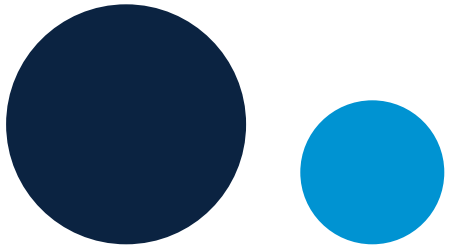
AUBURN UNIVERSITY
Samuel Ginn College of Engineering
*Chemical Engineering*

# RECENT DEVELOPMENTS AND OPPORTUNITIES IN MESOSCALE MODELING OF COLLOIDAL SUSPENSIONS

MICHAEL P. HOWARD

# MODELING COLLOIDAL SUSPENSIONS

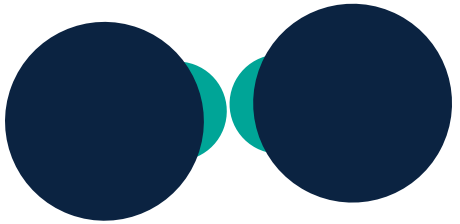
**polydispersity**



**roughness**

**shape anisotropy**

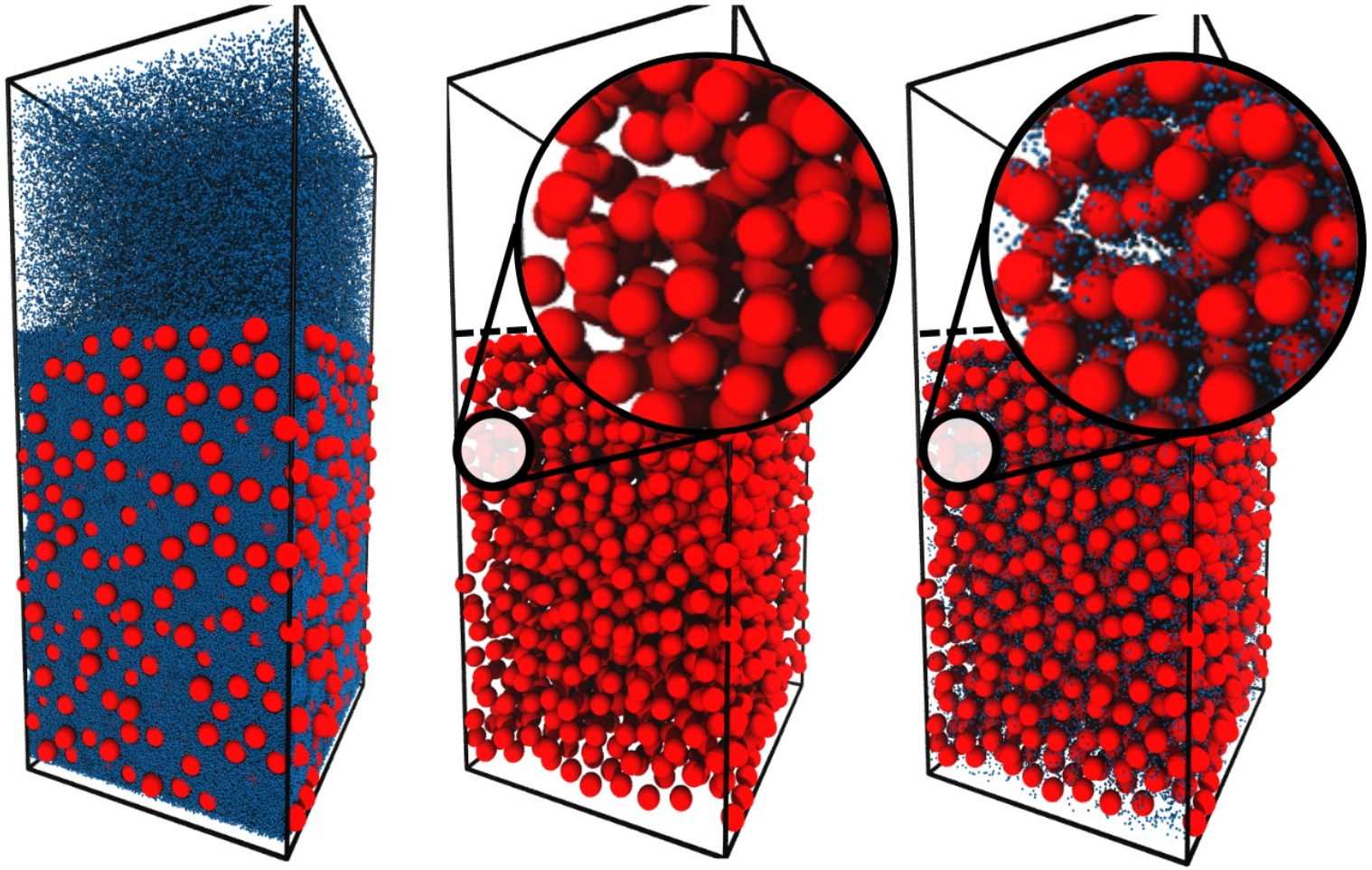
**interaction anisotropy**



## Challenges

- Describe the **direct interactions** between particles.
- Capture the indirect **hydrodynamic interactions** between particles that are mediated by the solvent.

# HYDRODYNAMIC INTERACTIONS



For Brownian particles:

- Explicit solvent
  - Molecular dynamics
- Implicit solvent
  - Free-draining dynamics
  - RPY dynamics
  - Stokesian dynamics
  - Fast lubrication dynamics
- Mesoscale solvent
  - Dissipative particle dynamics
  - Lattice Boltzmann
  - Multiparticle collision dynamics

# HYDRODYNAMIC INTERACTIONS

## STOKESIAN DYNAMICS

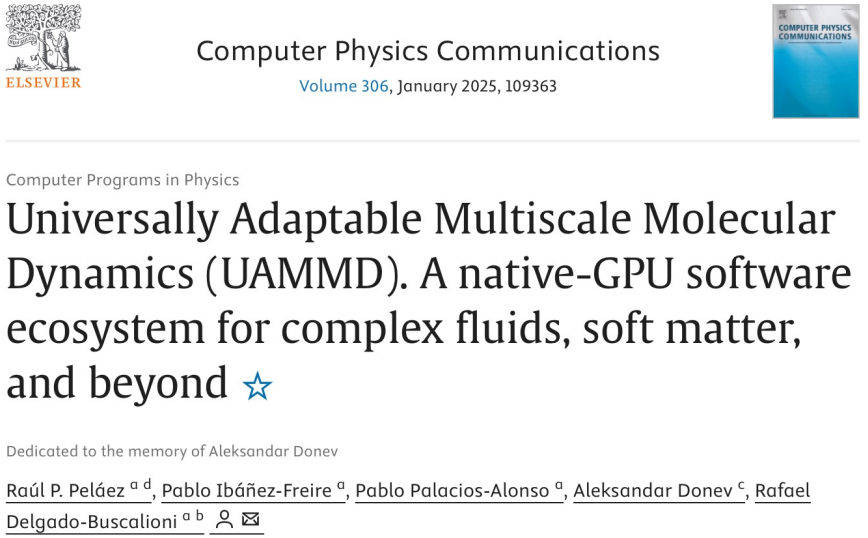
- Tensor-based hydrodynamics (combining near-field and far-field), often considered “gold standard” for suspensions.
- Method is mathematically difficult and simulations are expensive, so it has been difficult for new users to adopt and to scale.
- Fast implementation developed by A. Fiore (*J. Fluid Mech*. **878**, 544) for HOOMD-blue in 2019, but code is unfortunately not maintained.
- **Developments:** New implementations by W. Torre (thanks to IFPRI!) and R.P. Peláez are available open-source and achieve good performance.


SciPost

SciPost Phys. Codebases 56 (2025)

**Python-JAX-based fast Stokesian dynamics**

Kim William Torre[1⋆], Raoul D. Schram[2†] and Joost de Graaf[1‡]


ELSEVIER

Computer Physics Communications

Volume 306, January 2025, 109363

Computer Programs in Physics

**Universally Adaptable Multiscale Molecular Dynamics (UAMMD). A native-GPU software ecosystem for complex fluids, soft matter, and beyond ☆**

Dedicated to the memory of Aleksandar Donev

Raúl P. Peláez [a d], Pablo Ibáñez-Freire [a], Pablo Palacios-Alonso [a], Aleksandar Donev [c], Rafael Delgado-Buscalioni [a b]

# HYDRODYNAMIC INTERACTIONS

## STOKESIAN DYNAMICS

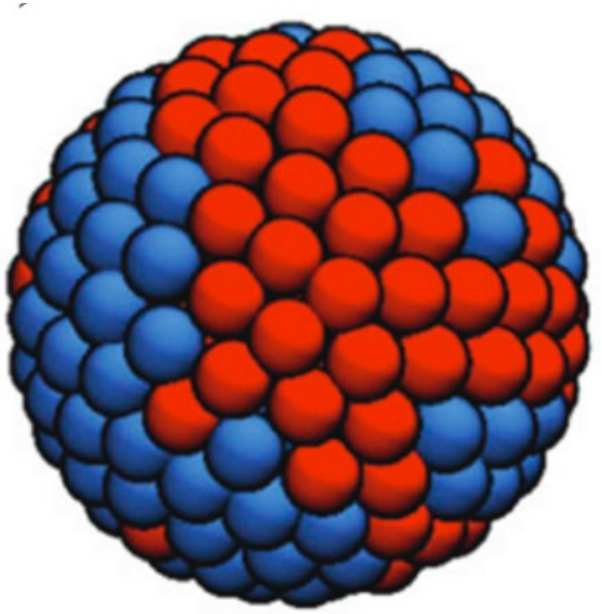
- Discrete particle models extend SD to other particle shapes.
  - Also called SD for rigid assemblies, composite bead model, and multiblob method.
- **Opportunities:** extend existing SD (and related method) codes to support discrete particle model and polydispersity, new codes likely need a long-term home.

PHYSICAL REVIEW FLUIDS **10**, 100701 (2025)

Perspective | Invited Articles

**Modeling complex particle suspensions: Perspectives on the rigid multiblob method**

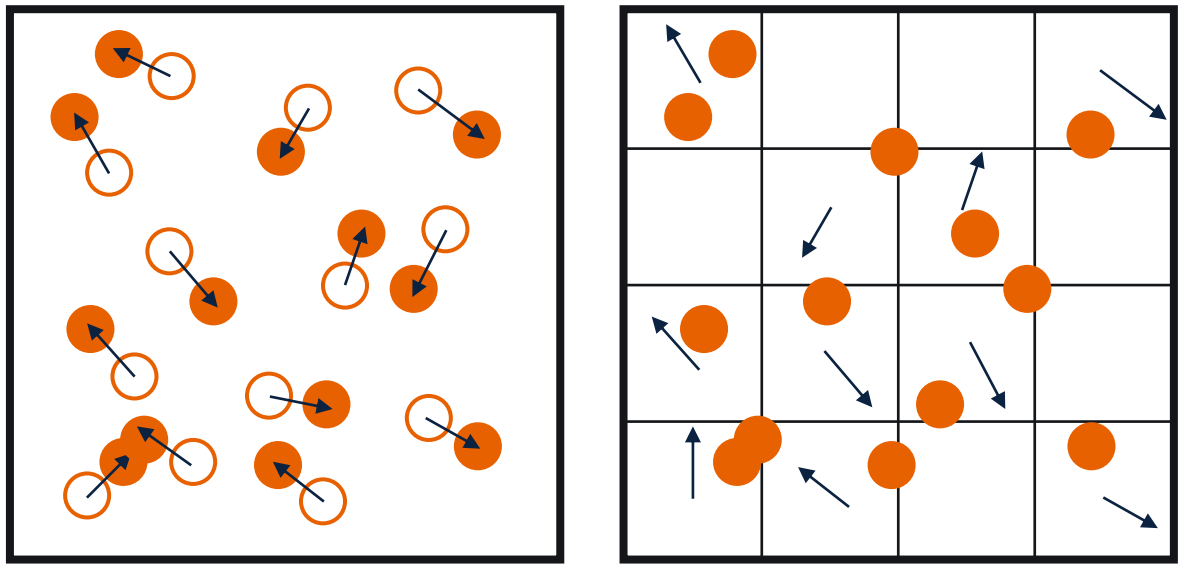
Blaise Delmotte [1,*] and Florencio Balboa Usabiaga [2,†]



# HYDRODYNAMIC INTERACTIONS

## MULTIPARTICLE COLLISION DYNAMICS

- Incorporates hydrodynamic interactions through an explicit solvent that has small computational cost because there are no pair forces between solvent particles.
- Available open-source in HOOMD-blue with active support, LAMMPS to a lesser extent.



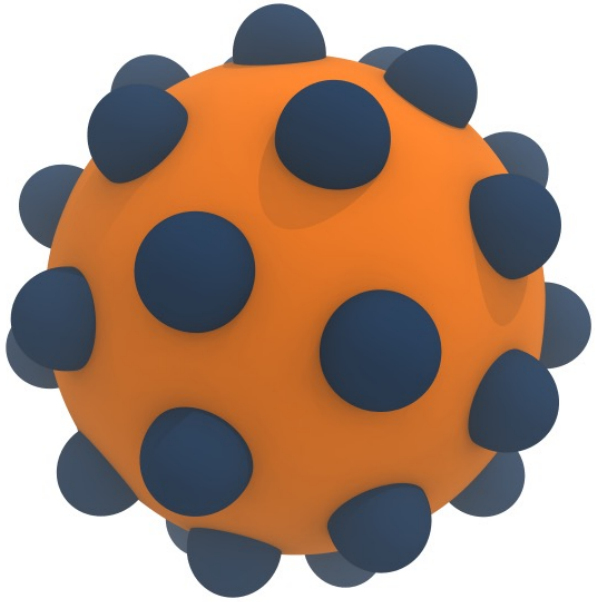
**stream** **collide**

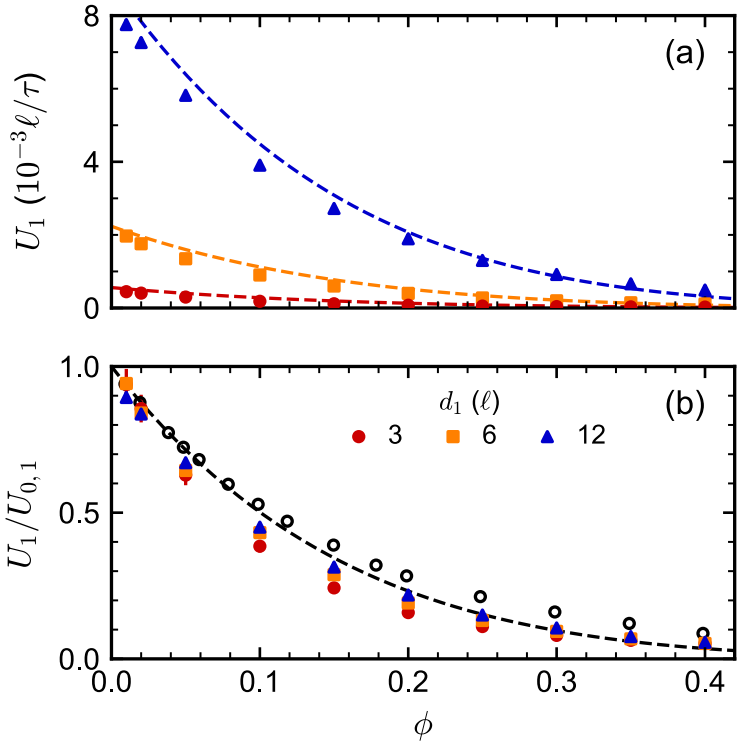
A. Malevanets and R. Kapral. *J. Chem. Phys.* **110**, 8605 (1999).
M.P. Howard, A.Z. Panagiotopoulos, and A. Nikoubashman. *Comput. Phys. Commun.* **230**, 10 (2018).

# HYDRODYNAMIC INTERACTIONS

## MULTIPARTICLE COLLISION DYNAMICS

- Represents colloidal particles using discrete particle model.
- Works well for monodisperse colloidal suspensions.





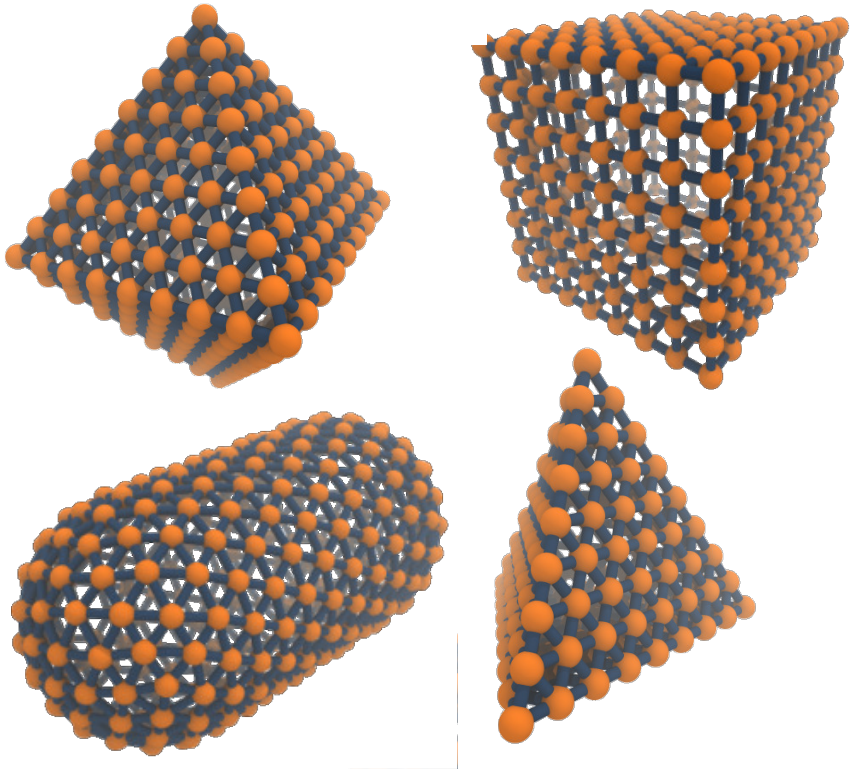


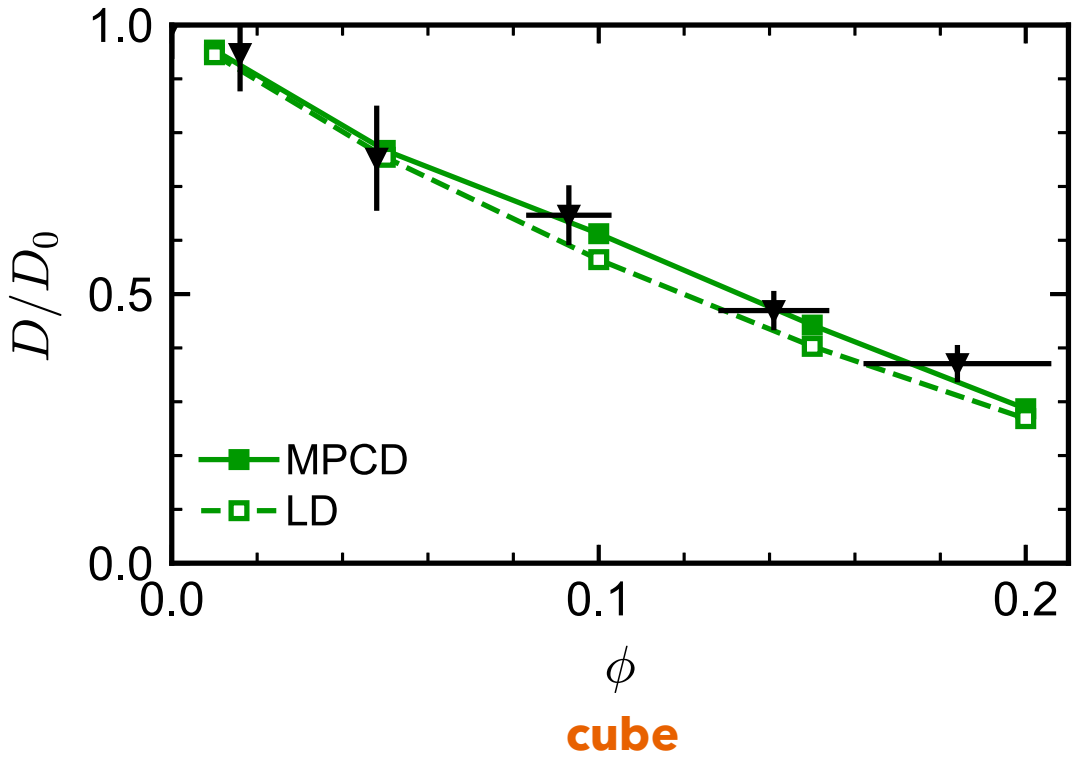
Y.M. Wani, P.G. Kovakas, A. Nikoubashman, M.P. Howard. *J. Chem. Phys.* **156**, 024901 (2022).
M.P. Howard. *in preparation* (2026)

# HYDRODYNAMIC INTERACTIONS

## MULTIPARTICLE COLLISION DYNAMICS

- **Developments:** Works well even with different particle shapes.





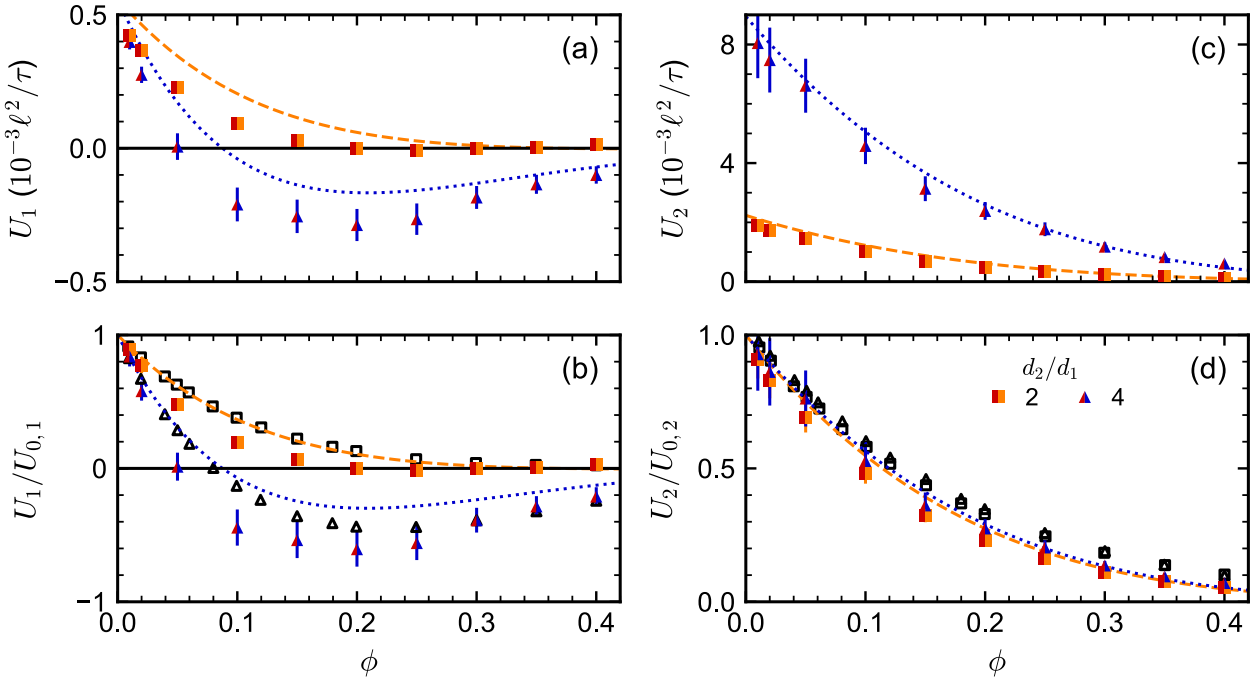

**cube**

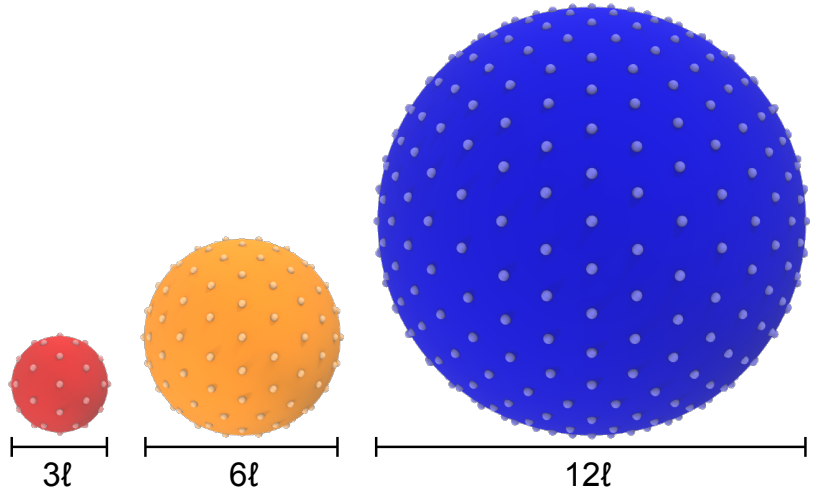
Y.M. Wani, P.G. Kovakas, A. Nikoubashman, and M.P. Howard. *Soft Matter* **20**, 3942 (2024).

# HYDRODYNAMIC INTERACTIONS

## MULTIPARTICLE COLLISION DYNAMICS

- **Developments:** Works well even with different particle sizes (thanks to IFPRI!).



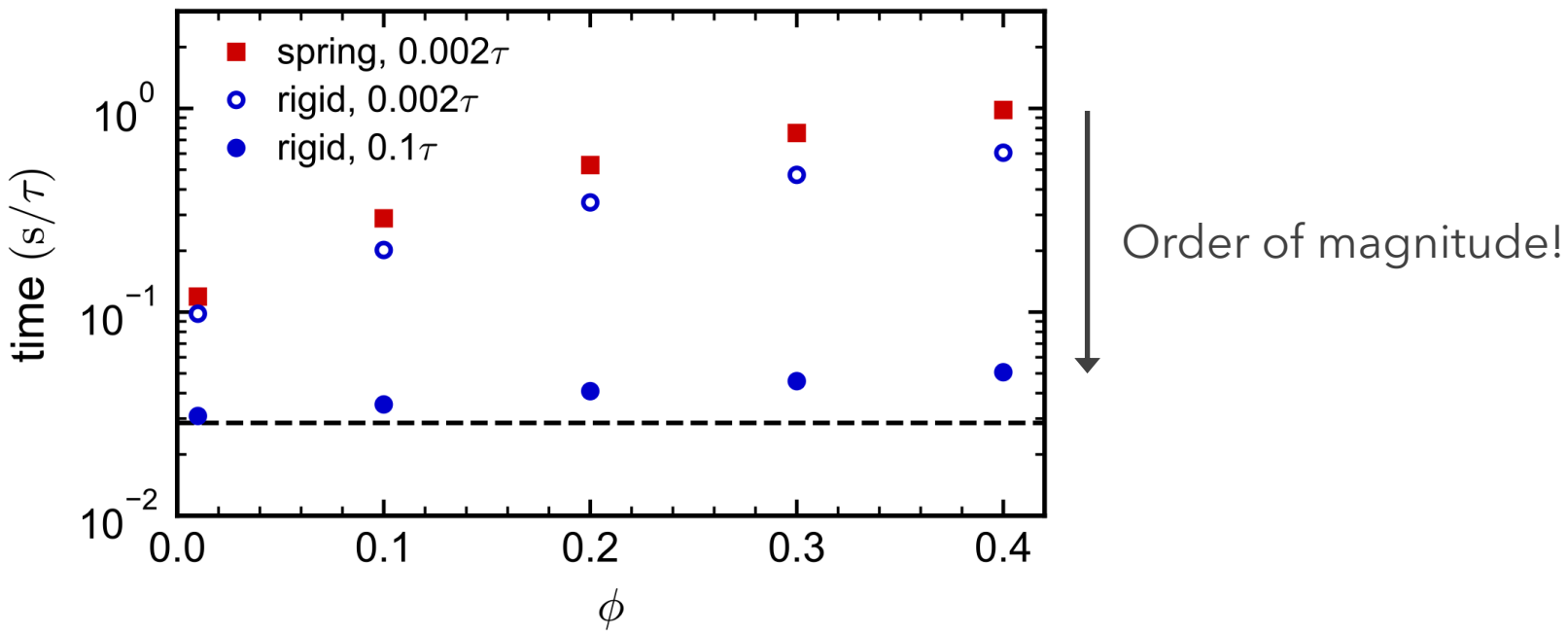




M.P. Howard. *in preparation* (2026).

# HYDRODYNAMIC INTERACTIONS

## MULTIPARTICLE COLLISION DYNAMICS

- **Developments:** New rigid-body coupling enables ~10x speedup.



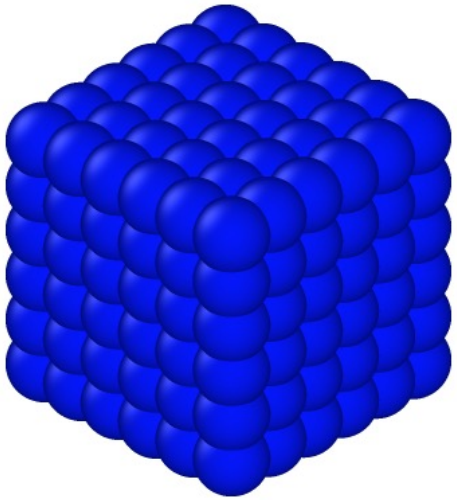

- **Opportunities:** Identify best strategy to discretize particles, handle lubrication / high volume fractions accurately.

M. Bush, J.C. Palmer, and M.P. Howard. *in preparation* (2026).

# PARTICLE INTERACTIONS

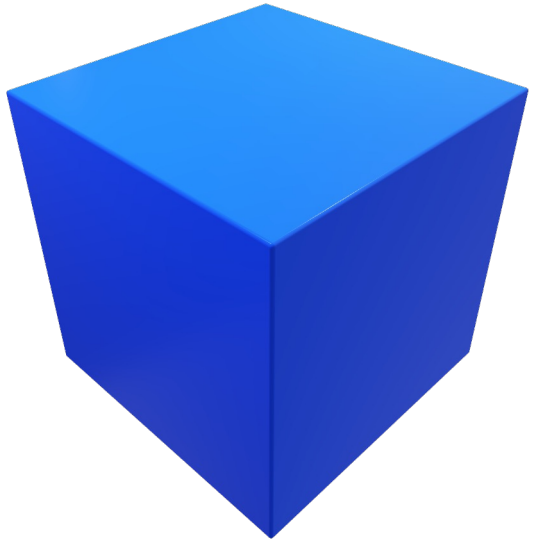
- Would like to be able to model the interactions between large, complex objects efficiently.
- Discrete particle models can also be useful for this purpose! But, there is potentially a large computational cost to doing so.

$\mathbf{r}^n$



$O(n^2)$ interactions per pair

$\mathbf{R}, \boldsymbol{\Omega}$

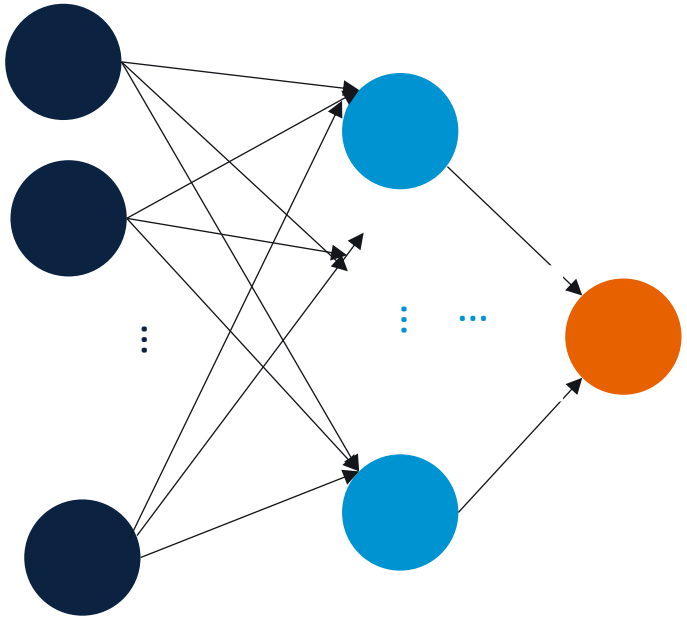


$O(1)$ interactions per pair

# PARTICLE INTERACTIONS

## MACHINE LEARNING

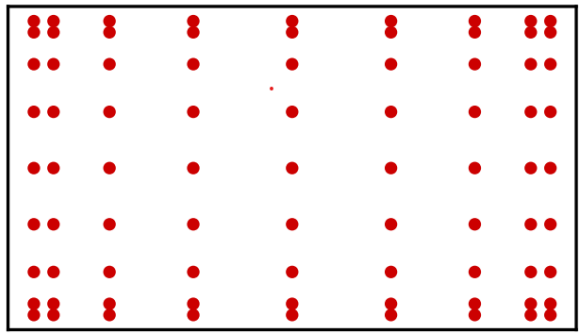
- Goal is to create a mathematical model that approximates the potential energy (or corresponding forces / torques) that are computed from a physics-based model.
- Generic machine-learning (ML) methods need:
  - Descriptors (inputs)
  - ML regression model
  - Training data
- **Developments:** ML methods can work really well for this purpose!
  - Argun et al. used particle coordinates [*J. Chem. Phys.* **160**, 244901 (2024)] or point clouds [*J. Chem. Phys.* **163**, 234120 (2025)] with neural networks.
  - Wilson and Huang [*J. Chem. Phys.* **159**, 024110 (2023)] used mathematically invariant coordinates with neural networks.
  - Campos-Villalobos et al. [*npj Comput. Mater.* **10**, 228, (2024)] used pre-processed descriptors with simple linear regression.
- One drawback: training requires alot of data (millions of configurations).



# PARTICLE INTERACTIONS

## MULTIVARIATE POLYNOMIALS

- **Developments:** We have developed a framework to approximate anisotropic pair potentials using multivariate Chebyshev polynomial interpolation with minimal training data.
  - Sampling strategy + functional form of potential work together
  - Also use physics-informed transformations to improve sampling efficiency further



sampling strategy

$$\hat{f}(\mathbf{x}) = \sum c_i \psi_i(\mathbf{x})$$

functional form

M. Fakhraei, C.A. Kieslich and M.P. Howard. *J. Phys. Chem. B* **125**, 6985 (2025); *under review* (2026).

  - Achieve comparable accuracy to ML models with 2–3 orders of magnitude less data!

- **Opportunities:** Use sparse and/or adaptive sampling, difference learning to reduce data requirements further, implement as software achieving same performance as ML models

# THOUGHTS ON OPPORTUNITIES

- Non-spherical particles (deformation? adhesion?)
- Rough particles (boundary conditions? friction?)
- How to systematically add hydrodynamic interactions to methods when they are known to be missing / incompletely captured?
- Can data-driven models be used for modeling other interactions that are hard to compute but haven't been considered yet (e.g., lubrication, friction, adhesion)?
- Can we capture true polydispersity in both particle interactions and hydrodynamic interactions, not just discrete particle populations? Does it matter?

# ACKNOWLEDGEMENTS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