Multiscale framework to simulate interactions in food systems from the chemical to the mechanical space: a step towards in-silico digestion

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Food's physicochemical and mechanical breakdown during oral processing and digestion is invariably complex. Many scales must be considered simultaneously: macroscale for hydrodynamics, mesoscale for structures, and microscale for thermodynamically- and composition-driven phenomena. The soft matter community has developed a wealth of Lagrangian simulation methods, but they fail to meet the time and length scales of food and oral processing. We propose to map the efficient smoothed particle hydrodynamics (SPH) framework onto more detailed ones capturing chemical details. The SPH methodology has several flavors adaptable to solid and liquid behaviors. They offer dramatic performance gains and predictions in the mechanical space of food (flow, macroscopic mixing, and fracturing). In the chemical and physicochemical spaces, acceptable predictions can be recovered only after proper parameterization, either from experiments or detailed simulations. This work explores a parameterization from Dissipative Particle Dynamics (DPD) to recover adhesion, lubrication, and non-ideal behavior in the chemical space.

The conditions for shadowing DPD simulations with SPH ones are shown for different strategies involving pure SPH particles, rigid and soft particles interacting only via Hertz contacts in a virtual viscosimeter (to measure stress at wall and shear viscosity), tribometer (to recover a pseudo Stribeck curve) and back-extruder (global texture assessment). The capacity of mapped SPH simulations to effectively study complex phenomena in foods is illustrated on solid and soft suspensions under shear and compression. The tunning of interactions between solid particles enables to reproduce flocculation and, in some ways, gelation. The mechanical behavior of simulated Pickering emulsions obtained with SPH-DPD framework is compared with experimental results. The framework is available as an open-source project for LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator, Sandia Laboratories, USA): https://github.com/ovitrac/Pizza3. Finally, the key steps to simulate the breakdown of insoluble food pieces during mastication and bolus transport in the digestive tract are detailed.