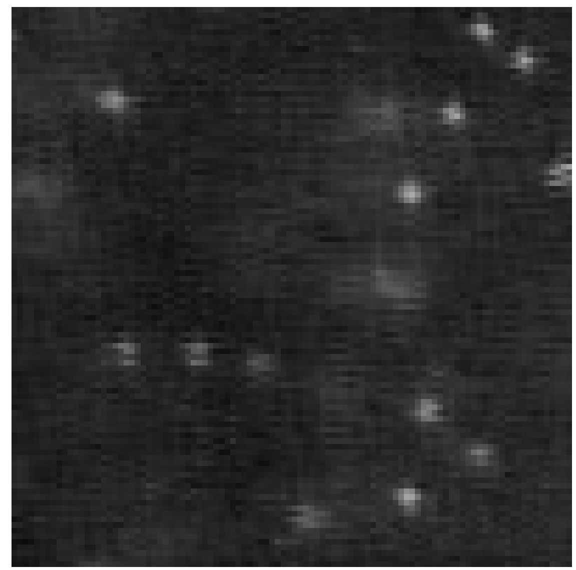
$$d\tilde{\mathbf{x}} d\tilde{\mathbf{x}}^T = 2k_B \mathbf{M} dt$$

Polymeric fluid: ***coarse-graining*** model

- SDPD: Coarse-grained viscoelasticity + Brownian motion

- Application: Passive microrheology
  (correct diffusional dynamics for a nanoparticle in a polymeric liquid)





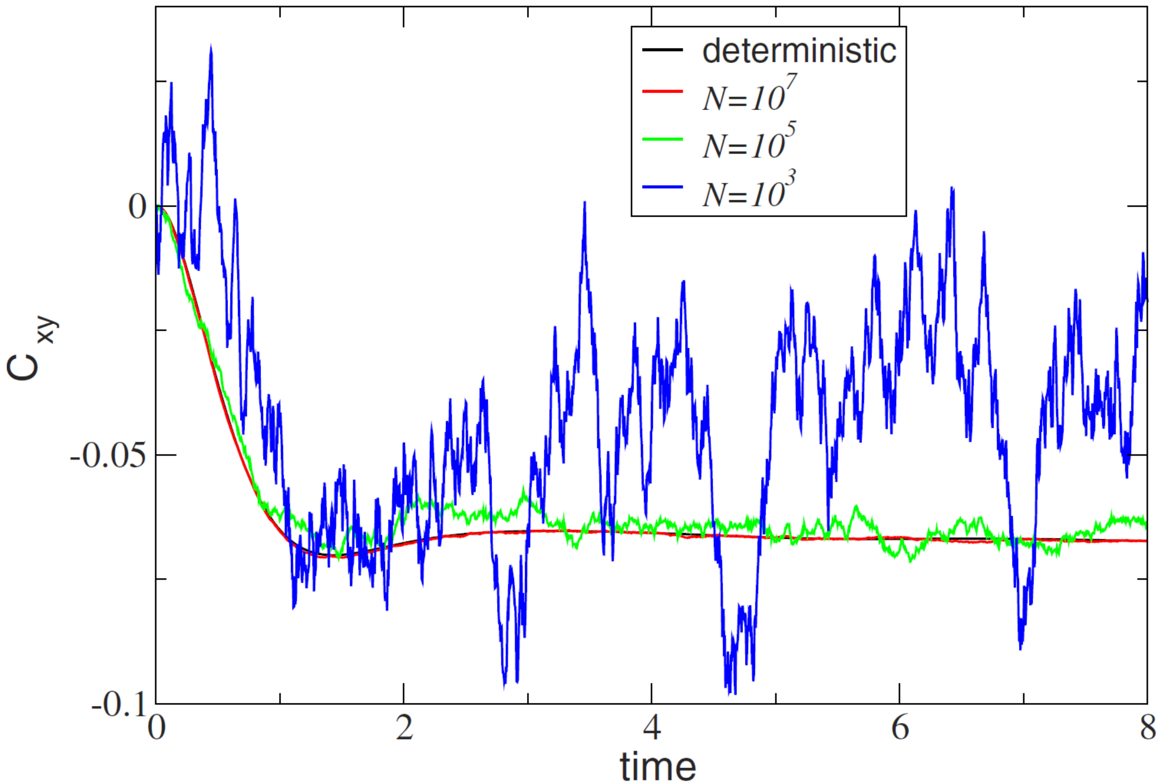
Vazquez, Ellero, Espanol, Microfluidics Nanofluidics **13**, 249-260 (2012)

III: Towards continuum

Polymeric fluid: ***coarse-graining*** model

Vazquez, Ellero, Espanol, Phys.Rev. E **79**, 056707 (2009)

$$\langle d\tilde{c}^{\alpha\beta} d\tilde{c}^{\alpha'\beta'} \rangle = \frac{dt}{N_p \tau} \left[c^{\alpha\alpha'} \delta^{\beta\beta'} + c^{\alpha'\beta} \delta^{\alpha\beta'} + c^{\alpha\beta'} \delta^{\beta\alpha'} + c^{\beta'\beta} \delta^{\alpha\alpha'} \right]$$



Polymeric fluid: ***macroscopic continuum*** model

$$d\mathbf{c}_i \;=\; -\mathbf{c}_i \cdot \left(\sum_j \mathcal{V}_j W'_{ij} \mathbf{v}_{ij} \mathbf{e}_{ij} \right) dt - \left(\sum_j \mathcal{V}_j W'_{ij} \mathbf{v}_{ij} \mathbf{e}_{ij} \right)^T \cdot \mathbf{c}_i \, dt + \frac{1}{\tau} \left[\mathbf{1} - \mathbf{c}_i \right] dt + d\tilde{\mathbf{c}}_i$$

$$\mathcal{V}_i = \left(\sum_j W_{ij} \right) \longrightarrow \infty \qquad \rightarrow 0$$

Fluid particle volume

$$\lim_{\mathcal{V}_i \to \infty} \text{ SDPD } = \text{SPH}$$

Polymeric fluid: ***macroscopic continuum*** model

$$d\mathbf{c}_i = -\mathbf{c}_i \cdot \left(\sum_j \mathcal{V}_j W'_{ij} \mathbf{v}_{ij} \mathbf{e}_{ij}\right) dt - \left(\sum_j \mathcal{V}_j W'_{ij} \mathbf{v}_{ij} \mathbf{e}_{ij}\right)^T \cdot \mathbf{c}_i \, dt + \frac{1}{\tau} \left[\mathbf{1} - \mathbf{c}_i\right] dt$$

SPH discretization

- **Oldroyd-B viscoelastic PDE** (conformation tensor representation: Huelsen et al. 1987)

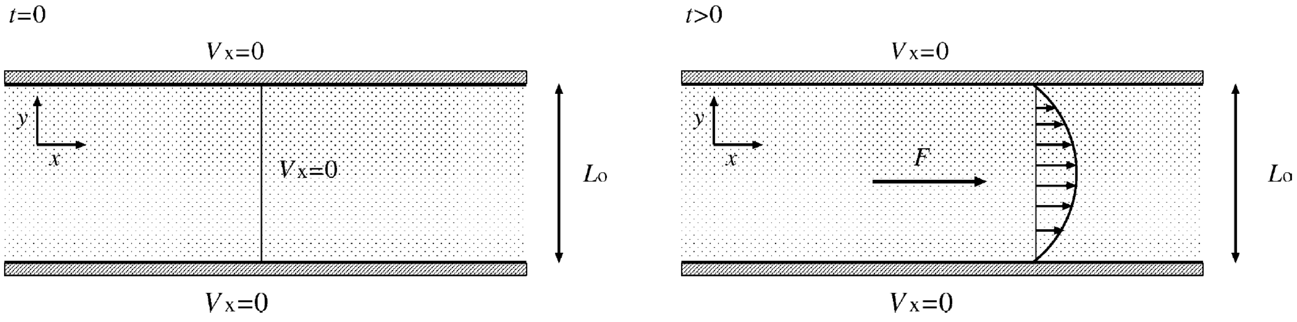
$$\frac{\partial \mathbf{c}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{c} = \underbrace{(\boldsymbol{\nabla} \mathbf{v})^T \cdot \mathbf{c} + \mathbf{c} \cdot (\boldsymbol{\nabla} \mathbf{v})}_{\text{flow stretching}} + \underbrace{\frac{1}{\lambda} \left[\mathbf{1} - \mathbf{c}\right]}_{\text{polymer relaxation}}$$

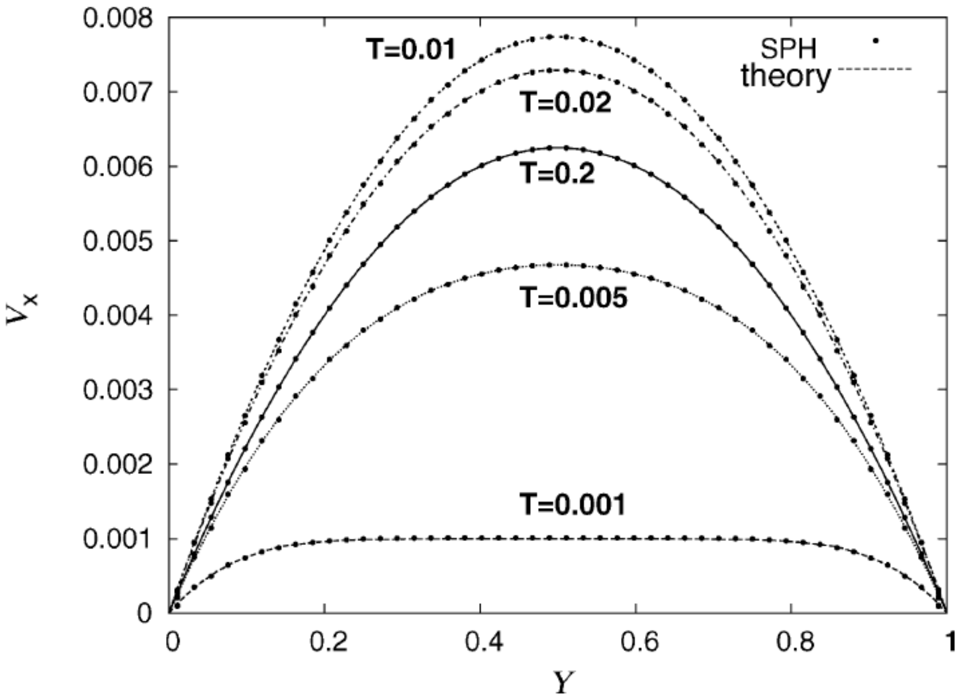
Oldroyd, James "On the Formulation of Rheological Equations of State".
Proceedings of the Royal Society of London, A, **200** (1063): 523–541 (1950)

Polymeric fluid: ***macroscopic continuum*** model

- **Oldroyd-B transient simulations**
  [start-up Poiseuille flow]

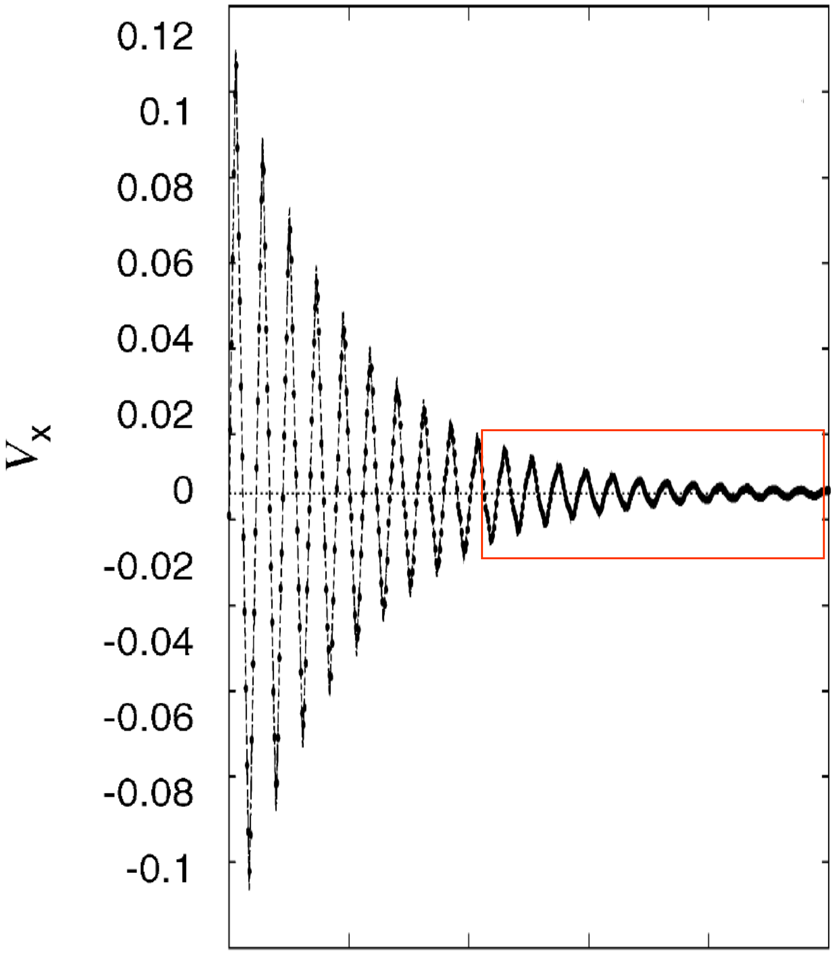
Ellero, Tanner, J. Non-NewtFluid. Mech. **132**, 61 (2005)
Smoothed Particle Hydrodynamics





Polymeric fluid: ***macroscopic continuum*** model

- **Oldroyd-B transient simulations**
  [start-up Poiseuille flow]



Ellero, Tanner, J. Non-NewtFluid. Mech. **132**, 61 (2005)
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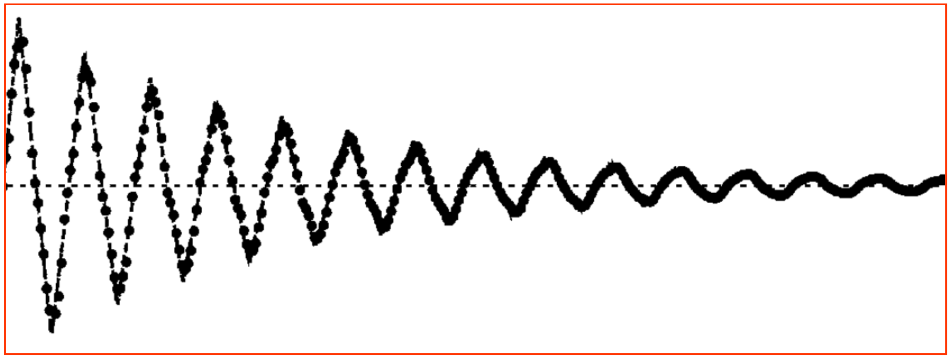
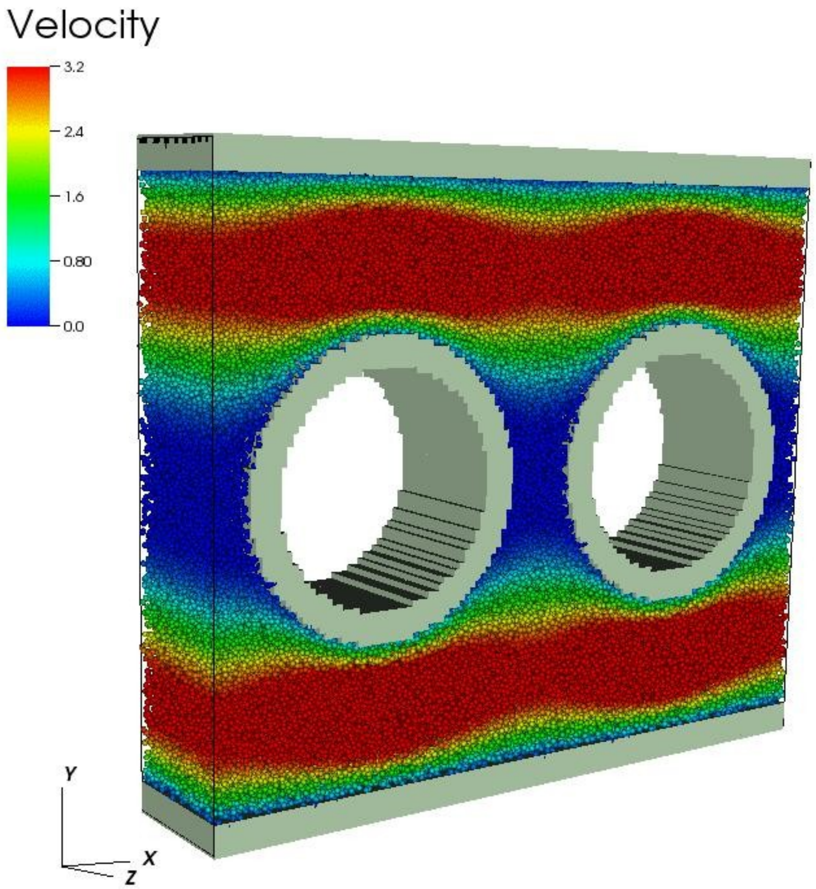


Polymeric fluid: ***macroscopic continuum*** model

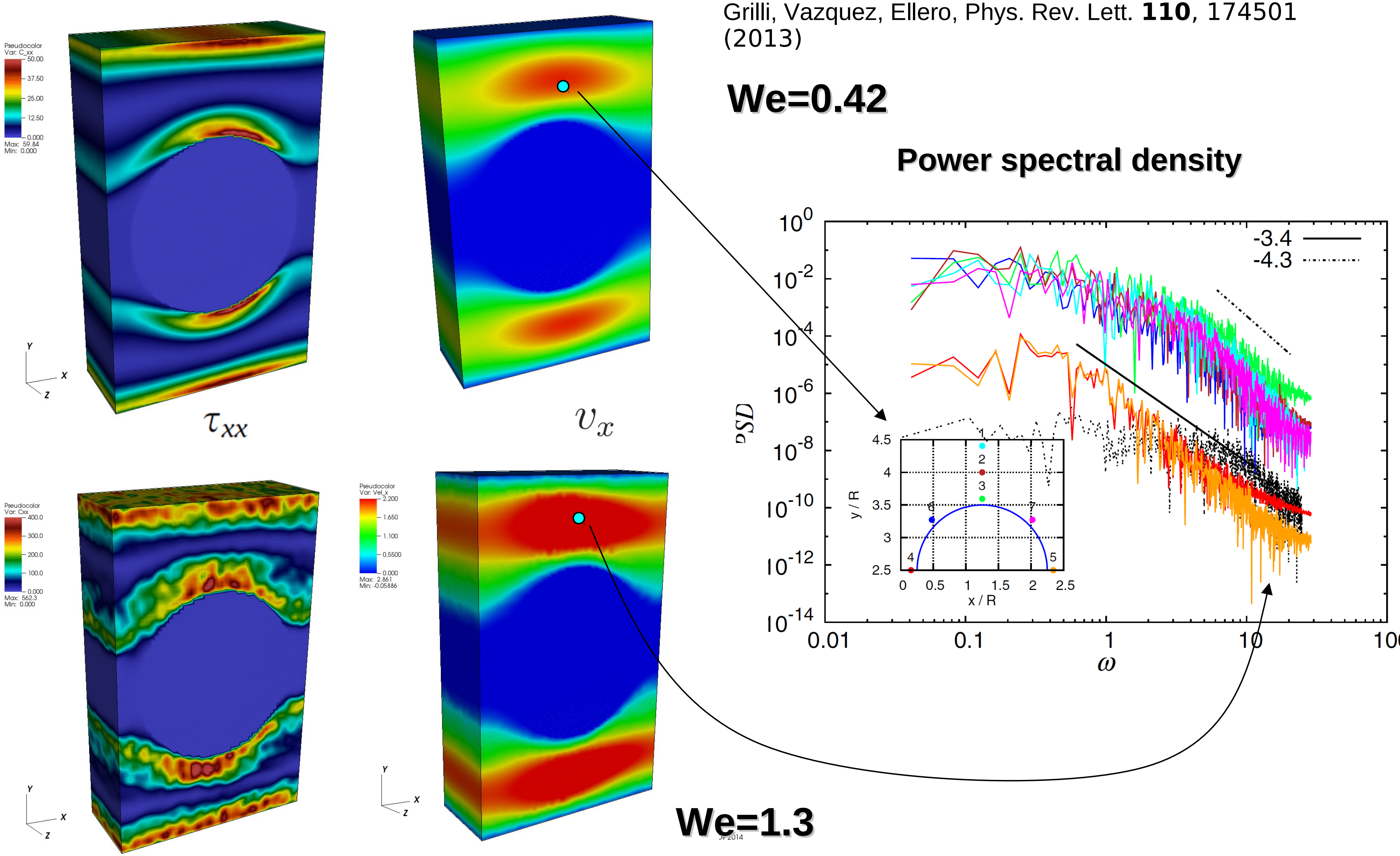
- **Flow in around micro-array of cylinders**

Grilli, Vazquez, Ellero, Phys. Rev. Lett. **110**, 174501 (2013)



Polymeric fluid: ***macroscopic continuum*** model

Grilli, Vazquez, Ellero, Phys. Rev. Lett. **110**, 174501 (2013)

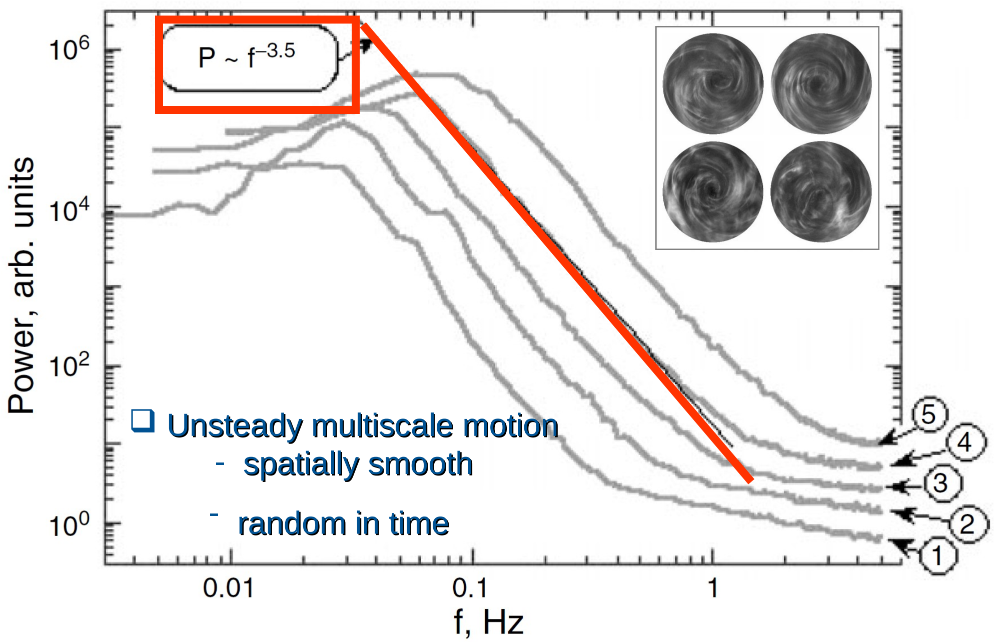


Elastic turbulence

NATURE | VOL 405 | 4 MAY 2000

Elastic turbulence in a polymer solution flow

A. Groisman & V. Steinberg



- Unsteady multiscale motion
  - spatially smooth
  - random in time

- Power-law decay
- Talyor‘s hypothesis: $E(k) \sim k^{-\alpha}$ α>3

- Lebedev PRE 2003 (theory→ >3!!)

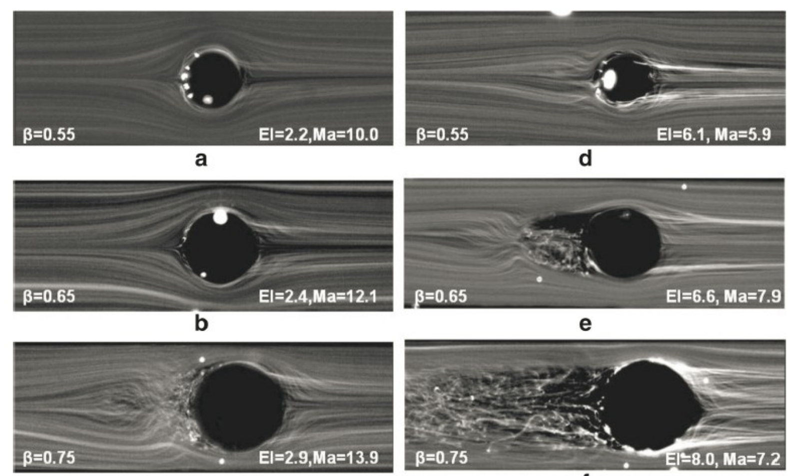
Rheol Acta
DOI 10.1007/s00397-015-0875-6

ORIGINAL CONTRIBUTION

Mechanisms of onset for moderate Mach number instabilities of viscoelastic flows around confined cylinders

Xueda Shi[1] · Stephen Kenney[1] · Ganesh Chapagain[1] · Gordon F. Christopher[1]

Received: 6 March 2015 /Revised: 20 August 2015 /Accepted: 24 August 2015



Conclusions

- **SDPD for simple Newtonian solvents: improved DPD version.**
  - control transport coefficients
  - arbitrary thermodynamic behaviour EOS, incompressibility
  - thermodynamic def. particle volume: resolution analysis straightforward

- **Consistent scaling of thermal fluctuations: SDPD→SPH : “large” particle volumes**

- **Complex fuids: SDPD versatile approach → hierarchical modelling**

- **Mesoscopic models possible as DPD (albeit with better defined solvent properties).**

- **Coarse-graining approach offer scale advantage (under some approx).**

- **Consistent scaling: SDPD→ SPH specific discretization continuum viscoelastic PDE**
  - e.g. Hookean spring dumbells → Oldroyd-B

- **Embedded in GENERIC: (i) 1st Law; (ii) 2nd Law; (ii) FDT exactly statisfied.**