Molecular Dynamics-like approaches and many-body forcefields as a universal strategy to simulate food from processing to deconstruction

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In the context of food, Molecular Dynamics (MD)-like methods assume that "food atoms" can be attached/detached, mixed, and react with other "food atoms" to build food structures, predict/visualize food fracturing, analyze the interactions between food and body fluids (saliva, bile salts), understand the critical steps of the contamination by food packaging substances... This lego-like interpretation of food science and engineering is poised to revolutionize the field by adapting coarse-grained models not designed to build systems at the irreducible atomistic scale but at meso to continuum scales.

The presentation shows the versatility of the approach to simulate complex structures and their evolutionary, transport, and reactivity properties in the presence of complex mixtures. The development of accurate forcefields is generally hampered by the need to encode the food's thermodynamic response and physical state in many interatomic potentials. Machine learning and many-body potentials are presented as a comprehensive and consistent alternative capable of providing dynamic simulations shadowing microscopic observations in near real-time. These new "food atom" potentials can be derived in two different ways: from numerical simulations conducted at a much lower scale (possibly with another coarse-grained but more detailed forcefield) or from displacement/deformation fields inferred from dynamic microscopic/macroscopic observations. It is shown that the first approach is preferable during digestion when the essential chemical information and micellar structures are not experimentally accessible and must be reconstructed from detailed simulations. The second approach works well on mechanical problems involving fluid-fluid (e.g., emulsions, foams) and solid-fluid (e.g., suspensions, gels) interactions but also for coupled flow-reaction problems, as exemplified in our study of thermooxidation during deep-frying. Various studies exemplify how our results can be transferred to various food contexts with reasonable computational power via our open-source project Pizza3 for LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator, Sandia Laboratories, USA). The project abstracts several food-specific tasks: converting experimental images into "food-atoms," setting food systems as a collection of "food-atoms" with desired shapes and distributions, and derivating new "food-atom" forcefields from existing ones. A static interpreter facilitates the implementation of programmatically defined complex moves and actions such as those met during food processing, oral processing, and digestion.