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APPLICATION OF NOVEL MESH-FREE TECHNIQUES FOR THE SIMULATION OF MECHANICAL PROBLEMS IN FOOD

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ABSTRACT

Mechanical modeling in foods and, more generally, food engineering has been challenging. The most commonly invoked difficulties are the lack of properties tabulated specifically for food problems and the presence of soft matter structures associated with weak molecular interactions. Mechanical descriptions are essential for predicting food deconstruction, such as texture perception and digestion. The complications are numerous: large deformations, free surfaces, colligative properties, coupling between mechanics (fracturing), and thermodynamics (dissolution, swelling) above and below the thermodynamic limit (TL). Eulerian descriptions coupled with continuum descriptions are difficult to implement when more than one scale is involved, and the number and geometry of domains evolve with time. The study presents a new and flexible framework to simulate free flows, rigid/deformable/breakable suspensions interacting with rigid walls or moving objects. The methodology relies on a smoothed particle hydrodynamics formulation with particles moving independently beyond a critical distance and an updated version to describe elastic and plastic deformations in solids. The framework is illustrated on three typical problems, and its predictions are compared to known theories. Its integration with approaches below TL is finally discussed.

INTRODUCTION

In the 60-years prior, many manufacturing industries have transformed their design processes to benefit from Computer-Aided Design (CAD) and Computer-Aided Manufacturing (CAM) techniques. However, the benefits are still not felt evenly across the board, and particular classes of problems cannot be fully addressed with such approaches. Solid and semi-solid chemical engineering products and bioproducts, including food products, exhibit several difficulties (Kalakul et al. 2018; Zhang et al. 2017). They are self-organized, and their macroscopic properties span over several scales.

The soft-matter properties of such products require the use of a particular branch of physics involving ongoing theories and statistical mechanics (van der Sman 2012). In short, the many-component and -phase problem slowdowns the convergence of microscopic properties to asymptotic ones. In addition, some free-energy-driven evolutions may alter the locality principles, as observed during swelling/shrinkage, fracturing/dissolution (Battiato et al. 2019). Closure problems remain particularly difficult, and formulations using two or more scales are generally poorly adapted and flexible in the logic of tailoring predictive approaches. In general, CAD and CAM approaches should be easier to implement than the trial-and-error approaches they are supposed to replace.

This work explores variations of Smoothed Particle Hydrodynamic (SPH) simulation techniques to simulate fluids-solids and free-surface interactions with Lagrangian formulations. A flavor developed at the Ernst Mach Institute coined SMD, or Smooth Mach Dynamics, implements a total-Lagrangian formulation well adapted to large deformations and fracturing of solids (Leroch et al. 2016). The advantages are multiple; a meshless MD-like “Molecular-Dynamics-like” formulation can be used interchangeably with transported solids, moving walls, and flows using massively parallel open-source packages like LAMMPS (Thompson et al. 2022). This repurposed package was chosen to build an integrated environment to simulate mechanical, mass transfer, and flows in foods above and below the thermodynamic limit (TL).

The manuscript presents the mesoscopic formulation above TL for three representative classes of problems, with the intent of evaluating the accuracy and possible deviations of the combined SPH+SMD framework. It is organized as follows. The following section introduces the three types of particles considered and their pair-interactions: SPH-type, SMD-type, and wall-type. The chosen case studies, inertial flow with free surfaces, back extrusion, and solid-in-liquid suspension, were chosen for their general interest in food and the existence of reference analytical solutions. Section three analyzes the performance and accuracy of the simulations. Finally, the last section summarizes the findings and future works.

NUMERICAL METHODS

Overview

Problems of multiphasic simulations remain very challenging, and highly dynamic systems with immiscible fluids or deformable and breakable solids are avoided. Eulerian mesh-based methods such as Finite Element and Finite Volume descriptions become prohibitively expensive to apply to rapidly evolving interfaces of multiphasic systems, and specific Lagrangian methods circumvent the problem.

Several Langrangian formulations exist to represent fluids, and soft matter, including DPD or Dissipative Particle Dynamics and its variant, Smoothed Dissipative Particle

Hydrodynamics (SDPD) (Español and Warren 2017), SPH or Smoothed Particle Hydrodynamics (Violeau and Rogers 2016) coupled or not with DEM or Discrete Element Methods (Cundall and Strack 1979). Recently, Karunasena et al. (2014) aggregated SPH-DEM-based individual cells to describe morphological changes of plant tissues during drying. The formulation requires defining seven types of force interactions: cell wall stiff forces, wall damping forces, wall-fluid attraction and repulsion forces, non-bonded wall-wall repulsion forces, forces due to the bending of the cell wall, and to concentrate cell wall during drying. These artificial or mesoscopic forces do not match macroscopic stresses and cannot be parameterized from bulk properties.

This work generates complex solid shapes by clustering particles/atoms, such as in DEM, but by keeping a continuum mechanics formulation. They can be subjected to elastoplastic behavior and even broken. All solids (rigid or deformable) interact with themselves or with fluids through Hertzian overlap potentials, directly related to Young's modulus for a solid body or the bulk modulus for a liquid. Three generic particles were considered:

- SPH particles represent Newtonian liquids such as water: the particles move almost independently (updated Lagrangian) under the constraint of an equation of state to simulate a weakly compressible fluid.
- SMD particles can be glued together to represent a continuous solid/object; they follow the object's global displacements/rotations and deformations (total Langrangian); fracturing may also occur if the mechanical stress reaches a threshold.
- Rigid wall particles are placed in a fixed configuration that can be static or translated/rotated during a simulation.

For the total Lagrangian SPH formulation adopted in SMD, each particle is defined by its position, velocity, Cauchy stress tensor, and Green-Lagrange strain tensor. An equation of state closes the system parameterization for computing the pressure (the diagonal terms of stress tensor) and a material model to compute shear stresses (the off-diagonal terms of the stress tensor). Damage and failure models can finalize the description of solids.

As for the updated Lagrangian SPH formulation, continuous bodies are represented by an ensemble of discrete particles:

- Particles have their mass and can move freely relative to each other; properties such as pressure are calculated at the center of each particle based on the weighted contributions of its neighbors
- As such, it directly calculates properties of the continuum and can completely forgo fluid boundary tracking, making it particularly advantageous for simulations with large boundary displacements
- The discretization process leads to specific difficulties, such as forming a smooth surface out of beads or capturing small geometry details in simulations

It is important to note that other meshless discretizations of continuum mechanics formulations exist (e.g., Peridynamics), but SPH has the advantage that the descriptions are readily implemented for both solid and fluid continuums, allowing consistency in processing and interpreting the results.

Smoothed Particle Hydrodynamics (SPH) formulation

SPH methodology can be seen as a variant of DEM methods for fluids instead of granular materials. The concepts of collisions are replaced by overlapping particles associated with weighted kernel functions. The quasi-compressible formulation adopted here is like the one described by Monaghan (2005). As discussed by Cleary Paul et al. (2013), it requires (i) a proper definition of the compressibility of the medium to avoid unphysical behaviors (local explosions at the free surface in regions under tensions); (ii) an artificial limitation of excess velocities to limit numerical diffusion and the jiggling of particles; (iii) fluids with similar densities due to the smoothing of pressure waves across interfaces.

Smooth Mach Dynamics (SMD) formulation

SMD is an analogous kernel-based collocation solver for elastoplastic solid problems. It has been described extensively by Ganzenmüller (2015) and by Ganzenmüller et al. (2016). In early implementations, it was noted that the number of integration nodes was insufficient to enable a stable integration of equilibrium equations. The total Lagrangian formulation resolves the issue whatever the arrangement of the particles and the type of mechanical deformation and even under large strains. The way materials points are connected does not change for elastic deformations, whereas the topology is updated for plastic deformations, and the reference coordinate system is reinitialized.

Implementation

The presented methodology is based on the USER-SMD package of LAMMPS, which uses the SPH formulation from continuum mechanics to model fluids and solids. The discretized equations take a form similar to those of molecular dynamics (MD), therefore making it possible to repurpose LAMMPS from a MD simulator. LAMMPS has been developed with the intention of performing massive MD simulations but is open-source, highly sophisticated, and designed to be extended, and the compromise is deemed acceptable the goals of the research.

The SPH, SMD, and rigid particle types are implemented natively in the USER-SMD package. A modification has been made to take advantage of restart files that allow launching a simulation from an initially equilibrated configuration. The initial configurations were made using the ATOMSK (Hirel 2015) package. Post-treatments were done by combining tools in MATLAB and Python with Ovito visualization capabilities.

CASE STUDIES

Mesoscopic modeling combined with SPH simplification is known to cause many approximations, which justify a systematic study of biases and errors. Among them, the considered SPH flavor and fluid-solid interactions implement only pseudo-viscosity. Hertz contacts do not enforce a no-slip condition at walls. The spherical symmetry of collocation kernels introduces a poor approximation of gradients close to boundaries and interfaces. The small number of particles may affect the preservation of momentum and numerical stability in narrow spaces. In the absence of surface tension, the continuity of fluid-air interfaces cannot be enforced.

Table 1. Details of case studies with increasing complexity

Case study	Type of particles	Ideal behavior	Non-ideal behavior	No. of part-icles	Comp. time (≤16 cores)
A. Torricelli tank flow	SPH and rigid wall (fixed)	Pure inertial flow (unsteady)	Pressure loss within the nozzle	3e5	1h
B. Back-extrusion	SPH and rigid wall (moving)	Incompress-ible flow with flow inversion	Slip at boundaries	5e5	1h
C. Shear of solid-liquid suspension	SPH, SMD, and rigid wall (moving)	Viscous flow	Percolation threshold	1.2e5	15m

The studied cases are summarized in Table *1* and illustrated in Figure *1*. Studies were chosen to exacerbate the specific effects in simulations while directly comparing exact solutions when they exist. They are presented in ascending complexity such that the equivalent simulation in an Eulerian scheme becomes less tenable.

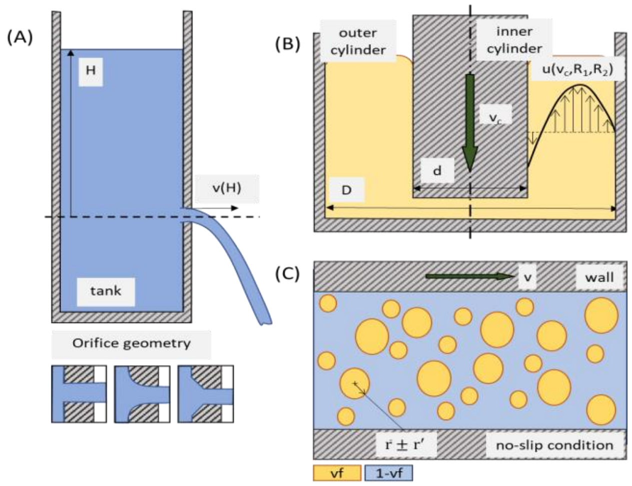

Figure 1. Case study (A): Overview of the flow configuration with different orifice geometries. The height H is measured from the centerline of the orifice. Case studies (B) and (C). See Table 1 for details.

Case-study A: Torricelli tank flow

Case-study A is a pure mechanics problem enabling the isolation of error sources when parameterizing SPH simulations. Based on Torricelli's law, it expresses the conservation of mechanical energy as the linear relationship between the outflow velocity, v, and the square root of the fluid height above the tank nozzle, H. The frictional losses at the orifice depend on the flow, shape, and roughness of the orifice. Finally, the discharge velocity reads:

$$v = C\sqrt{2gH} \qquad (1)$$

Where the coefficient of discharge, C, is a free parameter, typically ranging between 0.6 and 1.0 (see Figure *1*A and discussion in White (2016)). g is the gravitational constant.

Case-study B: back-extrusion

Case-study B mimics an experimental device and protocol used commonly to determine bulk viscous properties of food (Perrot et al. 2011). Fakhari and Galindo-Rosales (2021) developed the analytical solutions shown below for Newtonian flows. The Newtonian laminar velocity field between an axially shearing annular flow reads:

$$u = \frac{C_1}{2} r^2 + C_2 \ln(r) + C_3 \qquad (2)$$

$$C_1 = -8v_c \frac{D^2 - d^2 + 4d^2 \ln\left({}^{d}/_{D}\right)}{(D^4 - d^4)\ln\left({}^{d}/_{D}\right) + (d-D)^2(d+D)^2}$$

$$C_2 = v_c \frac{D^2 - 3d^2}{(D^2 - d^2)\ln\left({}^{d}/_{D}\right) + D^2 - d^2}$$

$$C_3 = v_c \frac{D^2(D^2 - d^2) + (D^4 - 4D^2d^2 + 3d^4)\ln(2) + 4D^2d^2\ln(d)}{(D^2 - d^2)^2 + (D^4 - d^4)\ln\left({}^{d}/_{D}\right)}$$

Case-study C: shear flow of a solid-in-liquid suspension

Case-study C was designed to represent a monodisperse suspension of solid particles in a shear flow close to the percolation threshold. The simulations were conducted in 2D to emphasize solid-solid interactions, whereas case studies A and B were simulated in 3D.

The following elements of validation and consistency were considered: flow rate with the decreasing heights (study A), radial velocity profiles within the gap (study B), fluctuations of normal stresses at rough walls (study C).

RESULTS

Case-study A: Torricelli tank flow

The simulation was executed with 300,000 SPH particles in a rigid container. Before the particles were allowed to leave the container, the system was relaxed from its initial state to form a static reservoir. The orifice was created with a diameter of ten times the particle diameter. The exit velocity was calculated as the mean x-velocity of the particles between the orifice exit and a half tank length from the orifice.

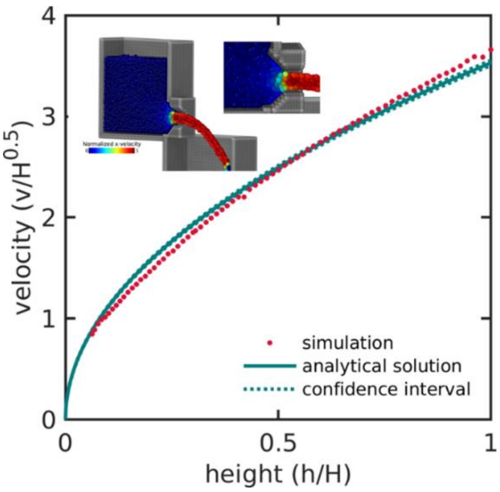

Figure 2. Normalized velocity $v(t)$ vs. the residual height $h(t)$ in the tank. The image shows a cross-section of the simulation and a closeup of the cone-shaped nozzle used.

Simulations and theory were in good agreement when the results were fitted to an effective discharge constant $C = 0.80$, and a normalized height $h/H > 0.1$. Equation 1 is predictive for cases where the velocity inside the tank is much smaller than v. When h approaches the vertical width of the orifice, causing a surface flow inside the tank, Eq. (1) breaks down, and simulation deviates from theory.

Case-study B: back-extrusion

Figure *3* presents the simulation of 500,000 SPH particles in a rigid cylindrical container, forming a tank of liquid subjected to back extrusion. The system is relaxed from its initial state until the fluid is static, then the inner cylinder is pushed into the liquid, forcing it to flow into the gap between the cylinders, where an annular flow develops. The relative downward displacement of the inner cylinder draws adhering particles in the opposite direction of the net mass flow upwards. Due to the low compressibility of the system, the net flow is equal to the displaced volume of the inner cylinder.

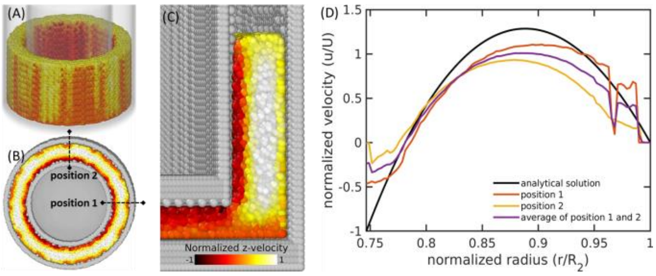

Figure 3. (A-C) Simulated configuration when 80% of the volume is extruded and velocity profiles back-mapped on particles and (D) radial z-velocity profiles in the gap in the vertical direction at 50% of the height.

The simulation shows some resemblance to the analytical solution, but velocity near the boundaries does not effectively reproduce the non-slip condition expected for the flow, and this is a well-known challenge when implementing the SPH method (Shadloo, Oger, and Touzé 2016).

Simulated velocity profiles fluctuated around the inner cylinder and were not perfectly axially symmetric. These deviations were associated with the slight compressibility of the SPH formulation and the generation of the surfaces from lattices, preventing constant friction at the wall. The absence of permanent contact with the surface causes the velocity of particles near walls to fluctuate. Remarkably, though the simulation does not implement tangential forces at the wall, the collisions with the beads representing the surface partially reproduced the no-slip condition without enforcing the concept of adhesion or surface energy. Similar effects are observed in MD simulations using purely repulsive forcefields. Elastic collisions transport momentum satisfactorily and lead to a realistic annular velocity profile presenting strong similarities with theory.

Case-study C: shear flow of a solid-in-liquid suspension

Figure *4* details a sheared 2-phased suspension consisting of 121,000 particles distributed as 56,000 SPH particles for the continuous liquid phase and 65,000 SMD ones for the dispersed elastic phase. The rough surface was prepared with rigid wall particles assembled in a sinusoidal pattern. The height and period of the pattern were smaller than the circular objects in suspensions representing either rigid globules or solid particles. Periodic boundary conditions enabled to simulate steady flows. The suspension concentration was close enough to the percolation threshold in 2D to observe correlated displacements between objects subjected to opposite displacements. Figure *4*A shows an example of frequent configurations, where close packaging allowed stress fluctuations to propagate through touching particles and across the flow. The transient configuration demonstrated that flowing objects could self-organize to dissipate stresses. These macro-clusters or strings could involve up to 12-15 objects, whose periodic impacts with the walls were recorded and shown in Figure *4*B and C. The effective medium, including SPH and SMD-based objects, behaved collectively as compressible flow subjected to shearing, as experimentally observed by Dbouk, Lobry, and Lemaire (2013). Simulations were highly consistent with experiments. Shear-induced particle/object migration and their contribution to normal stresses at the walls were carried by direct contacts even in the absence of thrust.

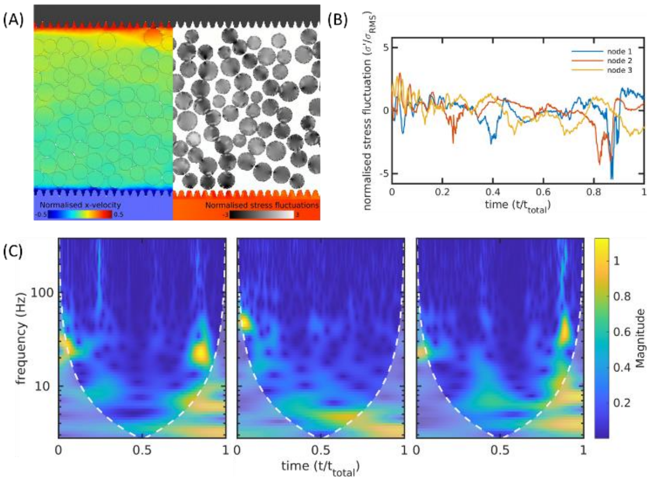

Figure 4. (A) the mid-frame of the simulation with a split color field, the left giving the x-velocity normalized by the velocity of the shearing walls. The right gives the stress fluctuations normalized by the root mean square of the stress fluctuations. (B) Von Mises stresses for three equidistant positions on the bottom wall. (C) Corresponding scalograms of mechanical signals at the wall.

CONCLUSIONS

The simulation scheme using three types of particles to represent unsteady flows in the presence of complex stresses and solid-fluid interactions is highly versatile and flexible. It reproduced the evolution of systems out of equilibrium remarkably. The systems could be made unstable either by the large amount of kinetic/mechanical energy dissipated in a short period or by the self-organization of heterogeneous systems. Generic molecular-dynamic-like codes such as LAMMPS offer a practical methodology to transfer momentum and preserve mass; SPH and SMD formulations bring additional concepts from continuum mechanics, including an explicit representation of stresses and strains. Simulations can be set up from any threshold images or 3D meshes for spatial resolutions ranging from micrometers to meters or more. Most computations can be set up in a couple of minutes and executed with reasonable computer power

(~16 cores) for up to one million SPH, SMD, or wall particles. Comparatively to MD-like techniques, coarse-graining and dimensionless formulation accelerate explicit integration by several orders of magnitude. Even in the absence of sophisticated formulations for viscous behavior (pseudo-viscosity) and interactions with solids (Hertz contacts), several relevant features such as the non-slip condition, pressure drop, interactions in the cluttered flows emerged from simulations. Therefore, the presented approaches are particularly suitable for describing the early stages of food deconstruction and digestion. The macroscopic behavior of dispersions of solids-in-fluid is well described below mechanical rupture. Changing the mechanical properties during simulation will open the possibility to simulate the change of states (solidification, partial crystallization), and aggregation.

PERSPECTIVES

The proposed description uses the concepts of continuum mechanics, and the described fluctuations do not have a thermodynamic origin but result from numerical artifacts related to the fluctuation of the density between the collocation points that represent the particles. The natural evolution of a fracture process towards a dissolution and swelling process requires combining the current description with refined descriptions below the thermodynamic limit. The low computational cost of the current mesoscopic simulation will allow SPH and SMD with localized simulations, where a small group of particles in a neighborhood is converted into smaller particles of type SDPD or DPD. The current work aims to develop a multiframework concept where particles obeying different scales and physical mechanisms are simultaneously simulated in replicates. An example of such constructions above and below the thermodynamic limit is sketched in Figure *5*.

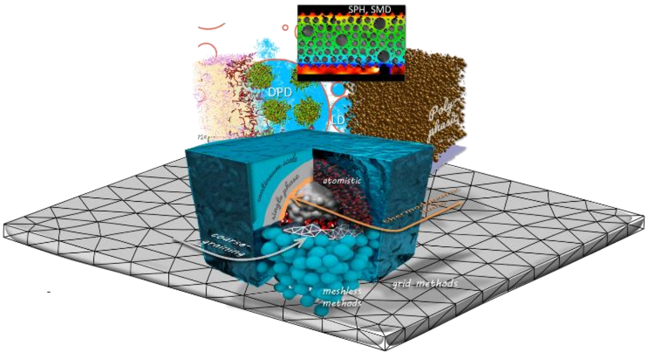

Figure 5. Example of concurrent simulations with particles describing the evolution of a system at different scales.

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