Complex Fluids Theory and Simulations

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Summary

- We use theory and simulations to relate microscopic dynamics and structure of complex fluids to their macroscopic properties.

- We collaborate with experimentalists to address mechanisms of phenomena that occur on nano to micro-scale and create tools to predict soft matter behavior.

- The complex fluids that we are interested are transient networks, nanocomposites, and jammed suspensions.

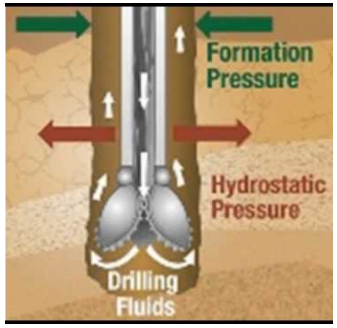
I. Micro-dynamics and macroscopic flow of soft solids

Personal care products

3D printing

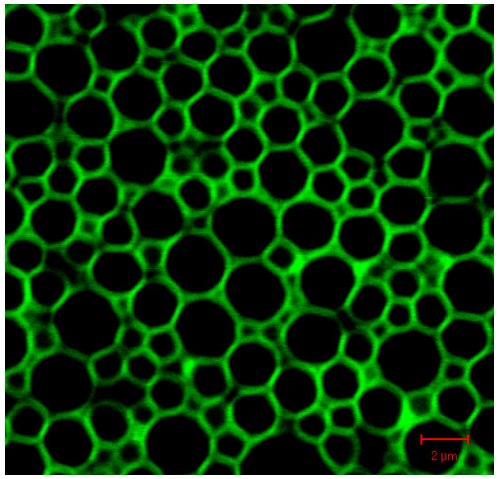
Delivering coatings to paper

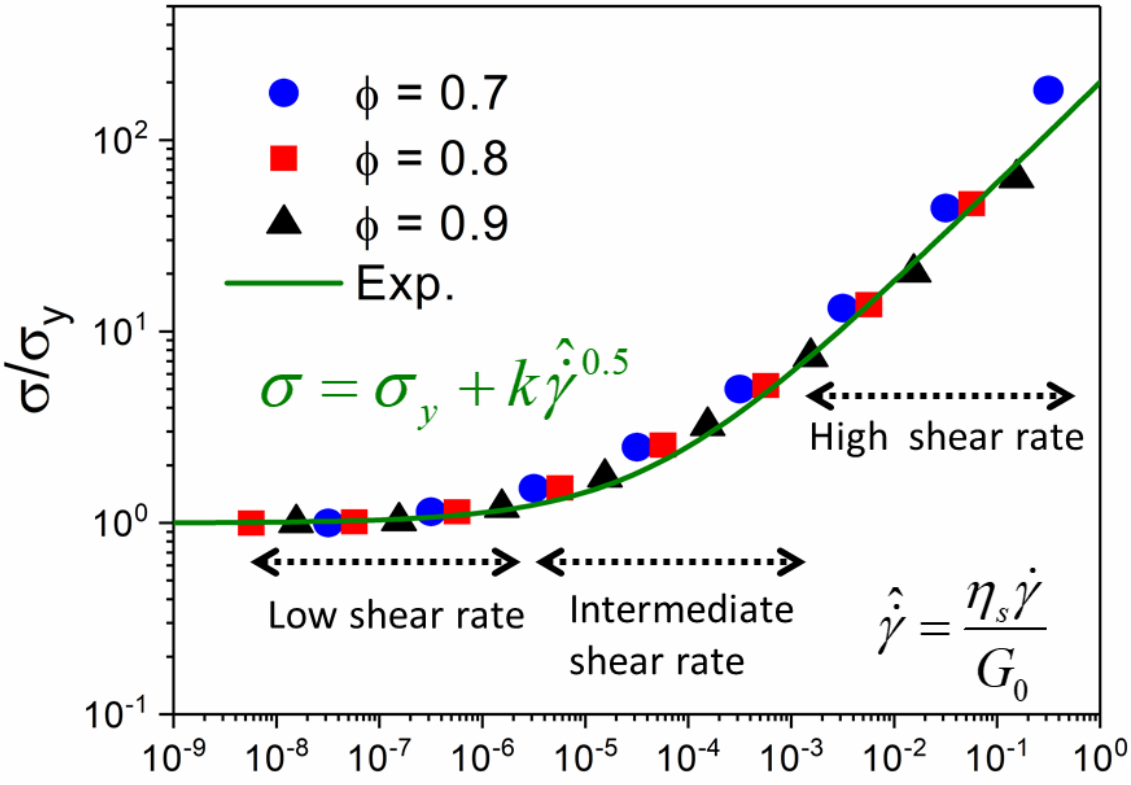
Drilling mud



- More than 10,000 tons for formulation applications
- Drilling fluid market: 1.07 Billion USD in 2017

II. Current understanding





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Liu et al. Soft Matter., 2018.
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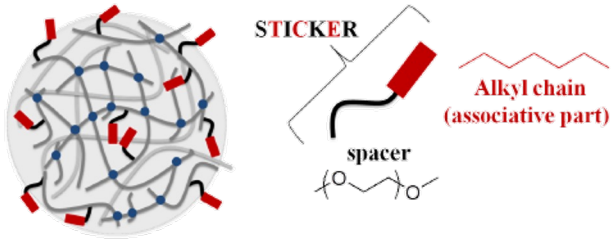
Bonnecaze et al. J. Rheol., 2020.
Khabaz et al. J. Rheol., 2021.
Liu et al. J. Rheol., 2021.
Khabaz and Bonnecaze, Phys. Fluids, 2021.
Di Dio et al. J. Rheol., 2022.

II. Micro-dynamics and macroscopic flow of soft solids

New microgels!



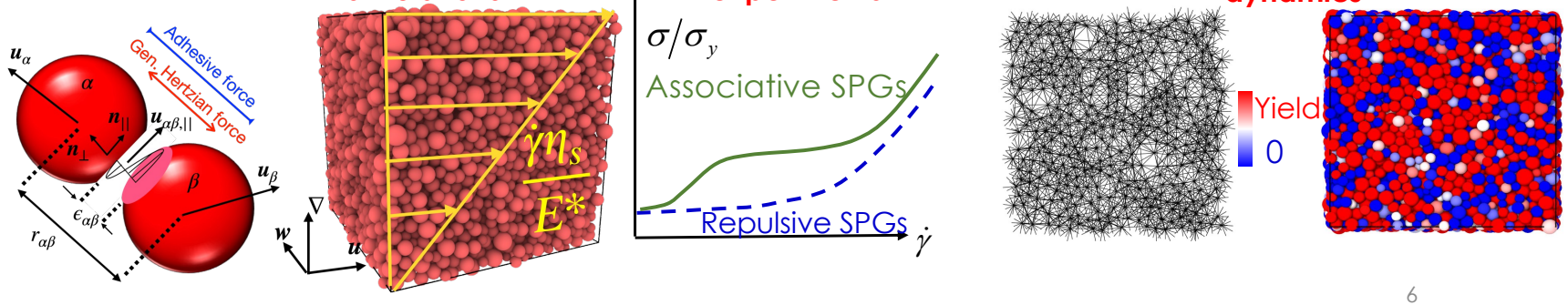
Key factors

- Adhesive forces
- Flow strength
- Residual stress
- Boundaries

Objectives →

- Predict flow curves
- Characterize role of residual stress on transient rheology
- Identify mechanism of DHs and plastic deformation
- Use trajectories to design an ML model to predict localized yielding from the structure SPGs

Build models → **Perform shear simulations** → **Compare with experiments** → **Understand the physics and predict dynamics**



II. NRT-HDR: Graduate traineeship on advances in materials science using machine learning

Goals:

- Discover materials with AI
- Skilled in digital data, AI, ML
- Effective team member in diverse group
- Work in multi-disciplinary setting

Research topics:

- Additive manufacturing of polymeric composites
- Batteries and solid-state polyelectrolytes
- Sustainable and recyclable polymers
- Tuning data management and machine learning tools

Lab rotation:

Collaborators: Profs. Jana, Wang, Duan, Tan, and Cheng

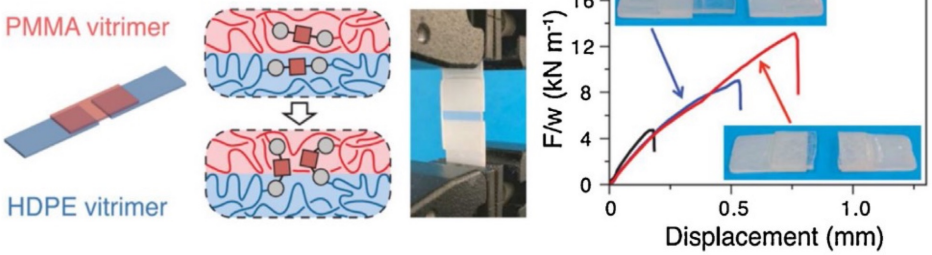
International partners: Germany , South Korea, Japan

External collaborators: AFRL, NASA, Eaton Corporation, Goodyear, Bridgestone

III. Vitrimers: Practical route for reprocessing thermosets

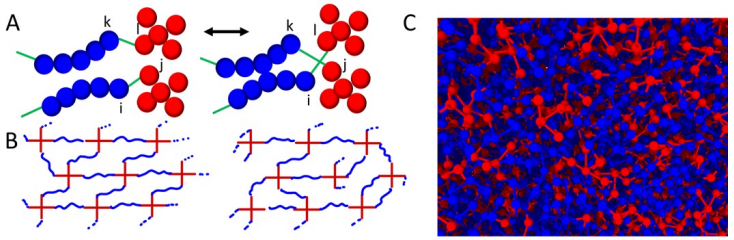
Thermoplastic Thermoset

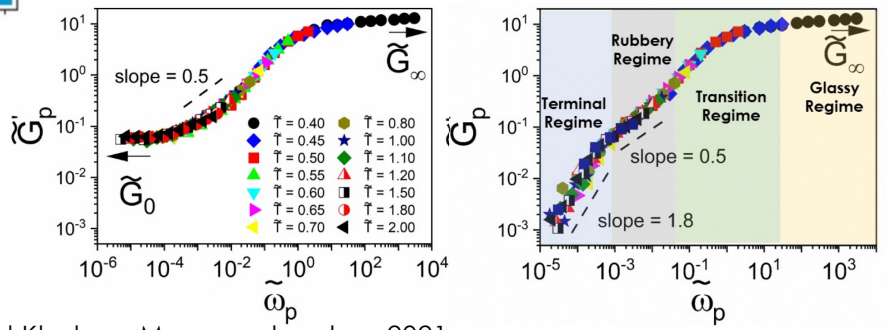
Rheology	Mechanics	Structure and dynamics
Dynamic moduli Flow behavior	Stress-strain behavior in linear and nonlinear regimes Failure and stress distribution	Microstructure under deformation Deformation-induced dynamics



Rottger et al., Science, 2017.

Hybrid MD-MC methodology





Perego and Khabaz, Macromolecules., 2021.
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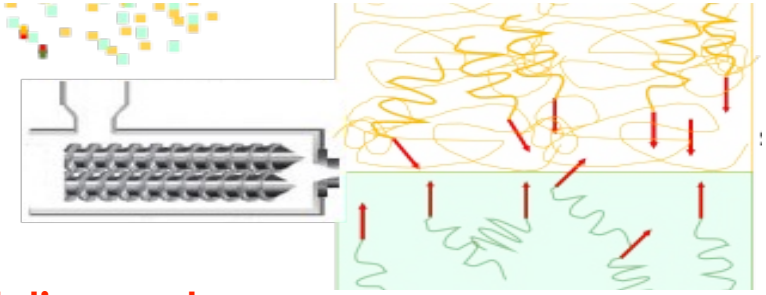
Perego and Khabaz, Macromol. Rapid Commun., 2022.
Perego, Lazarenko, Cloitre, and Khabaz, Macromolecules., 2022.

V. Plastic/rubber recycling: Engineering the interface of incompatible polymer blends

Incompatible polymers in recycled plastic waste stream

Compatibilizers diffuse and reinforce the interface



Simulation goals:

- Computational design of interface compatibilizers
- Dynamics of compatibilizers in immiscible blends
- Mechanics of interface

Other components of the project:

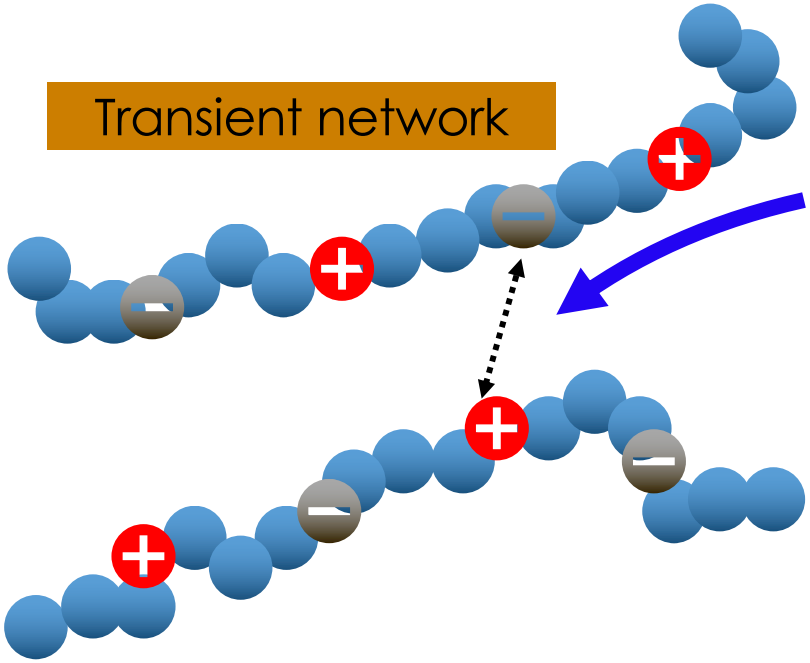
- Synthesis
- Physics of crystallization
- Morphology, crystallinity in the boundary of melt-extruded blends and compression molded laminates
- Mechanics
- Processing

UA: Profs. Jia, Dhinojwala, Khabaz, Jana, Eagan, Miyoshi, and Foster

Industrial collaborator: Braskem

IV. Thermodynamics of shape-memory ionomers

Goal: Understand the mechanism of shape changing and structural relaxation in these systems



How strong are these bonds?

What is the relaxation time of the bonds?

Collaborators: Prof. Cavicchi