Wet Systems Consultant Report 2020

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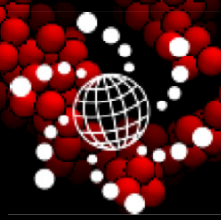
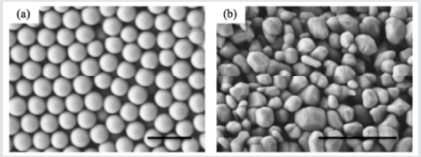
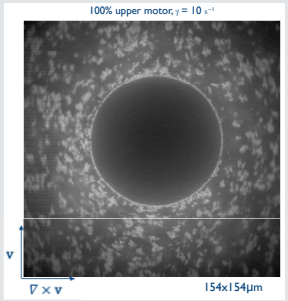


Prepared for

IFPRI

International Fine Particle Research Institute

Wet systems roadmap

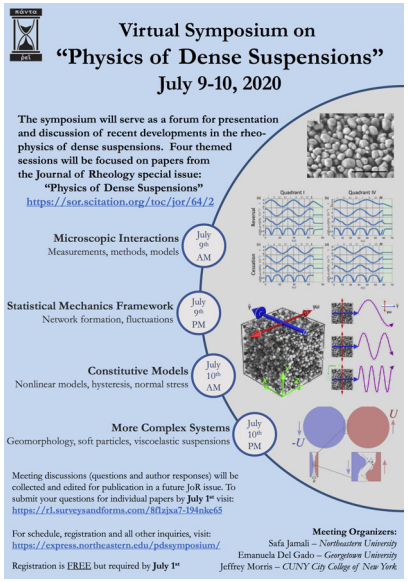
Need	Current work, opportunity, or need
Mechanisms of suspension rheology and stability How can rheology / flow / jamming be tailored, changed, altered, controlled? e.g. adsorbates, surface chemistry, physico-chemistry, particle properties (size distribution, shapes, roughness)	• Connecting structure, composition, particle characteristics to rheology and function (Slurry and Paste Rheology Project) • Tailored rheology with interactions, particle roughness (see SIFs project update)
Model formulations and **model validation** "Is your adhesive hard sphere index-matched monodisperse suspension truly representative of my system?" Effect of fines, polydispersity, roughness, shape, …  Lee et al., 2020	• SIFs project with Jan Vermant (year 1) • Collaboration with Lilian Hsiao (particle roughness)
Rheology and **stability (especially involving changes)** Aging, *formulation changes*, *sensitivity*, *feed variability* Predictable? "How close to edge" is a formulation? "What can go wrong" / "what just went wrong"? Informs accelerated testing? (*months / years* to *days / weeks*)	• Opportunity for **computational models** in close coordination with experiments
Processing flows and **processability** Extrusion, die slip, static zones Complex geometries and flows 	• Imaging dense suspension flows in complex geometries (see SIFs project update) • Opportunity for **computational models** • Microstructure changes in compression (Slurry and Paste Rheology Project)

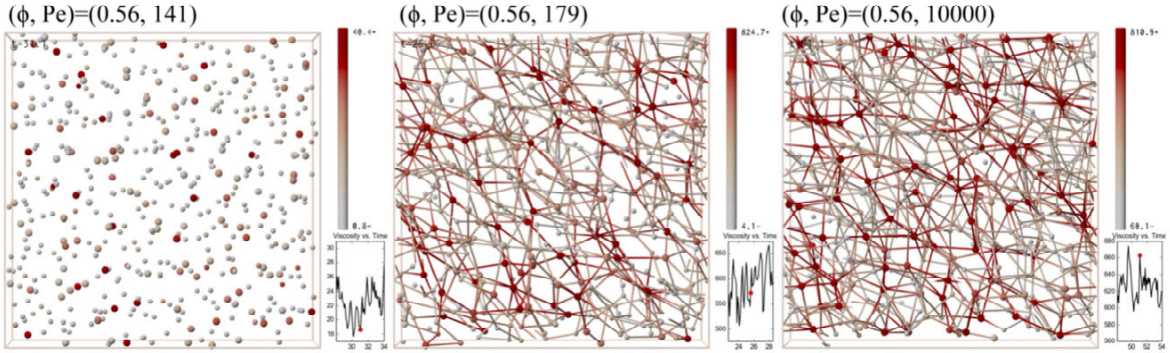
Recent fundamental advances in the field

- Concepts of particle contact, force chains, or force networks have come together in the study of suspensions
- Debate over role of (lubrication) hydrodynamics versus contact friction in discontinuous shear thickening
- New insights into the role of particle contacts, particle surface chemistry

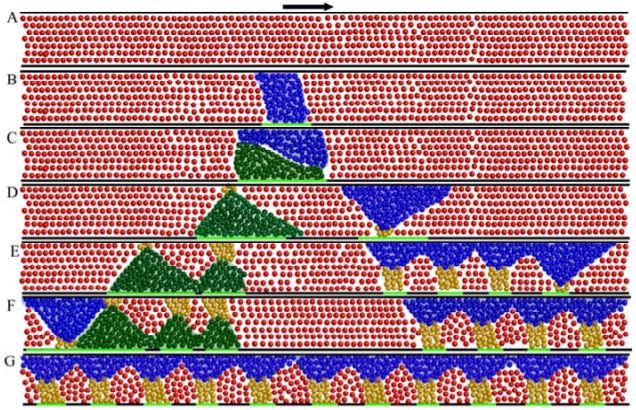
See: Journal of Rheology special issue on the Physics of Dense Suspensions
Volume 64, Issue 2, March 2020

Upcoming: Physics of Dense Suspensions Symposium, July 9-10, 2020
https://express.northeastern.edu/pdssymposium/

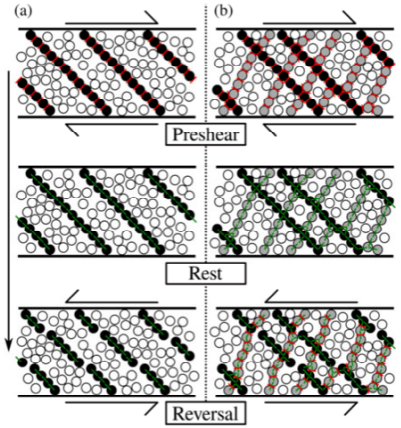




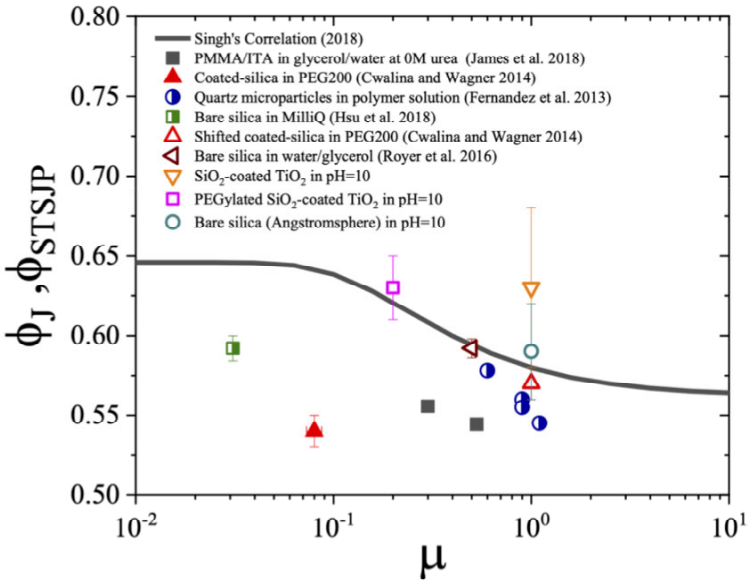
Wang, M., Jamali, S., & Brady, J. F. (2020). Journal of Rheology, 64(2), 379-394.



V. Rathee, D. L. Blair, J. S. Urbach, J. Rheol. 64, 299--307 (2020).



J.A. Richards et al., J. Rheol. 64, 405–412 (2020).



Y. Lee, Y. Luo, S. C. Brown, N. J. Wagner, J. Rheol. 64, 267--282 (2020).

Advances: computational modeling

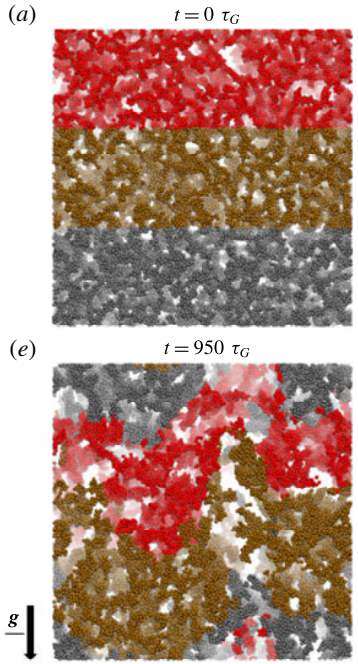
THE JOURNAL OF CHEMICAL PHYSICS **146**, 124116 (2017)

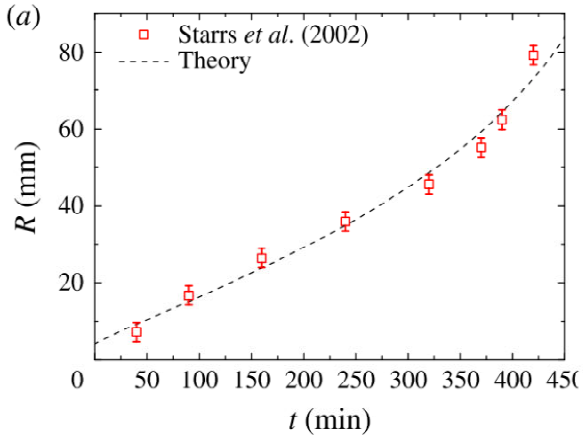
Rapid sampling of stochastic displacements in Brownian dynamics simulations

Andrew M. Fiore,[1] Florencio Balboa Usabiaga,[2] Aleksandar Donev,[2] and James W. Swan[1,a)]
[1]*Department of Chemical Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA*
[2]*Courant Institute of Mathematical Sciences, New York University, New York, New York 10012, USA*

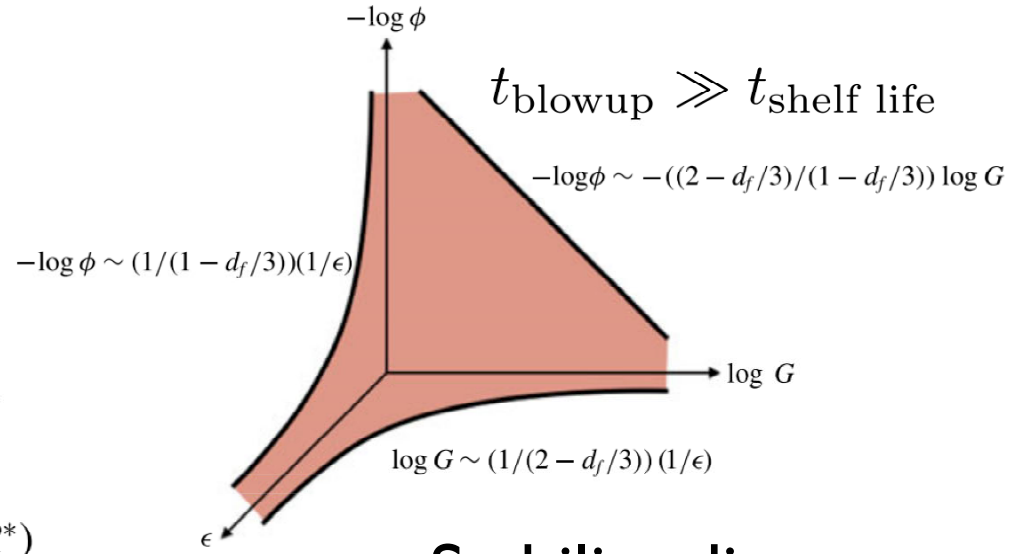
Stability / sedimentation of gels

Z. Varga, J. L. Hofmann, J. W. Swan, J. Fluid Mech. 856, 1014–1044 (2018).





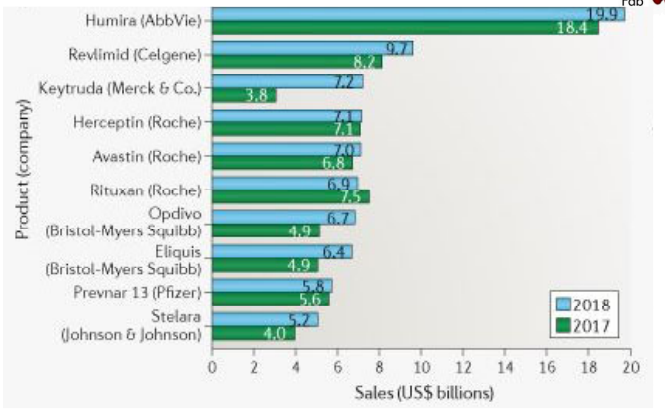
$$\frac{t_{blowup} - t}{t_{blowup}} = \frac{\Gamma(2 - d_f/3, R(t)/R^*)}{\Gamma(2 - d_f/3, 0)}$$

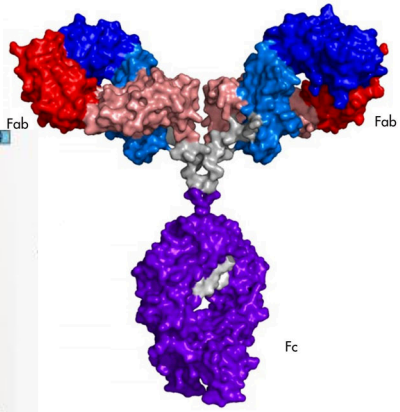


Stability diagram

Opportunity: MAb biologics

Global MAb market valued at ~$135.38 billion in 2018, expected to grow to ~$213 billion at a CAGR of 12.0% through 2022.

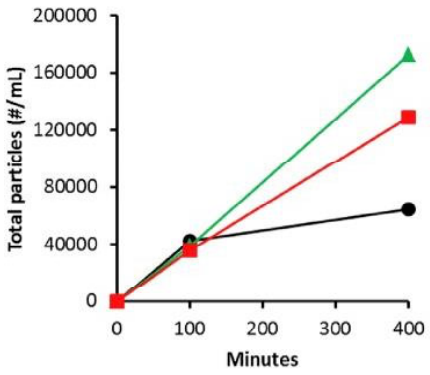


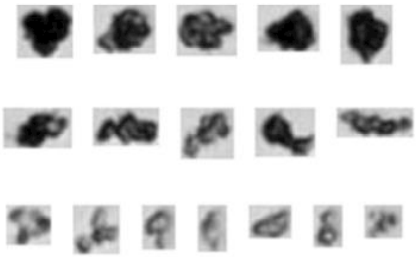


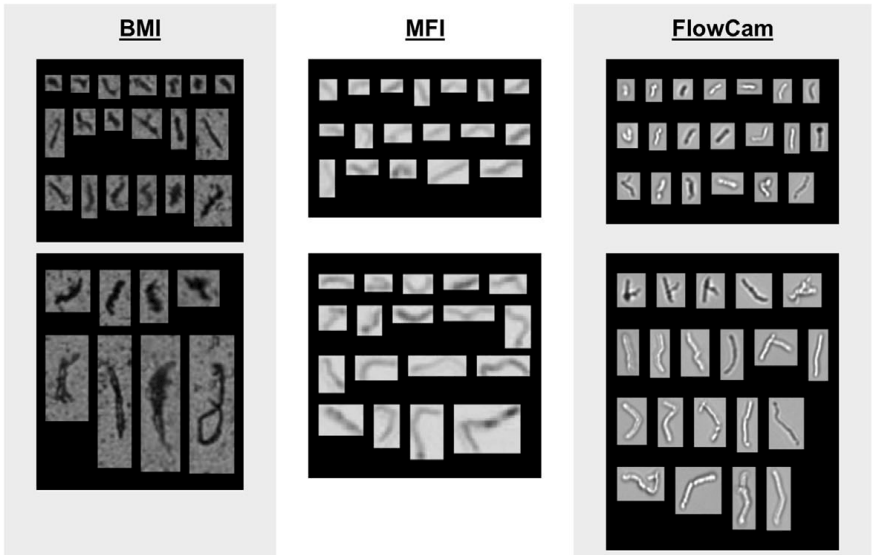
10 mg/mL antibody formulation particle formation

Kiese et al., J. Pharm. Sci., 97, 4347-4366 (2007)

Players in the area: Amgen, Genentech, Medimmune, Janssen, GSK, BMS, … in close supervision with regulatory bodies (e.g. FDA)







- Exogenous particle formation processes, kinetics
- Particle detection and particle characterization

IFPRI Investigators of Interest

PI	Institution	Research portfolio	IFPRI engagement
Lilian Hsiao*	North Carolina State University, Chemical and Biomolecular	Shaped colloids and functionalized surfaces	Active IFPRI collaboration with Vermant, 2019 proposal not selected
Lucio Isa*	ETH, Zürich, Materials	Colloid friction / tribology	Collaborator with Vermant / SIF project
James Swan*	MIT, Chemical Engineering	Computational modeling and theory	2018 Workshop attendee Potential collaboration SIFs
Roseanna Zia*	Stanford, Chemical Engineering	Computational modeling	2018 Workshop attendee
Roger Bonnecaze	UT Austin, Chemical Enigneering	Computational modeling, theory	2018 Report
Emanuela Del Gado	Georgetown, Physics	Modeling and theory of suspensions	None
Arthi Jayaraman	University of Delaware, ChBE/ MSEG	Computational modeling	None
Jeff Morris	City College of New York, Levich Institute	Computational modeling, theory	Wet tribology report (pending)
Dan Blair & Jeff Urbach	Georgetown, Physics	Friction and jamming in dense suspensions	2018 proposal not selected (Blair)
Xavier Chateau	Université Paris-Est / École des Ponts	Pastes, cements	None
Guillaume Ovarlez	Université de Bordeaux	Rheology, shear thickening, non-Brownian suspensions	None
George Petekidis	University of Crete / FORTH	Dense suspension rheology	2019 proposal not selected