Application of meshless simulation methods to study the micromechanics of flows in food systems

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Introduction

Many of the problems in modeling the mechanical behavior of food concern the complex interplay of forces and structures across a hierarchical scheme. In considering a basic emulsion, the inter-molecular forces, the heterogeneous structures, the rheology of constituent phases, the properties at the interfaces, are a few examples of the kinds of considerations needed in its mechanical description. Many problems are quickly reduced by relaxing the criteria for microscopic details or scale, and assumptions are introduced. But the study of food deconstruction (i.e., oral processing and digestion) stands out due to strong mechanical coupling across several magnitude orders of time and space remains important.

It is the purpose of this paper to show the capability of meshless numerical methods in applications of complex fluids and food deconstruction, particularly for considering the micromechanics and constituent morphology in a flow. A smoothed particle hydrodynamics (SPH) numerical method is presented and is applied to a sweep of parameters typically studied in the rheology of complex fluids (volume fraction, mechanical properties of constituent phases) and, when appropriate, the results are compared to analytical models. Additionally, the micromechanics and the interactions of solids to form force chains are interpreted. Finally, the advantages of an all-particle framework over mesh-based methods are discussed.

Methodology

Forces acting on particles are summed over the neighboring particles based on a kernel collocation method close to the original smoothed-particle hydrodynamics (SPH) technique [Monaghan 2005]. The total Lagrangian SPH (TLSPH) computes stresses from an approximated strain tensor and attaches particles to a reference frame to apply plastic deformation criteria. The Langrangian implementation with an hourglass correction permits large elastic and plastic deformations for modeling of soft and hard solids [Ganzenmuller 2014]. The simulations are carried out in LAMMPS [Thompson et al. 2022] and the developments are included in an open-source project, Pizza3 (github.com/ovitrac/Pizza3). Simulations, as shown, typically contain 100,000 particles and are executed in less than 30 minutes across 16 cores.

Results

The typical results on shearing suspensions are illustrated in Fig. 1, showing solid-solid and solid-fluid interactions. Deformable solids can be directly simulated (Fig. 1 (a-b)) or can be part of a multiphase system. More material properties are accounted for in the description of the solids than would be achieved with even a sophisticated discrete element method, and stress fields in the particles and at the walls arise spontaneously. Stress signals from nodes at the wall are analyzed to study the relationship between local wall events and system micromechanics, such as the presence and size of solid force chains.

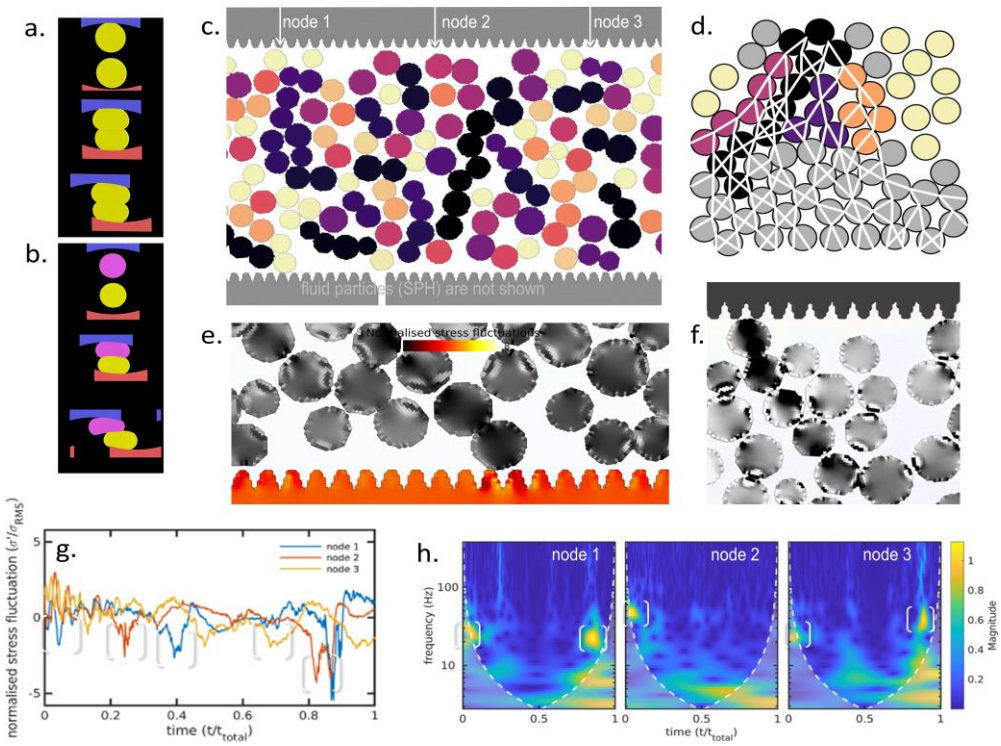

Figure 1 : (a-b) two extreme behaviors of solid deformable particles (a=adhesion, b=slip); (c-d) principles of force chain transmission in the suspension. (e-f) Details of stress fluctuations at the wall within particles. (g-h) Time-frequency stress response at nodes 1,2,3

Conclusions and Perspectives

Using entirely Langrangian-based methods to fully describe multiphasic flow is more commonly considered in the context of molecular dynamics (MD) simulations and thus sub-micron scales. The high level of research activity around Lagrangian methods from a continuum discretization combined with the growing fields of applications can partly be attributed to the ease of applying them to problems with complex boundary dynamics – typically challenging for mesh-based methods. The use of particles also simplifies massive parallelization with mature computational techniques from MD.

The SPH technique alone, applied to complex flows, simulates rheological and micromechanical phenomena to a level of detail not typically studied. Future work will explore the ability to leverage an all-particle description by transforming one particle species to another (e.g., solid to fluid). Predicting these transformations through a concurrent multiscale simulation approach is key in recovering details of forces from lower scales and coupling the microscopic and macroscopic phenomena, one such example being considered is to use Dissipate Particle Dynamics to model interface surfactants.

References

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