Franco-American project Group Modeling and Computational Engineering

Ph.D. Thesis offer 2022 | Funded by a Franco-American project

Microscopic images converted into dynamic mesoscopic models: application to mechanical food deconstruction

Summary

Microscopic 4D (x,y,z,t) or 5D (dynamic spectral images) techniques and mesoscopic modeling are becoming versatile techniques. This Ph.D. thesis proposes to combine the two approaches to parameterize mesoscopic models of food constituents that would allow the direct simulation of the mechanical deconstruction of food. The central idea is to convert the deformation or velocity field observed in the field of a confocal microscope into parameters of hybrid models mixing **updated and total Lagrangian SPH** (*smoothed hydrodynamic particles*) methods. The work aims at optimizing the mechanical solicitation protocol and the microfluidic cell to maximize the identifiability of soft matter mechanical behaviors.

Research context

With high-performance and cloud computing development, modeling and simulation are thought to play an increasing role in almost all manufacturing activities. The food industry and products case may look anecdotal, but it is not. The success of homo sapiens as a biological species came from our capacity to feed and sustain its population and environment. The food industry is the leading manufacturing industry and the first industrial employer in developed countries. As shown in **Figure 1**, food engineering and its prediction tools contributed to reshaping this industry. The next frontier links sensory, nutritional values, well-being, and health. **Mesoscopic modeling is the cornerstone of new approaches enabling us to foresee the fate of food inside our digestive tract.**

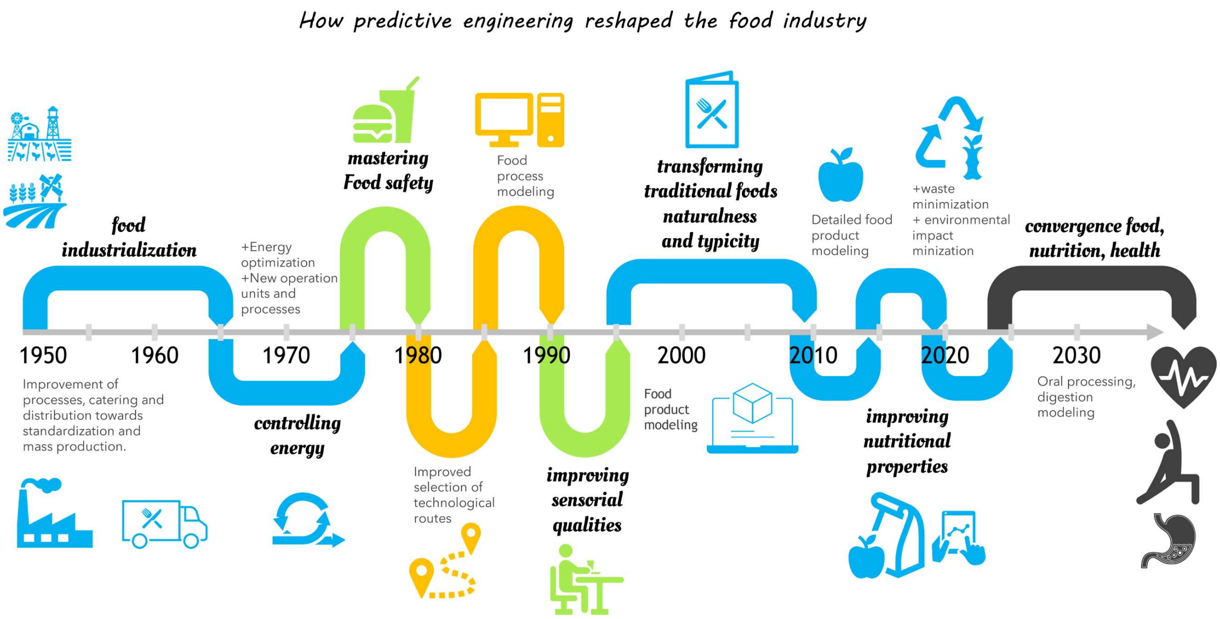

Figure 1. Timeline of the use of predictive modeling and engineering in the food industry.

Hosting group

The group modeling and computational engineering (**MODIC** : *MODélisation et Ingénierie par le Calcul*) of the joint research unit **SayFood** 0782 “ *Paris-Saclay Food & Bioproduct Engineering* ” brings together chemical engineers, physicists, and mathematicians to explore new modes of food transformation (*e.g.* , efficient industries, short supply chains, less packaging waste) and personalized foods (minimally processed foods, protein substitution, food formulation for aged or allergic people, etc.). The group is also part of the Ile-de-France network in porous solids science **RESPORE** and its research axis “towards *modeling at all scales* .” The emerging paradigm is multiscale modeling, where several scales are concurrently or sequentially considered in the food. Indeed, foods are first transformed into objects (*e.g.* , French baguette) before being deconstructed down to individual molecules and finally used as energy or building material by the human body. The zig-zag molecules-to-food-back to-molecules tremendously challenge modeling, particularly for the top-down branch associated with food deconstruction. **Mesoscopic descriptions aim at working below the continuum limit but above the thermodynamic one to keep the hierarchical self-organization of food at all stages of its deconstruction**.

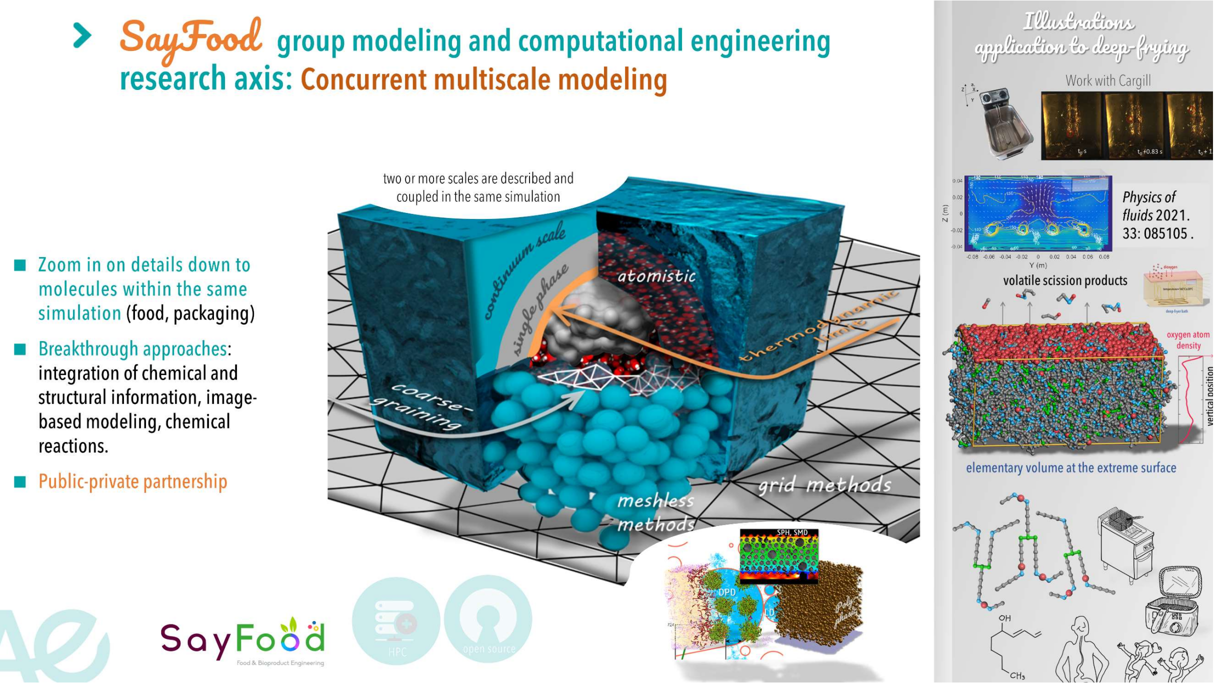

Figure 2. Illustration of the group MODIC axis multiscale modeling, after Ref. [**1** , **2**]. The right panel shows a recent application on modeling the flow and oxidation reaction kinetics within a deep fryer both at the scale of oil bath (process scale) and molecular scale [**3**]. Similar multiscale applications have been developed for food packaging [**4**].

A collaborative project on the mesoscopic modeling of oral processing

Food physics obeys soft-matter principles with cohesion dominated by weak and non-covalent interactions: entangled polymers, self-organized colloids, and surfactants. Saliva and mechanical work contribute to overcoming the cohesive internal energy. Mesoscopic modeling offers the best compromise between preserving physicochemical details (local composition and supramolecular structures, phase organization) and continuum mechanics. In food deconstruction, the assumptions of an effective medium are poorly verified: the interface quantities between phases increase considerably with fractal dimensions much greater than unity; the resulting properties vary with history, and the boundary conditions are essentially unknown. On the opposite side of the scale, simulations at the atomistic scale are not appropriate to study systems evolving far from thermodynamical equilibrium in the presence of mechanical stresses and composition gradients.

> *Take-away*
>
> **Mesoscopic modeling is an umbrella encompassing a broad range of meshless techniques, including or not chemical details.** They are promising as they could potentially fill the gap between a continuum description of foods and their constituents. The proposed Ph.D. program is part of a Franco-American project involving two Ph.Ds. in parallel. The first one already initiated focuses on developing the coupling between two techniques, Smoothed Particle Hydrodynamics (SPH) and Dissipative Particle Dynamics (DPD), on both sides of the thermodynamic limit. The second Ph.D. will focus on the validation and parameterization of mesoscopic methods (forces and forcefields, kernels) based on microscopic observations and stress measurements.

Problem statement

We are designing several simulation frameworks capable of describing flows, mechanical ruptures, and their subsequent evolutions under entropy-driven phenomena (dissolution, diffusion) at mesoscopic scales. at the upper scale, updated and total Lagrangian SPH techniques are the preferred methodologies for liquids and solids, respectively. DPD and its variants share the same concepts of blurred particles at the lowest scale. The latter is subjected to soft repulsive interactions but explicitly incorporates temperature effects. These principles made designing DPD- or SPH- fluids and solids possible by assembling and possibly connecting beads/particles. Many elemental particle types (water/saliva bead, oil droplet, solid, gel, tooth, tongue, etc.) are required to describe the behavior of foods during oral processing. We will focus on foods' mechanical fragmentation and rheological properties related to their perception.

> *Take-away*
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> **As in classical molecular dynamics, mesoscopic models involve radial forces depending on pair-parameterization will determine how macroscopic properties emerge and whether objects (e.g., droplet, chewing-gum-like) will associate/mix or fragment (see examples in Figure 3c)**. We propose to explore a parameterization from the dynamic observation of interactions between micrometric objects (droplet, rigid) and surfaces (tooth, tongue, palate) and between them. Since strains and displacements are more easily measurable and comparable with simulations, a direct comparison between acquired image sequences and dynamic simulations under periodic mechanical solicitations is sought.

Project description

Experimental work

The Ph.D. will design microfluidic experiments to provoke interactions between objects (stabilized droplets, gel particles) with controlled characteristics and surfaces. The interactions will include shearing, crowding, compression, and impact in the presence of a continuous phase (water, saliva simulant). The effects of physical state (*e.g.* , melting, miscibility) will also be explored. Observations will be carried out under a visible light microscope operating in different acquisition modes: confocal, phase contrast, epifluorescence, and fast Raman imaging (to get chemical details). Perturbations will be applied with typical frequencies ranging from 0.1 to 100 Hz to reach mesoscopic scales. Interactions with walls, including mechanical stresses, will be reconstructed from the deformation of structured surfaces. A suggestion of experiments is shown in **Figure 3**.

Transforming static pixels into animated "3D beads" and objects

The simulated and observed resolutions coincide. Our toolbox Pizza3 [5] for LAMMPS [6] already implements some capabilities to convert pixels from thresholded images into animated 3D beads and objects. The beads move according to the combination of two causes: external stresses (imposed pressure, force, velocity, flowrate) and mesoscopic forces, which require parameterization. In other words, the simulated objects should reproduce the acquired image sequences by knowing only the external causes. Several assumptions are needed to transform localized observations in the focal plane (FP): 3D reconstruction of the objects in the observation direction (perpendicular to FP) and outside the observation field. Both tasks will be carried out by repeating the observations at different magnifications.

Since our final intent is to reconstruct mechanical behaviors, validation should emphasize stress measurements. They are, however, much more challenging to assess microscopic scales than other properties such as local chemical composition, morphology, strain rate, and displacement fields. We prefer, therefore, to target validations by comparing simulations with velocity fields and viscous, elastic, and plastic deformation of materials with known properties. The dynamic observations (periodic or not) need to be sufficiently detailed to enable the adjustment of several parameters (*e.g.* , up to 12 in **Figure 3C**). Considerations inherent to the mesoscopic representation (stability, feasibility, and computational cost) will be used to restrict the search and accelerate the identification process.

Since we propose to evaluate mesoscopic properties between " *grains* " that have no immediate physical reality in the image, the proposed approach is closer to image learning. The typical procedure will include correlative microscopy, image registration, and a numerical identification procedure involving concurrent image mesoscopic simulation. Several 3D simulations will be launched on our cluster or in the cloud with different sets of parameters in parallel. Each explored branch will be refined or terminated according to the criteria of reliability to be defined.

> *Take-away*
>
> **Mesoscopic model matching observations** will be designed using the abstraction layer Pizza3 [5], enabling programming in LAMMPS [6] and running simulation on our computer cluster from abstract concepts. Depending on the results, one or several optimization methods, including machine learning, will be used to accelerate the parameterization from microscopic observations. This first work should preclude the construction of a future digital twin scheme enabling change, automatically the perturbation strategy based on the difficulty of optimizing simulation parameters. We anticipate the emergence of the first collaborative database of mesoscopic properties of food.

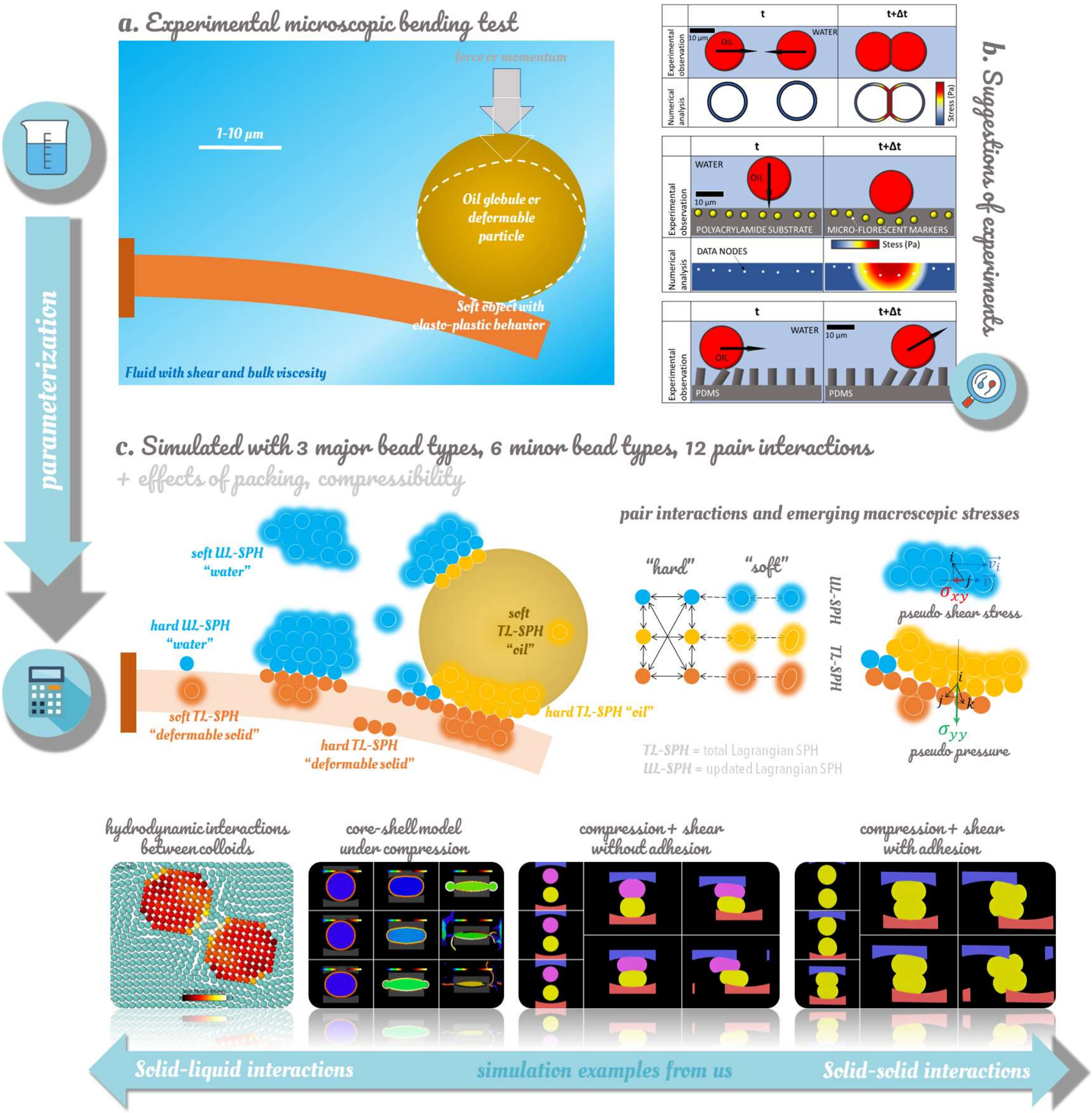

Figure 3. Principles of the parameterization of mesoscopic models.

- *(a) Typical mechanical testing under a microscope.*
- *(b) Examples of experimental setups to recover micro-stresses in an oil-in-water microfluidic chip:* `Ex. 1` *active contour or edge detection model to estimate the local curvature and relate it to stress with the Young-Laplace equation;* `Ex. 2` *deformable walls with known mechanical properties are embedded with markers, and stresses are recovered by approximating the wall as a Boussinesq half-body or with a finite element approximation;* `Ex. 3` *point forces are computed from the deflections of elastic posts with the Euler-Bernoulli beam theory.* `Ex. 1-3` *are implemented in Refs. [7], [8] and [9].*
- *(c) Equivalent simulation using our framework (under development) in Pizza3 using total and updated Lagrangian descriptions. Some of our simulations are shown at the bottom; color gradients map stresses.*

Role of the Ph.D. candidate

The Ph.D. candidate will design and execute experiments, including preparing reference systems, observations, and acquisition. In strong collaboration with the development team, he/she will program in Python (and Matlab) optimization routines, enabling mesoscopic simulation refinement. He/she will analyze the results critically and provide mechanistic interpretations of the experiments and simulations. He/she will participate in the writing of scientific publications and contribute to scientific communications at international conferences.

Application and recruitment

Application details

Contract	**Public contract (contrat doctoral) – Doctoral student for 36 months starting 1st October (≈ 1950 € gross salary)**
Workplace	Université Paris-Saclay, 22 place de l'Agronomie, 91120 Palaiseau, France
Supervisors	Dr. Olivier Vitrac (Director), Pr. Denis Flick, Dr. Murielle Hayert
Deadline to apply	31st August 2022
Keywords	microfluidics, mesoscopic physics, image analysis, multiscale modeling, soft matter, food deconstruction

Prerequisites and procedure

- [ ] ***The applicant should have or be working towards a Master's degree in microfluidics, physics, physical chemistry, soft matter physics, material sciences, fluid mechanics, chemical engineering, or similar.***
- [ ] **Strong English (and some French) or a clear willingness to improve your level will be essential.**
- [ ] A prior experience in image analysis and programming will be appreciated.
- [ ] Send your application to Dr. Olivier Vitrac: **olivier.vitrac@agroparistech.fr** (contact E-mail)
- [ ] Cc. **murielle.hayert@agroparistech.fr** **denis.flick@agroparistech.fr** **william.jenkinson@agroparistech.fr**
- [ ] *Please include your CV, cover letter, two recommendation letters, and undergraduate and Masters' transcripts.*

Figure 4. Our campus AgroParisTech-INRAE at the University of Paris-Saclay and our research group (July 2022).

References

[1] Vitrac O, Nguyen P-M, Hayert M. In Silico Prediction of Food Properties: A Multiscale Perspective. *Frontiers in Chemical Engineering* . 2022;**3**:1-38 **https://doi.org/10.3389/fceng.2021.786879** .

[2] Vitrac O, Hayert M. Modeling in food across the scales: towards a universal mass transfer simulator of small molecules in food. *SN Applied Sciences* . 2020;**2**:1509 **https://doi.org/10.1007/s42452-020-03272-2** .

[3] Touffet M, Allouche MH, Ariane M, Vitrac O. Coupling between oxidation kinetics and anisothermal oil flow during deep-fat frying. *Physics of Fluids* . 2021;**33**:085105 **https://doi.org/10.1063/5.0055873** .

[4] Nguyen P-M, Guiga W, Vitrac O. Molecular thermodynamics for food science and engineering. *Food Research International* . 2016;**88**:91-104 **https://doi.org/10.1016/j.foodres.2016.03.014** .

[5] Vitrac O. 2022 2022/07/10; Available from: **https://github.com/ovitrac/Pizza3** .

[6] Thompson AP, Aktulga HM, Berger R, Bolintineanu DS, Brown WM, Crozier PS, in 't Veld PJ, Kohlmeyer A, Moore SG, Nguyen TD, Shan R, Stevens MJ, Tranchida J, Trott C, Plimpton SJ. LAMMPS - a flexible simulation tool for particle-based materials modeling at the atomic, meso, and continuum scales. *Computer Physics Communications* . 2022;**271**:108171 **https://doi.org/10.1016/j.cpc.2021.108171** .

[7] Molino D, Quignard S, Gruget C, Pincet F, Chen Y, Piel M, Fattaccioli J. On-Chip Quantitative Measurement of Mechanical Stresses During Cell Migration with Emulsion Droplets. *Scientific Reports* . 2016;**6**:29113 **https://doi.org/10.1038/srep29113** .

[8] Tang X, Tofangchi A, Anand SV, Saif TA. A Novel Cell Traction Force Microscopy to Study Multi-Cellular System. *PLOS Computational Biology* . 2014;**10**:e1003631 **https://doi.org/10.1371/journal.pcbi.1003631** .

[9] Tan JL, Tien J, Pirone DM, Gray DS, Bhadriraju K, Chen CS. Cells lying on a bed of microneedles: An approach to isolate mechanical force. *Proceedings of the National Academy of Sciences* . 2003;**100**:1484-9 **https://doi.org/10.1073/pnas.0235407100** .

$last\ revision - 2022 - 07 - 14$
