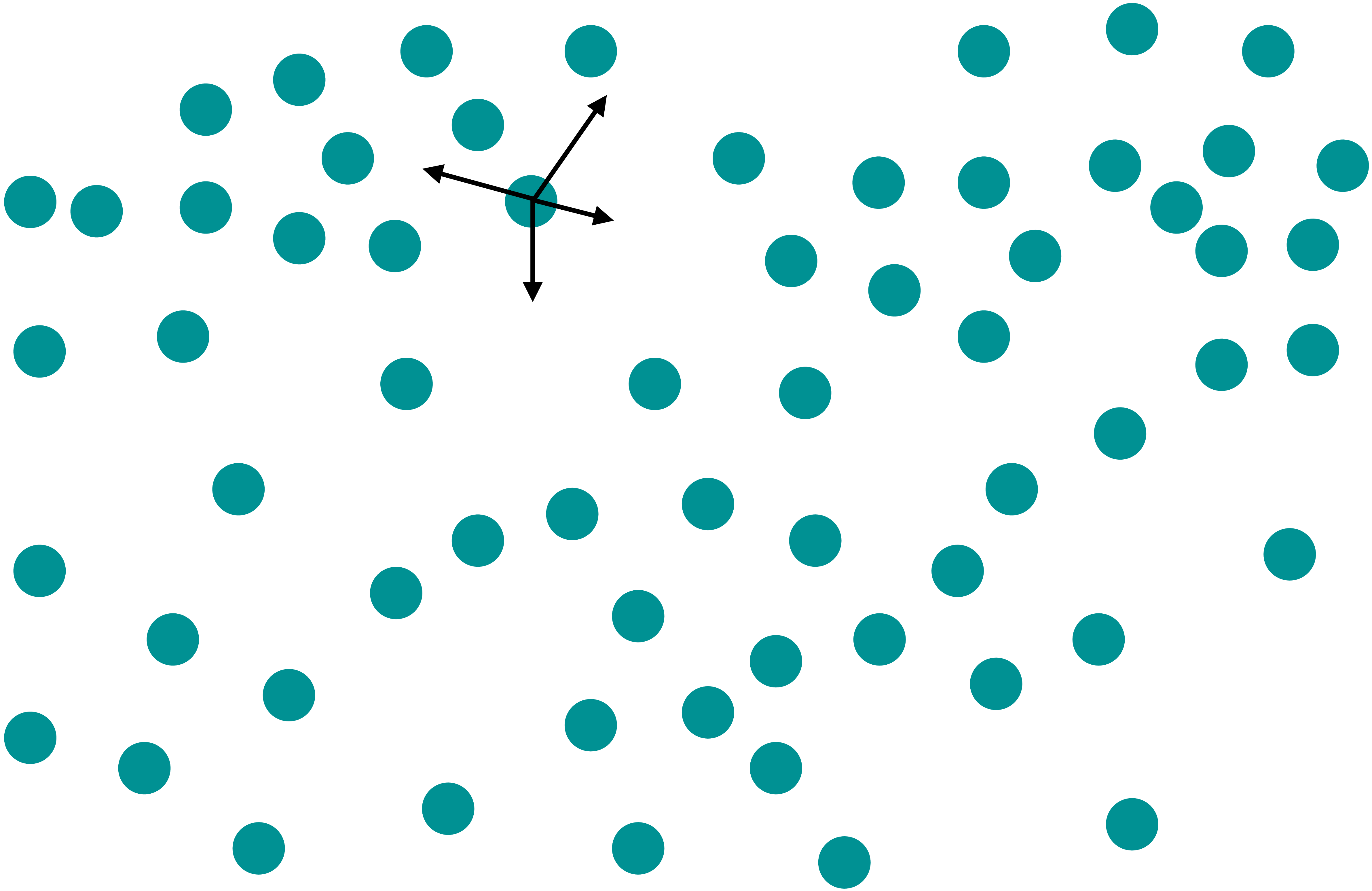
# Large Scale Simulation of Colloidal Hydrodynamics: Heterogeous Particles, Structures and Flow Patterns

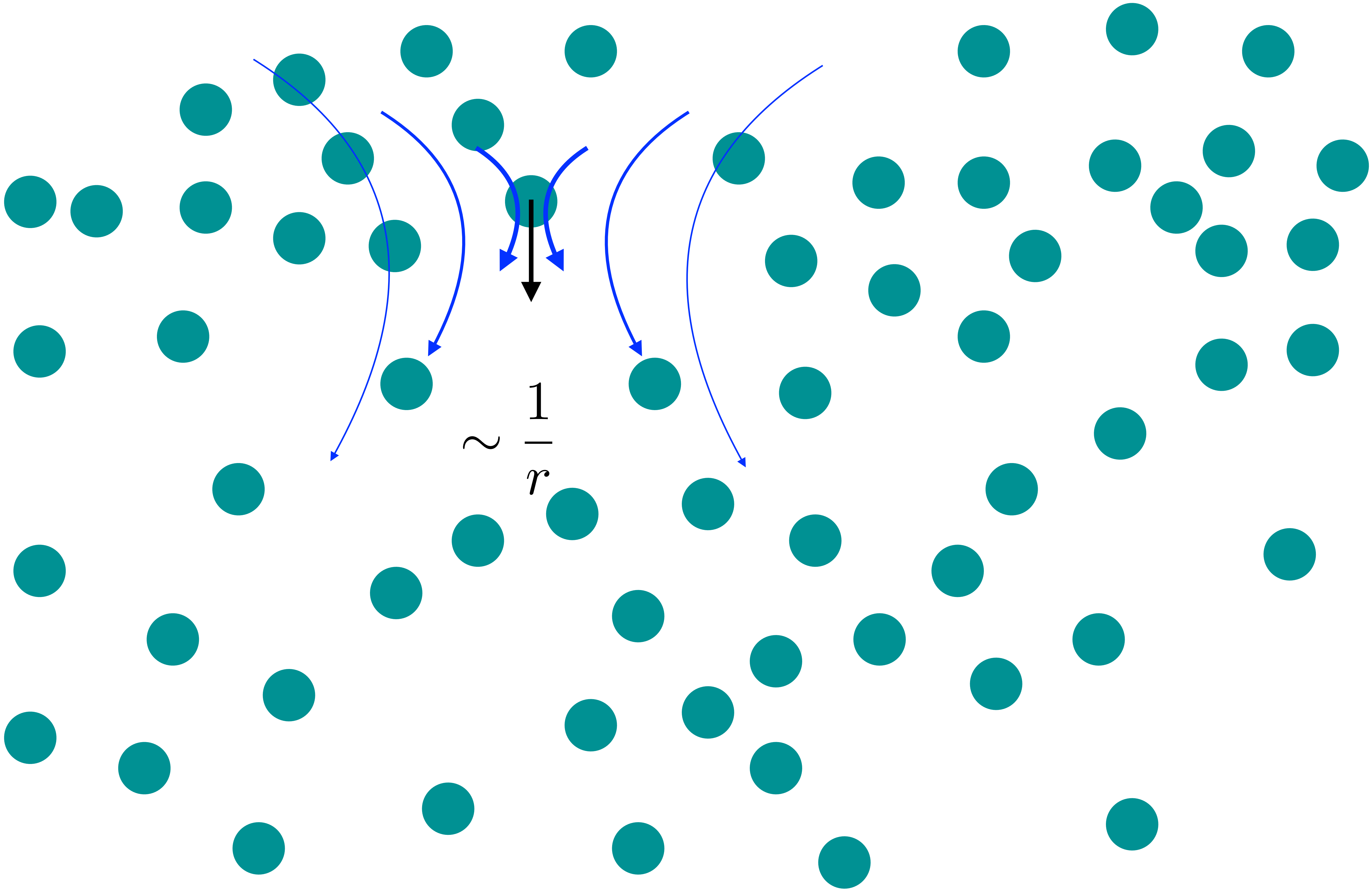

**James W. Swan**

**Department of Chemical Engineering**

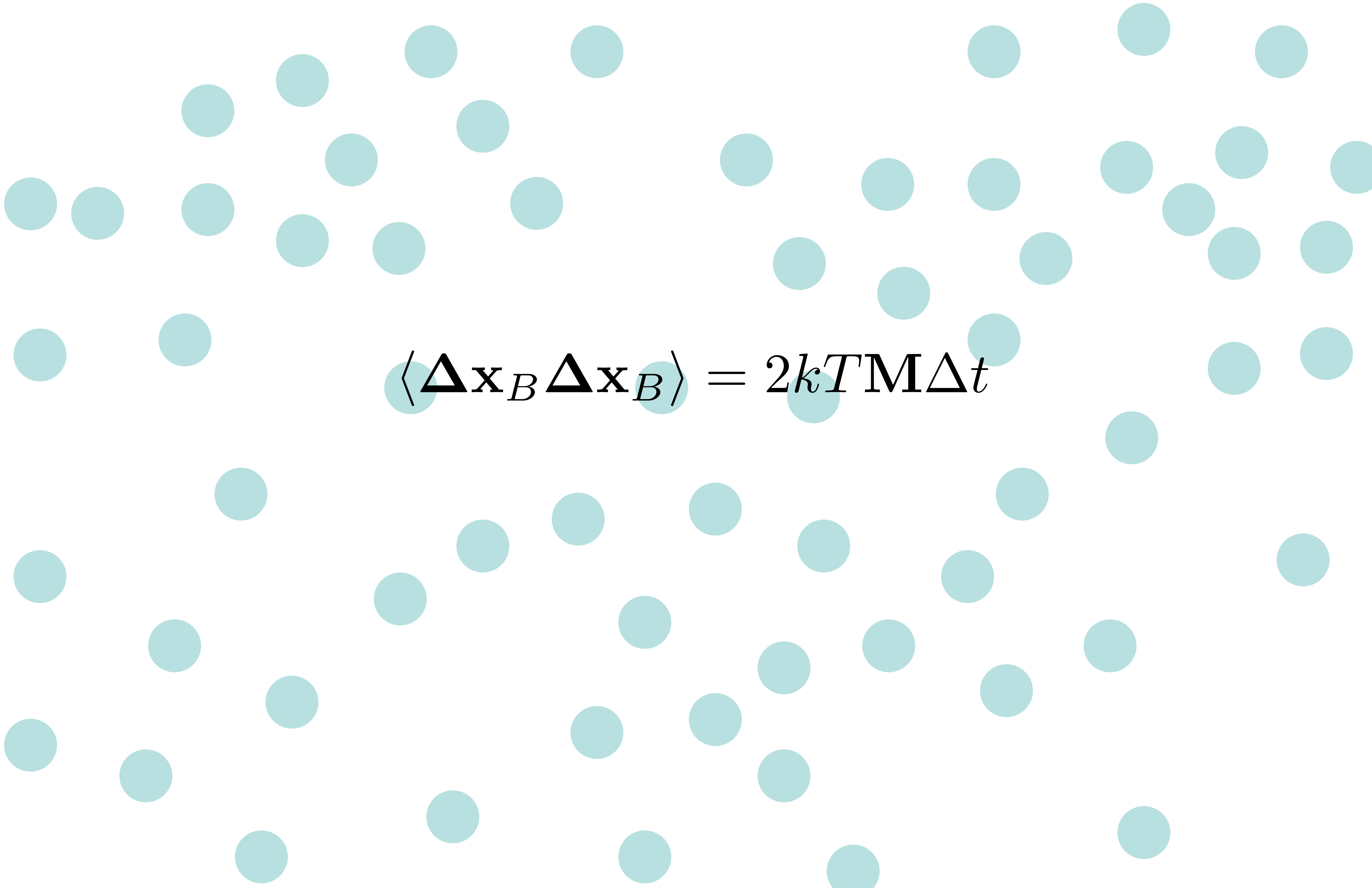
# Colloidal Hydrodynamics



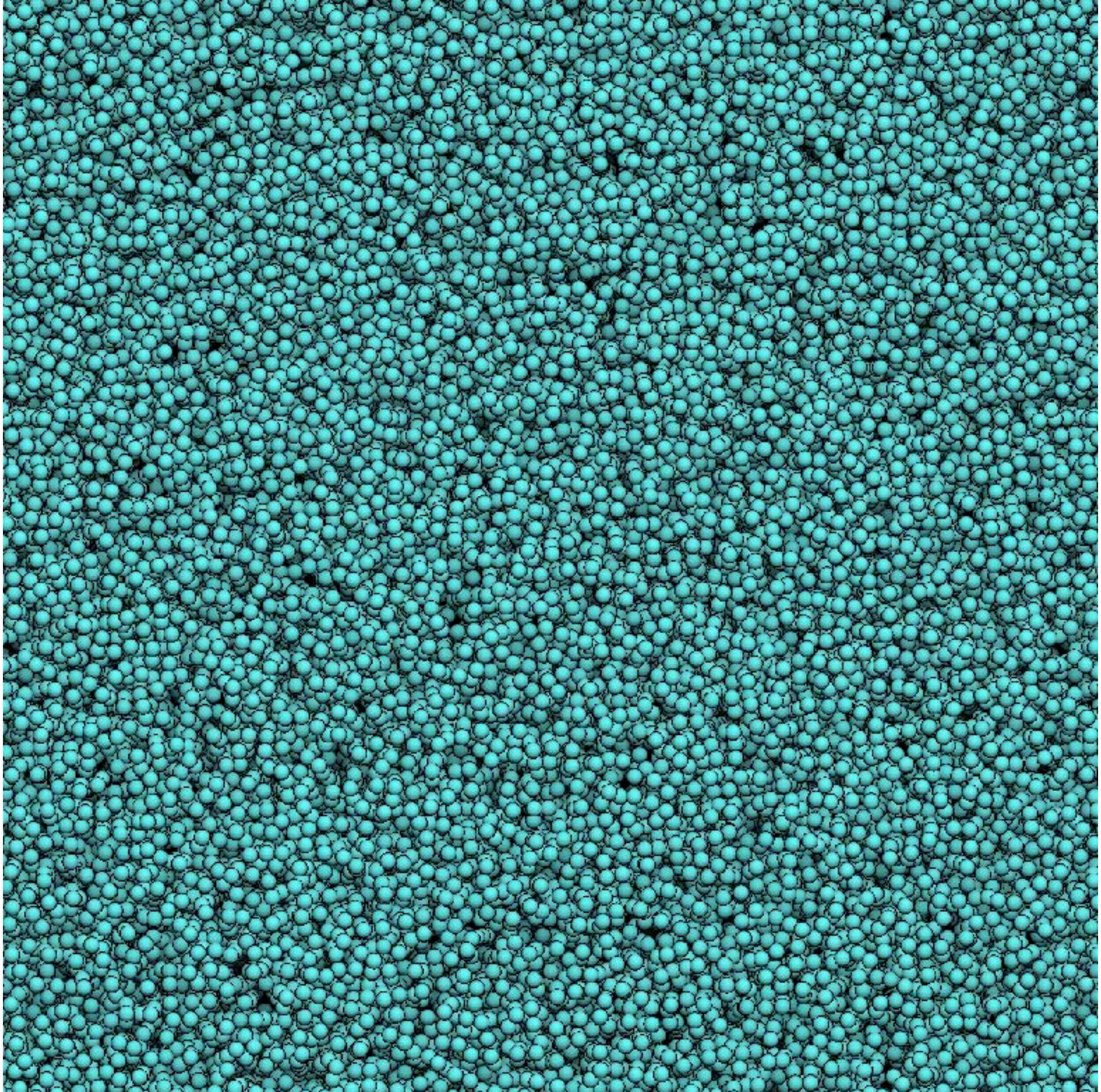
# Colloidal Hydrodynamics



# Colloidal Hydrodynamics



$$\langle \boldsymbol{\Delta}\mathbf{x}_B \boldsymbol{\Delta}\mathbf{x}_B \rangle = 2kT\mathbf{M}\Delta t$$




# HOOMD-blue

Fiore, Balboa, Donev, and Swan. J. Chem. Phys. 2017

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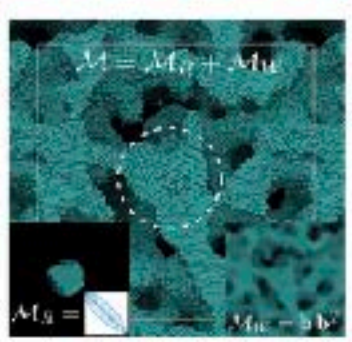
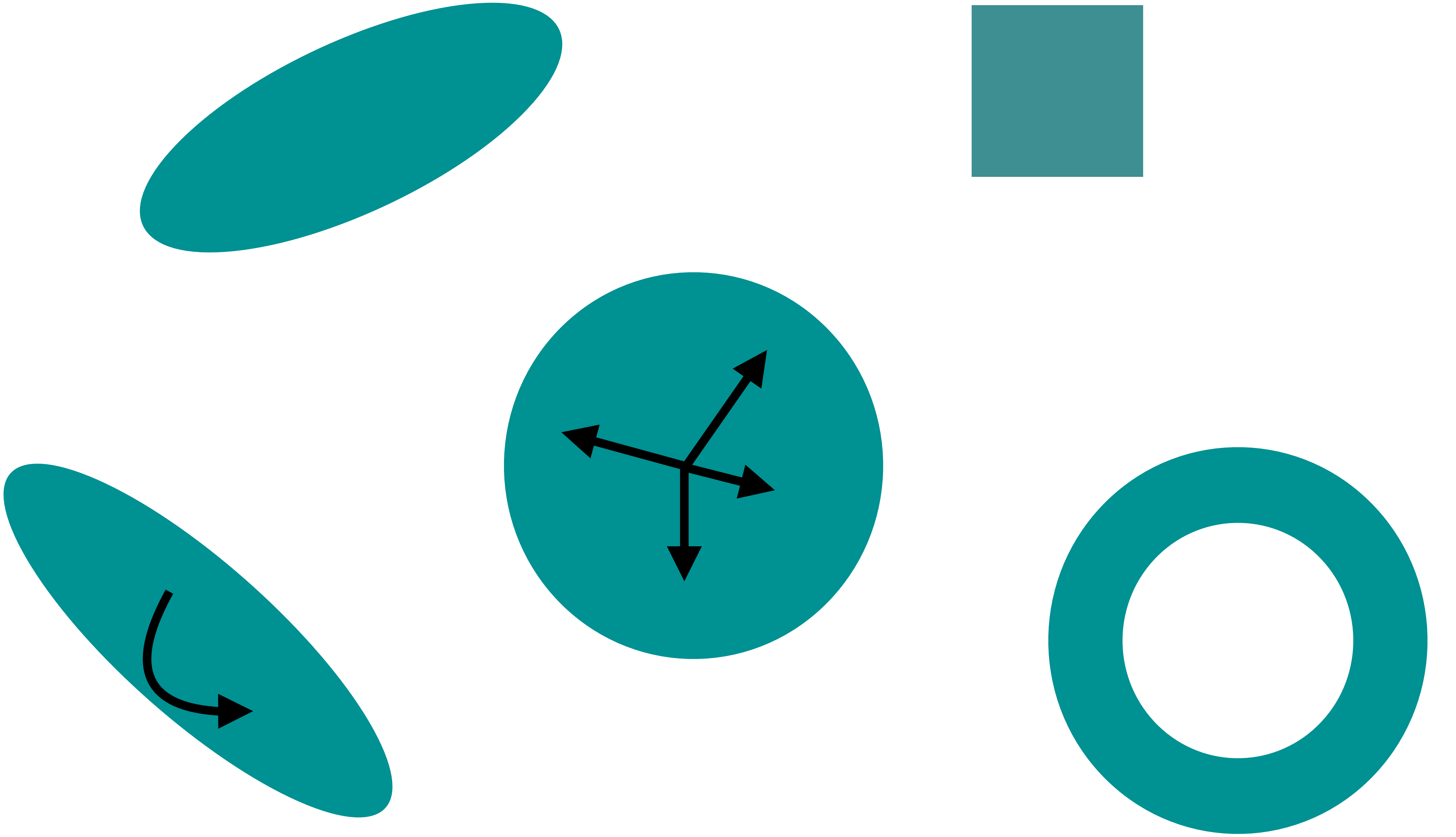
## Software

### Positively Split Ewald (PSE) Algorithm for RPY Hydrodynamics

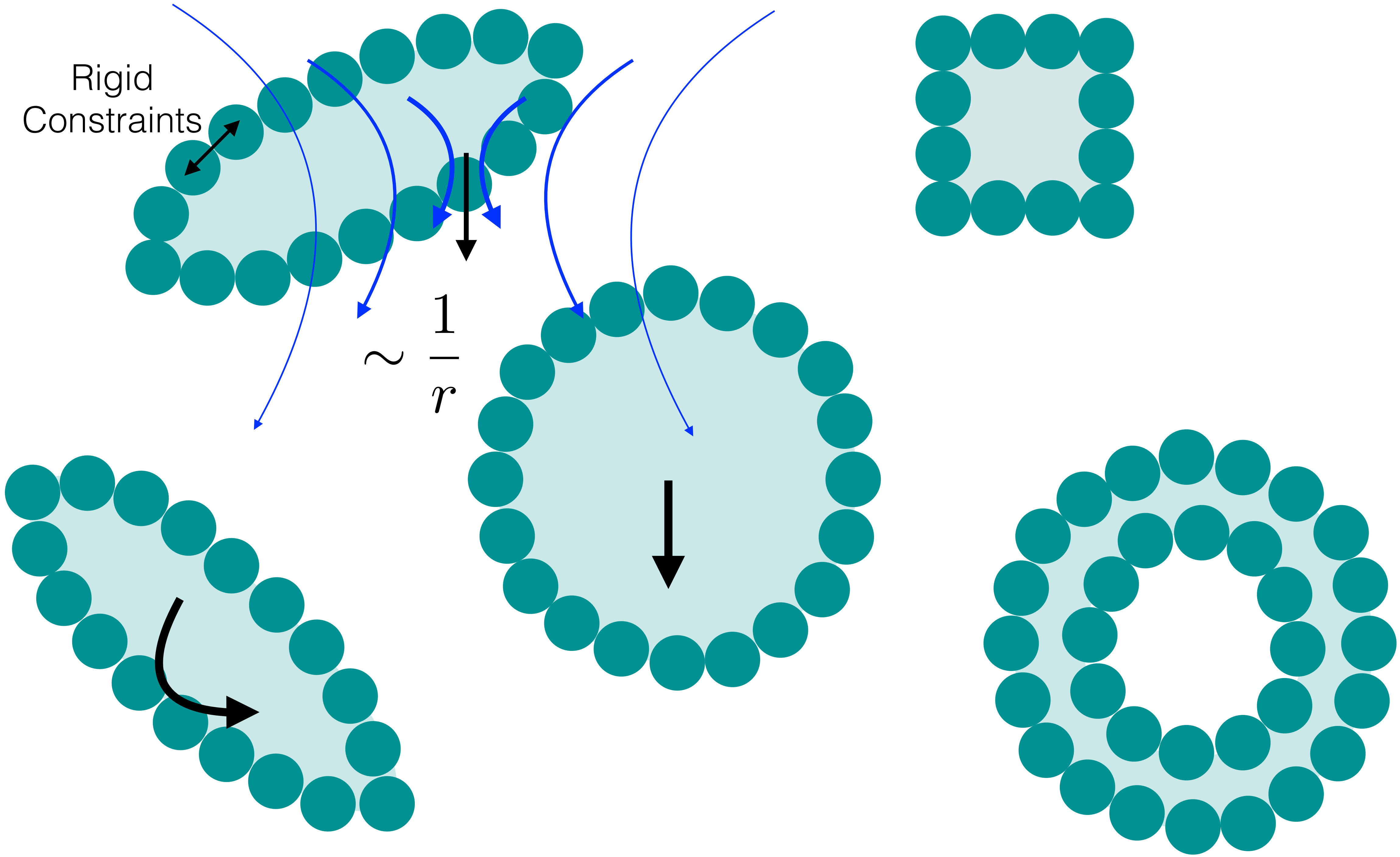


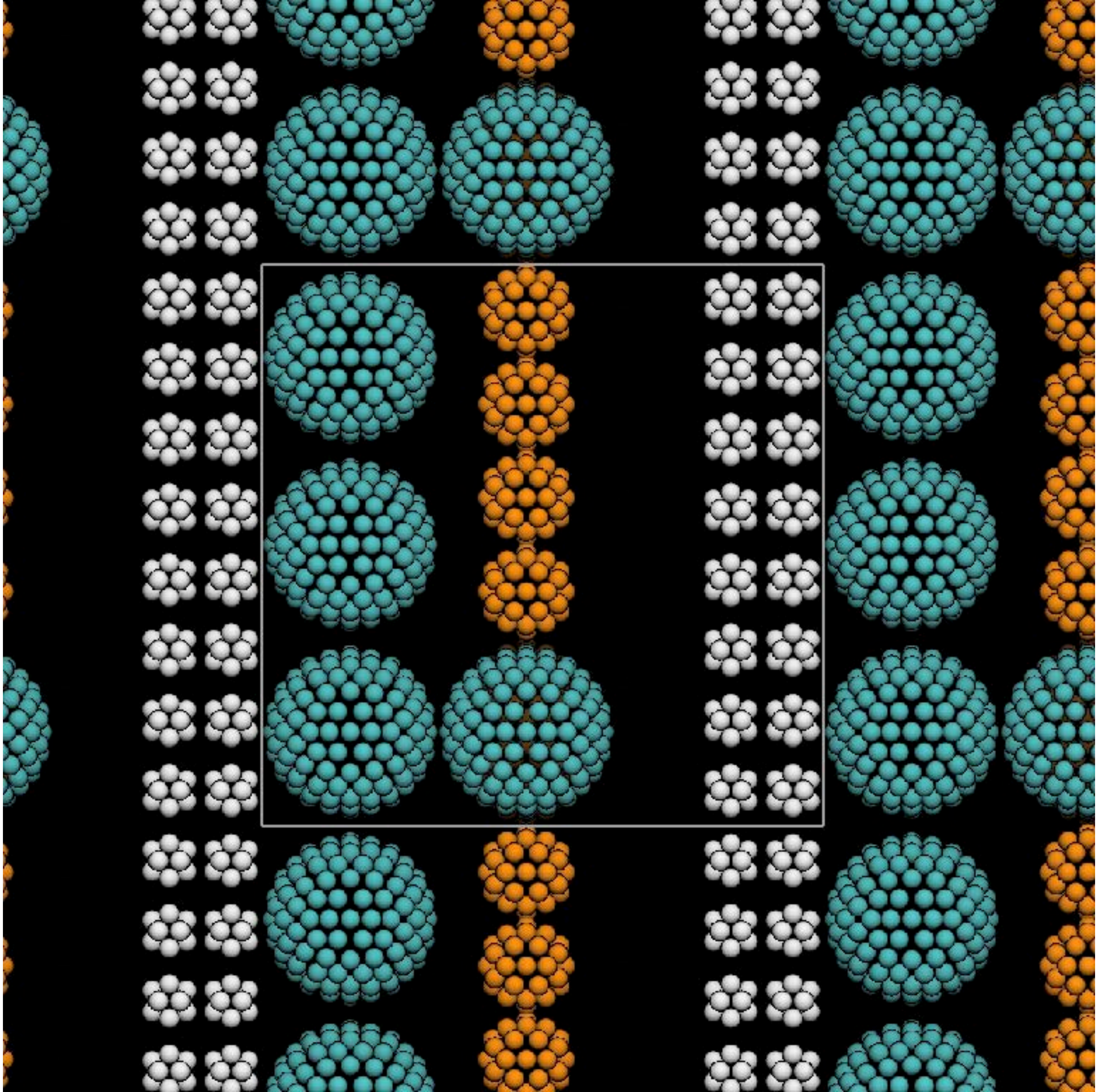
In the article 'Rapid sampling of stochastic displacements in Brownian dynamics simulations', Fiore et al. present a new technique for sampling the stochastic thermal displacements in Brownian Dynamics simulations with hydrodynamic interactions represented at the Rotne-Prager-Yamawaka (RPY) level of approximation. This technique, called Positively-Split Ewald sampling, samples the Brownian displacements from a superposition of two indepedent distributions: a wave space (far-field or long-ranged) contribution, computed using techniques from fluctuating hydrodynamics and non-uniform fast Fourier transforms; and a real space (near-field or short-ranged) correction, computed using a Krylov subspace method. The total computational complexity of the algorithm scales linearly with the number of particles modeled. The PSE algorithm enables simulations of up to 4 million colloidal particles. A high-performance implementation of the PSE algorithm on graphics processing units (GPUs), written as a plugin for the software package HOOMD-blue is freely available on GitHub.

# Colloidal Hydrodynamics



# Immersed Boundary Colloidal Hydrodynamics






HOOMD-blue

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Swan and Wang. Phys. Fluids 2016

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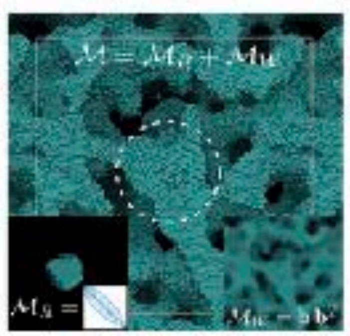
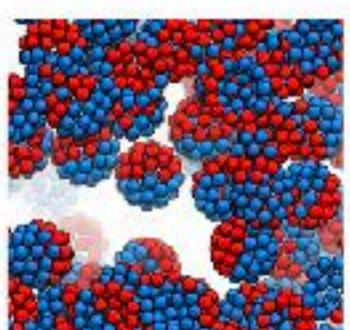
## Software

### Positively Split Ewald (PSE) Algorithm for RPY Hydrodynamics

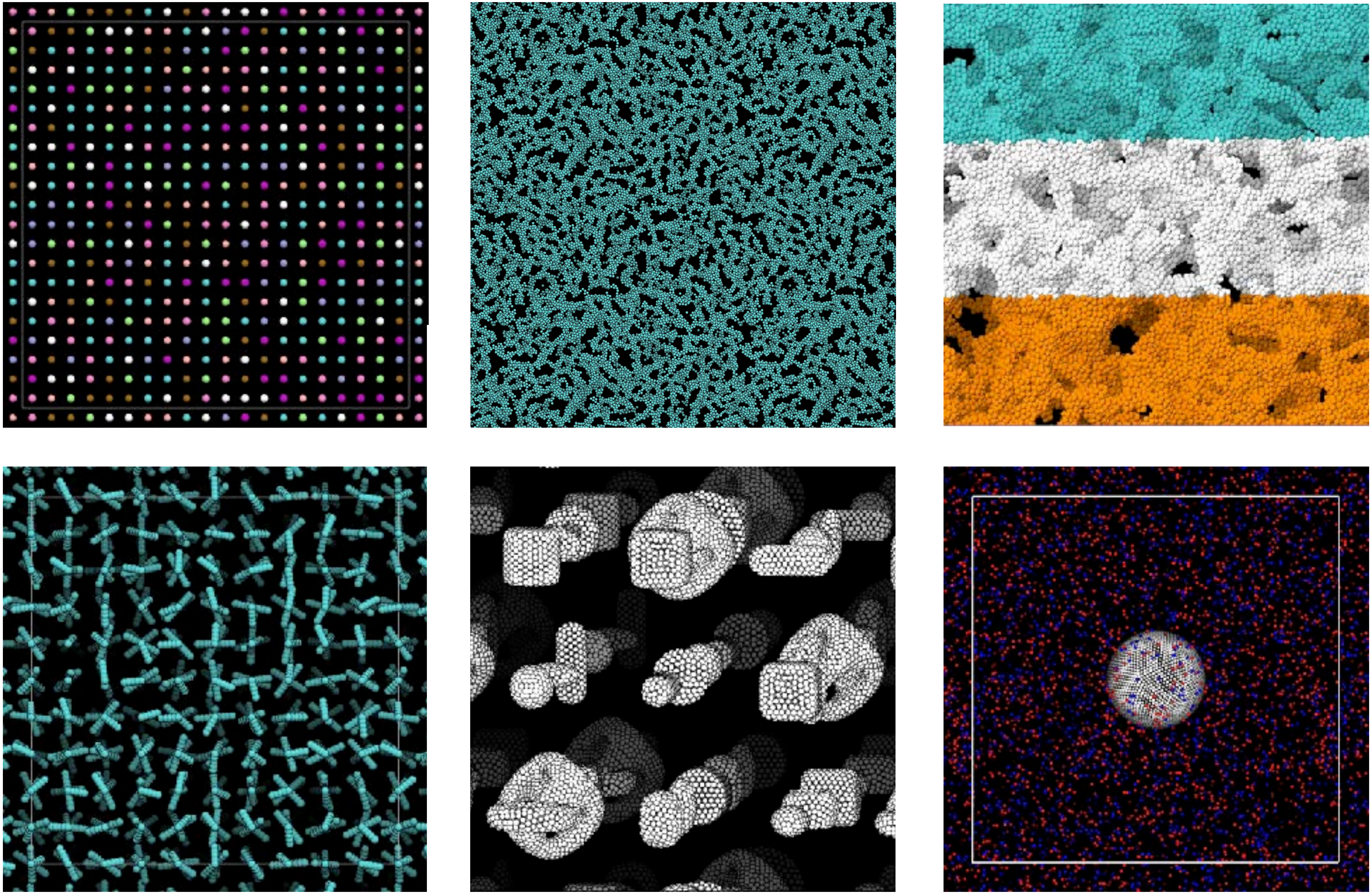


In the article 'Rapid sampling of stochastic displacements in Brownian dynamics simulations', Fiore *et al.* present a new technique for sampling the stochastic thermal displacements in Brownian Dynamics simulations with hydrodynamic interactions represented at the Rotne-Prager-Yamakawa (RPY) level of approximation. This technique, called Positively-Split Ewald sampling, samples the Brownian displacements from a superposition of two indepedent distributions: a wave space (far-field or long-ranged) contribution, computed using techniques from fluctuating hydrodynamics and non-uniform fast Fourier transforms; and a real space (near-field or short-ranged) correction, computed using a Krylov subspace method. The total computational complexity of the algorithm scales linearly with the number of particles modeled. The PSE algorithm enables simulations of up to 4 million colloidal particles. A high-performance implementation of the PSE algorithm on graphics processing units (GPUs), written as a plugin for the software package HOOMD-blue is freely available on GitHub.

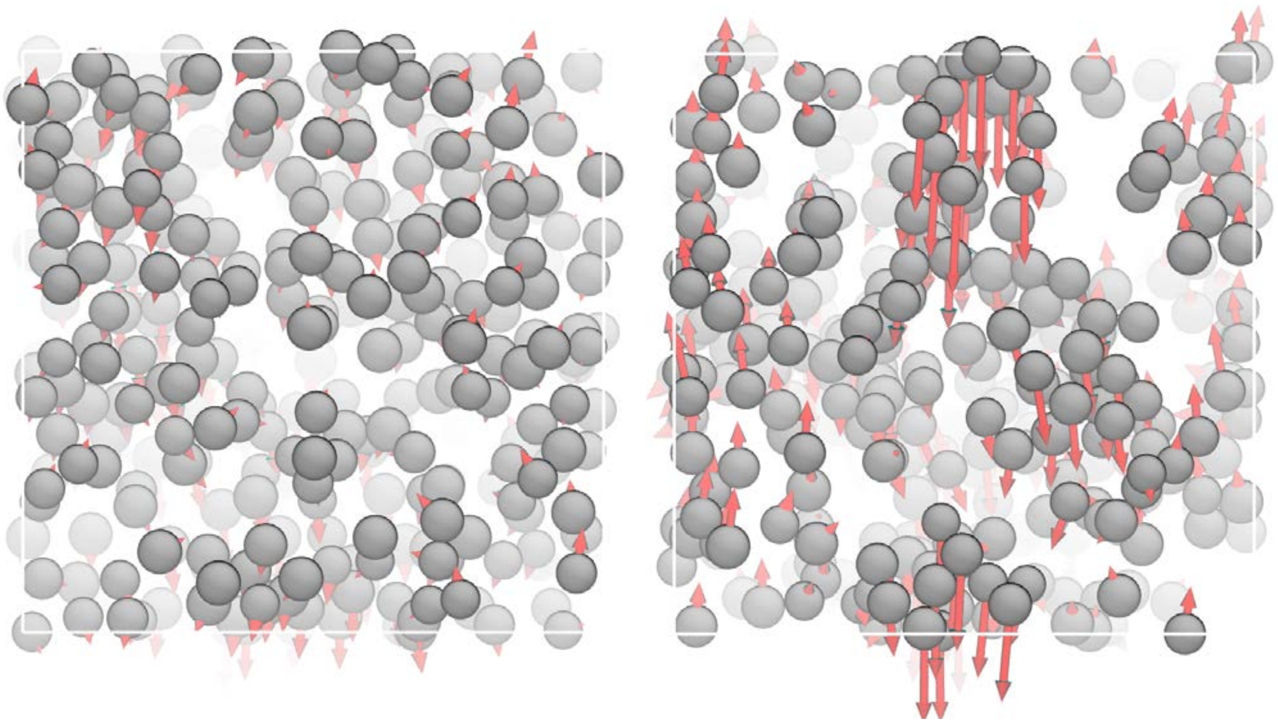
### Brownian Dynamics of Rigid Bodies

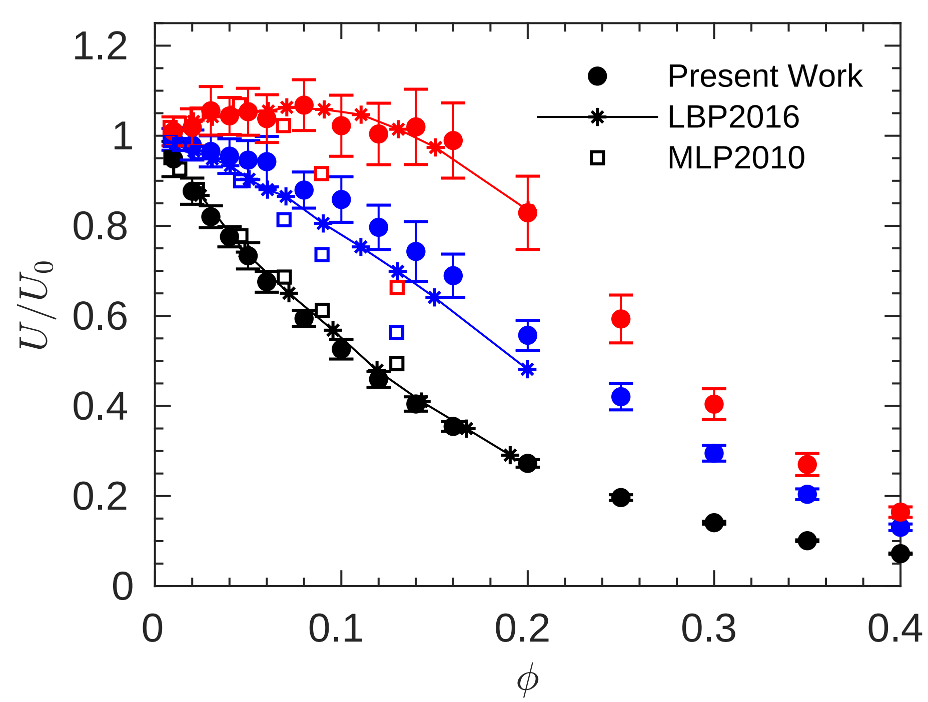


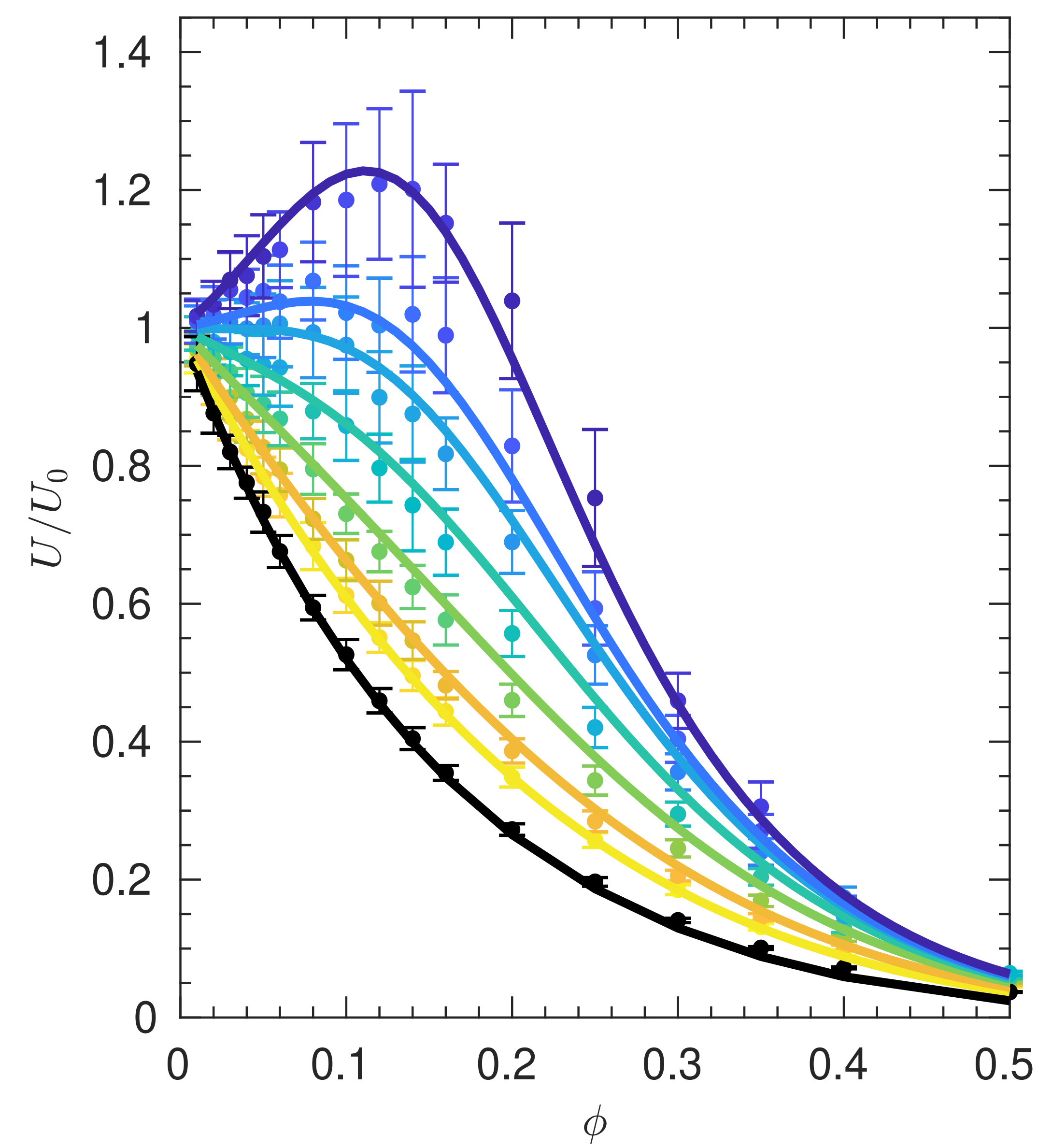
A GPU algorithm for Brownian Dynamics of composite-bead rigid particles is implemented. Arbitrarily shaped colloidal particles or macromolecules can be modeled as rigid assemblies of beads from surface tessellation. Hydrodynamic interactions among the beads are modeled with RPY tensor applying the PSE algorithm. Correct hydrodynamic and transport properties are successfully captured as demonstrated in the article "Rapid calculation of hydrodynamic and transport properties in concentrated solutions of colloidal particles and macromolecules". The software package can be downloaded here.



# How Do You Know It Works? (for not hard spheres)

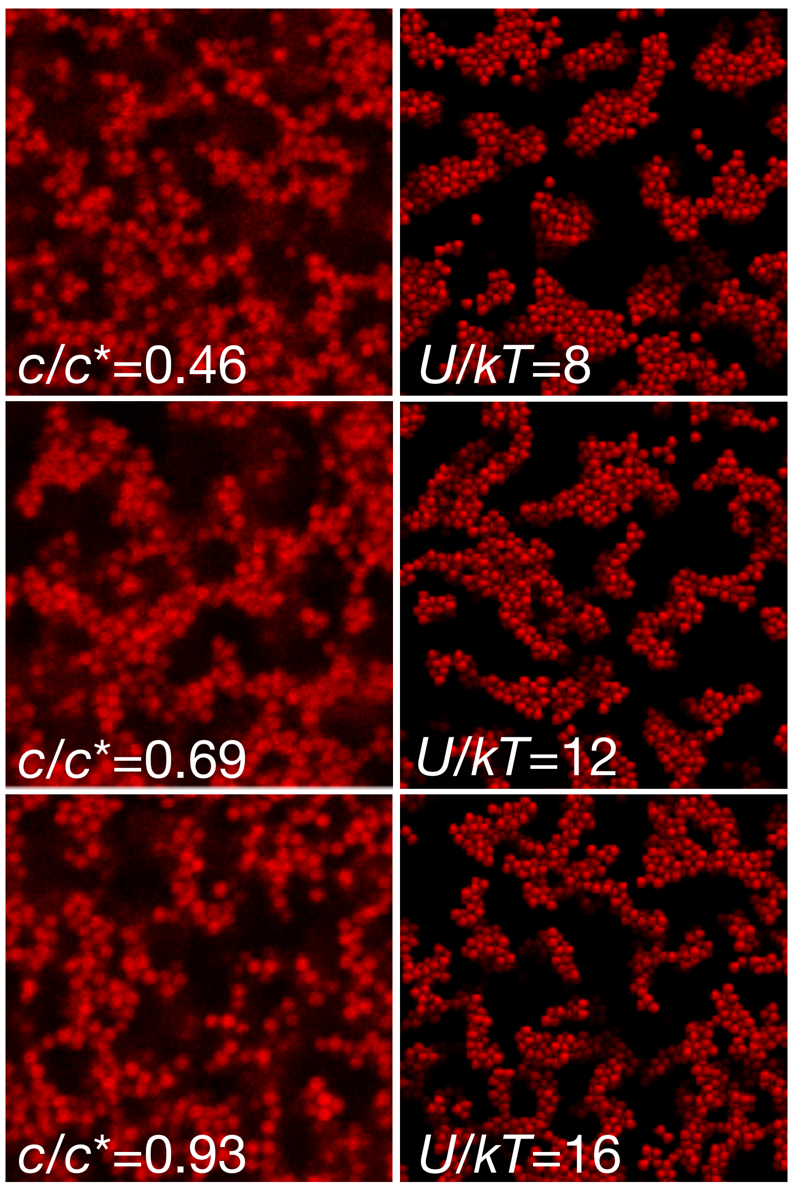


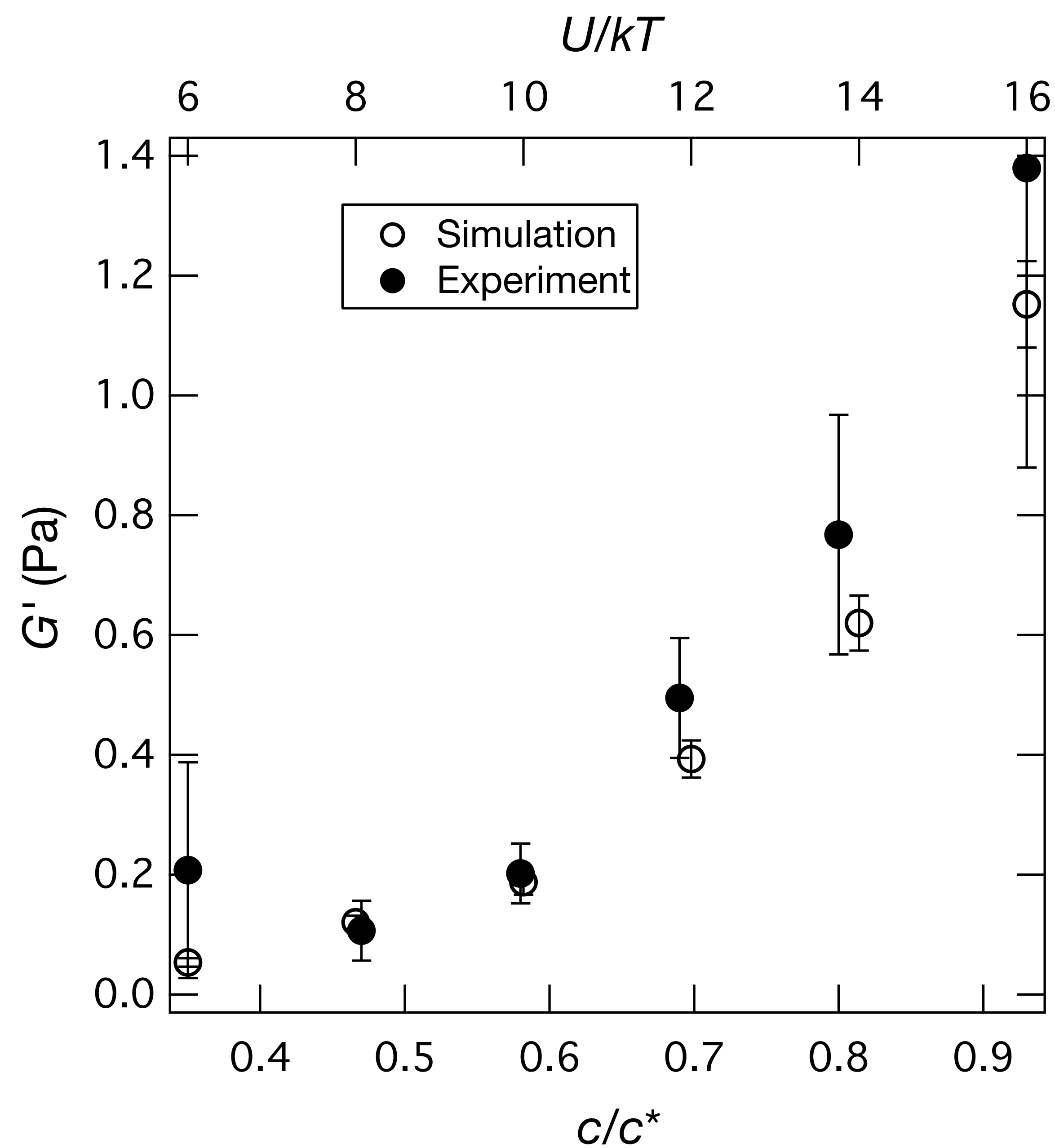



Fiore, Wang, and Swan. Phys. Rev. Fluids, 2018.

# How Do You Know It Works? (for not hard spheres)




Whitaker, Hsiao, Varga, Solomon, Swan, and Furst. submitted.

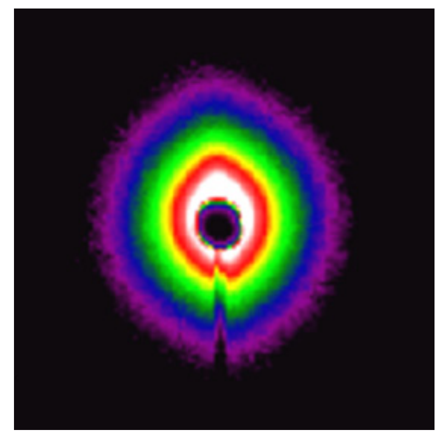
# Heterogeneous Structures and Flows

## Structure factor in an imposed shear flow

### Polyelectrolytes

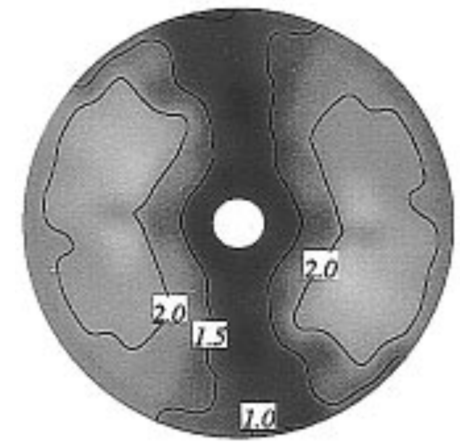
Villetti et al.,
Macromol. 2000

### Nanotubes



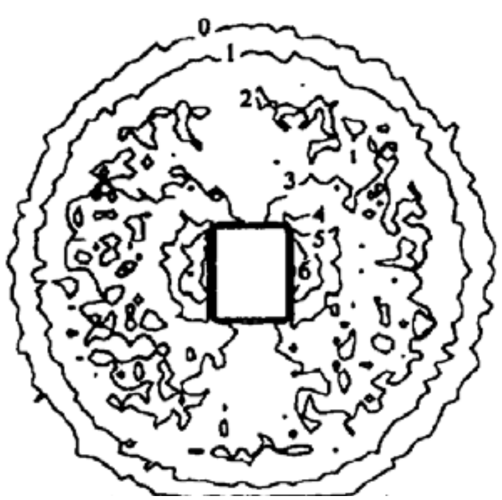
Pujari et al.,
J. Rheol. 2011

### Polymer solutions

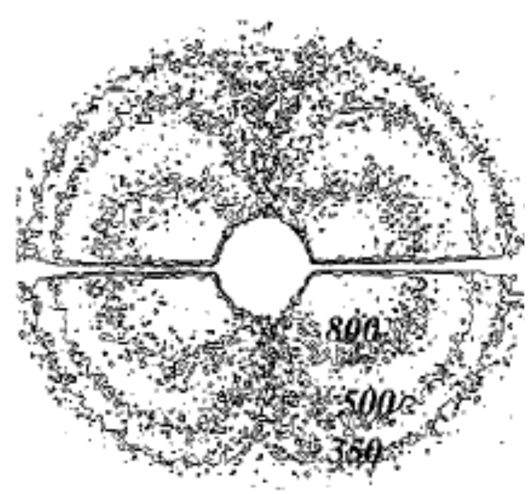



Miller et al.,
Macromol. 1996

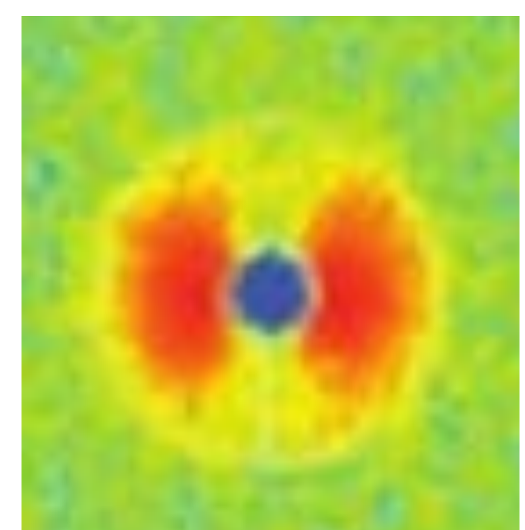
### Colloidal gels



Wouterson et al.,
J. Rheol. 1993



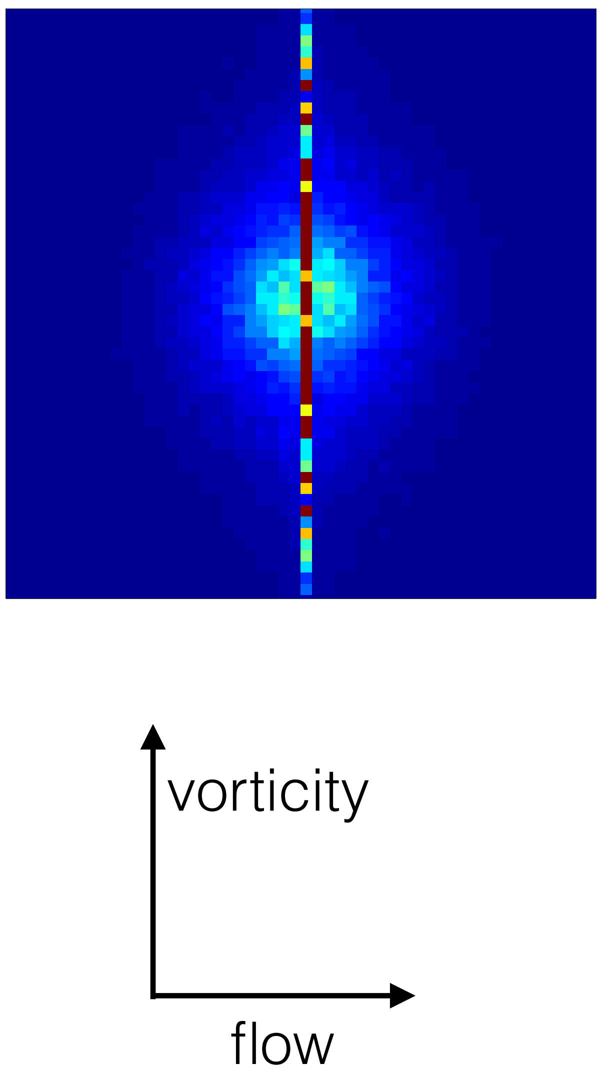

Varadan and Solomon
Langmuir 2001

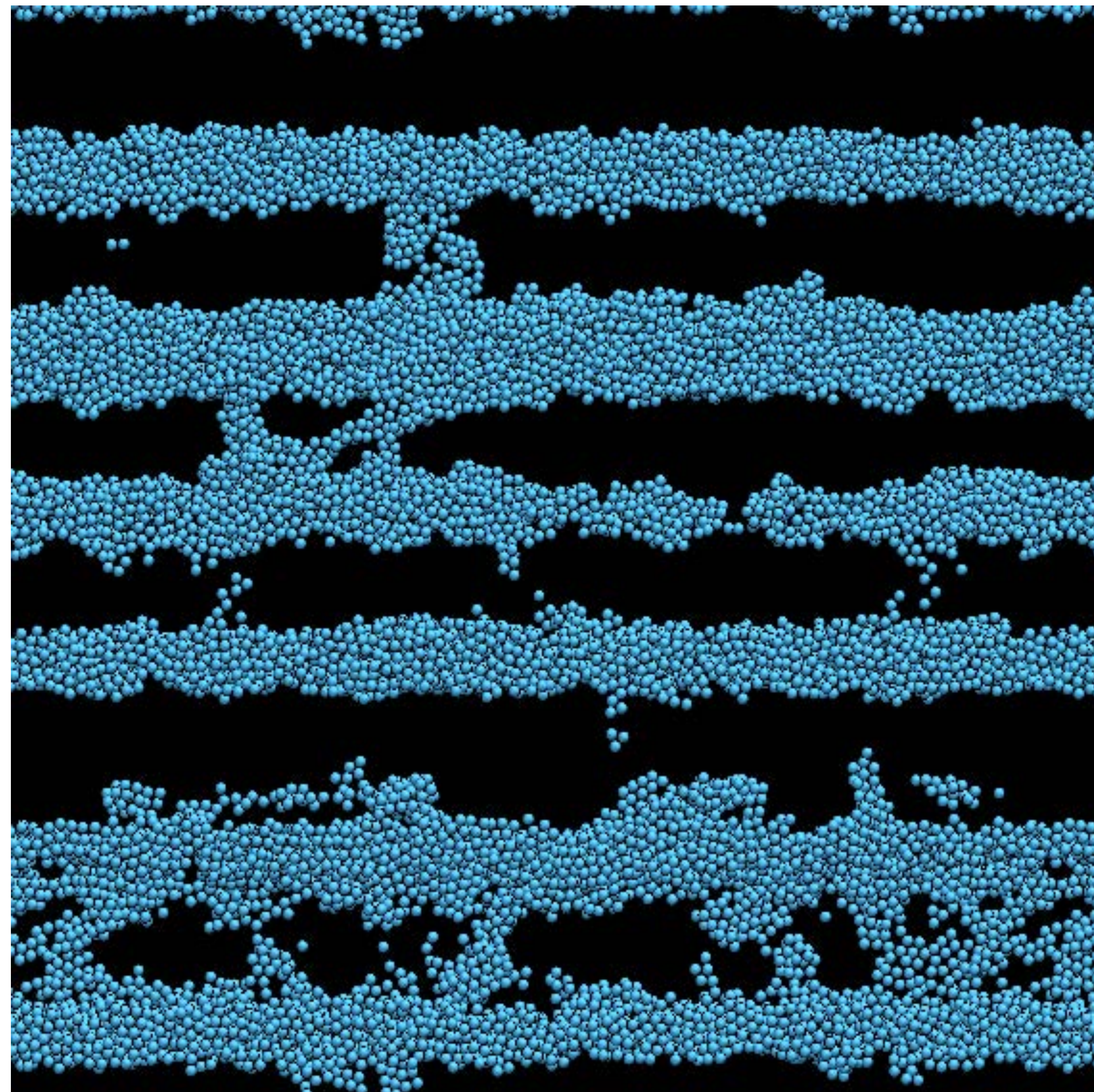


Kim et al.,
J. Rheol. 2014

# Colloidal Hydrodynamics Affect Structuring in an Imposed Flow

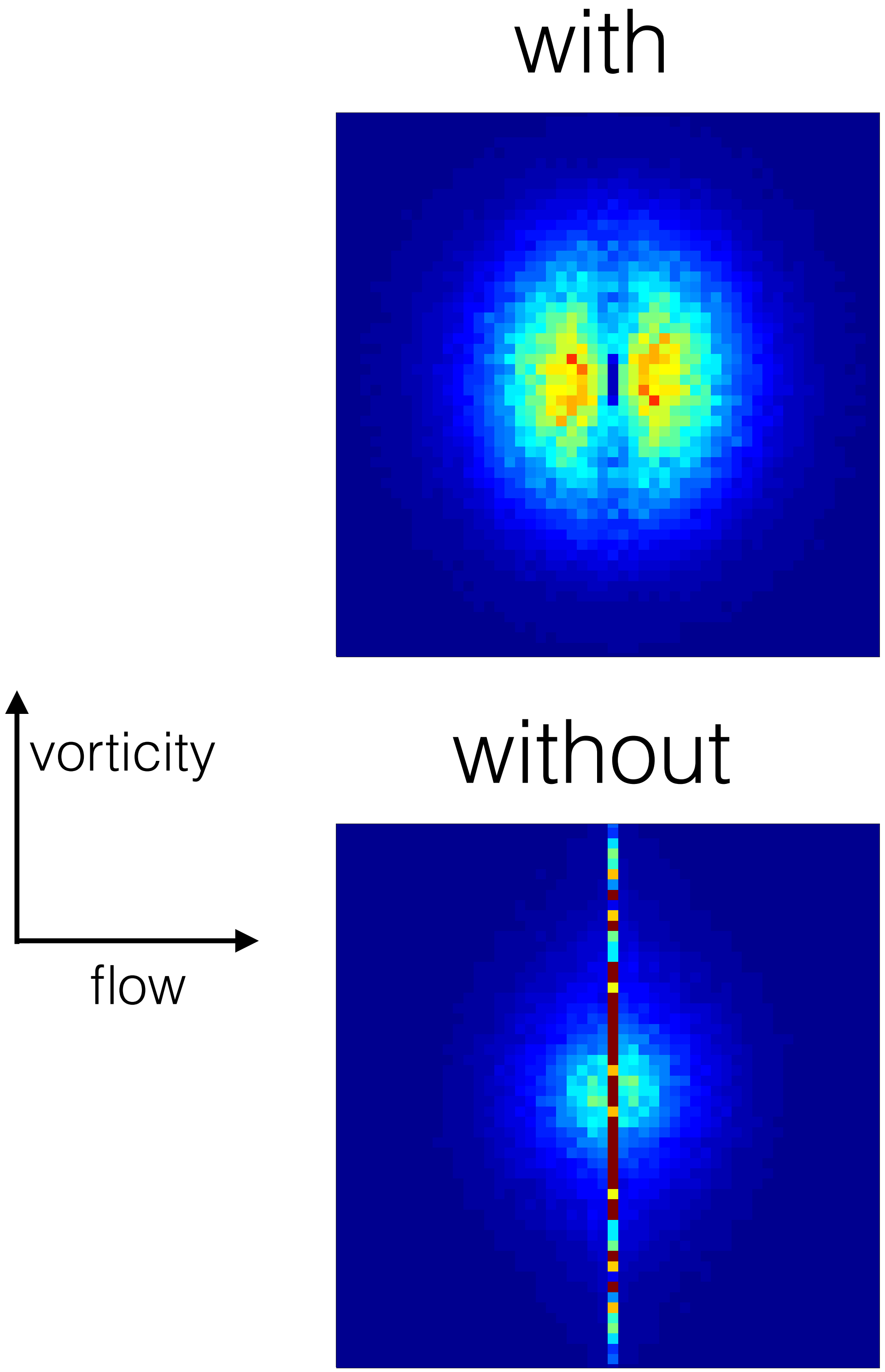
## No hydrodynamic interactions

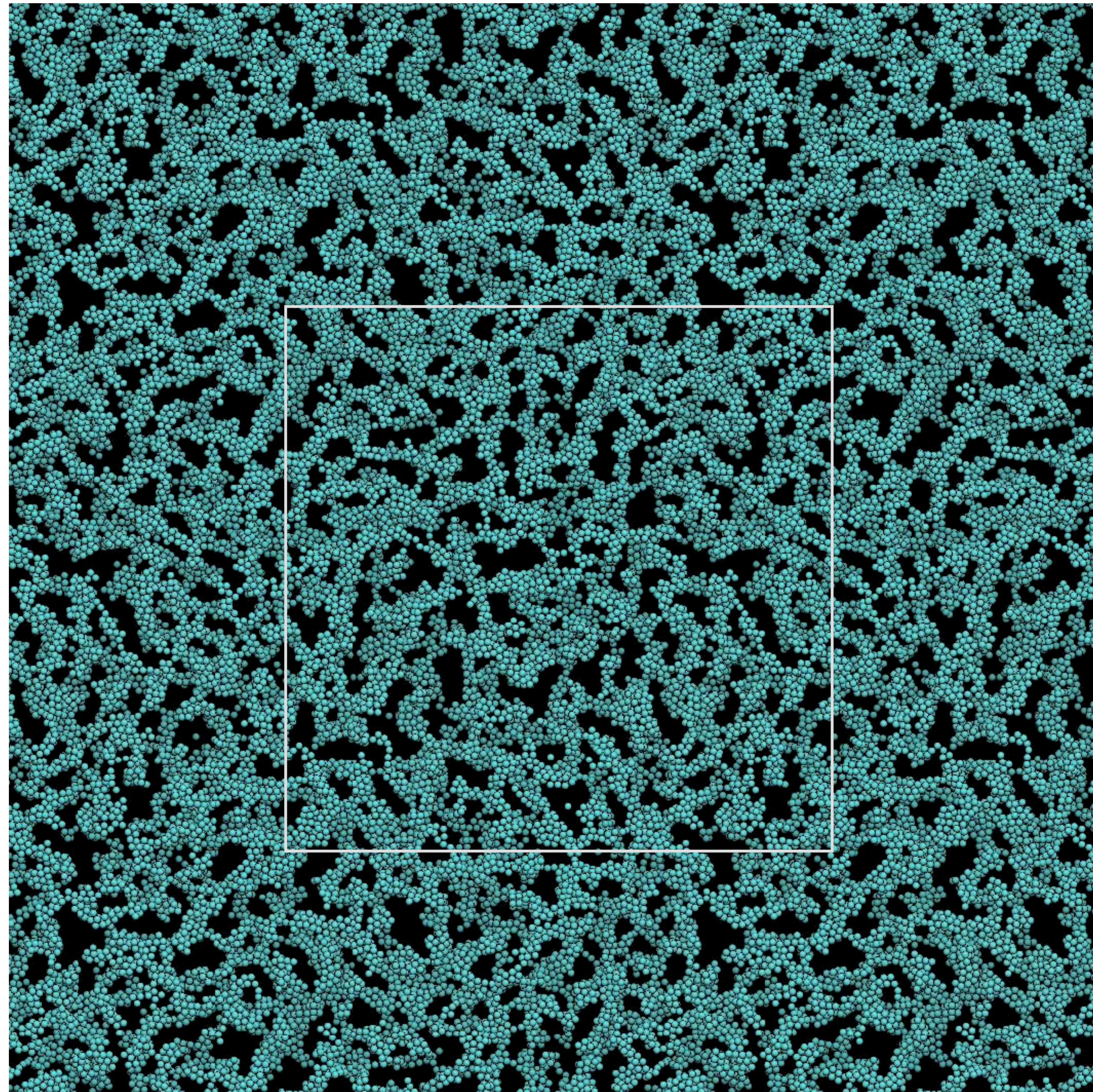


Silbert et al., J. Rheol.. 1999
Dong et al., J. Rheol. 2016

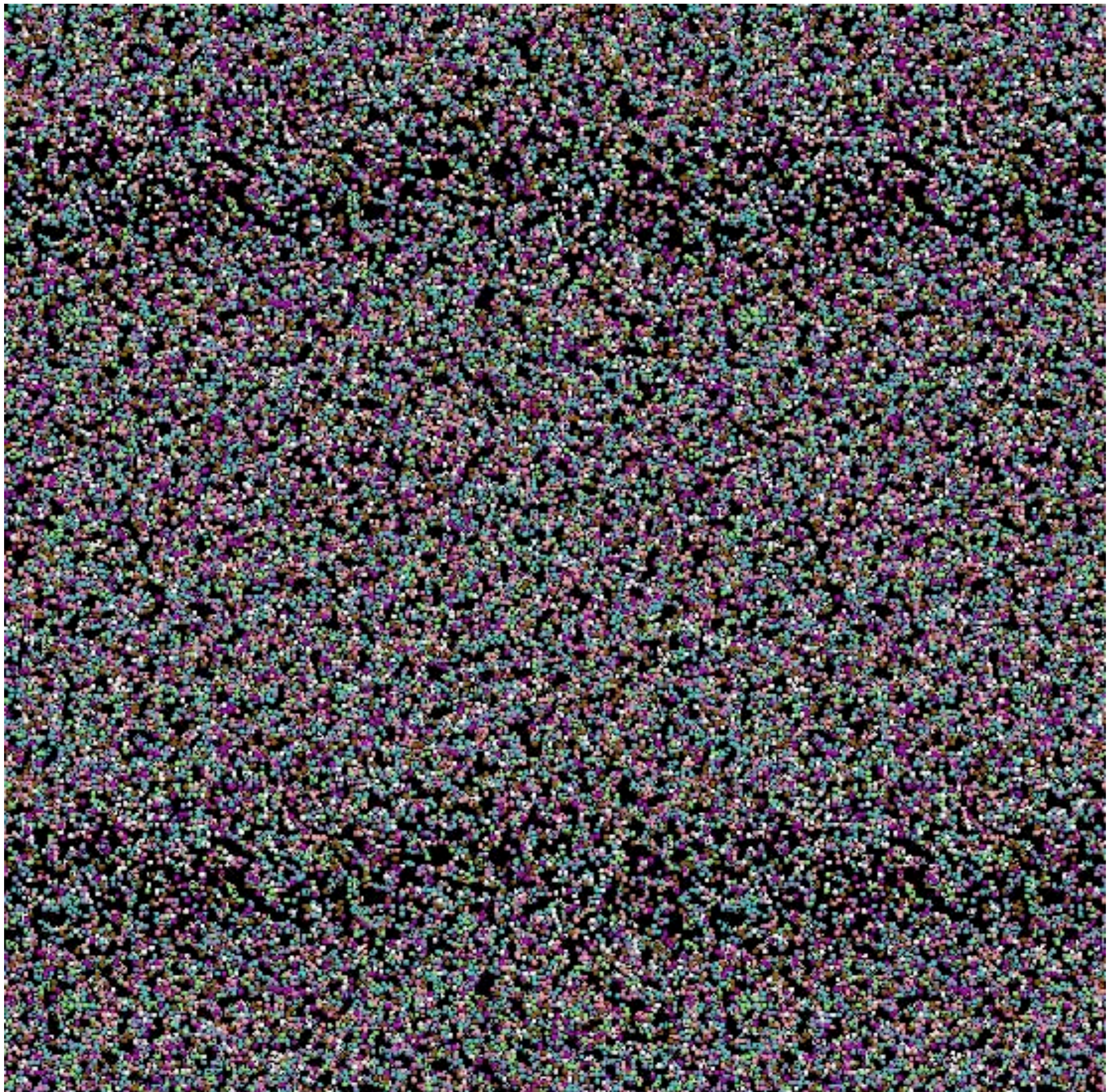
# Colloidal Hydrodynamics Affect Structuring in an Imposed Flow

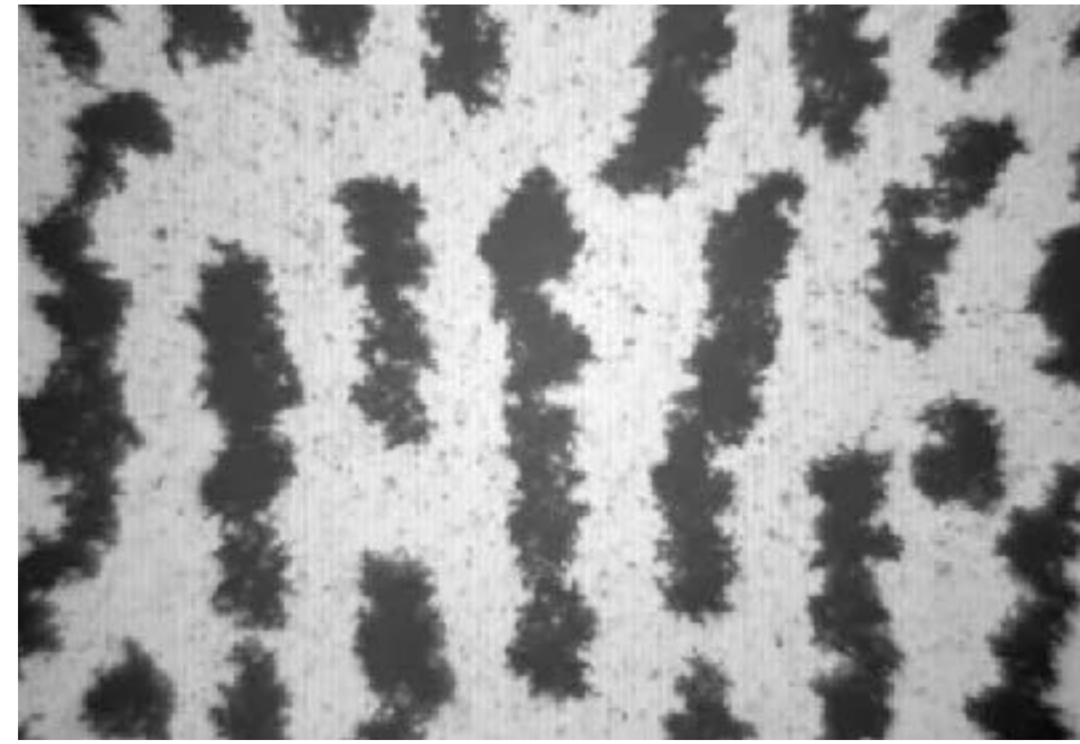


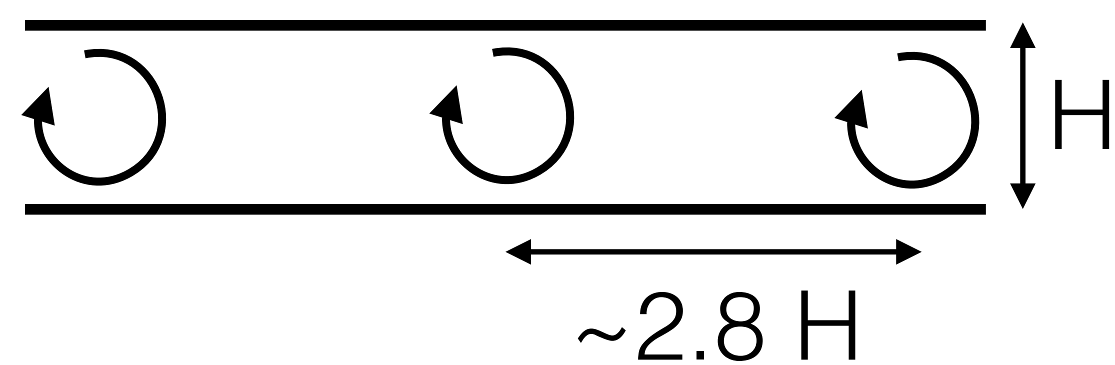
Varga and Swan. J. Rheology, 2018.

# Colloidal Hydrodynamics Affect Structuring in an Imposed Flow





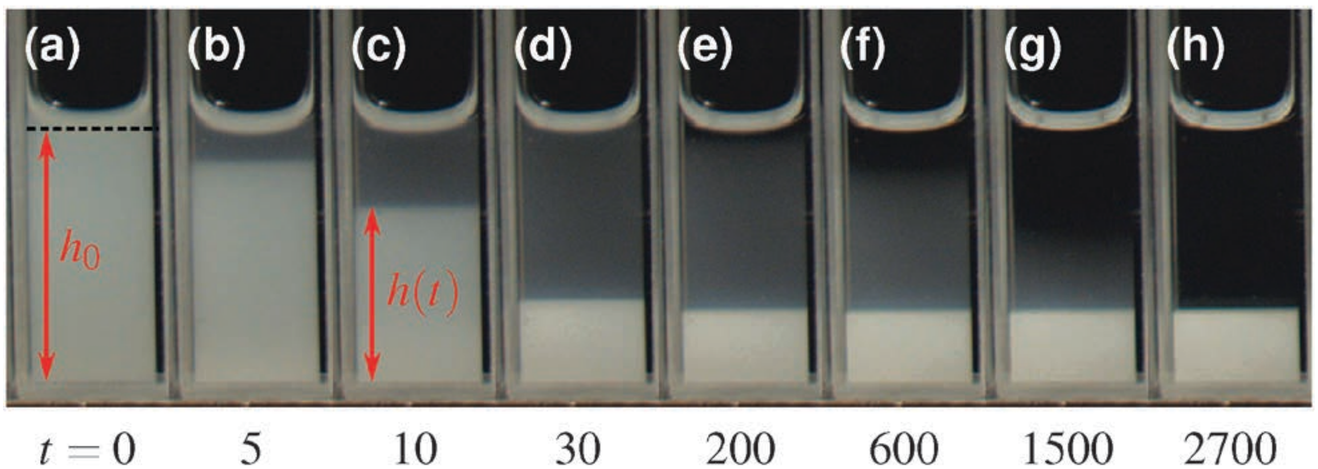
Grenard et al., Soft Matter 2011

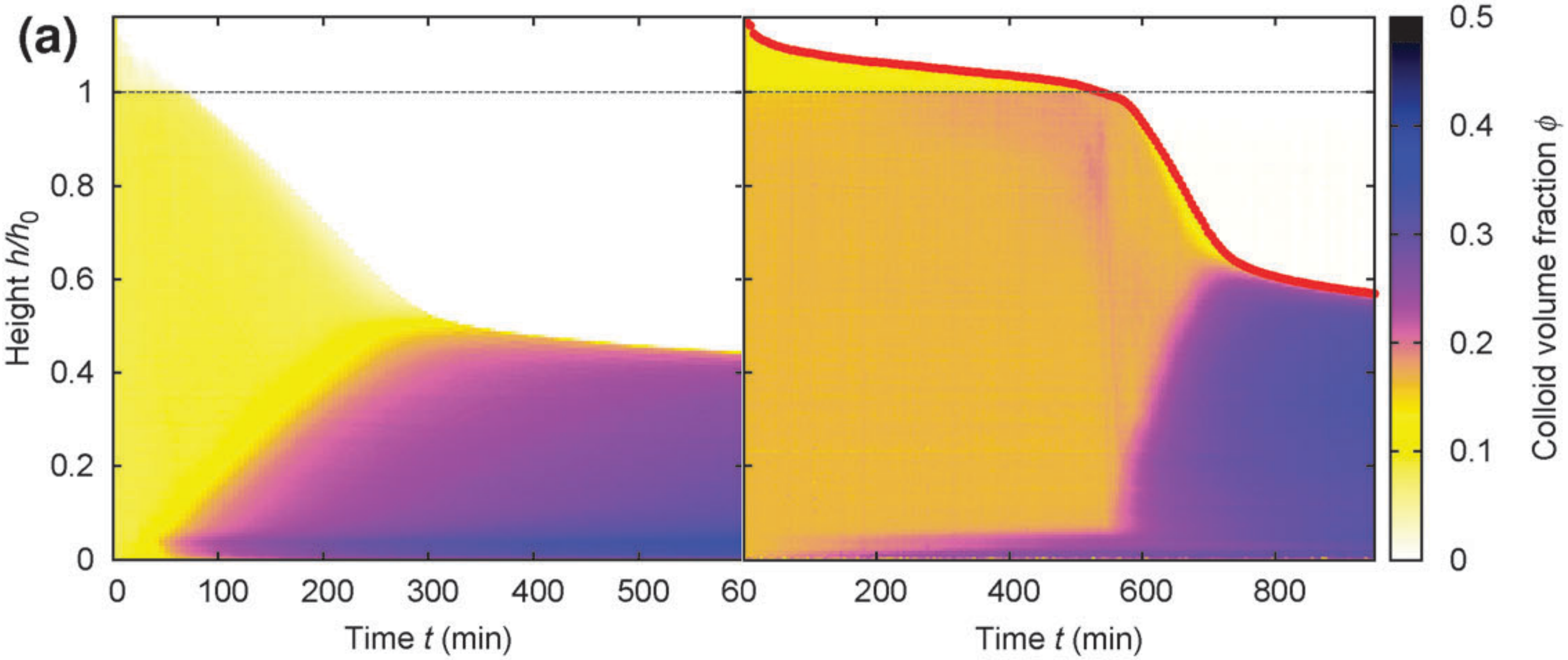



H/a=20

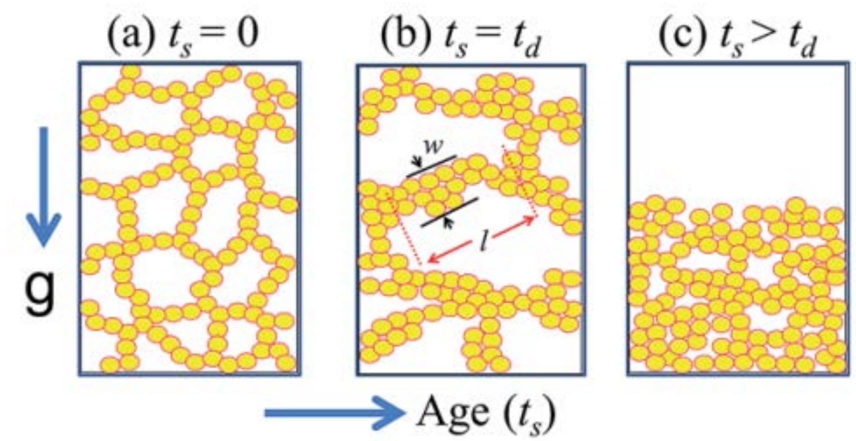
Divoux, Varga, Manneville, McKinley and Swan. in preparation

# Heterogeneous Structures and Flows

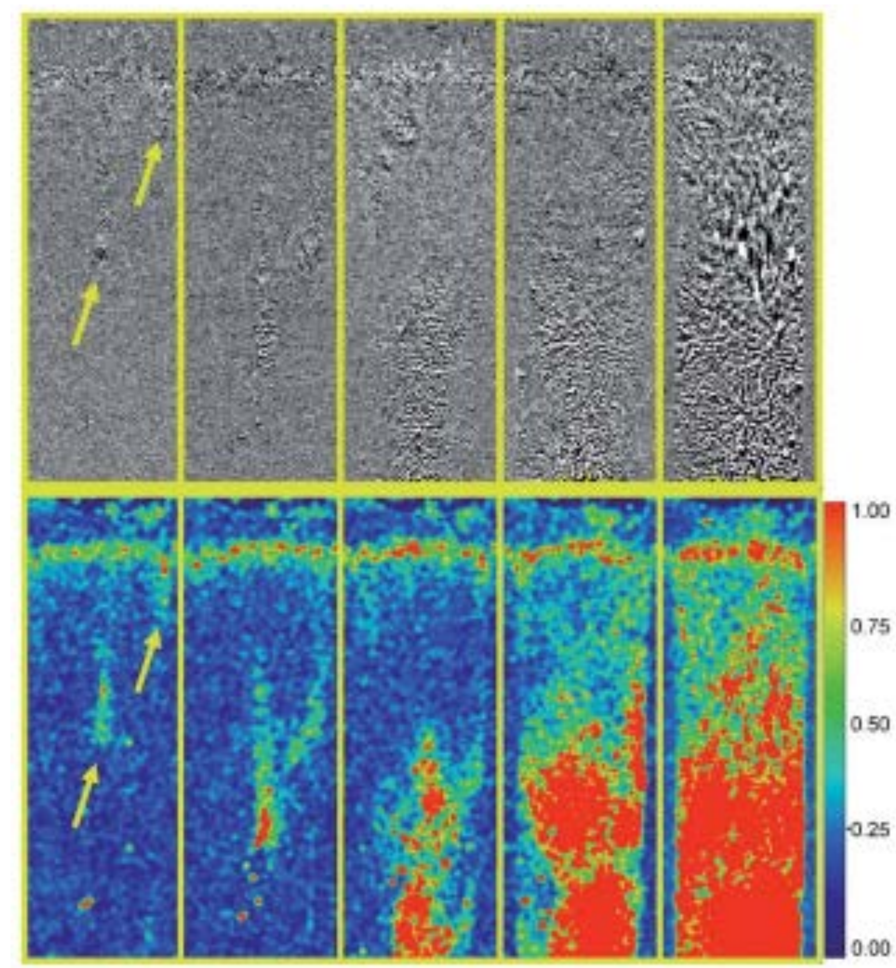



Harich et al., Soft Matter 2016

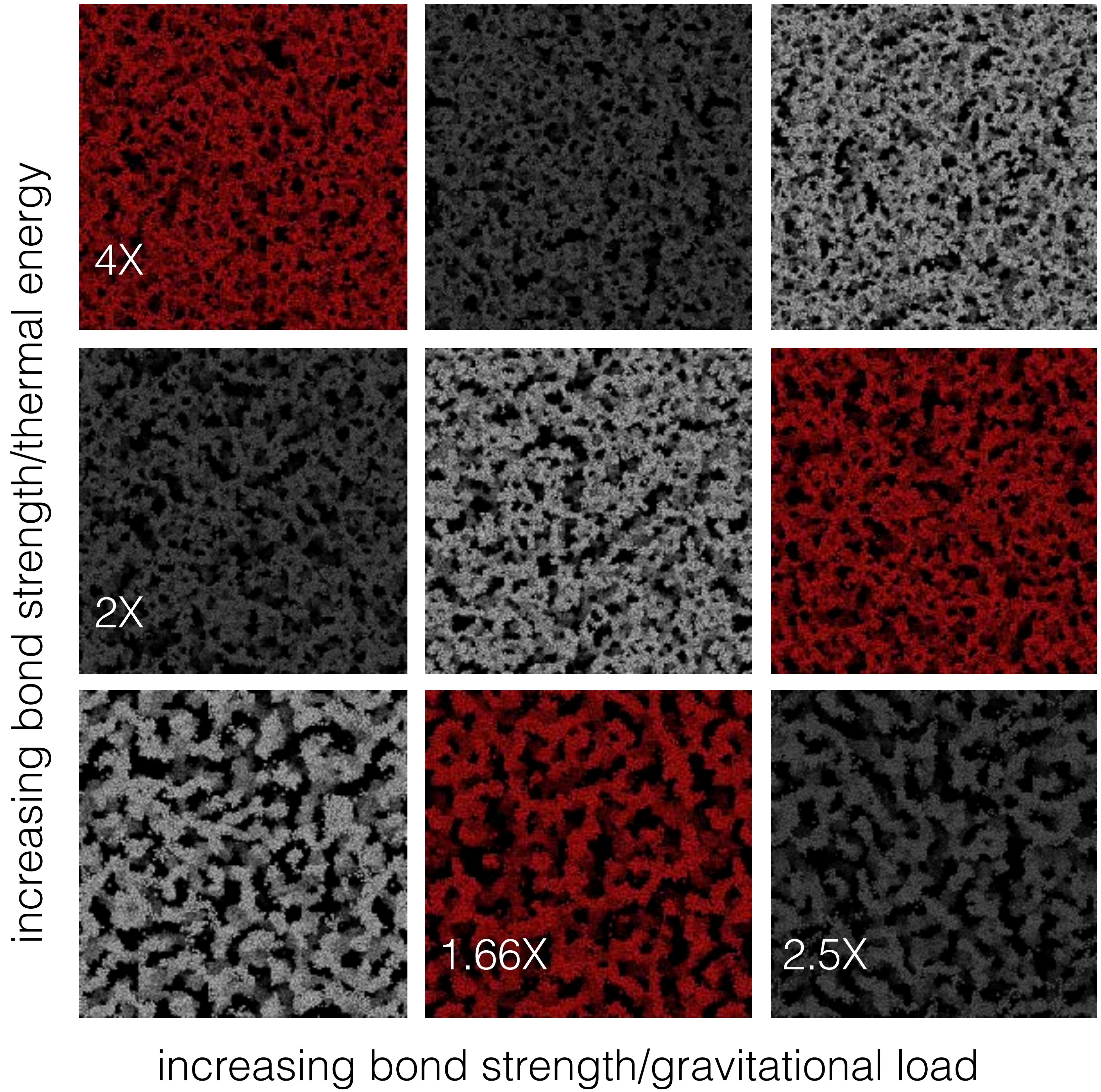



Ali and Bandyopadhyaym FD 2016

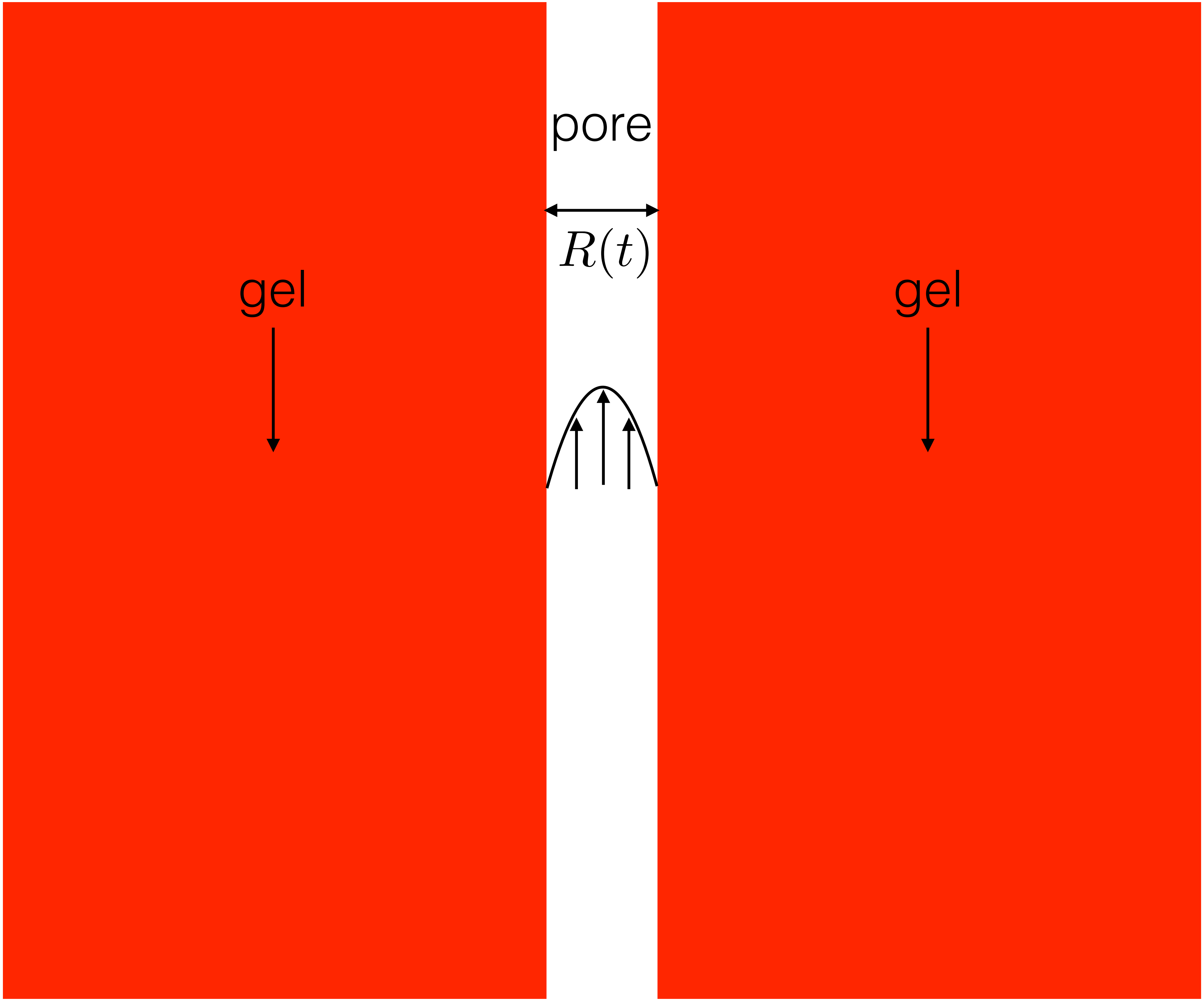


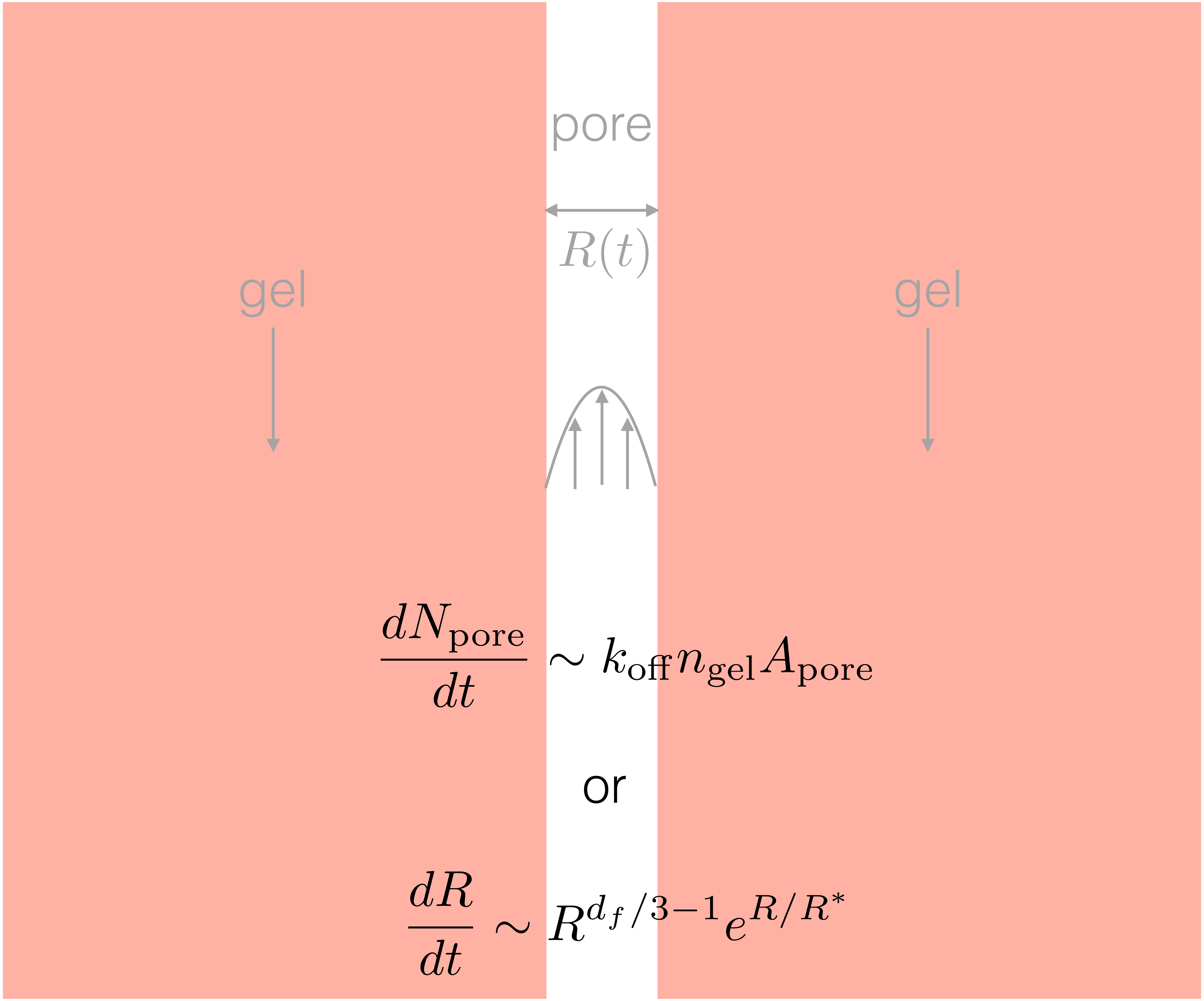

Sechhi et al., Soft Matter 2014

# Colloidal Hydrodynamics Affect Stability




Varga, Hoffman and Swan, J. Fluid Mech. submitted

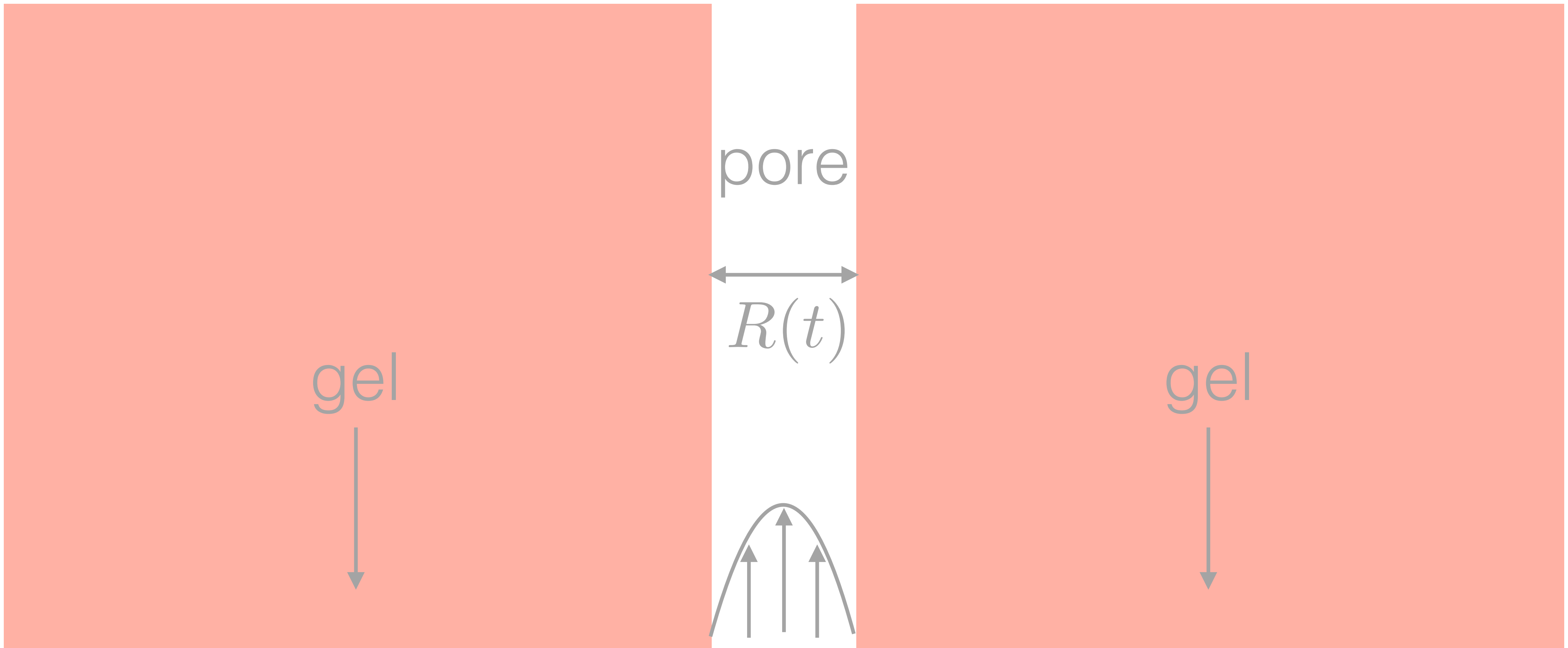

pore
$R(t)$
gel
gel




$$\frac{dN_{\mathrm{pore}}}{dt} \sim k_{\mathrm{off}} n_{\mathrm{gel}} A_{\mathrm{pore}}$$

or

$$\frac{dR}{dt} \sim R^{d_f/3-1} e^{R/R^*}$$

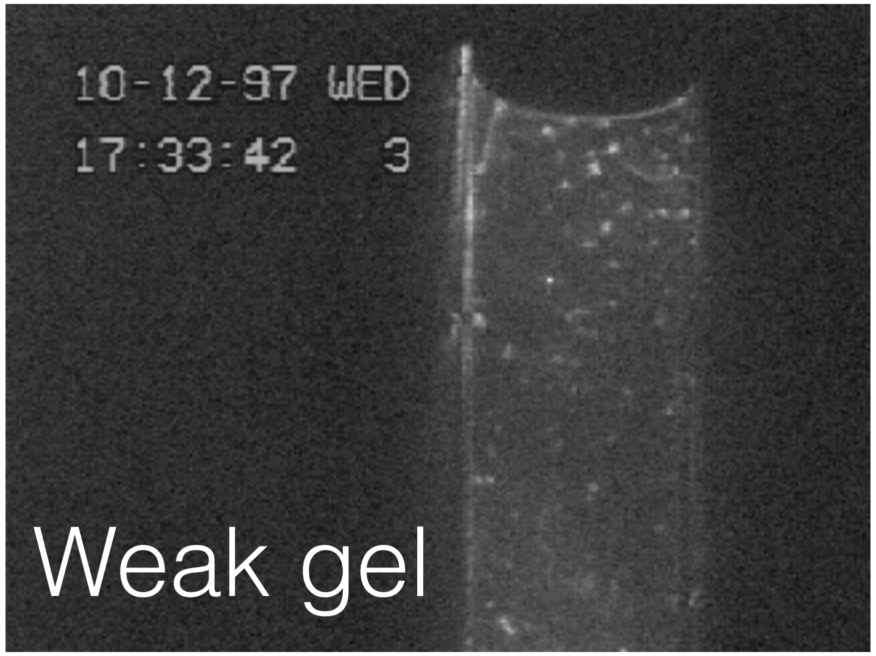


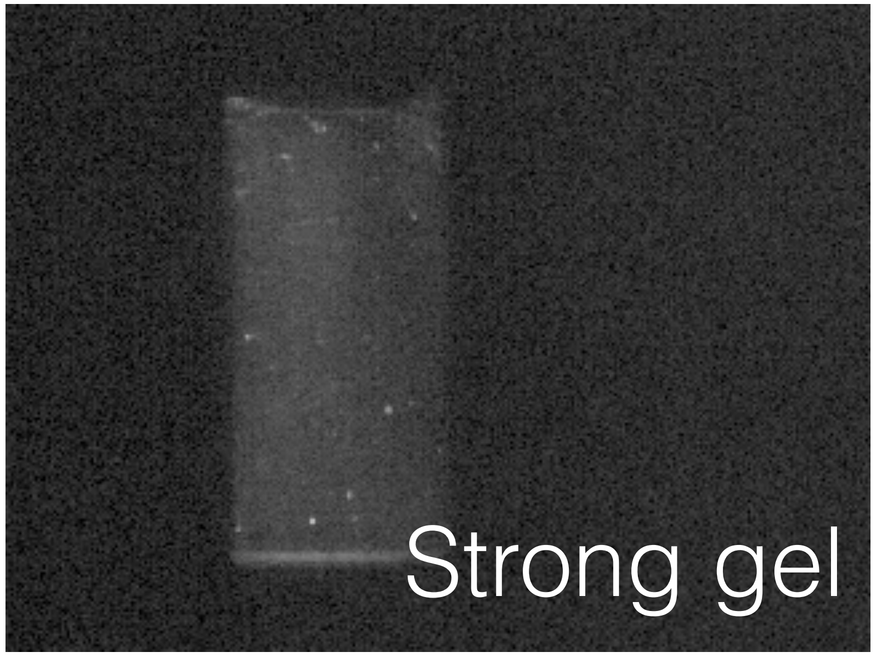

$$\frac{dR}{dt} \sim R^{d_f/3-1} e^{R/R^*}$$

Exhibits finite-time blow-up singularity

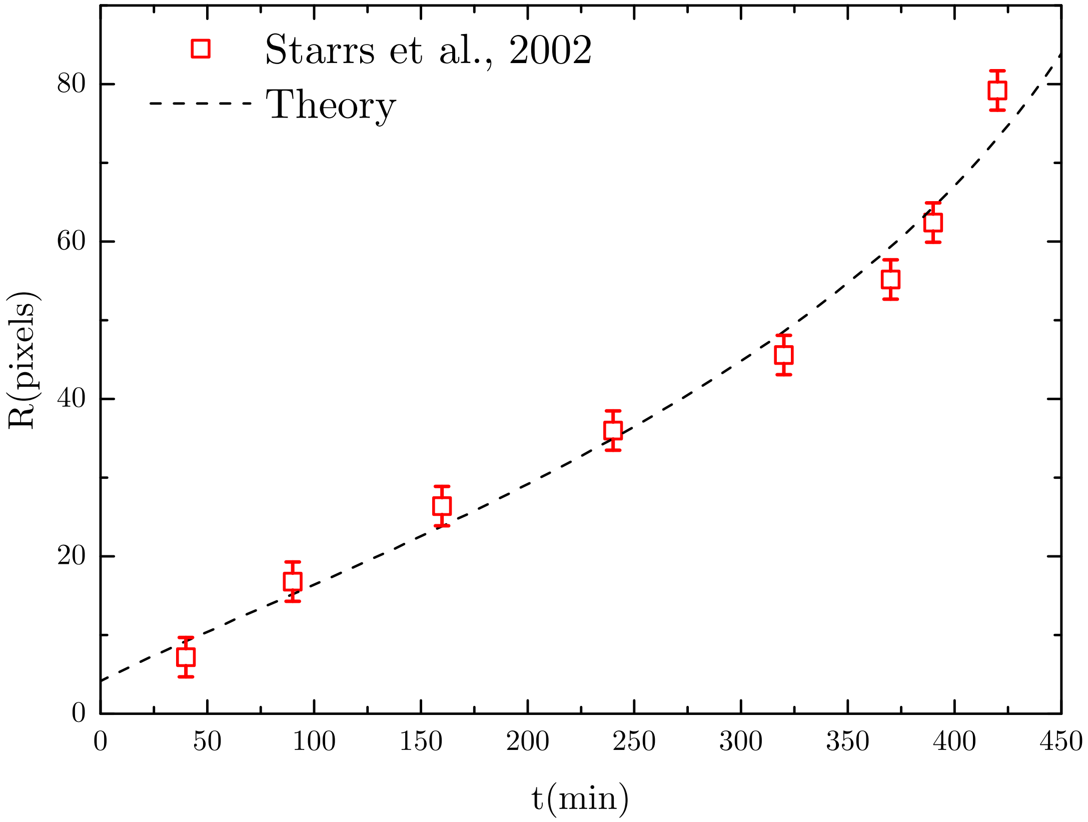
$$R \to \infty, \quad t \to {R^*}^{2-d_f/3} \Gamma(2 - d_f/3)$$

# Colloidal Hydrodynamics Affect Stability




$$t_{\text{blow-up}} - t \sim {R^*}^{2-df/3}\Gamma\left(2-\frac{df}{3}, \frac{R(t)}{R^*}\right)$$




Actual blow-up time: 570 min.
Best fit to model: 586 min.
From sim. parameters: 623 min.

Starrs, Poon, Hibberd, and Robins J. Physics: CM 2002

# Thank you

Andrew Fiore
Gang Wang
Zsigmond Varga

**For fast hydrodynamic interactions see:**

Fiore, Balboa, Donev and Swan, J. Chem. Phys. 2017

**HOOMD-blue plug-in:**

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