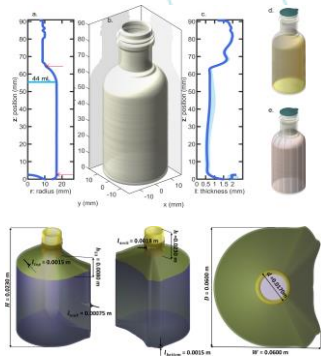
http://mol12.agroparistech.fr/fitness/external/AgroParisTech/MasterGP/

Food computer-aided engineering new perspectives from research

Olivier Vitrac, senior scientist INRAE
olivier.vitrac@agroparistech.fr



COMPUTER-AIDED FOOD ENGINEERING

Our recent review

but our old views

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Review Article | Published: 03 November 2022

Computer-aided food engineering

Ashim Datta, Bart Nicolaï, Olivier Vitrac, Pieter Verboven, Ferruh Erdogdu, Francesco Marra, Fabrizio Sarghini & Chris Koh

Nature Food **3**, 894–904 (2022) | Cite this article

603 Accesses | **1** Citations | **4** Altmetric | Metrics

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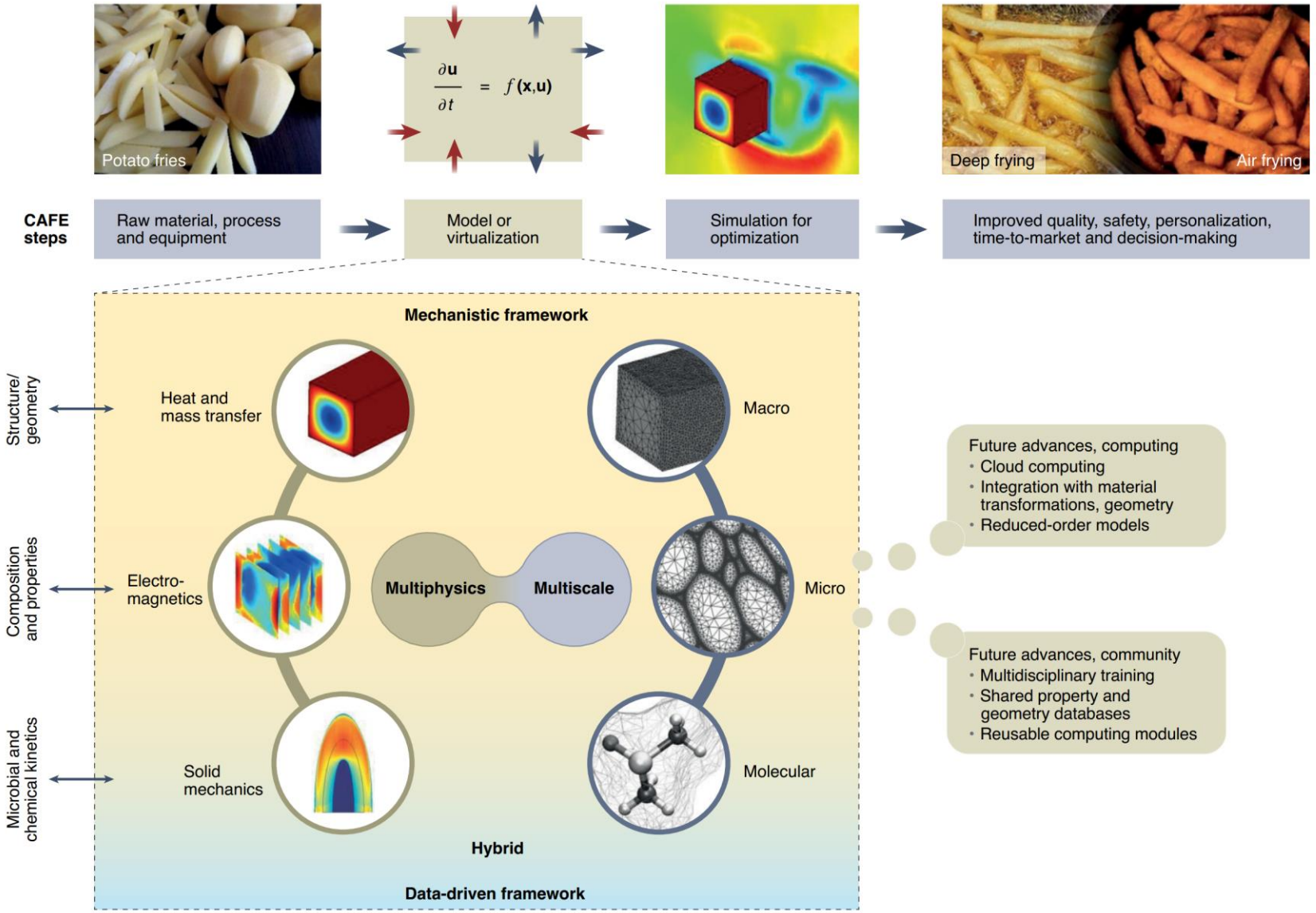

COMPUTER-AIDED FOOD ENGINEERING

Our recent review:
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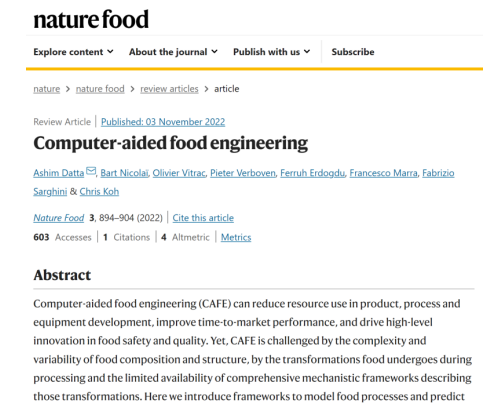
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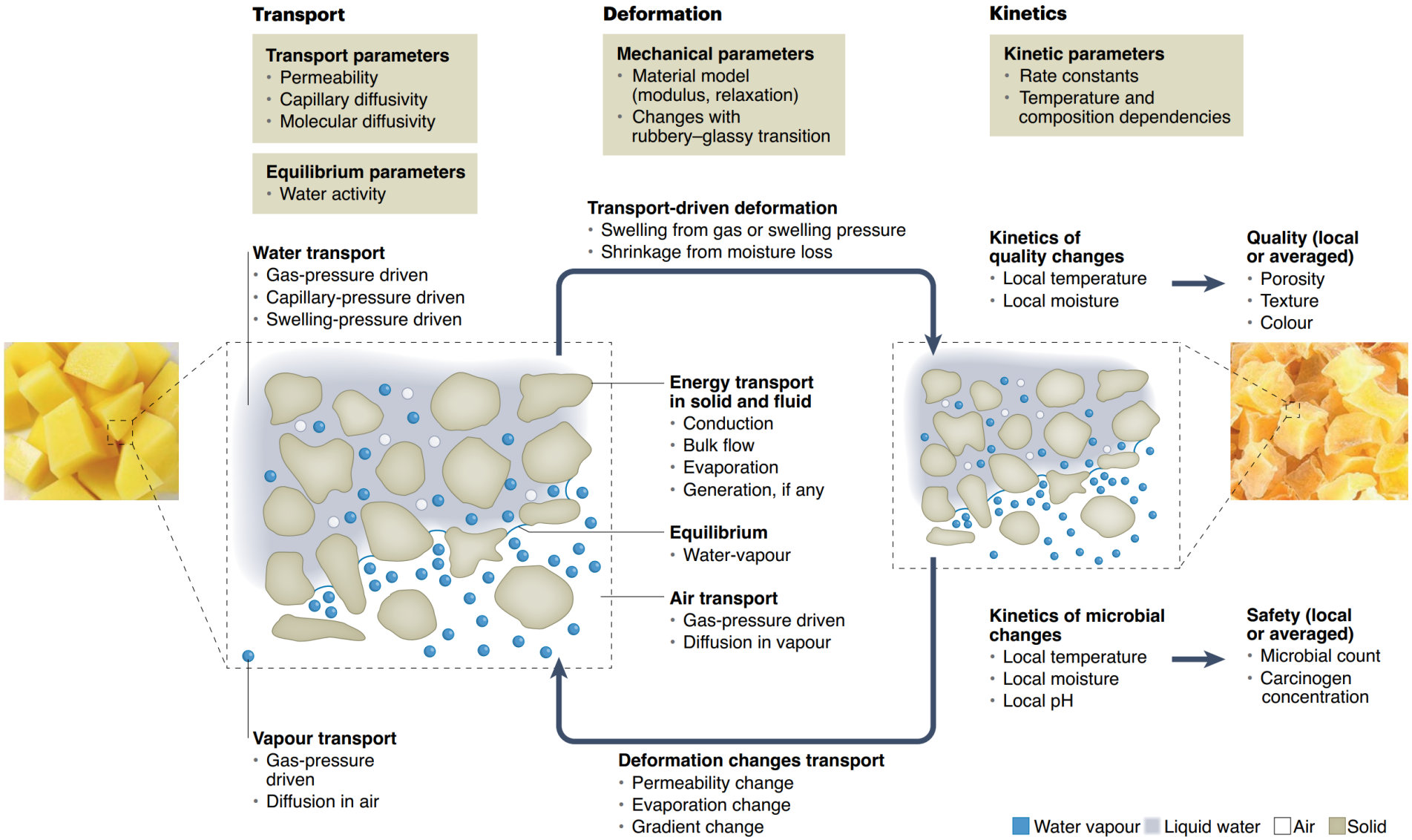
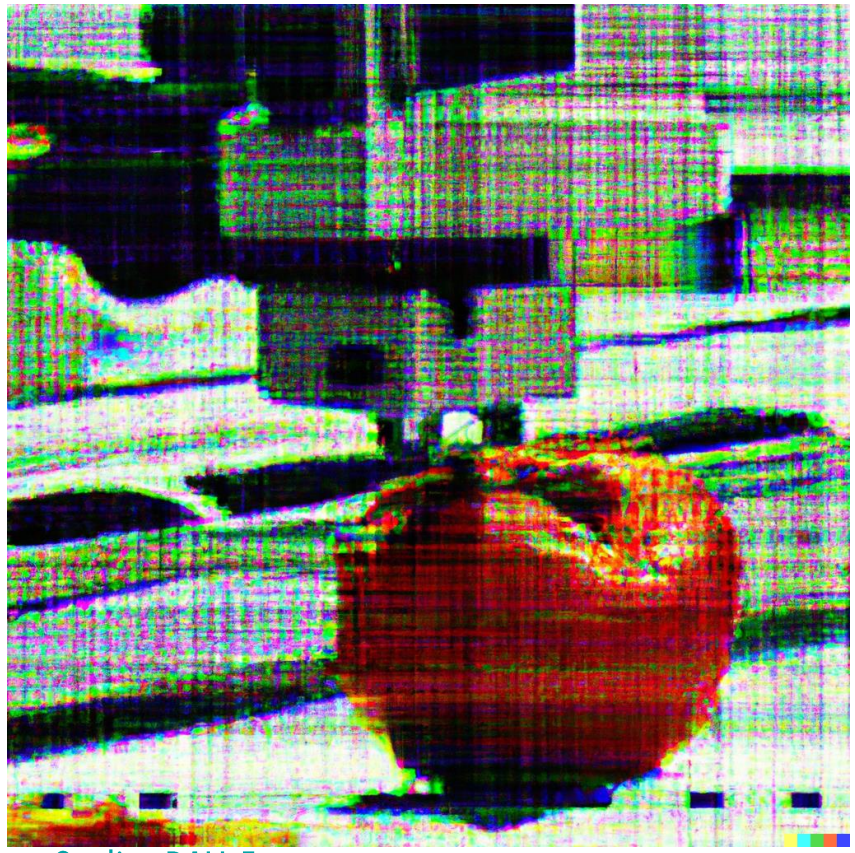
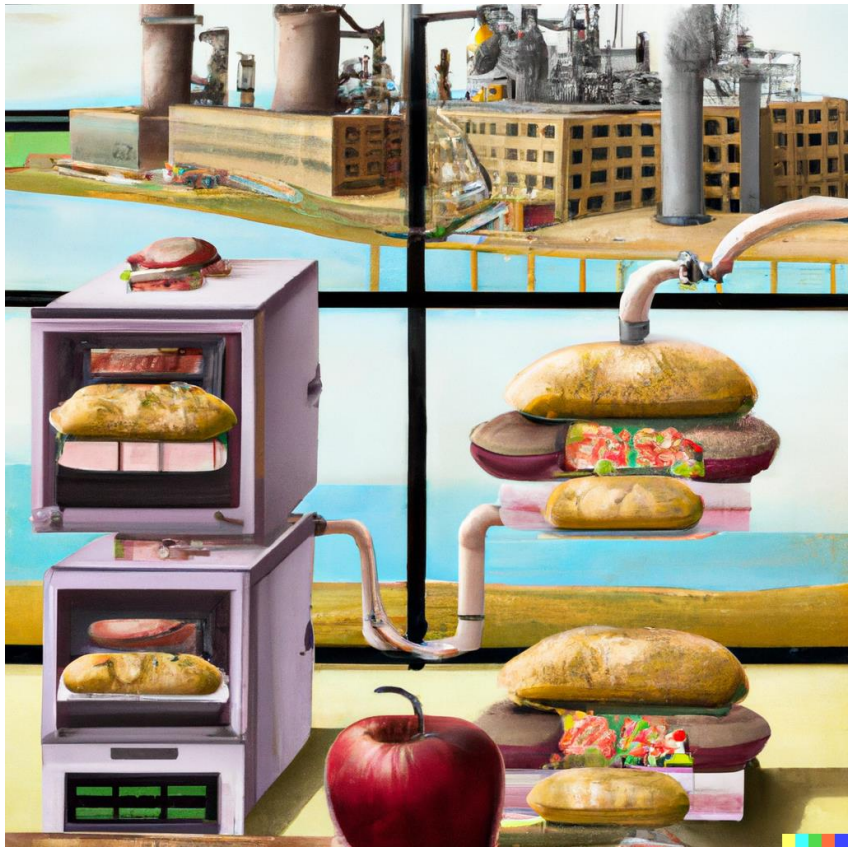


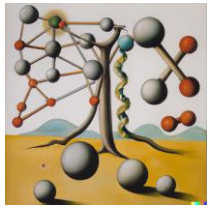
BEYOND

Can the computer create models? Or at least learn from experiments/on-line measurements?



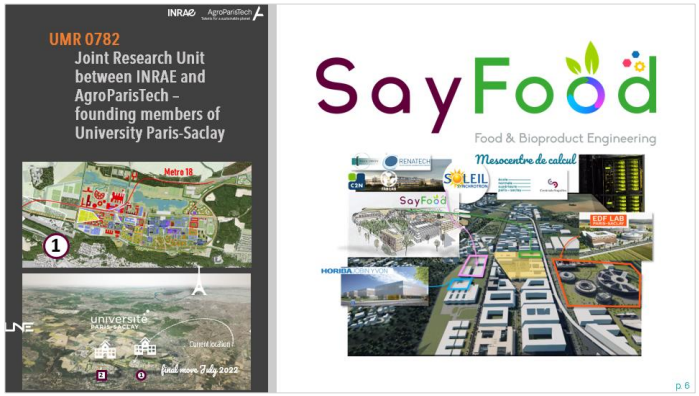


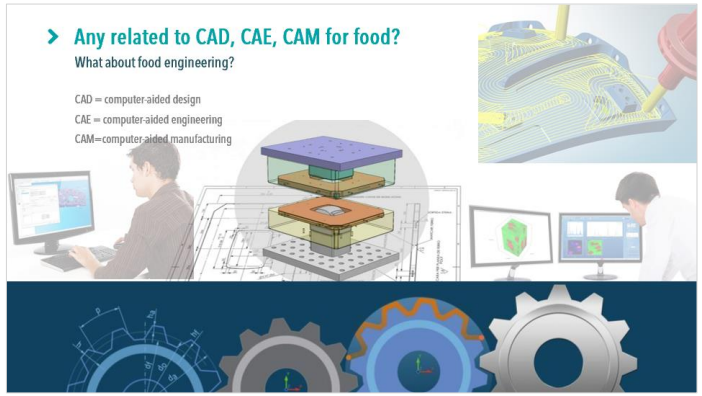
Credits: DALL-E

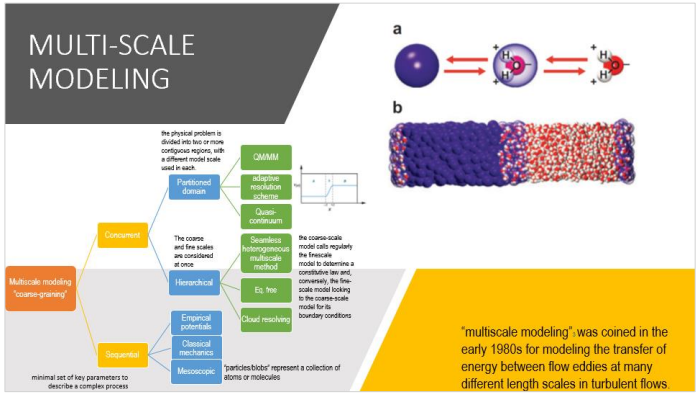


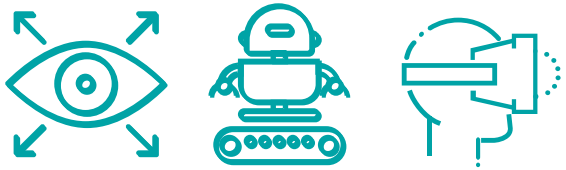
OVERVIEW

TOWARDS THE FUTURE





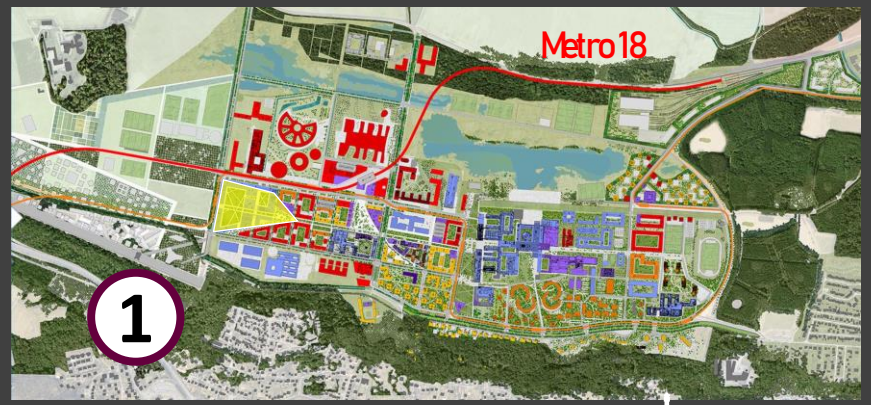


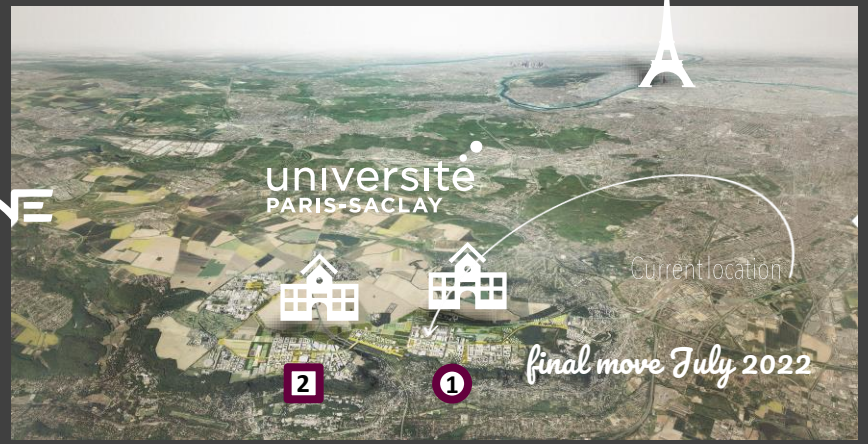


INRAE AgroParisTech
Talents for a sustainable planet

UMR 0782

Joint Research Unit between INRAE and AgroParisTech – founding members of University Paris-Saclay





SayFood

Food & Bioproduct Engineering

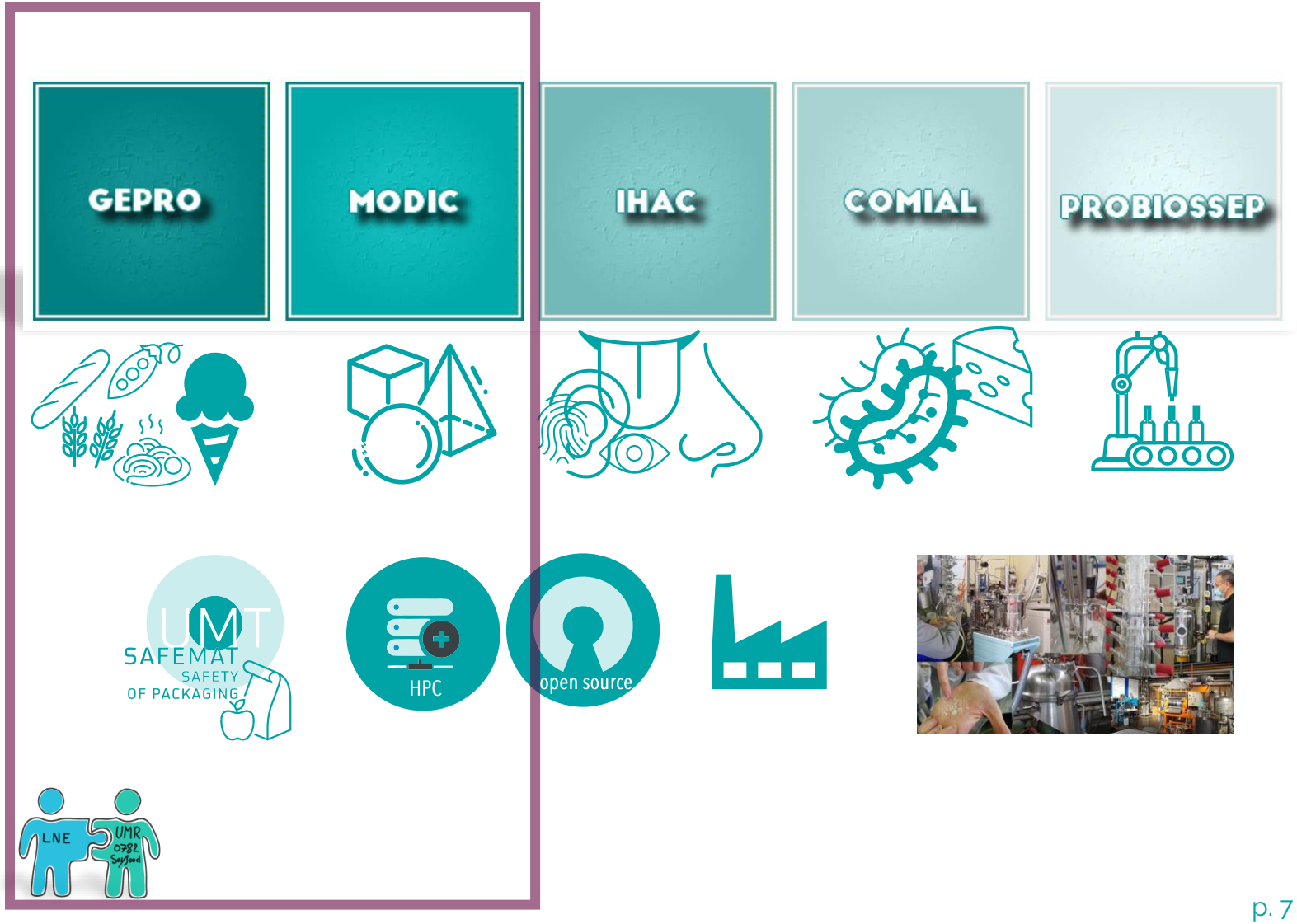
Overview of Unit SayFood

180 persons, ~40 PhD students and post-docs

SayFood

Food & Bioproduct Engineering

- Product Engineering (GePro)
- Modeling and Computational Engineering (ModIC)
- Human-Food Interactions for Design (IHAC)
- Food Microbial Communities (CoMiAl)
- Microbiological Processes, Stabilization, Separation (ProBioSSep)



Multidisciplinary research teams

SayFood
Food & Bioproduct Engineering

CoMiAl

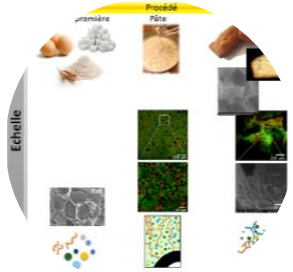
Food microbial ecosystems

ProBioSSep

Microbial processes, stabilization, separation

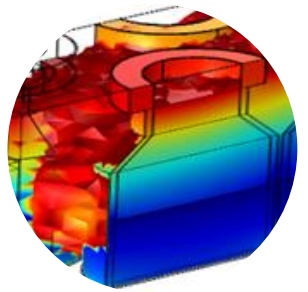
IHAC

Human-food interactions, from conception to consumption



GéPro

Product engineering



MIC

Modeling and computational engineering

Biochemistry

Physico-chemistry

Sensory analysis

Chemistry

Biochemistry

Physico-chemistry

Applied mathematics

Microbiology

Consumer sci.

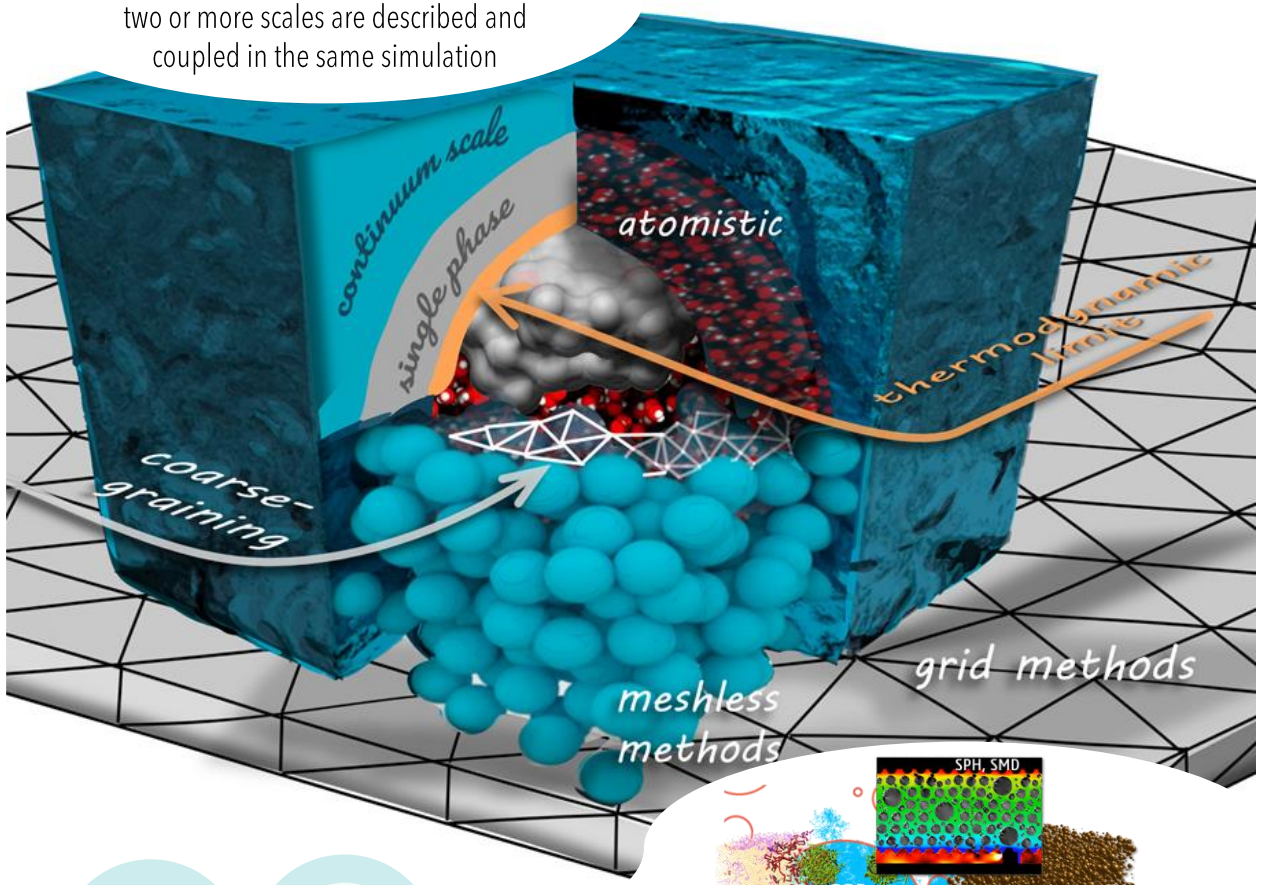
Genomics

Food process engineering

SayFood group modeling and computational engineering research axis: Concurrent multiscale modeling

- **Zoom in on details down to molecules within the same simulation** (food, packaging)
- Breakthrough approaches: integration of chemical and structural information, image-based modeling, chemical reactions.
- Public-private partnership

two or more scales are described and coupled in the same simulation



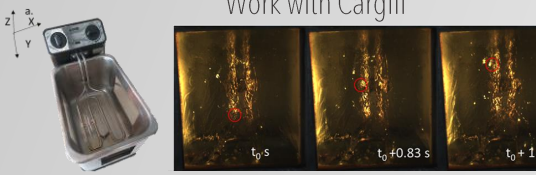
SayFood
Food & Bioproduct Engineering

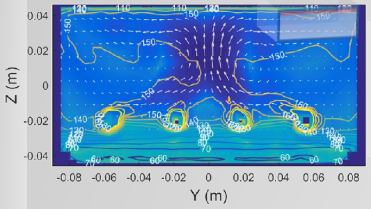
HPC

open source

Illustrations application to deep-frying

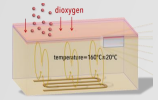
Work with Cargill

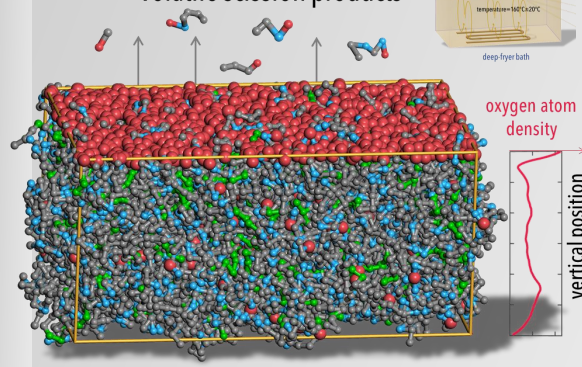




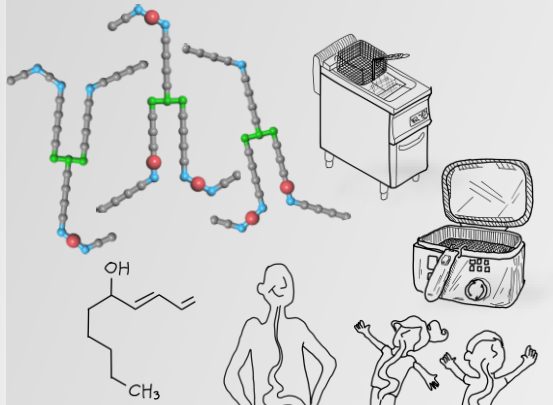
Physics of fluids **2021.** 33: 085105 .

volatile scission products



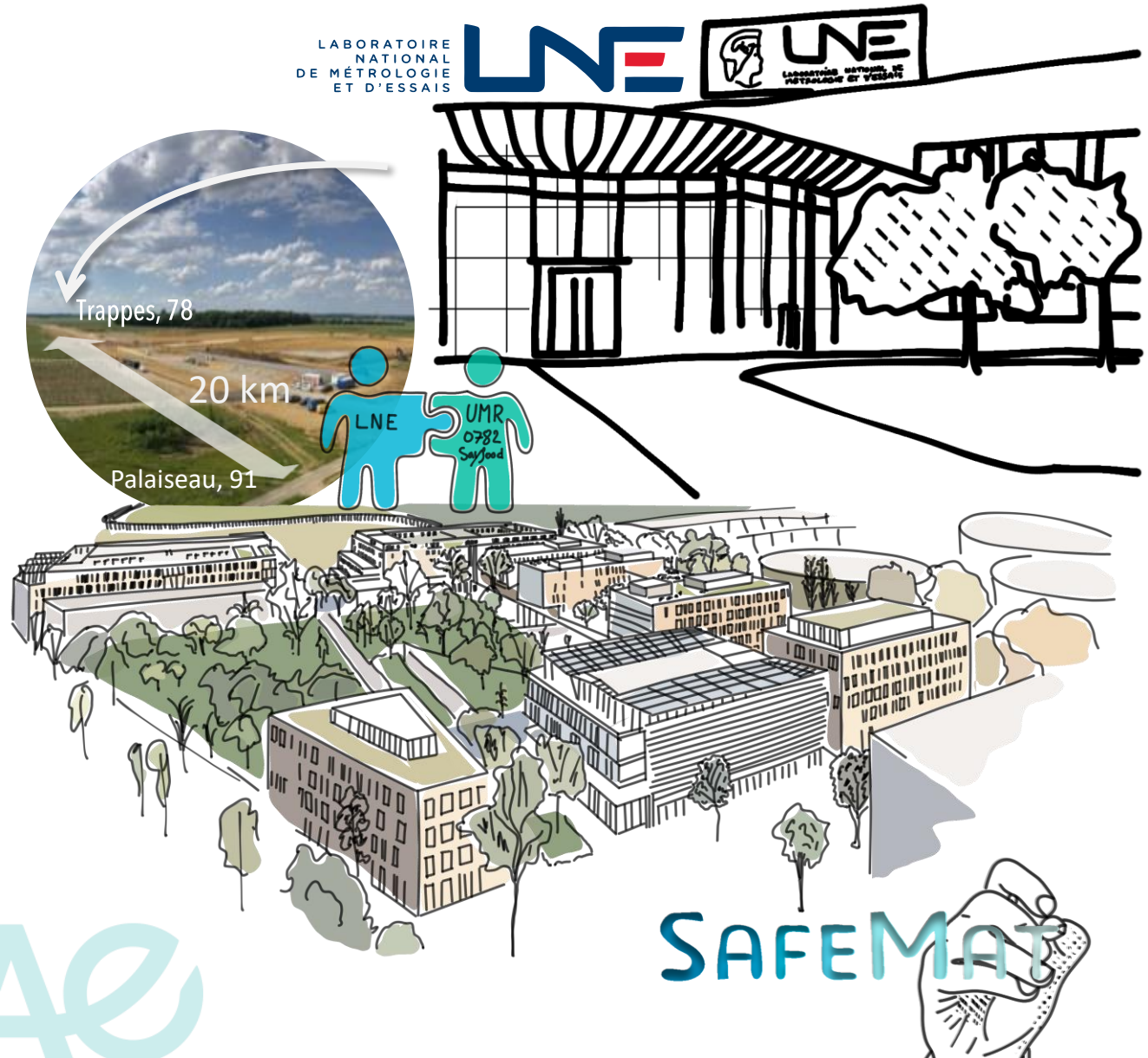


elementary volume at the extreme surface



A common laboratory between LNE and UMR SayFood

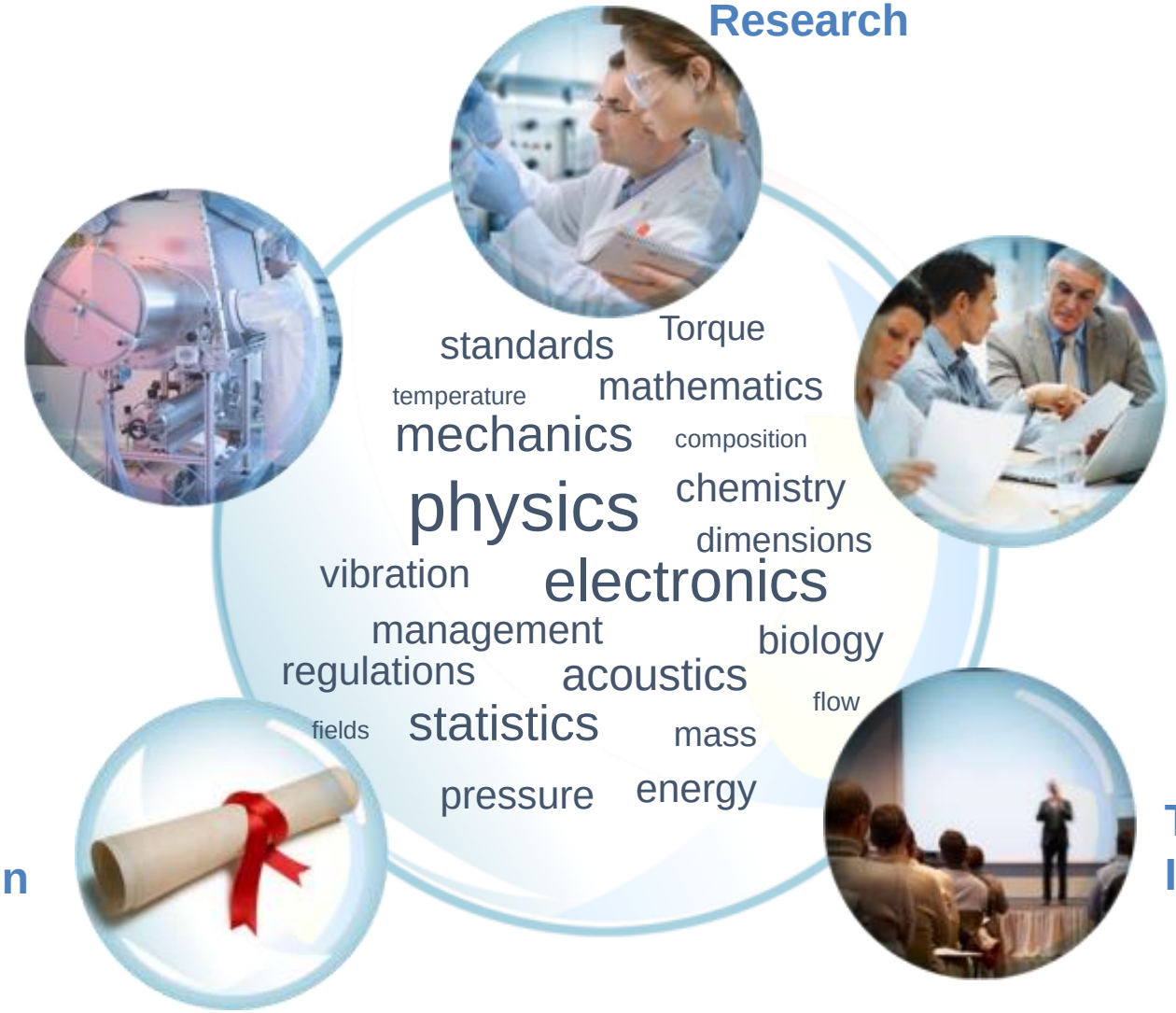
UMT ACTIA 22.07 SAFEMAT « Safe Materials for Food Contact »



UMT SAFEMAT SAFETY OF PACKAGING

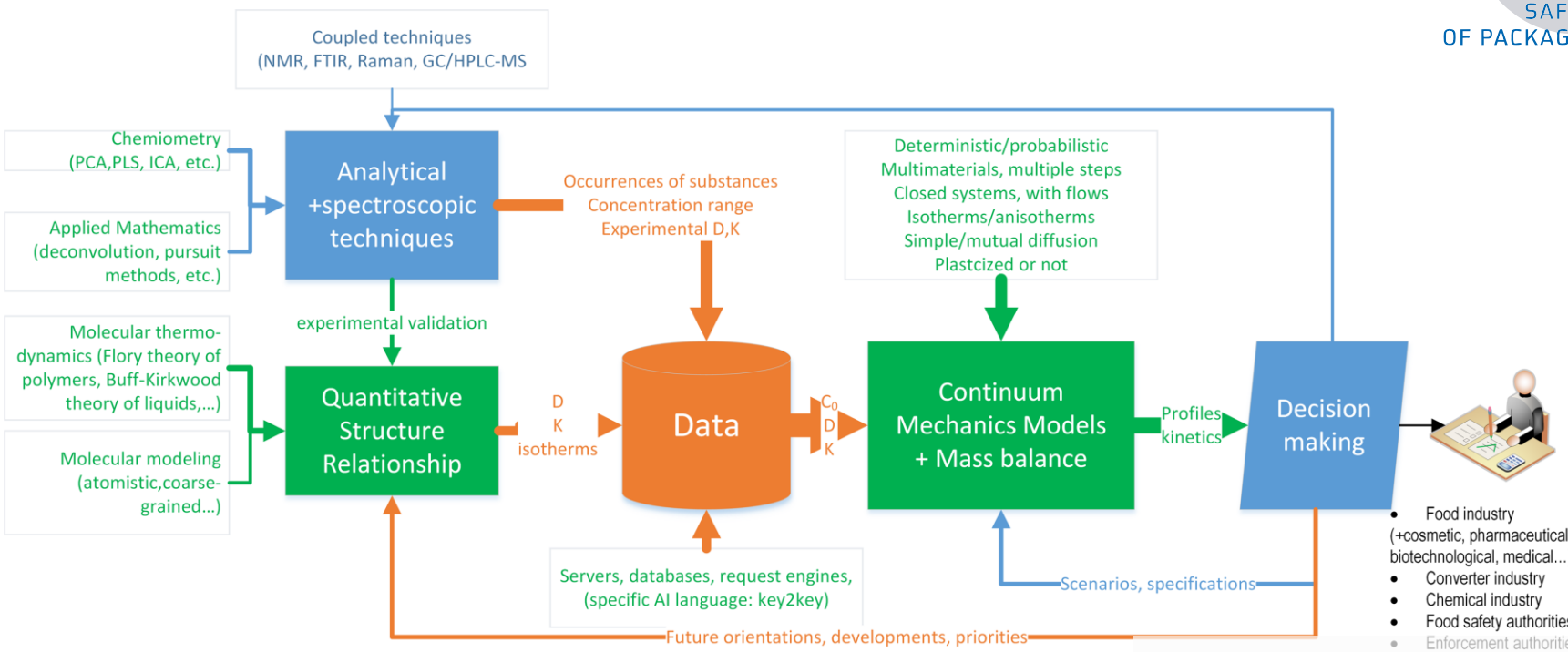
- accredited by the French ministry of Agriculture and Food (since 2017)
- Competent organization for EFSA (for both LNE and INRAE) on food contact materials
- **LNE = national reference laboratory** for food contact materials
- Complementarity of means (computation, analytical chemistry), two groups of SayFood involved
- **24 persons (9.5 full-time eq.)**
- Administrative coordinator Jean-Mario Julien (LNE)
- Scientific coordinator **Olivier Vitrac (INRAE)**

LNE: EXTENSIVE SCIENTIFIC AND TECHNOLOGICAL EXPERTISE



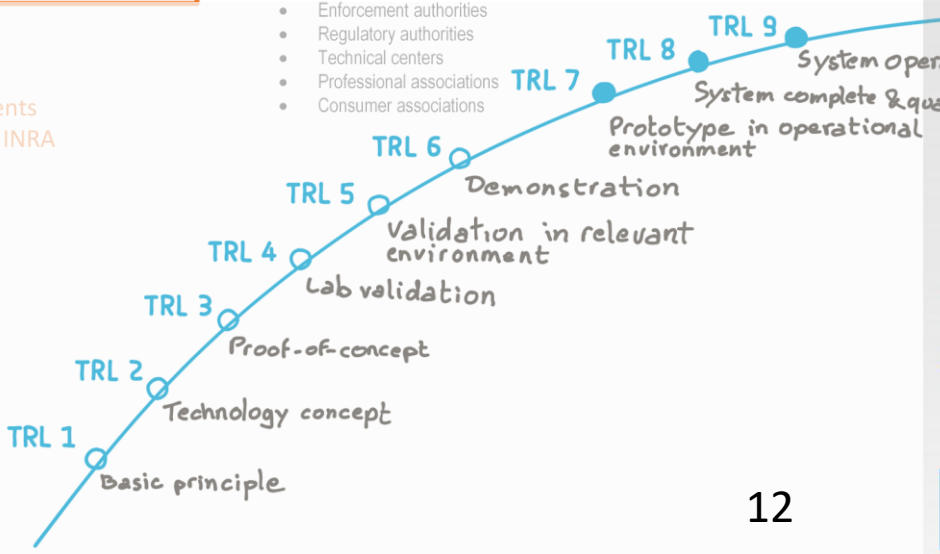
OUR STRATEGY

UMT SAFEMAT SAFETY OF PACKAGING



- Food industry (+cosmetic, pharmaceutical, biotechnological, medical...)
- Converter industry
- Chemical industry
- Food safety authorities
- Enforcement authorities
- Regulatory authorities
- Technical centers
- Professional associations
- Consumer associations

Main contributors: LNE, INRA, Joint developments between LNE and INRA



PERFORMANCE PLASTICS

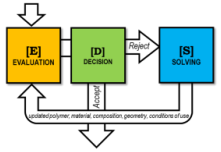
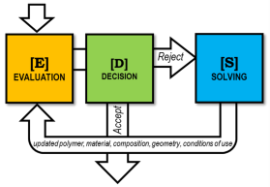
sartorius · PlasticsEurope Association of Plastics Manufacturers · valspar · Pernod Ricard · McCain · SEB · Casino supermarchés · food watch die essensretter · IFV Institut Français de la Vigne et du Vin · anses · IRSN Institut de radioprotection et de sûreté nucléaire · SCL Service commun des laboratoires · Fraunhofer IVV · Michigan State University · BfR Risiken erkennen – Gesundheit schützen · ECHA European Chemicals Agency · efsa European Food Safety Authority · Joint Research Centre JRC · FDA

Our priorities

ANTI-WASTE LAW for a circular economy

UMT SAFEMAT SAFETY OF PACKAGING

Objectives UMT 22.07

Public Service Mission	Recycle	Reduce	Reuse
Support the evolution of European regulations + anti-waste decrees		No contribution	
Supporting the substitution of materials			
Secure the product and ensure the performance of the packaging			

Objectives of the 3Rs Decree

Safemat project built around 3 R&D axes (TRL 1-7)

AXIS 1
FOOD GRADE
RECYCLATES

AXIS 2
AGING OF
RECYCLED MATERIALS,
REUSED, REEMPLOYED,
COMPOSTABLE

AXIS 3
ENGINEERING
INTEGRATING THE COUPLE
PACKAGING-PRODUCT

Mission of public interest, support the evolution of regulations, reconcile safety and performance

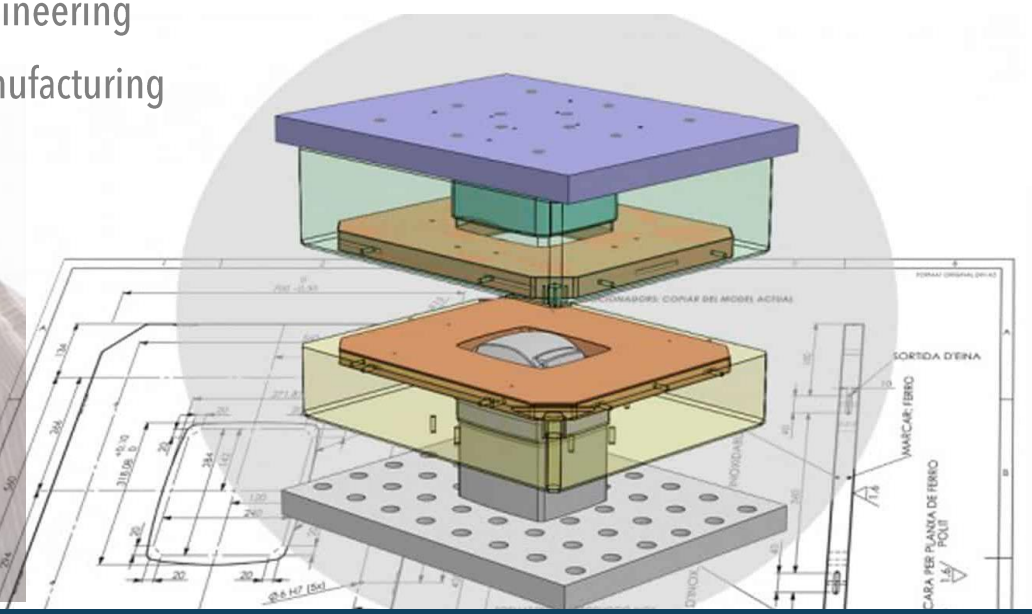
Any related to CAD, CAE, CAM for food?

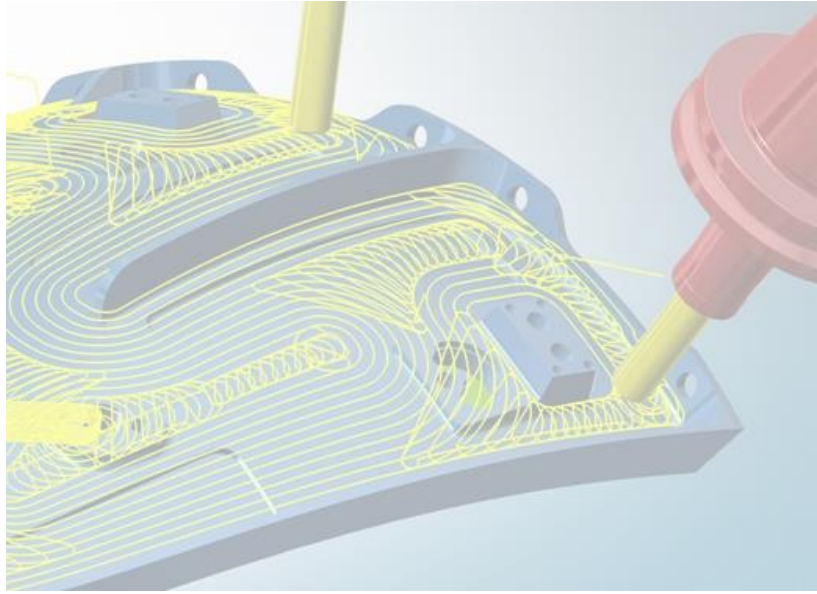
What about food engineering?

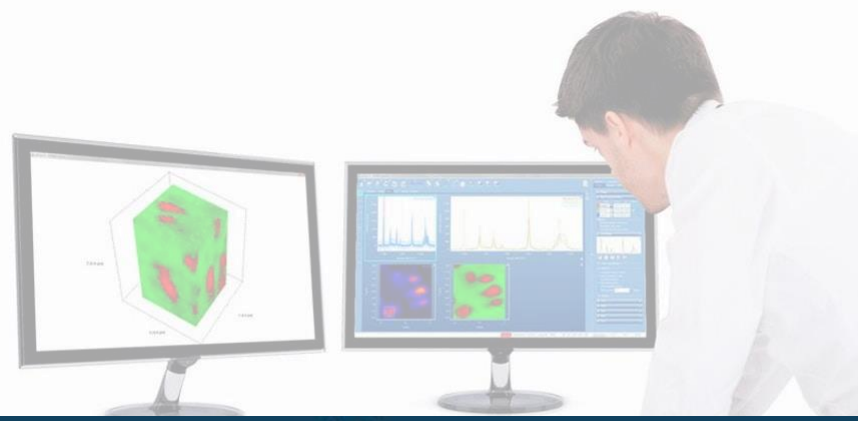
CAD = computer-aided design

CAE = computer-aided engineering

CAM=computer-aided manufacturing





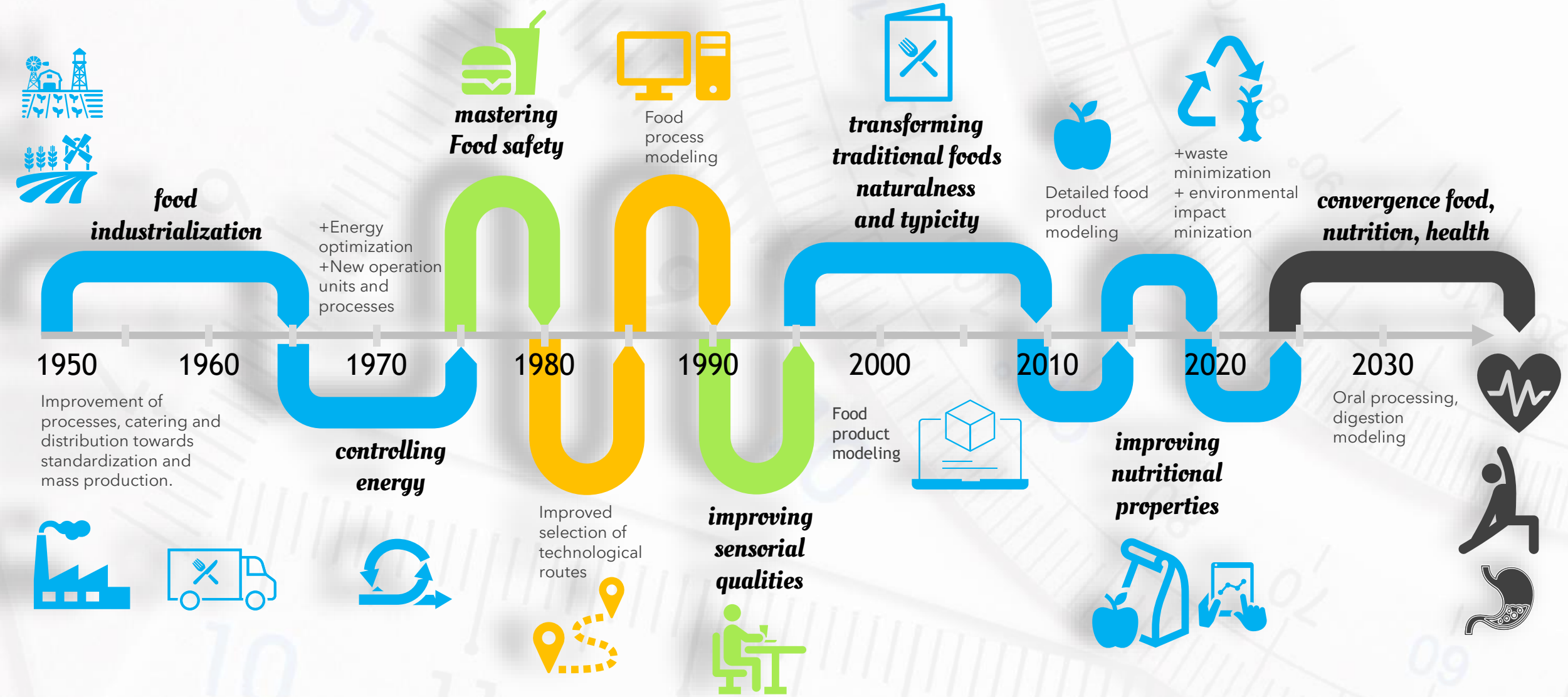


Computer design for food?

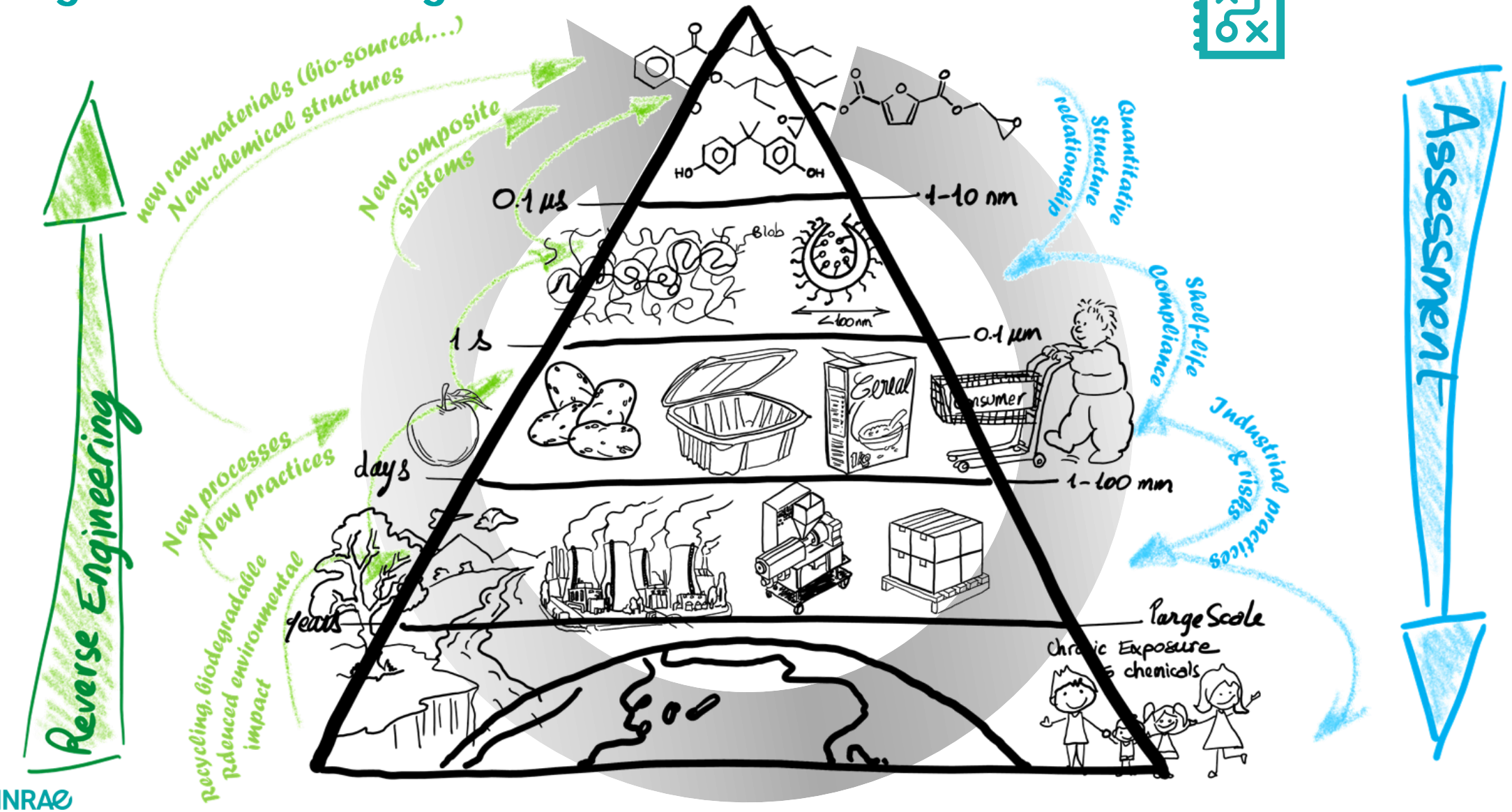
Computer design for food?

Computer design for food?

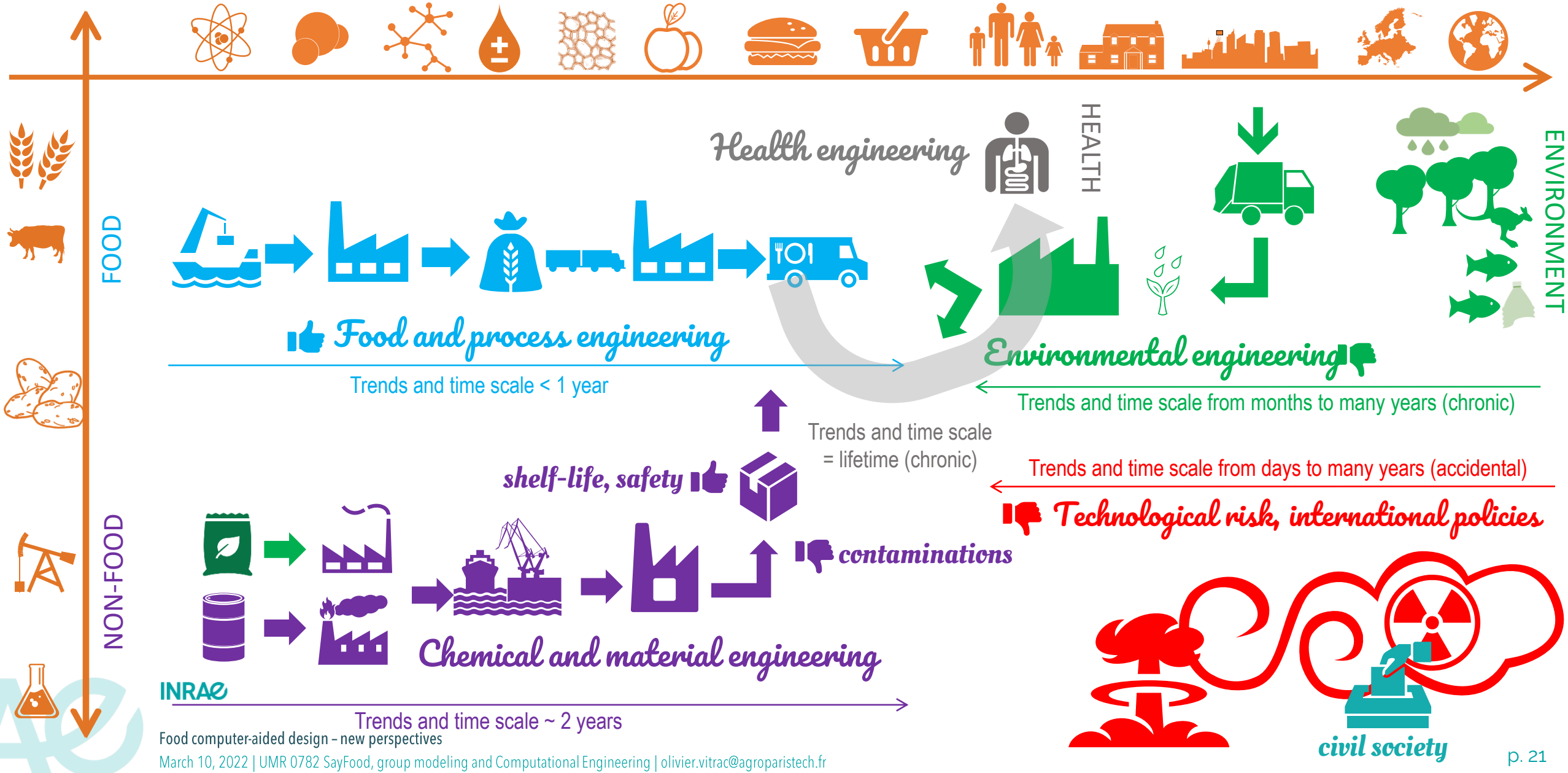
How predictive modeling reshaped/reshapes food engineering



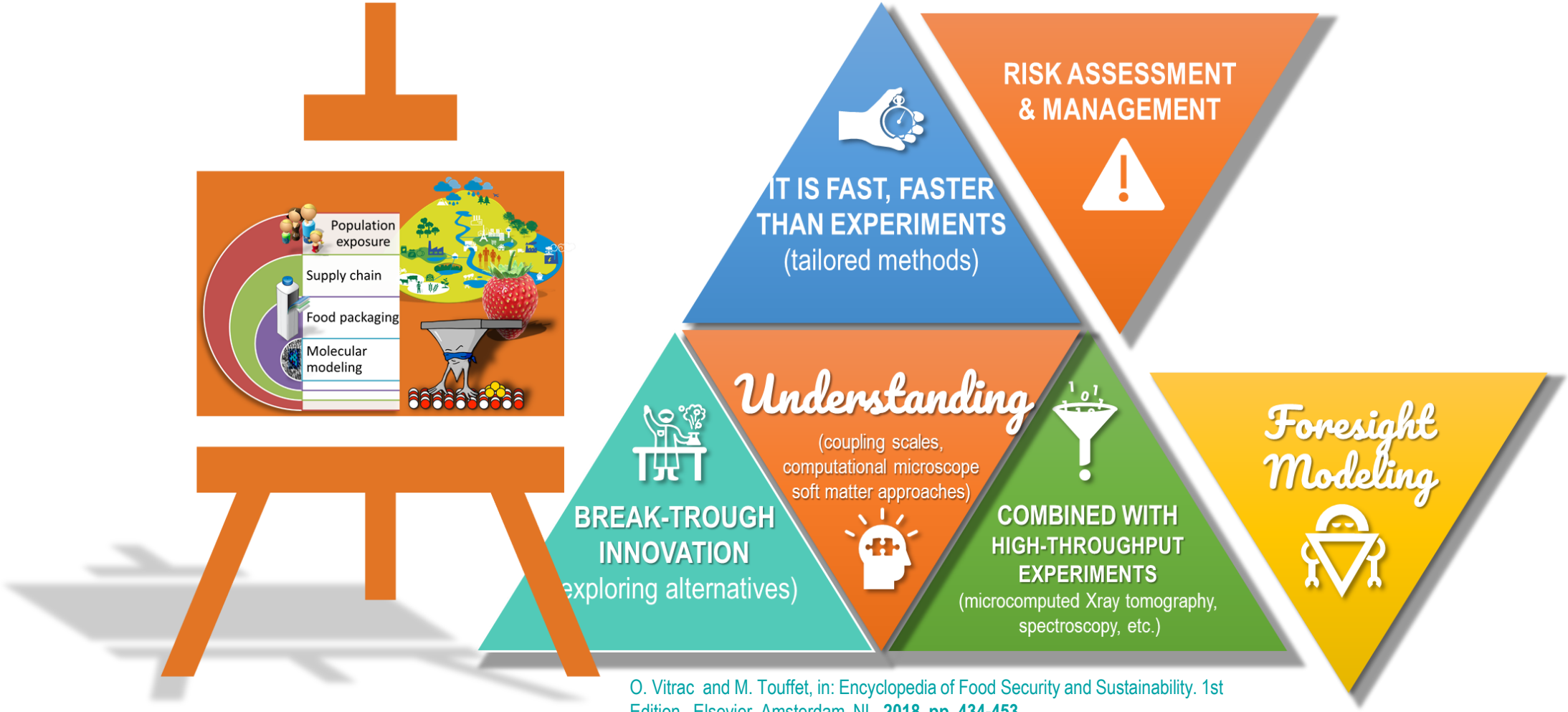
Large scale modeling: the next frontier



My contribution: modeling for global challenges *(linked scales and decisions)*

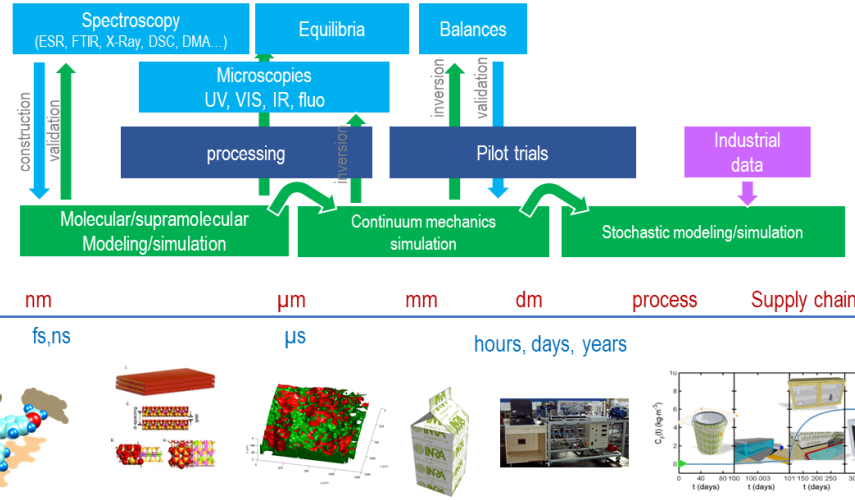


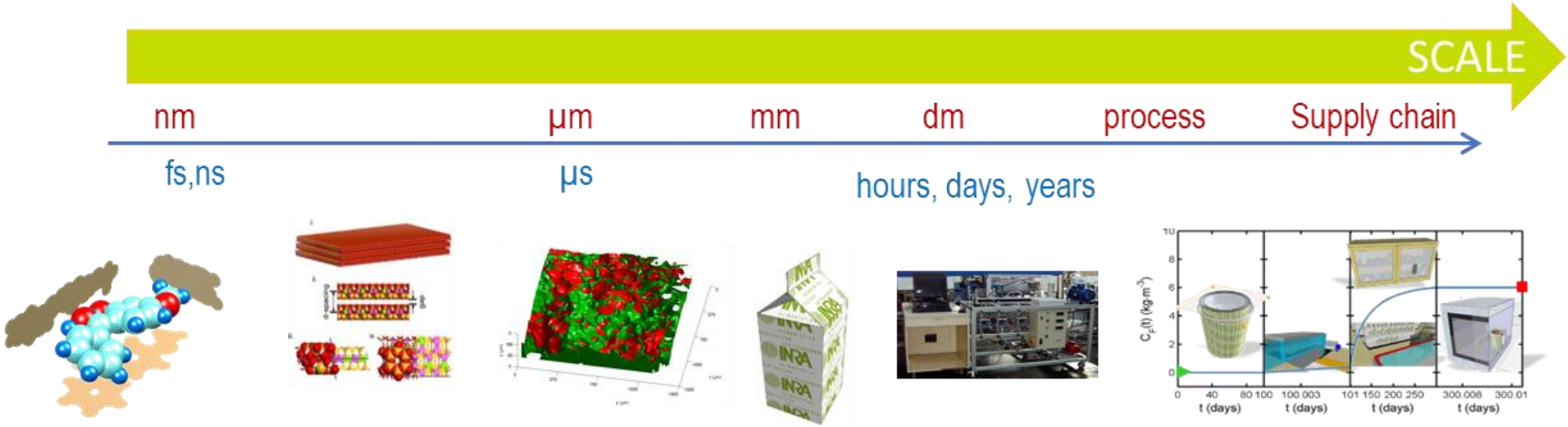
Modeling, predictions, foresight



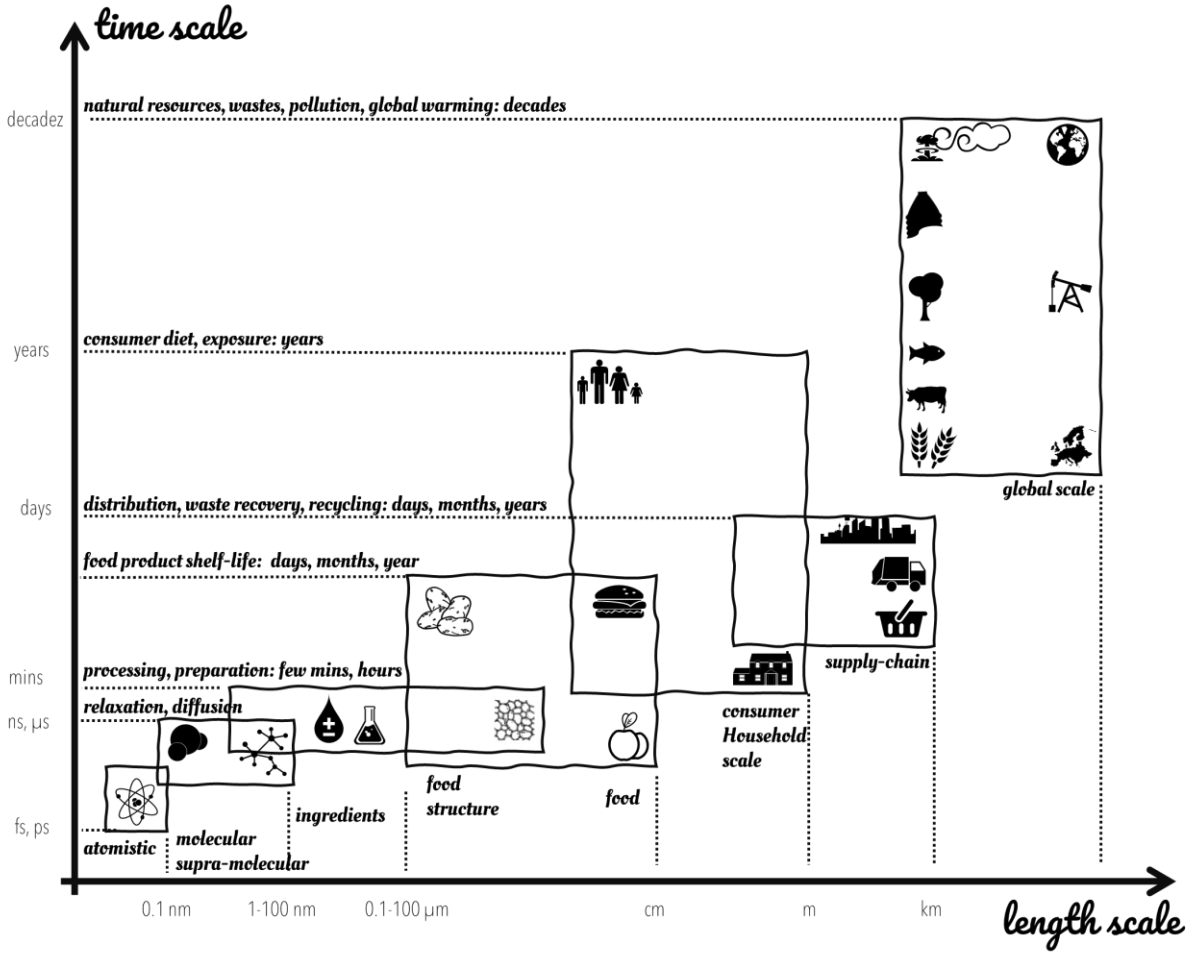
O. Vitrac and M. Touffet, in: Encyclopedia of Food Security and Sustainability. 1st Edition., Elsevier, Amsterdam, NL, **2018, pp. 434-453.**

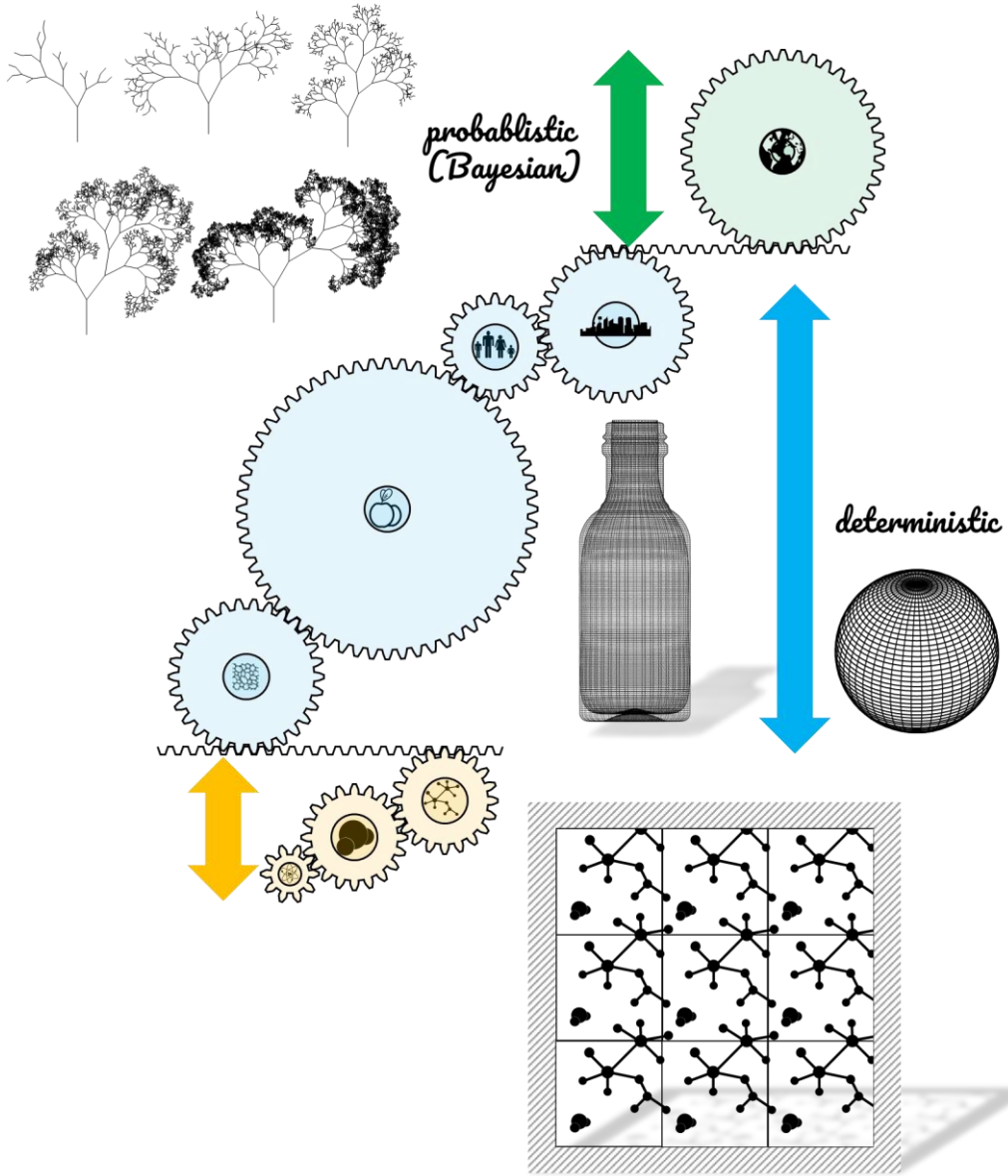
A first description of the scale problem



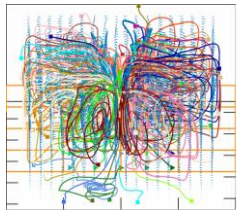


The scale problem





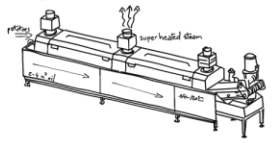
DEEP-FRYING



CONSUMER
(safer and healthier foods)

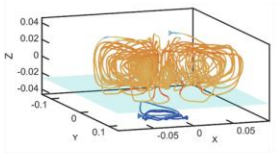
PROCESS SCALE

new deep-fryer designs and controls
(lower oil abuse, less fouling and smells)



new products, less fatty fried products

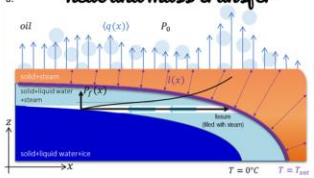
anisothermal flows



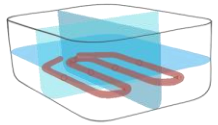
deep-fryer

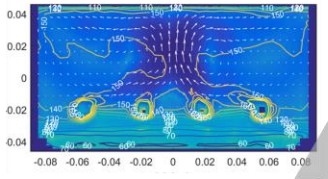
food product

heat and mass transfer



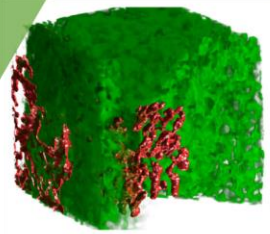
anisothermal flows

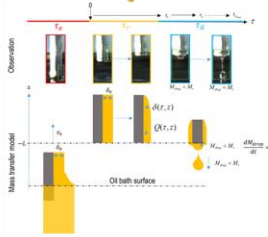




flow

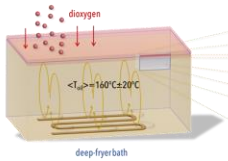
tissue

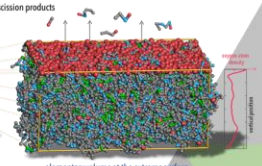


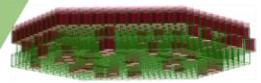


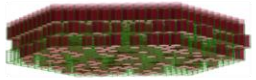
oil adhesion
oil dripping

oxygen dissolution - chemical transport

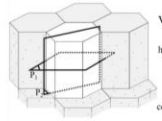


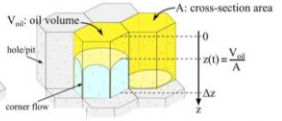






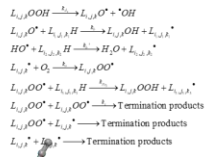
isolated cells



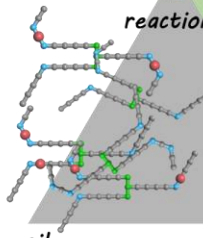


oil and air penetration

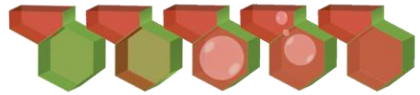
thermooxidation mechanism

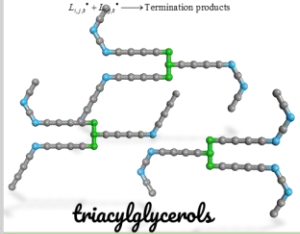


reactions



hydroperoxides

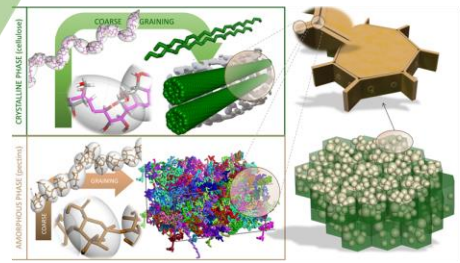




triacylglycerols

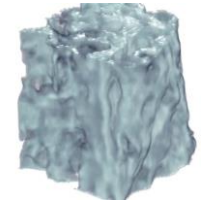
oil consituents

food constituents



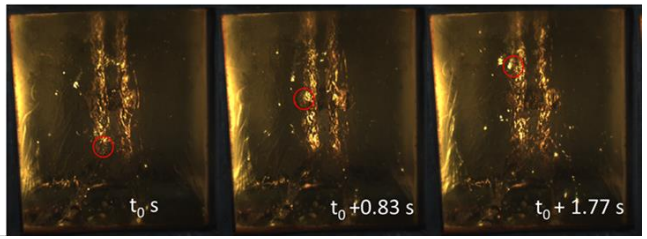
transformation of food constituents

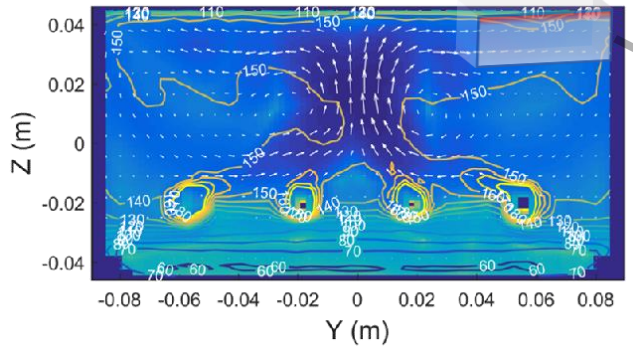
FOOD SCALE

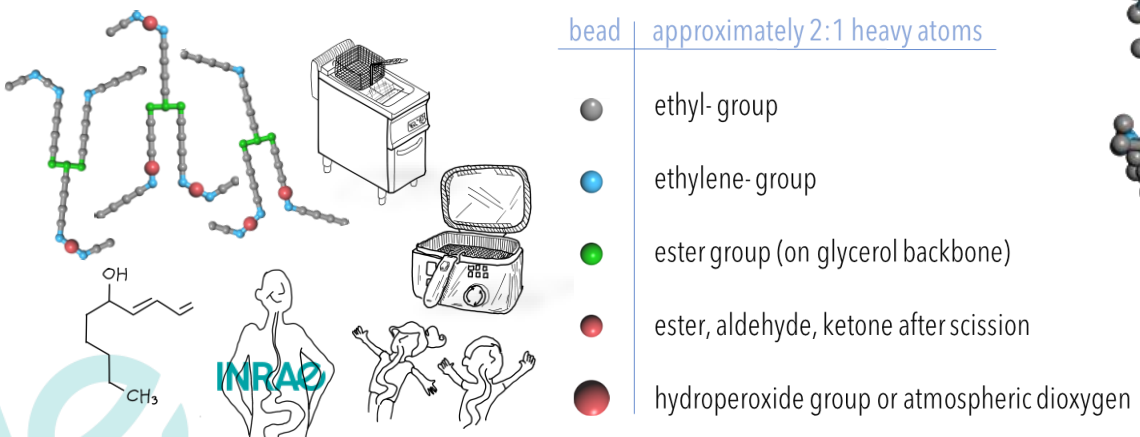


Example: detailed oil oxidation at molecular scale during deep-frying

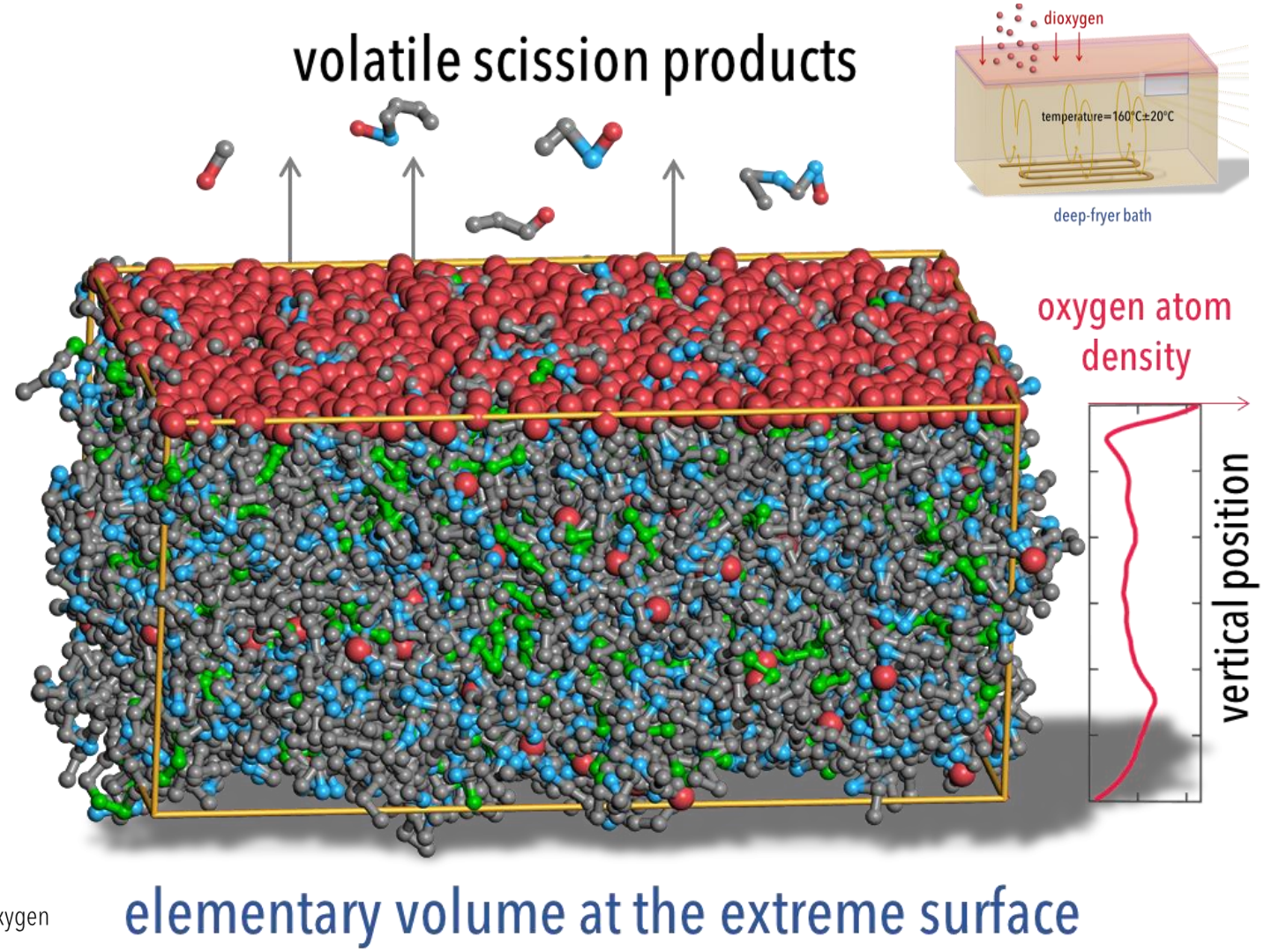
Touffet *et al*. Coupling between oxidation kinetics and anisothermal oil flow during deep-fat frying. *Physics of Fluids*. **2021**, 33, 085105



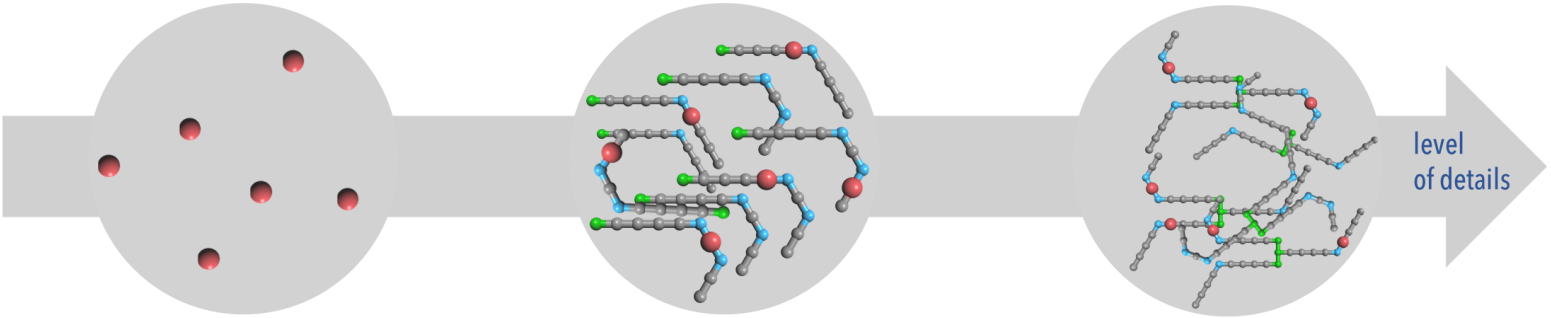




bead	approximately 2:1 heavy atoms
	ethyl- group
	ethylene- group
	ester group (on glycerol backbone)
	ester, aldehyde, ketone after scission
	hydroperoxide group or atmospheric dioxygen



MESOSCOPIC MODELING at process scale (oil oxidation> 2 hours) relating process design and control with chemistry



balance in hydroperoxide chemical functions or equivalent O_2:

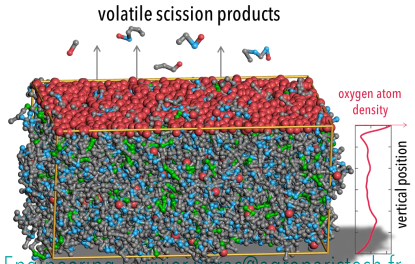
- balance of labile hydrogens
- average reactivity
- no specific thermal activation
- no effect of TAG composition
- no ability to predict the profile of oxidation products

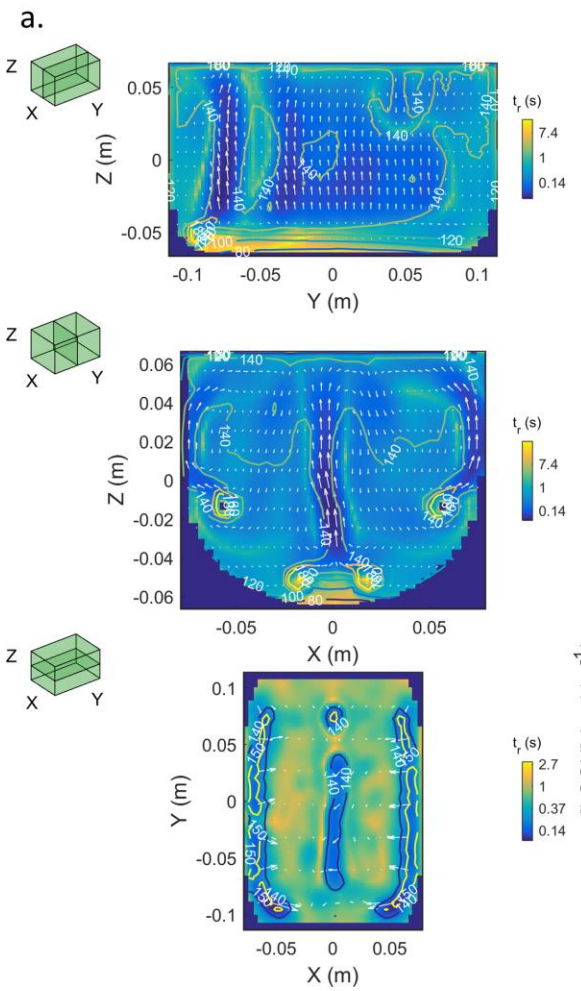
balance in fatty esters (FE) oxidized or not

- specific reactivity based on FE composition
- specific thermal activation
- effect of TAG composition
- lineage of oxidation products
- no correlated transport for FE attached to the same glycerol backbone

balance in triacylglycerols (TAG) oxidized or not

- realistic description
- correlated transport of FE attached to the same glycerol
- profile of oxidized TAG.
- possibility to add mono- and diacylglycerols.

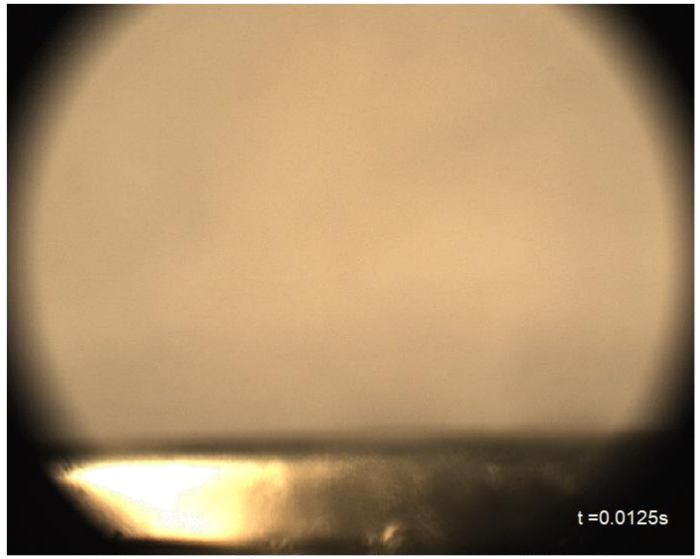


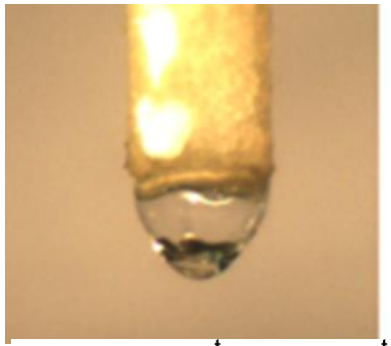


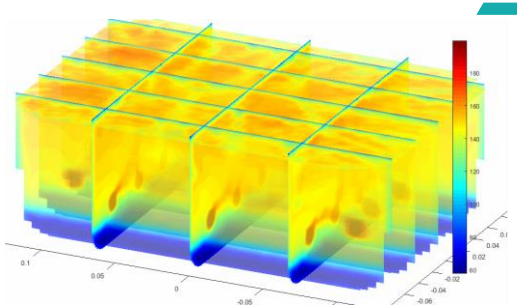
How to combine phenomena and scales

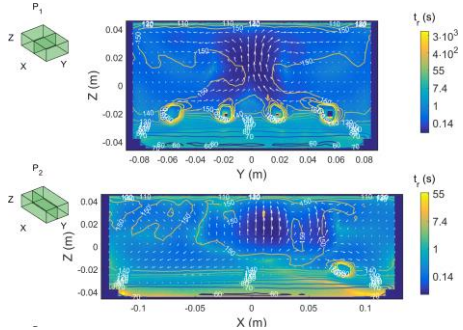
- Dimensionless (when possible)
- ***Coupling (expensive)*** vs ***nesting (inexpensive)***

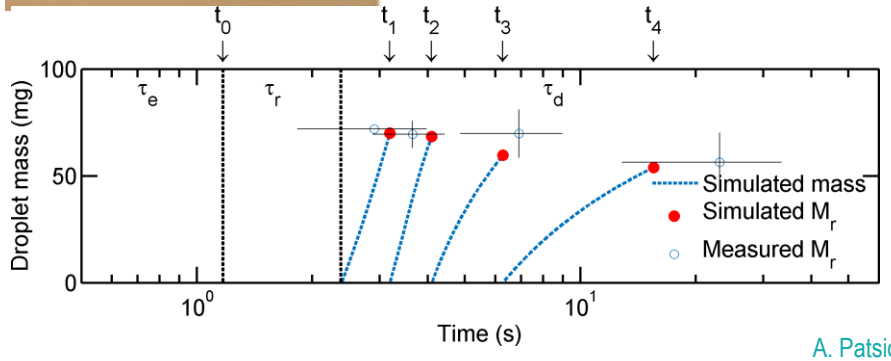
Oil dripping process (cooling)



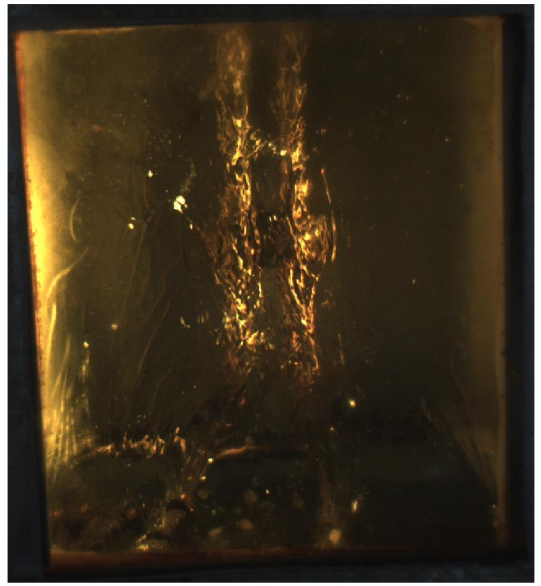


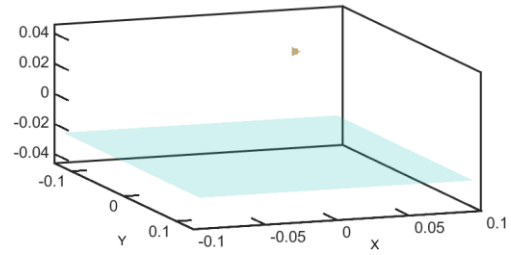






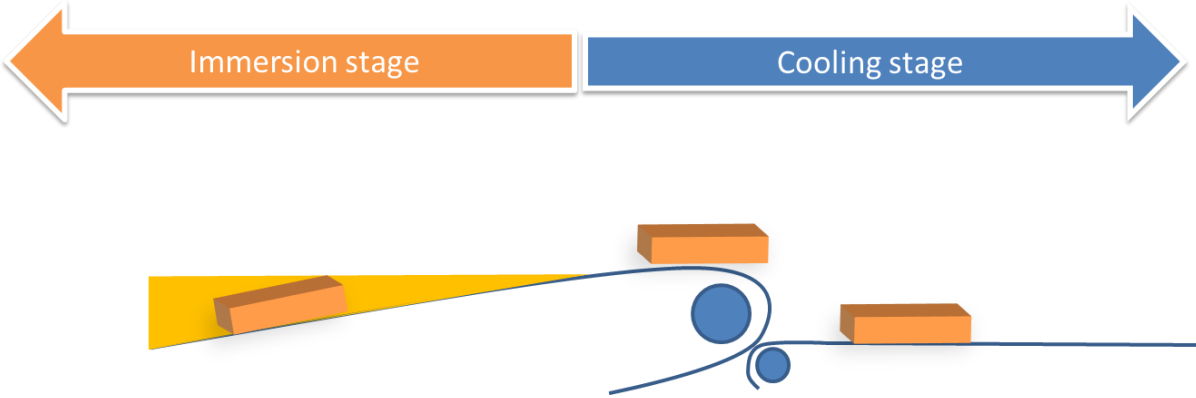
Oil oxidation during deep-frying





A. Patsioura, *et al*, *Food and Bioproducts Processing* ***2017, 101, 84-99.***
M. Touffet *et al.*, *Journal of Food Engineering* ***2018, 224, 1-16.***
M. Touffet *et al.*, *Physics of fluids* ***2021, 33, 085105***

Principles of deep-frying: beyond conventional descriptions



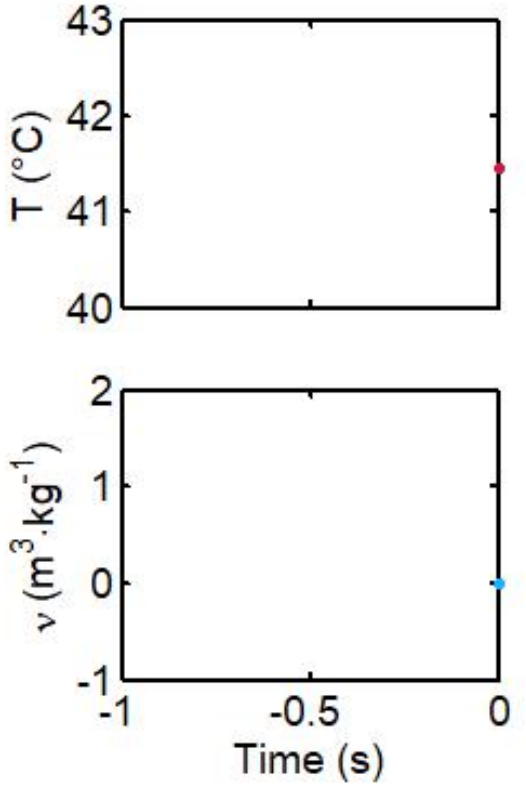
- Solid phases = starch, cell walls (cellulose pectins)
- Liquid phase = **WATER** (almost no oil)
- Gas phase = **PURE STEAM**

$=$ $\neq$ $\neq$

- Solid phases = starch, cell walls (cellulose pectins) + reaction products
- Liquid phases = water + **OIL**
- Gas phase = mixture **AIR** + residual water vapor

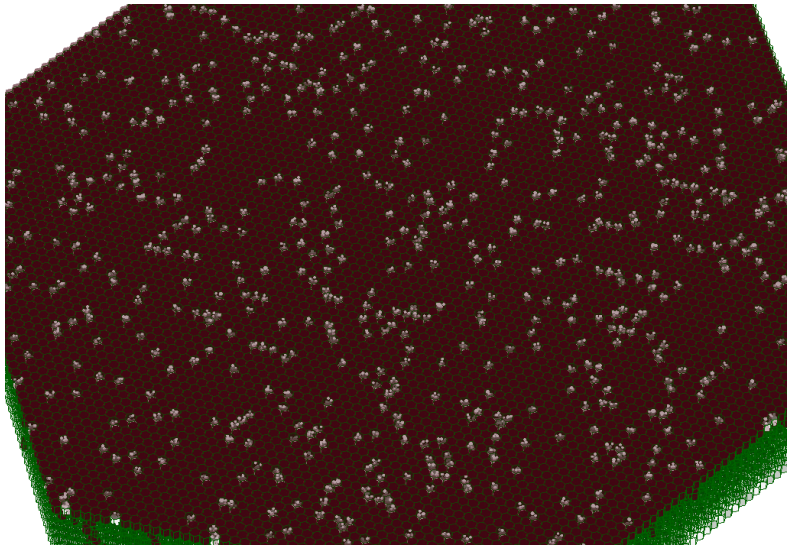
t=0s, T=41.454°C

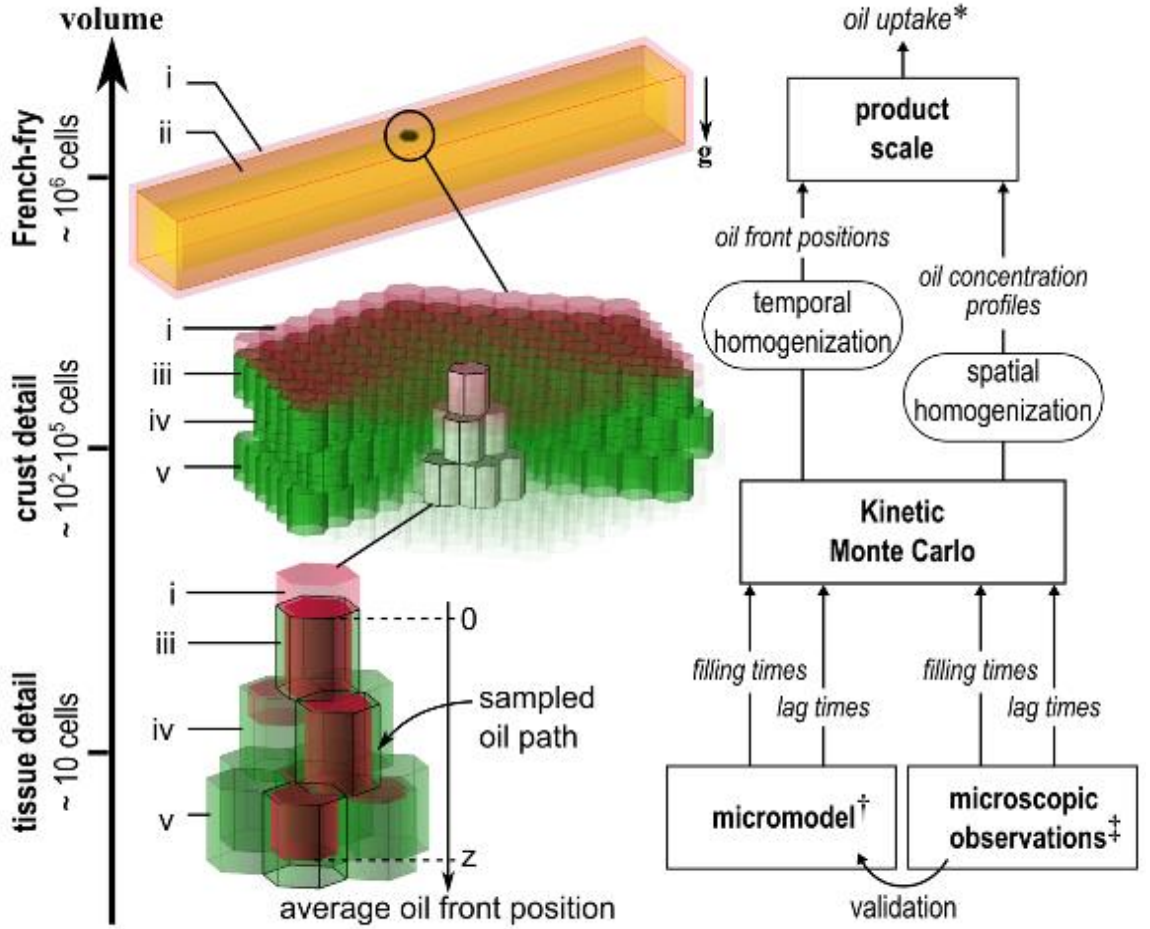
u = 0.001111 $m^3 \cdot kg^{-1}$



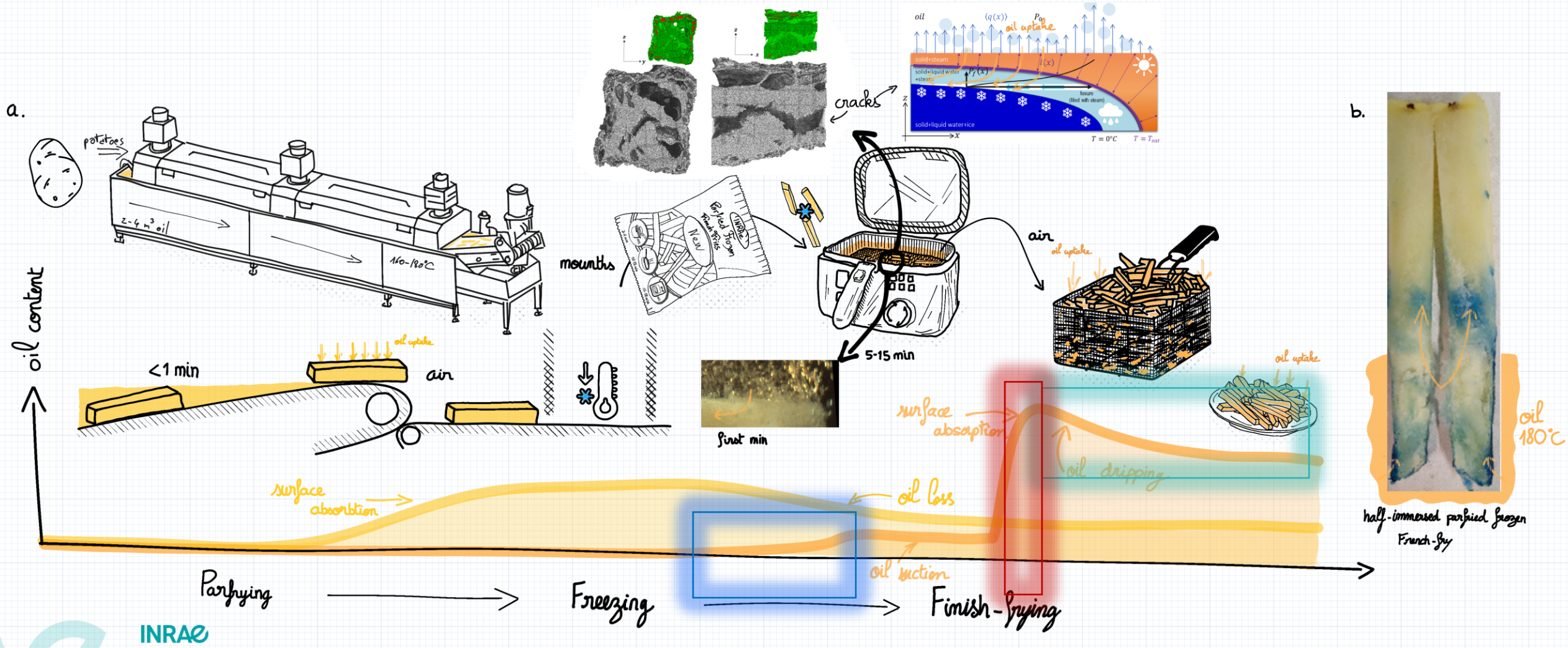
How to combine phenomena and scales

- ***Chaining*** ●→◆→●→■
- ***Looping***
- ***Ensemble averaging*** (very important) $x = \sum w_i \cdot x_i \,/\, \sum w_i$
- ***Serialization of scenarios***
- ***Piping*** (CFD, chemistry, mass transfer, thermodynamics models)
- ***Standards and good modeling practices***





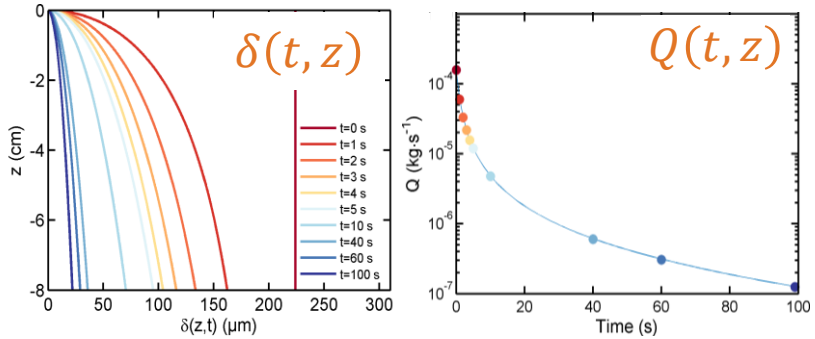
Multiscale model to describe oil uptake

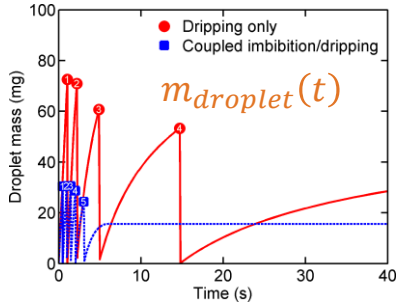


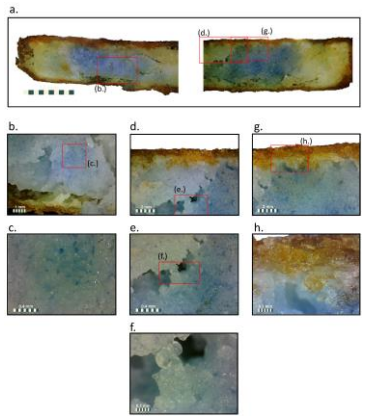
INRAE

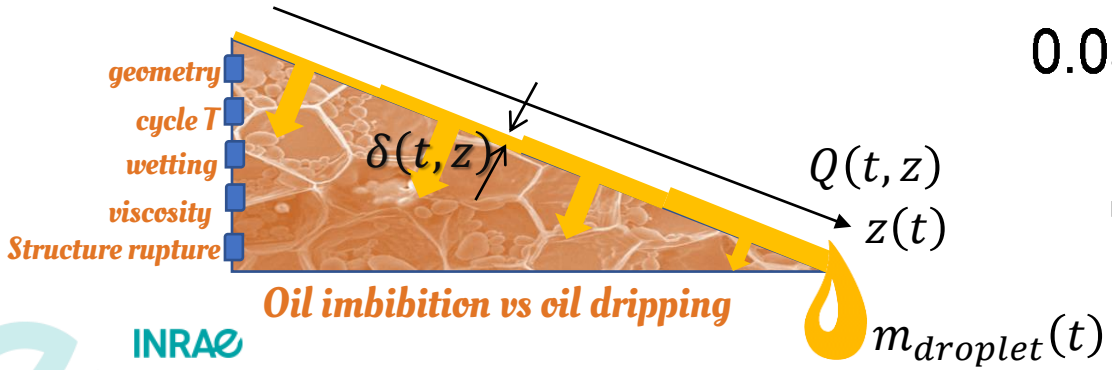
Touffet et al., Food Bioprod Process, 2020, 123, 14–30

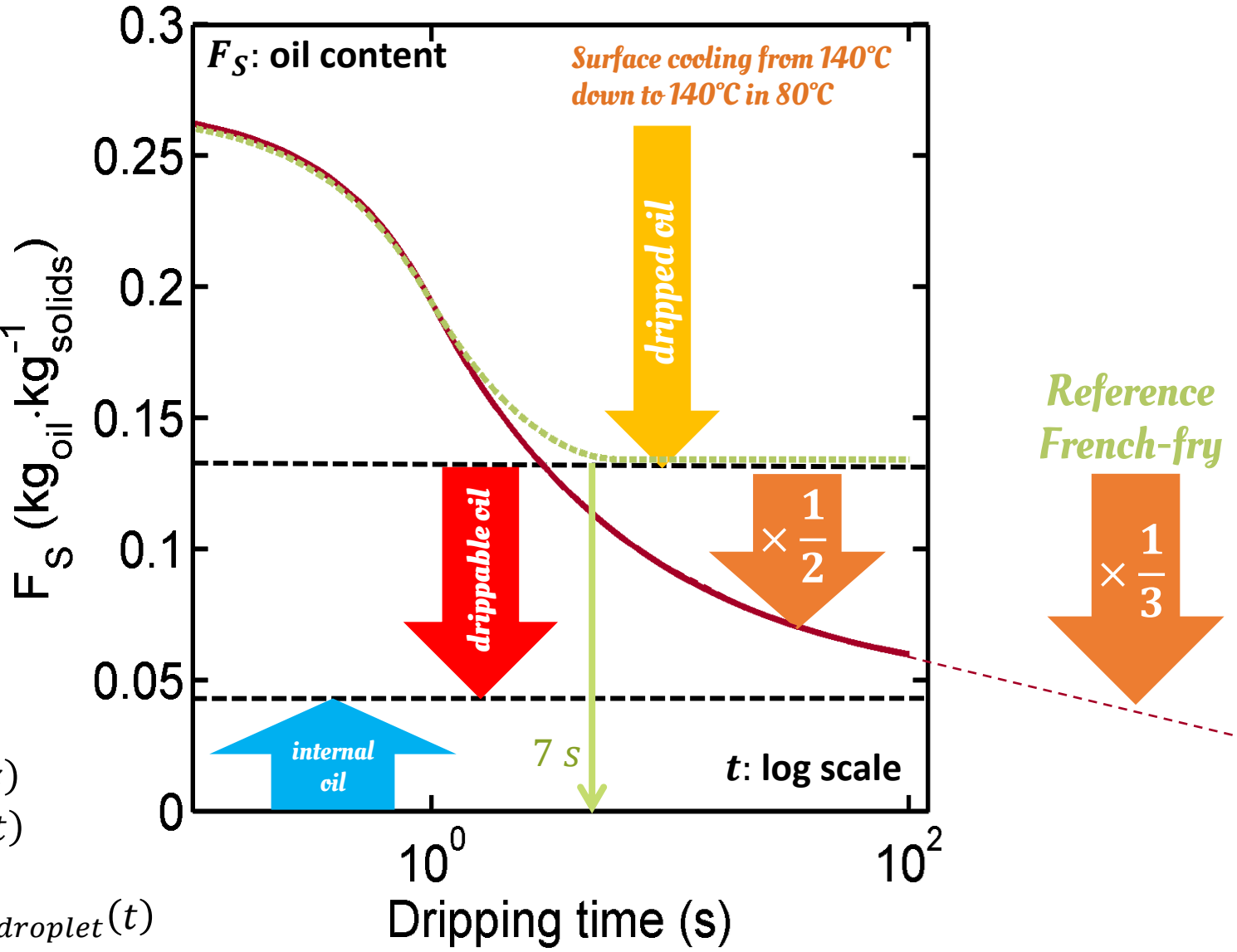
Oil penetrating and dripping process











Food Packaging

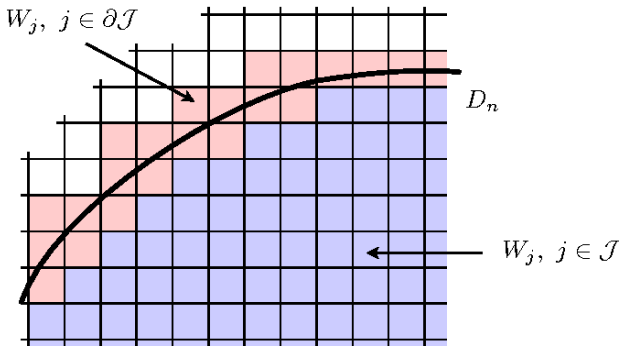
We are sleeping on a volcano… A wind of revolution blows, the storm is on the horizon.

Alexis de Tocqueville (1848, just prior revolutions in Europe).

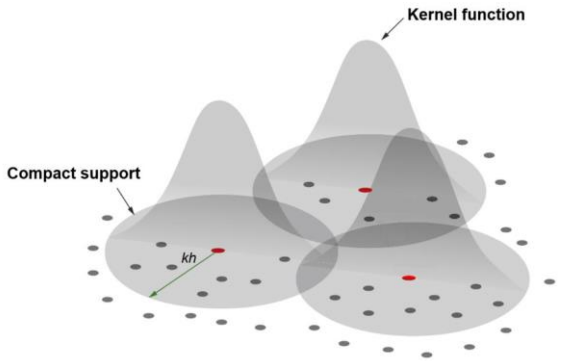
Beyond macroscopic description

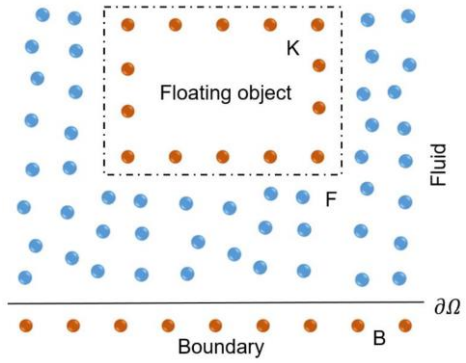
Continuum thermodynamic limit

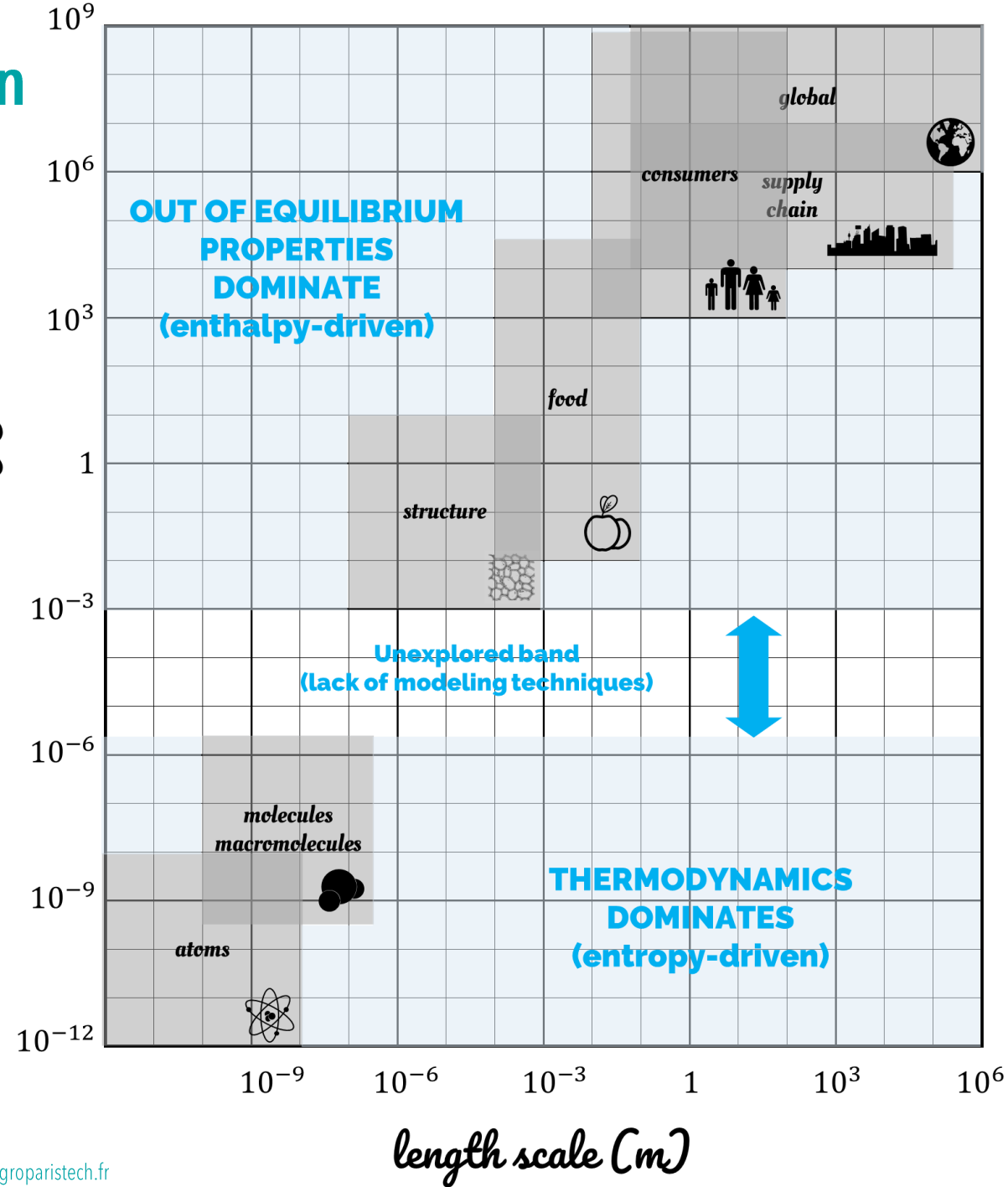
$$E, N, V, \Lambda \to \infty \quad \text{such that} \quad \frac{E}{N} \to e\,, \quad \frac{N}{V} \to n \quad \text{with } e, n \text{ finite.}$$



Continuum Mechanics limit



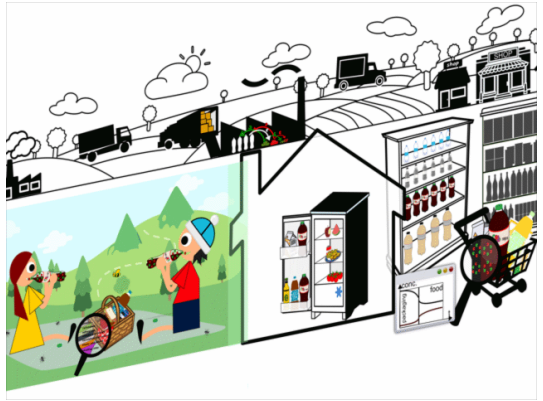


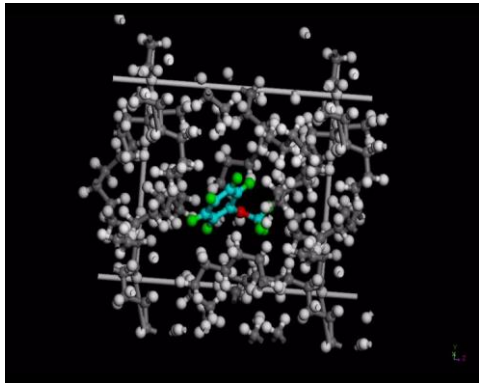


Food packaging

Property (transport, thermodynamics)

Statistical-Physics (equilibrium)



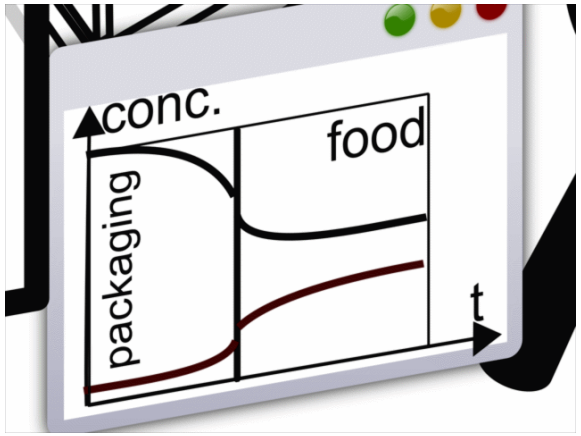


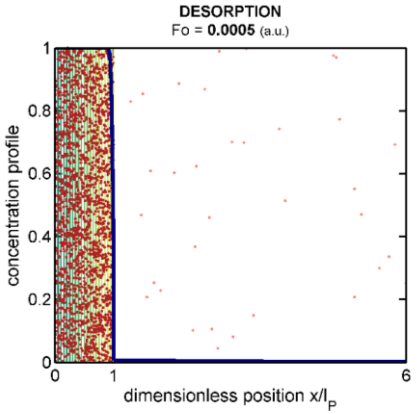
Free energy perturbation

$$\exp\left(-\frac{F_1 - F_0}{k_B T}\right) = \left\langle \exp\left(-\frac{U_1 - U_0}{k_B T}\right)\right\rangle$$

Fluxes, flows, kinetics

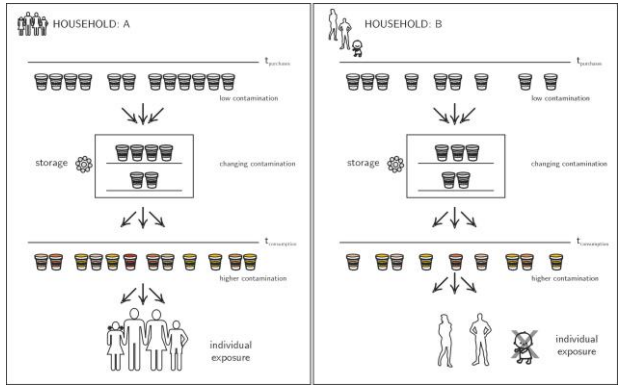
Deterministic, probablistic





Risk assessment

Probabilistic (no equilibrium)

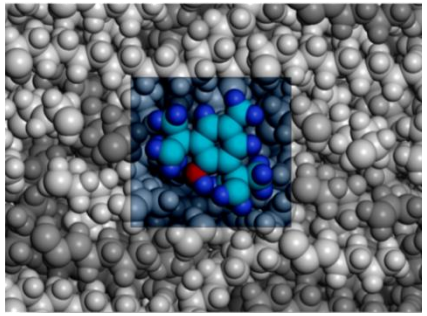


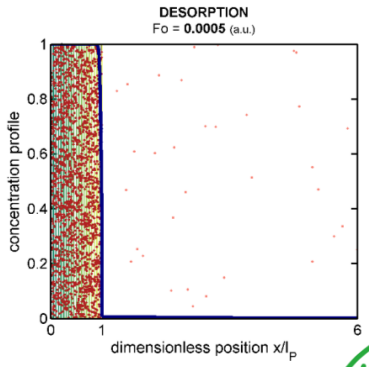
Industrial & Engineering Chemistry Research **2010, 49, 7263-7280.**
Industrial & Engineering Chemistry Research **2017, 56, 774–787.**
Food Research International **2017, 88, Part A, 91-104.**

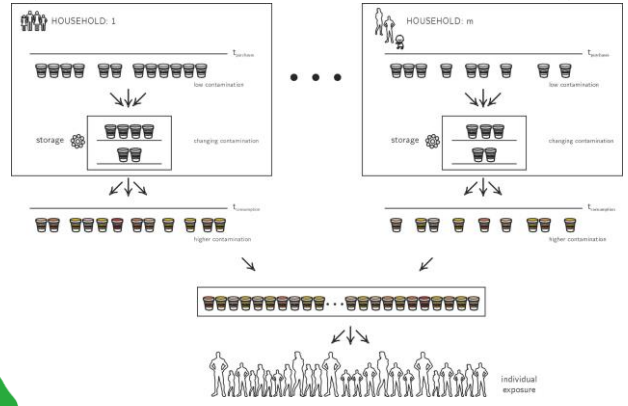
Food packaging

property | Contamination scenarios | consumer exposure

Probabilistic (equilibrium) | Probablistic/deterministic | Probabilistic (no equilibrium)

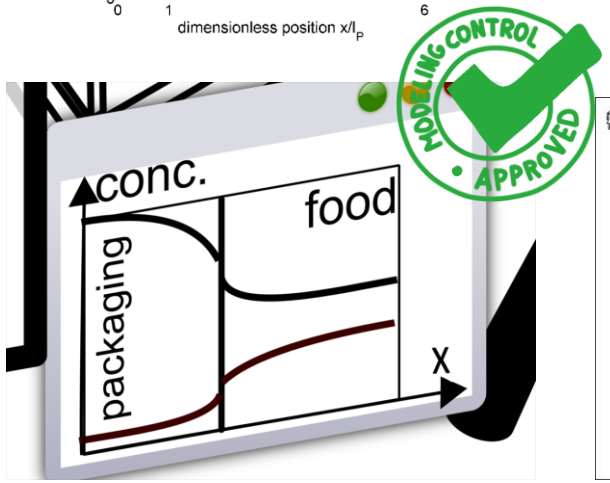


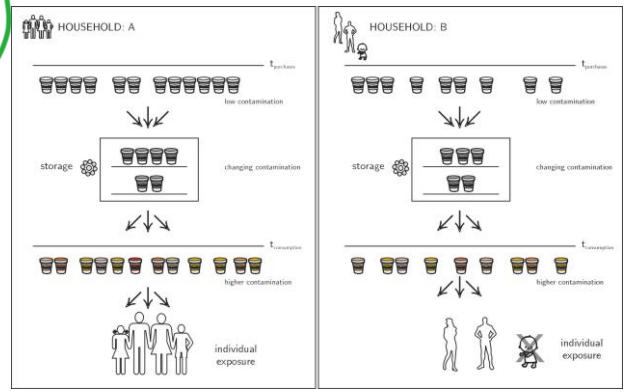


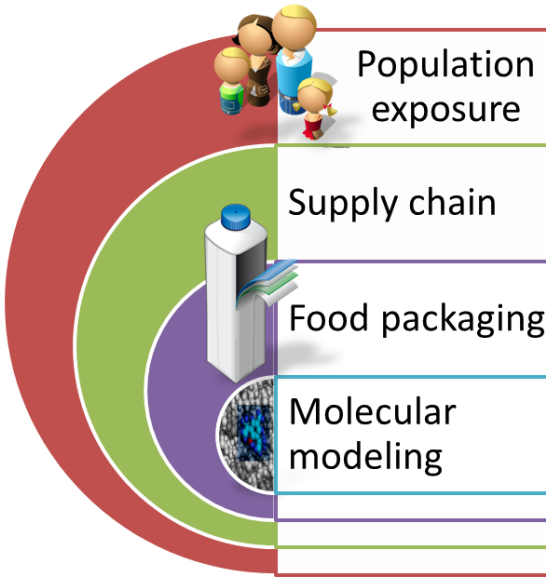


Free energy perturbation

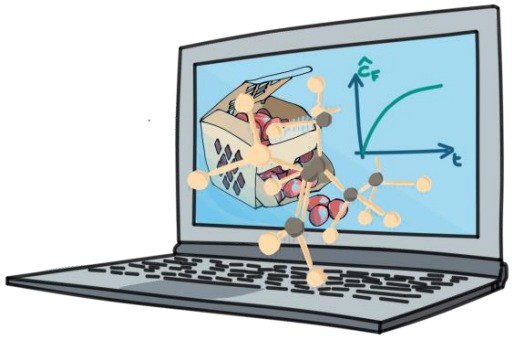
$$\exp\left(-\frac{F_1 - F_0}{k_B T}\right) = \left\langle \exp\left(-\frac{U_1 - U_0}{k_B T}\right)\right\rangle$$





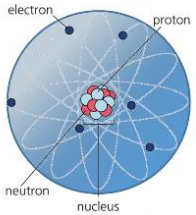


Molecular and supramolecular modeling



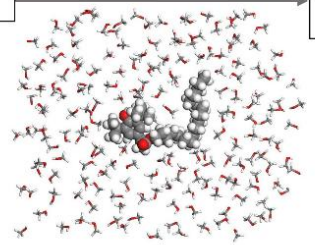
Excess mixing enthalpy: atomistic scale

Excess mixing Entropy: coarse grained repre-sentations



All-atomic model

MD simulation



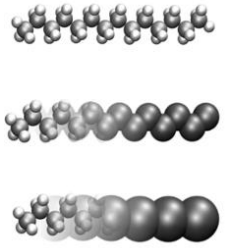
Full information
(but limited scale)

Coarse-graining – simplified model

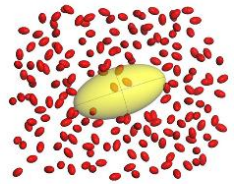
RDFs for selected degrees of freedom

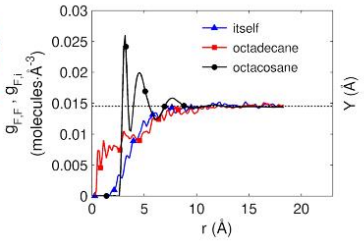
Boltzmann inversion
$U(r) \propto k_B T \ln[RDF(r)]$

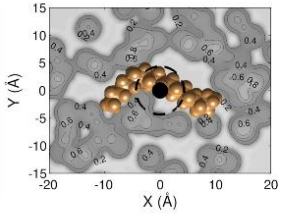
Effective potentials for selected sites



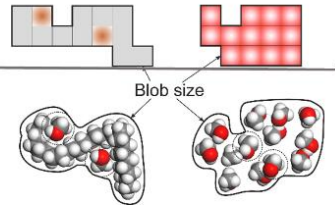
Increase scale







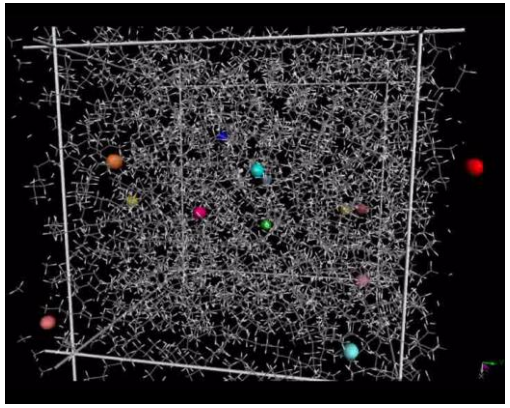
Effective potentials

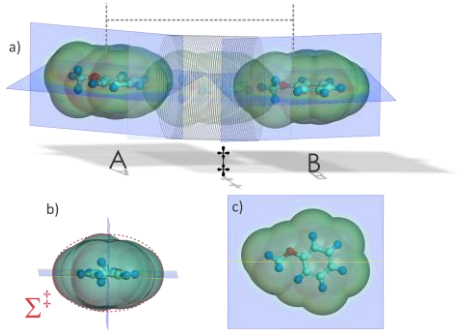


Properties on a larger length/time scale

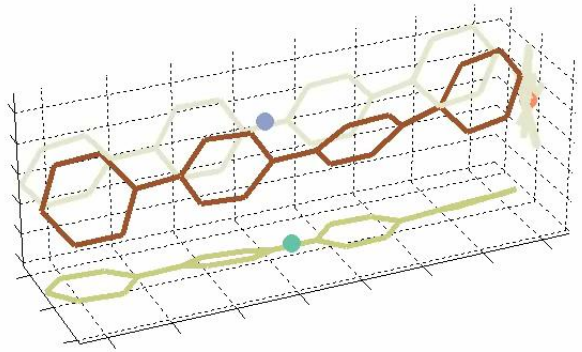
Identification of molecular mechanisms

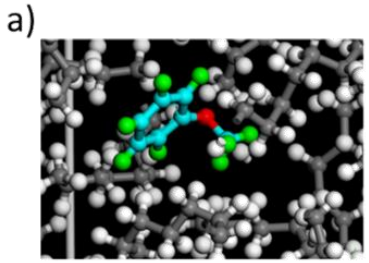
Vitrac et al. Front. Chem. Eng., 21 January 2022
https://doi.org/10.3389/fceng.2021.786879

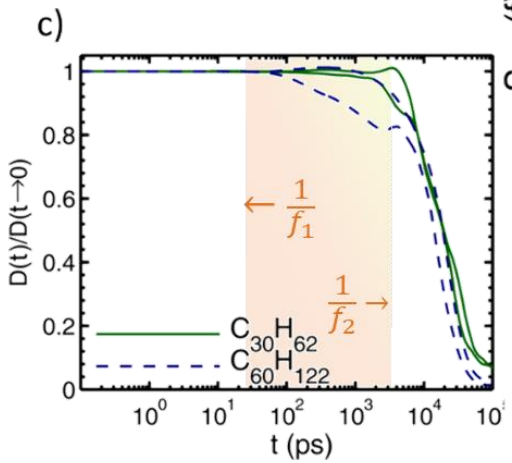




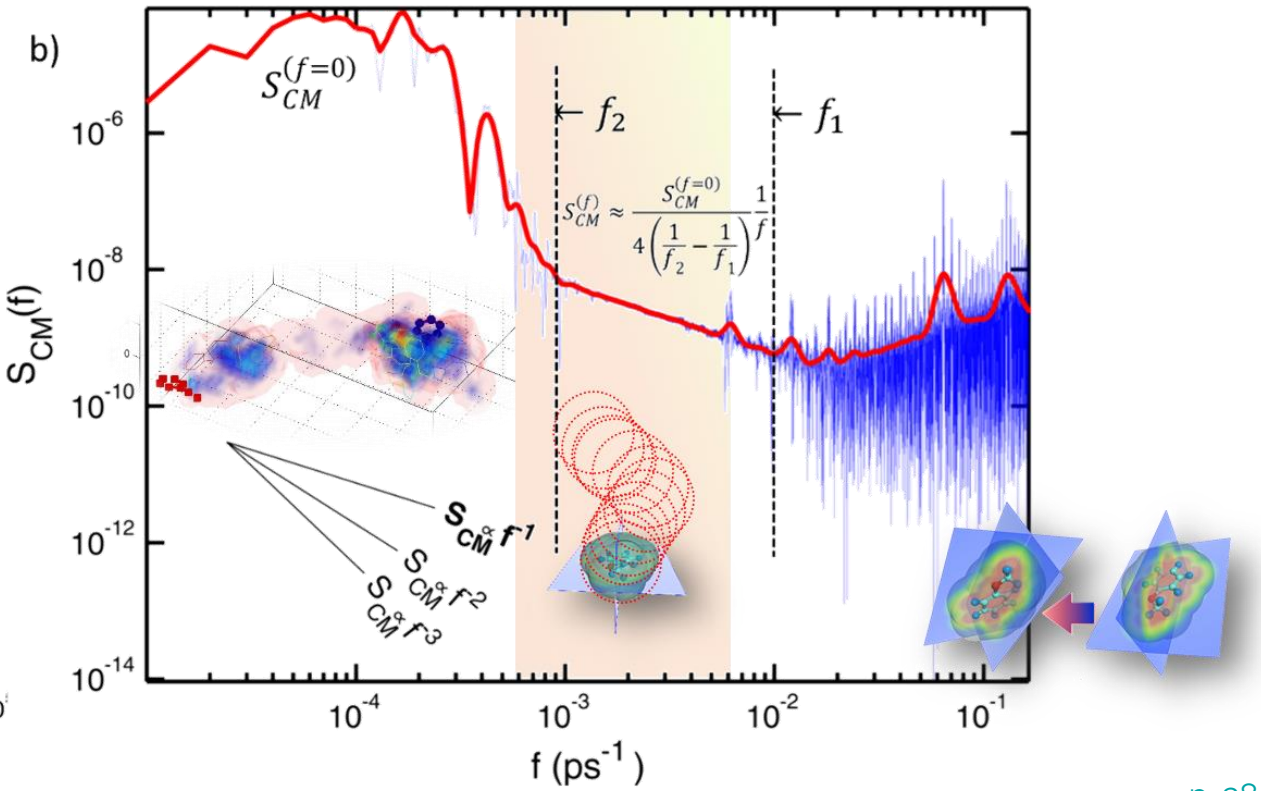
$$f_2 \leq f \leq f_1$$





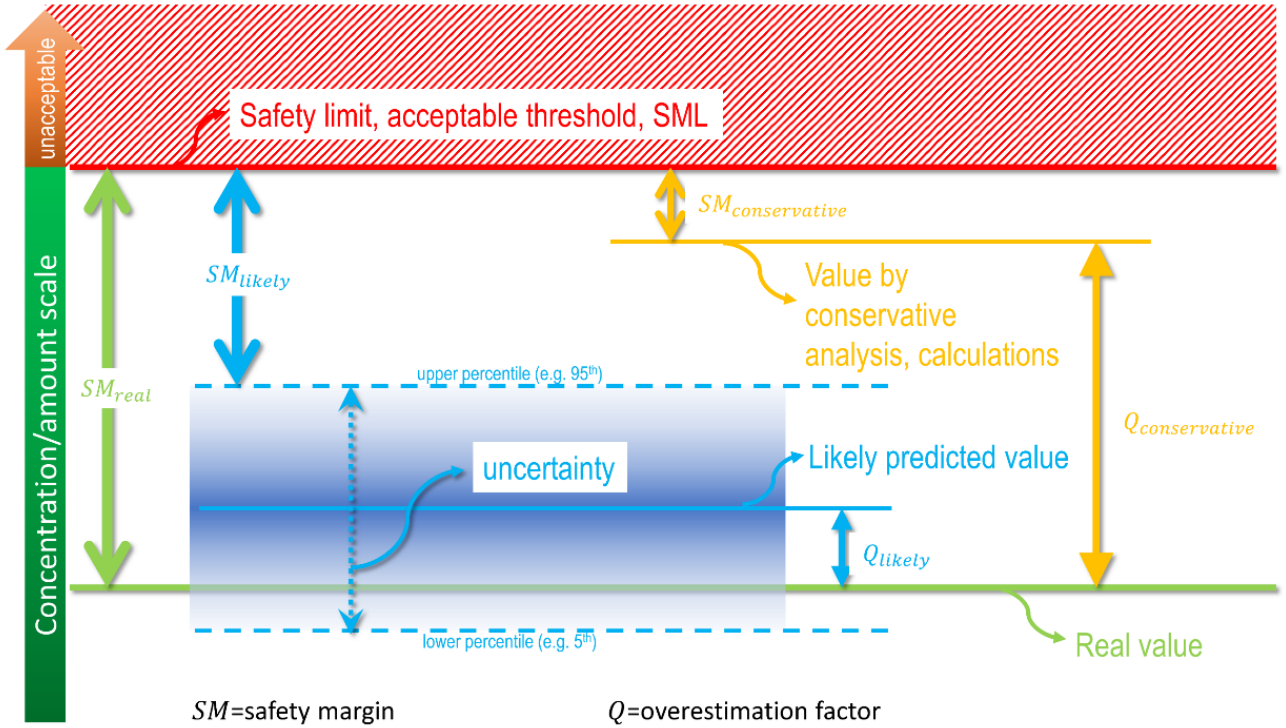


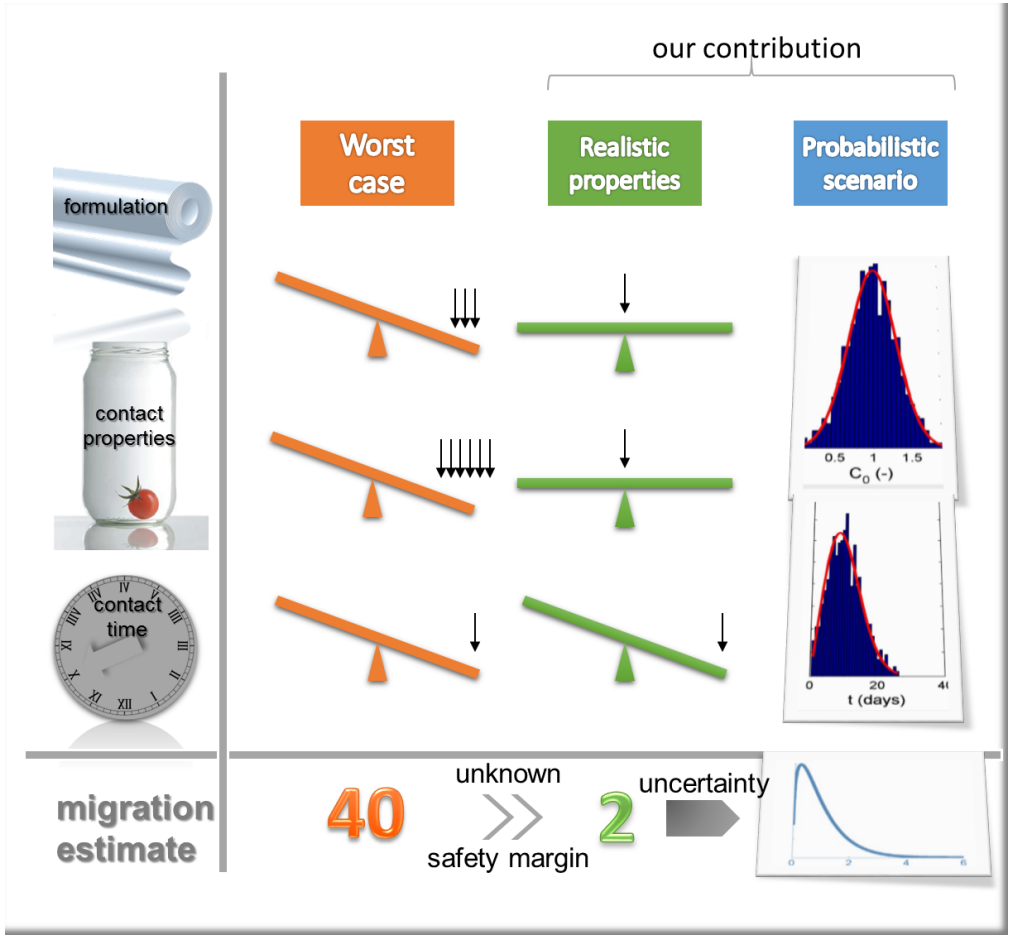
Spectral density of $\frac{1}{\pi}\frac{\partial}{\partial t}\langle\|\boldsymbol{x_{CM}}(t)-\boldsymbol{x_{CM}}(0)\|^2\rangle$, denoted $S_{CM}(f)$



Uncertainty vs Ignorance

- "*scientia*" (science) vs "*opinio*" (belief)
- Conventional modeling assumes complete knowledge and epistemologic transformation of information into knowledge.
- How to code "vagueness", "skeptism", "error", "doubt"





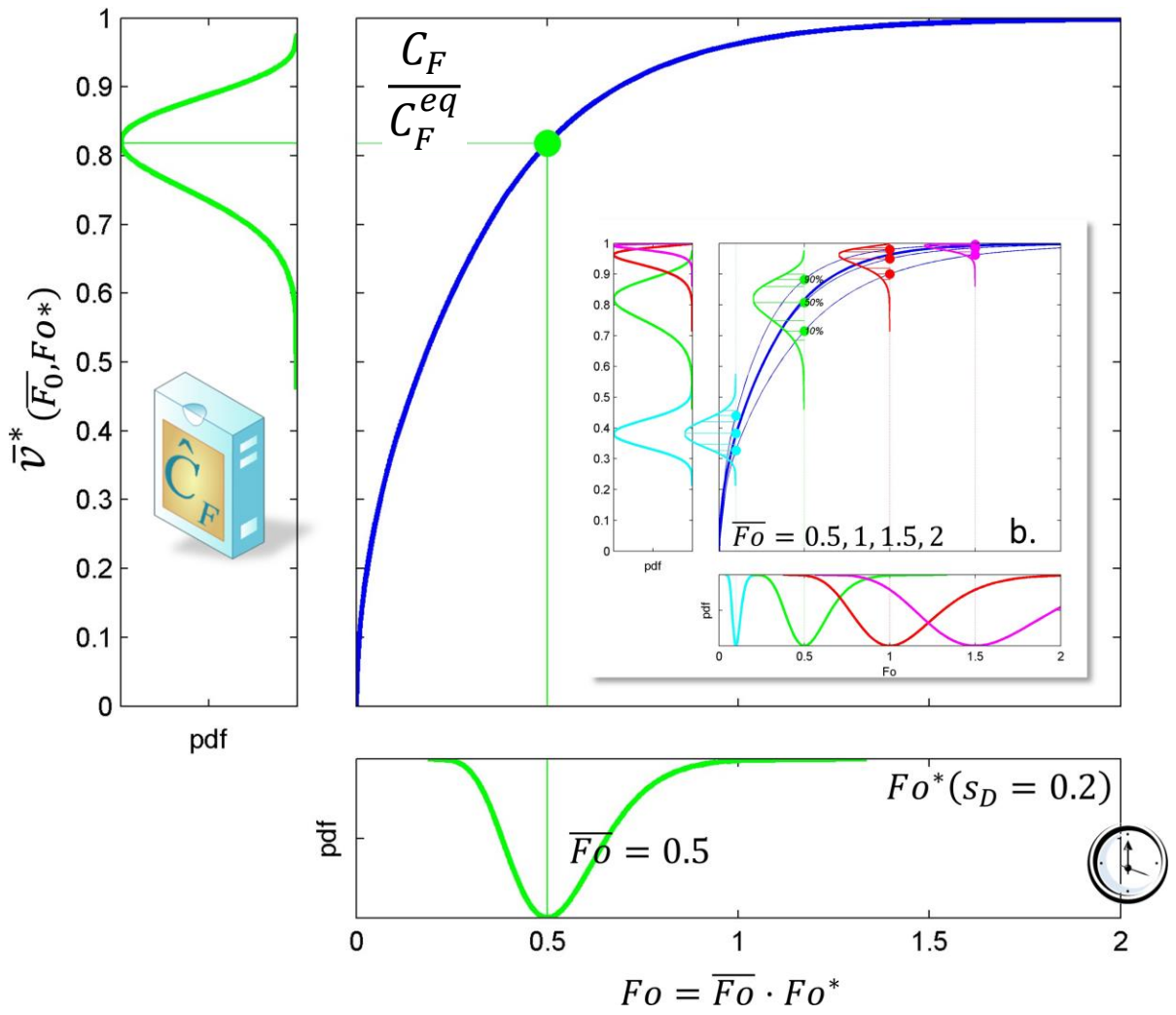
Y. Zhu, P.-M. Nguyen and O. Vitrac in: G. Robertson (Ed.): Elsevier Food Science Reference Module, Elsevier, Amsterdam, NL, 2019, pp. 64.

Probabilistic modeling

- Part of best practices
- "Mandatory" for risk assessment
- Uncertainty ≠ variability, it can be reduced by additional knowledge or model details.
- Monte-Carlo sampling can be avoided in several situations to reach almost real time simulation.

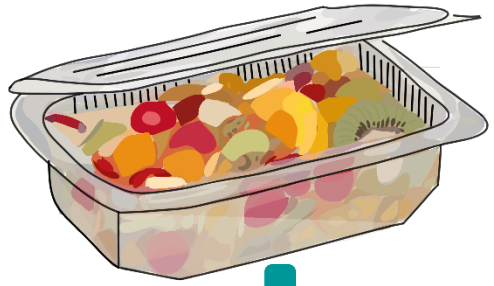
$$f_{\bar{v}^*}(v) = \sum_{k=1}^{p} f_{Fo}\left(\bar{v}^{*-1}\big|_{Fo\in Y_k}(v)\right)\left|\frac{d}{dv}\bar{v}^{*-1}\big|_{Fo\in Y_k}(v)\right|^{-1}$$

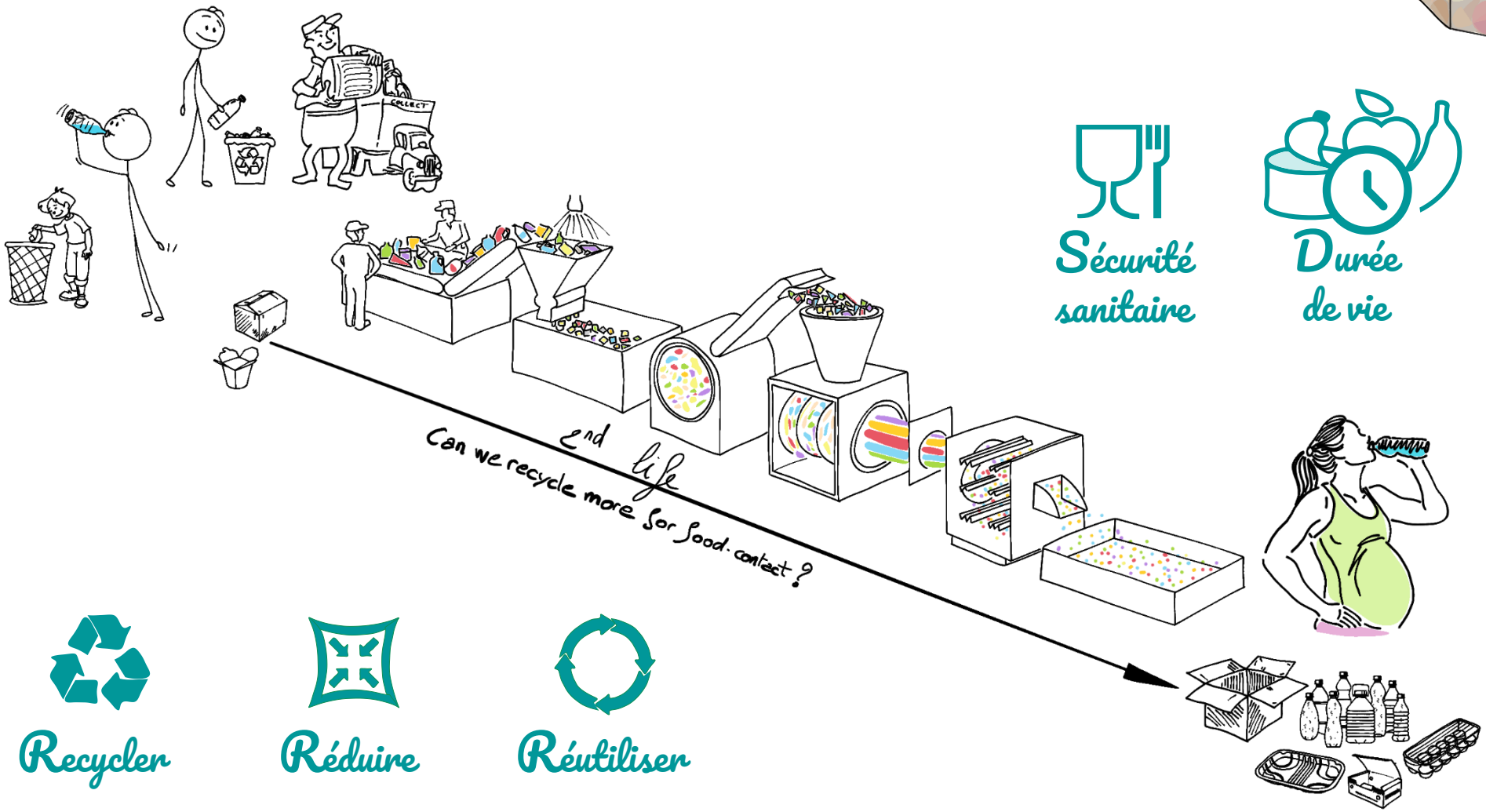
e.g., monotonic model



O. Vitrac and M. Hayert, *Aiche Journal* ***2005, 51, 1080-1095.***
O. Vitrac, B. Challe, J.-C. Leblanc and A. Feigenbaum, *Food Additives and Contaminants t* ***2007, 24, 75-94.***

Un problème d'ingénierie sous contraintes





Sécurité sanitaire

Durée de vie

Résistance mécanique

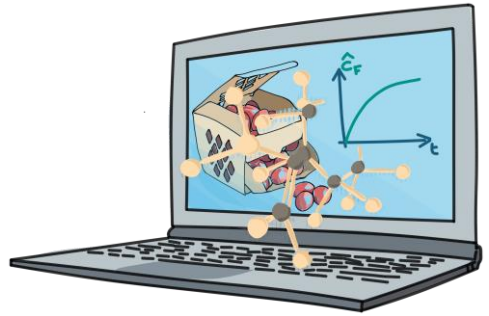
c&en Oct 2021, p. 28

Recycler

Réduire

Réutiliser

Des procédures de calcul acceptées en EU, USA, Chine



1990

EPA 560/5-85-015
September 1990

METHODS FOR ASSESSING EXPOSURE
TO CHEMICAL SUBSTANCES

Volume 11

Methodology for Estimating the Migration of Additives
and Impurities from Polymeric Materials

by

Arthur D. Schwope
and
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and

Robert C. Reid
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EPA Contract No. 68-D9-0166

Project Officer

Thomas Murray
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Office of Toxic Substances
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U.S. ENVIRONMENTAL PROTECTION AGENCY
OFFICE OF PESTICIDES AND TOXIC SUBSTANCES
WASHINGTON, D.C. 20460

https://nepis.epa.gov/Exe/ZyPURL.cgi?Dockey=P100BCMB.TXT

2015

European Commission

JRC TECHNICAL REPORTS

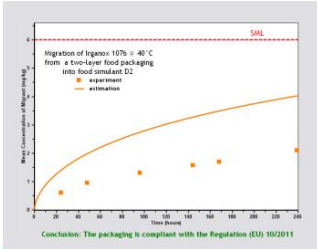
Practical guidelines on the application of migration modelling for the estimation of specific migration

In support of Regulation (EU) No 10/2011 on plastic food contact materials

Eddo J. Hoekstra (Ed.), Rainer Brandsch, Claude Dequatre, Peter Mercea, Maria-Rosaria Milana, Angela Störmer, Xenia Trier, Olivier Vitrac Annette Schäfer and Catherine Simoneau

2015

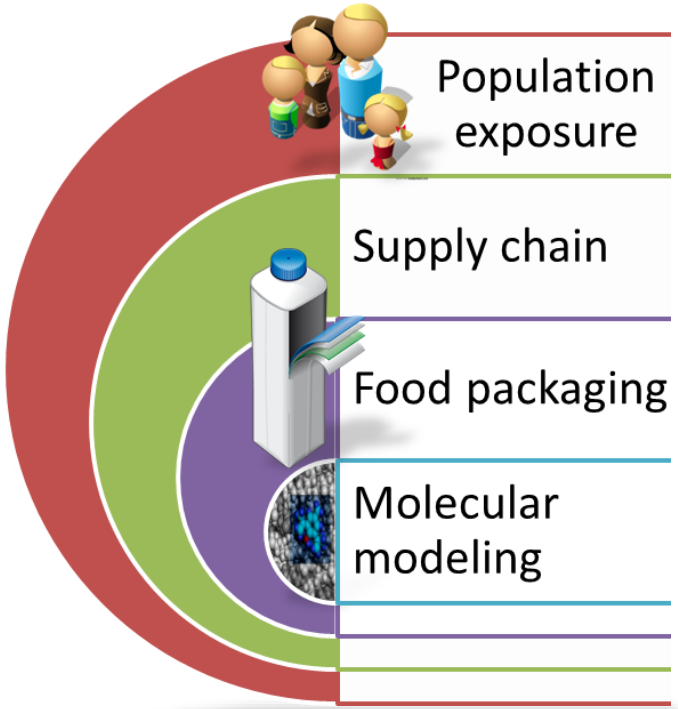
$$\frac{C_i^{n+1} - C_i^n}{\Delta t} = D\frac{C_{i+1}^n - 2C_i^n + C_{i-1}^n}{h^2}$$



Joint Research Centre

EUR 27529 EN

http://publications.jrc.ec.europa.eu/repository/handle/JRC98028

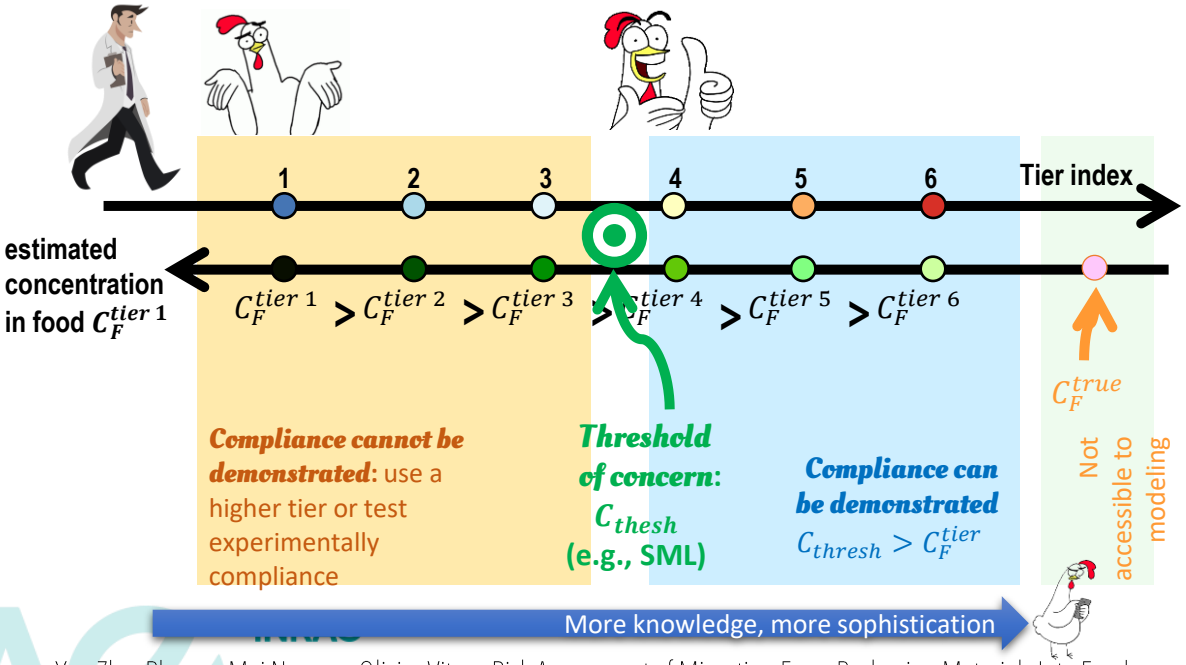


Parsimony vs. sophistication

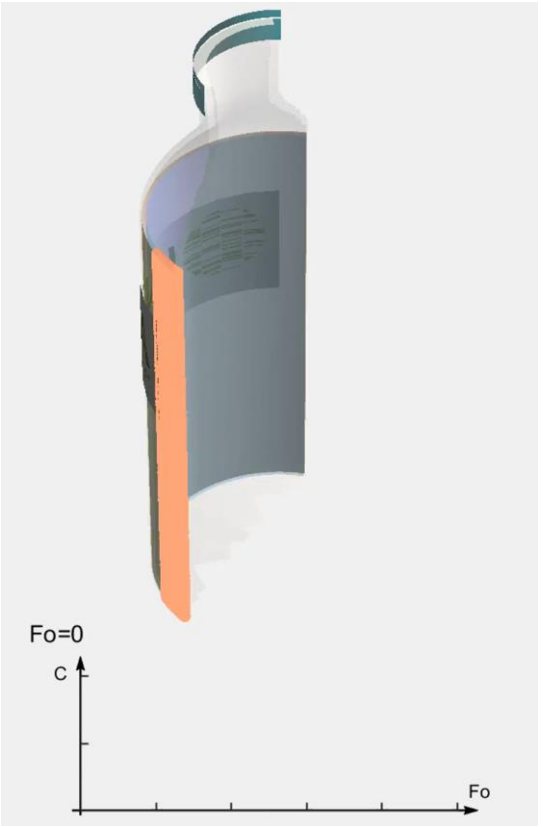
During the last decade migration modeling became high throughput, multiscale and connected to chemometric approaches

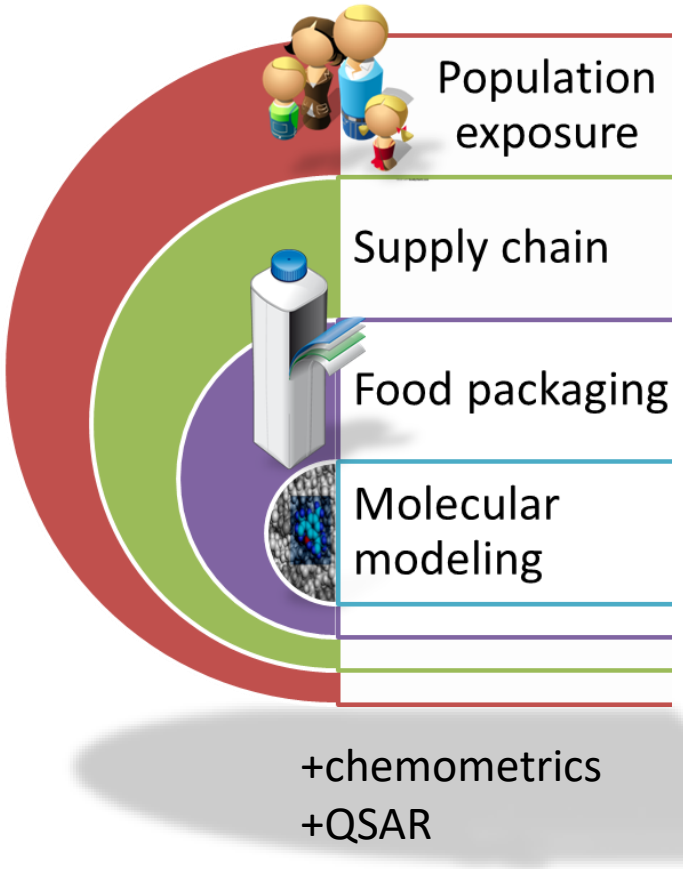
What is the goal?

The art of migration modeling consists in building a sequence of scenarios so that the last scenario provides a value lower than the threshold of concern while being large than the real concentration (unknown).



Multiscale modeling



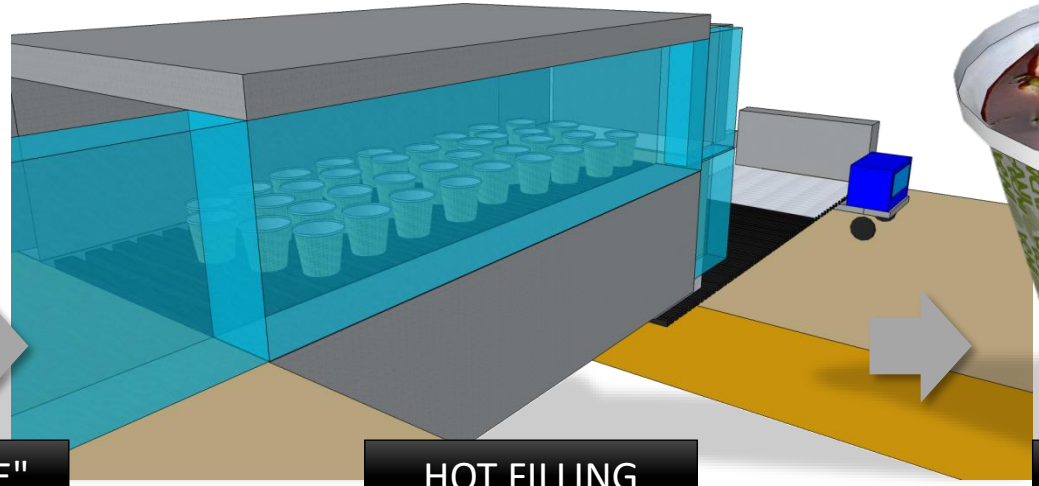


Yan Zhu, Phuong-Mai Nguyen, Olivier Vitrac, Risk Assessment of Migration From Packaging Materials Into Food, Reference Module in Food Science, Elsevier, 2019, https://doi.org/10.1016/B978-0-08-100596-5.22501-8.

Food Computer-Aided design: new perspectives

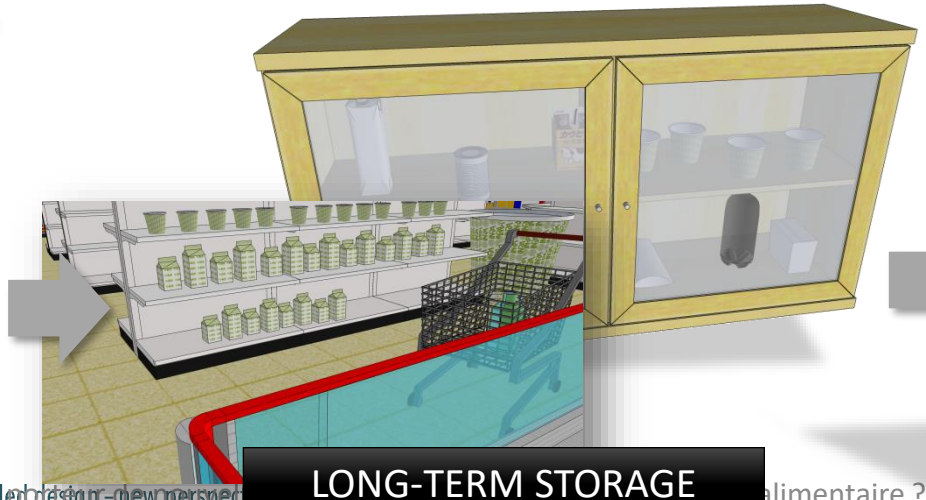
Des complexités arbitraires

STORAGE "BEFORE USE"



HOT FILLING

FATTY CONTACT



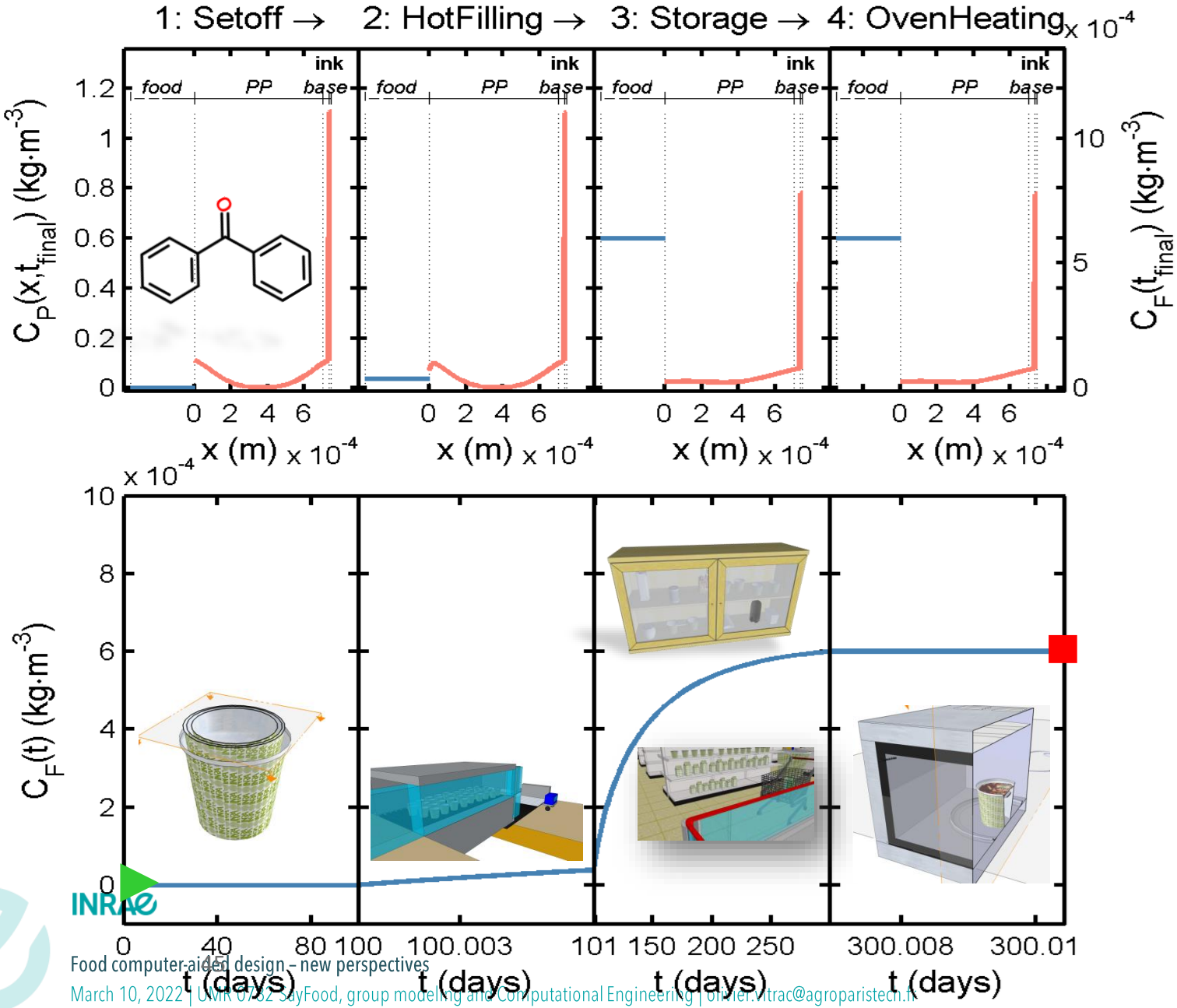
LONG-TERM STORAGE

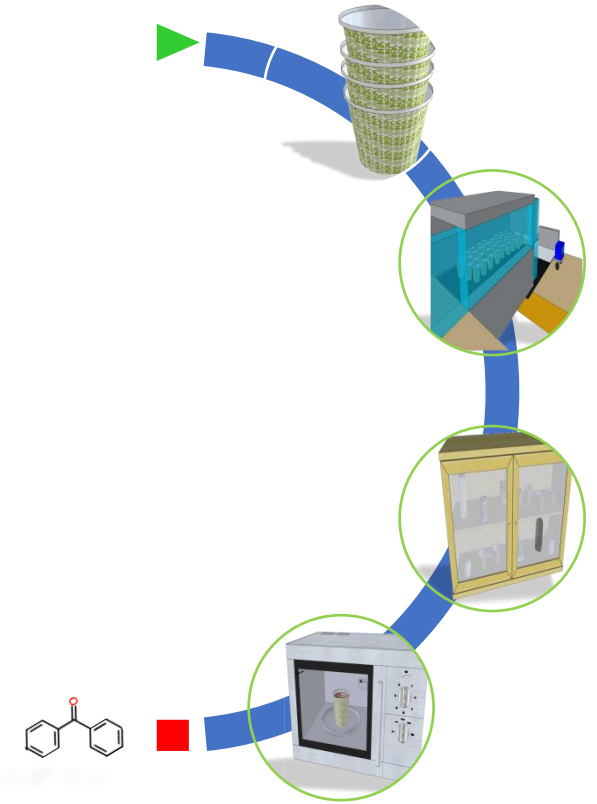
MICROWAVE OVEN HEATING

Nguyen, P.-M., Goujon, A., Sauvegrain, P., et Vitrac, O. (2013). A Computer-Aided Methodology to Design Safe Food Packaging and Related Systems. AIChE Journal, 59(4), 1183-1212.

CHAINED STEPS

UV-curing printing ink

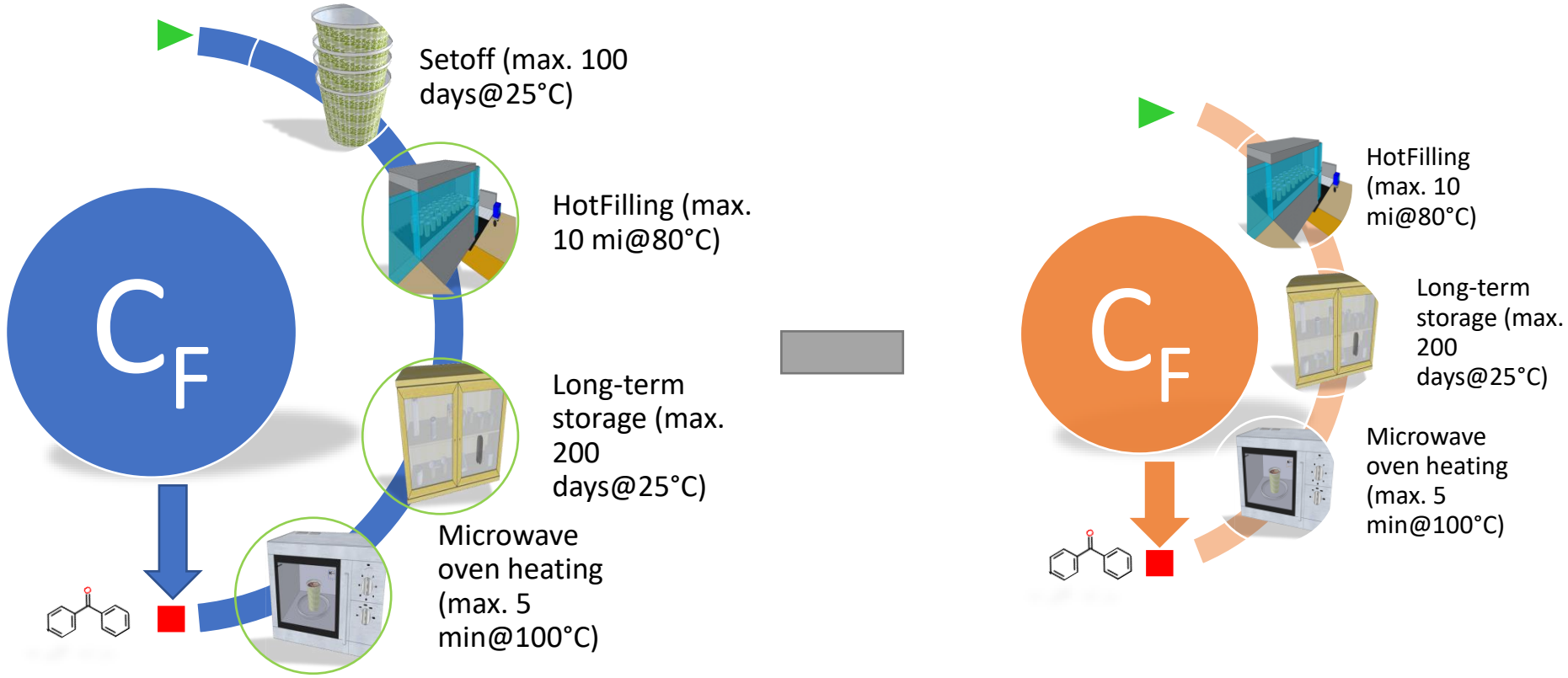




AIChE Journal, 59(4), 1183-1212

ASSESSING THE SEVERITY OF A SINGLE STEP

CASE OF "SETOFF" STEP



$$\text{Severity}\left(\hat{C}_F(step\,i)\right) = f\left(\max\left(C_{F_M}|_{1\to2\to\cdots\to M} - C_{F_M}|_{1\to2\to\cdots\to M/i}, C_{F_i}|_i\right)\right)$$

comparison with step i alone

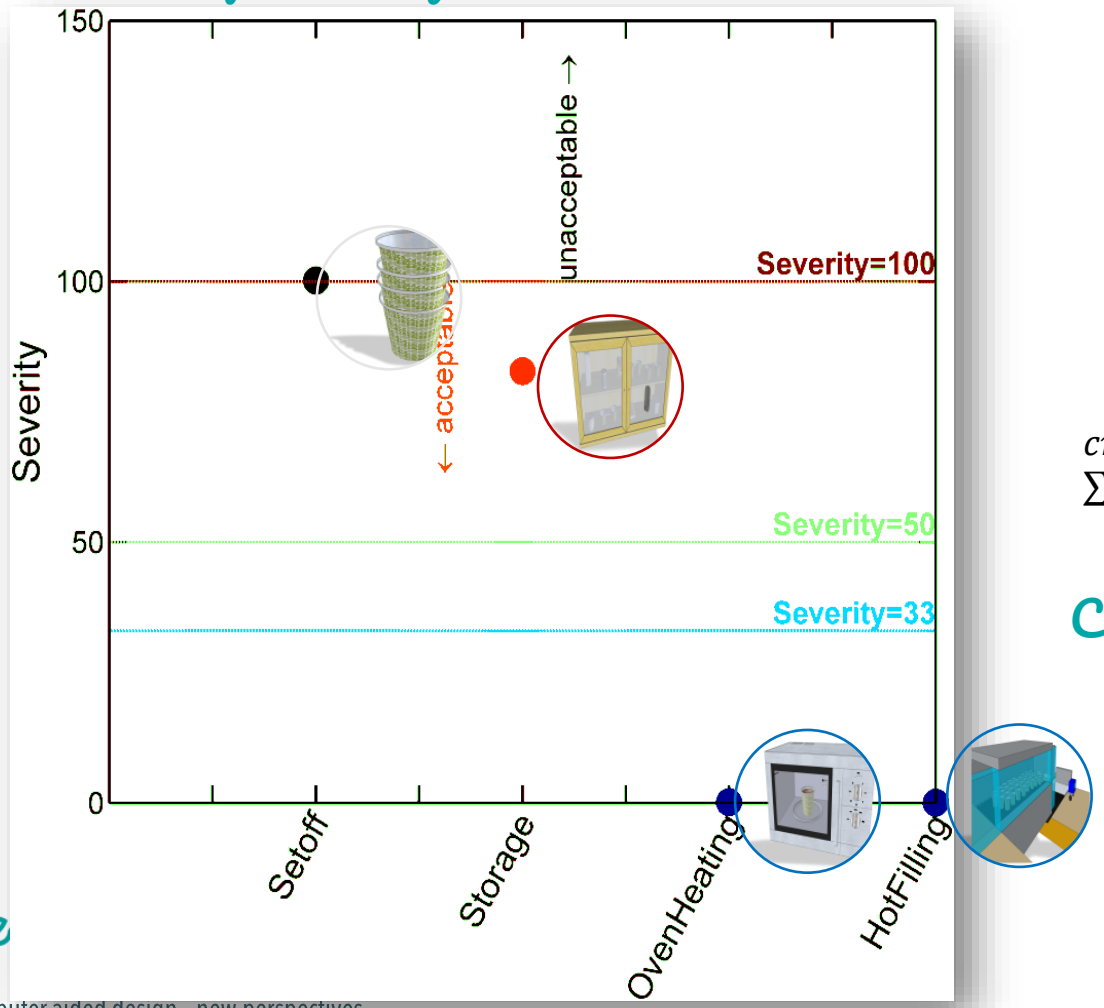
comparison with step i removed

CONCURRENT ENGINEERING: COMPARING THE SEVERITY OF SEVERAL STEPS, PACKAGING DESIGNS, SUBSTANCES…

AIChE Journal, 59(4), 1183-1212

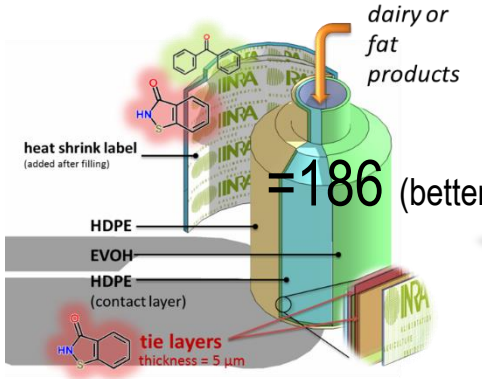
$$severity = 100 \times \frac{C_F}{SML}$$

Critical step (severity scale)



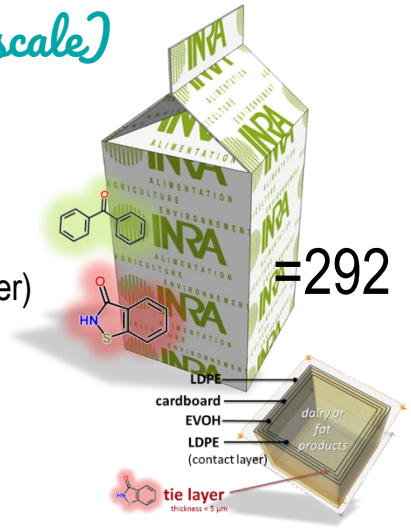
Unacceptable when $severity > 100$

Concurrent design (criticality scale)



=186 (better)

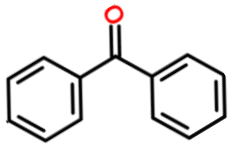
tie layer = EVA



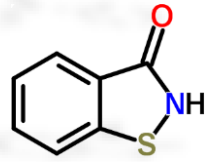
=292

$$criticality = \sum_{all\ components} \sum_{all\ substances} \sum_{all\ modalities} pr(modality) \times severity$$

Critical substance

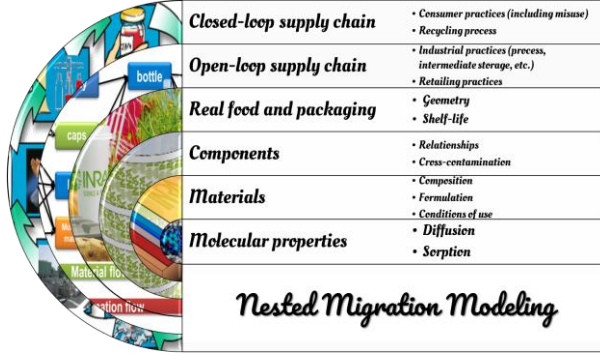


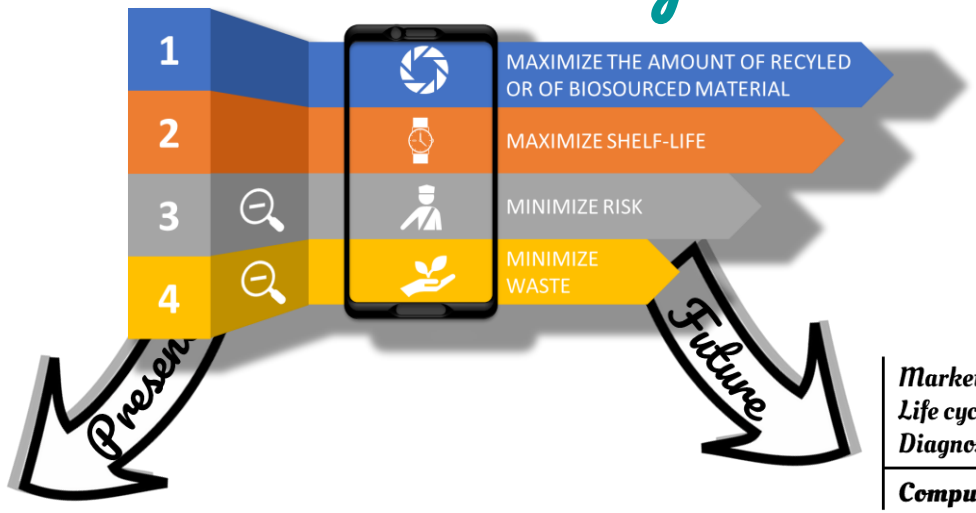
=115
(almost acceptable)



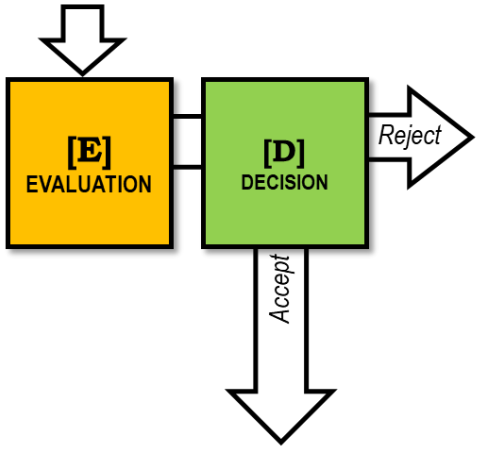
=124

De l'ingénierie concurrente à l'ingénierie intégrée





New substance
New material
New recycling process
New food packaging

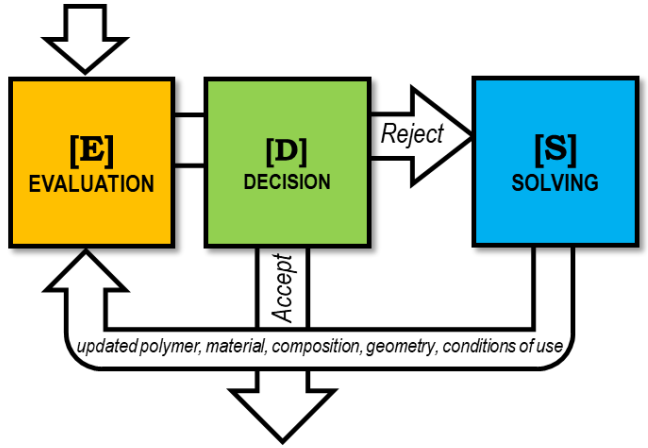


Experimental testing

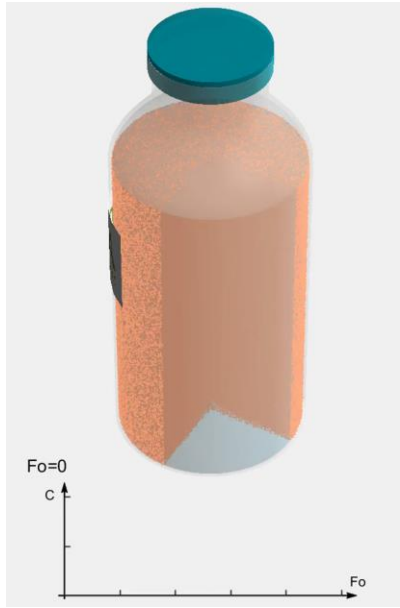
Compliant food contact material (FDA, EU, Chinese rules)

Market demand, new food products
Life cycle analysis considerations
Diagnostic from root cause analysis, seek of preventive actions

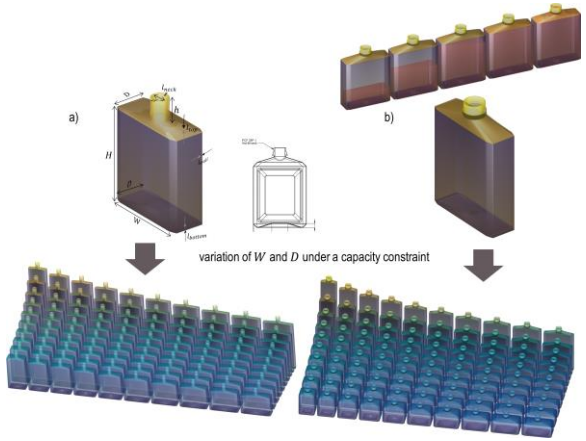
Computer-aided drafting



Rapid prototyping and compliance
Good manufacturing and design practices
Safer food products
Improved shelf-life
Eco-designed packaging

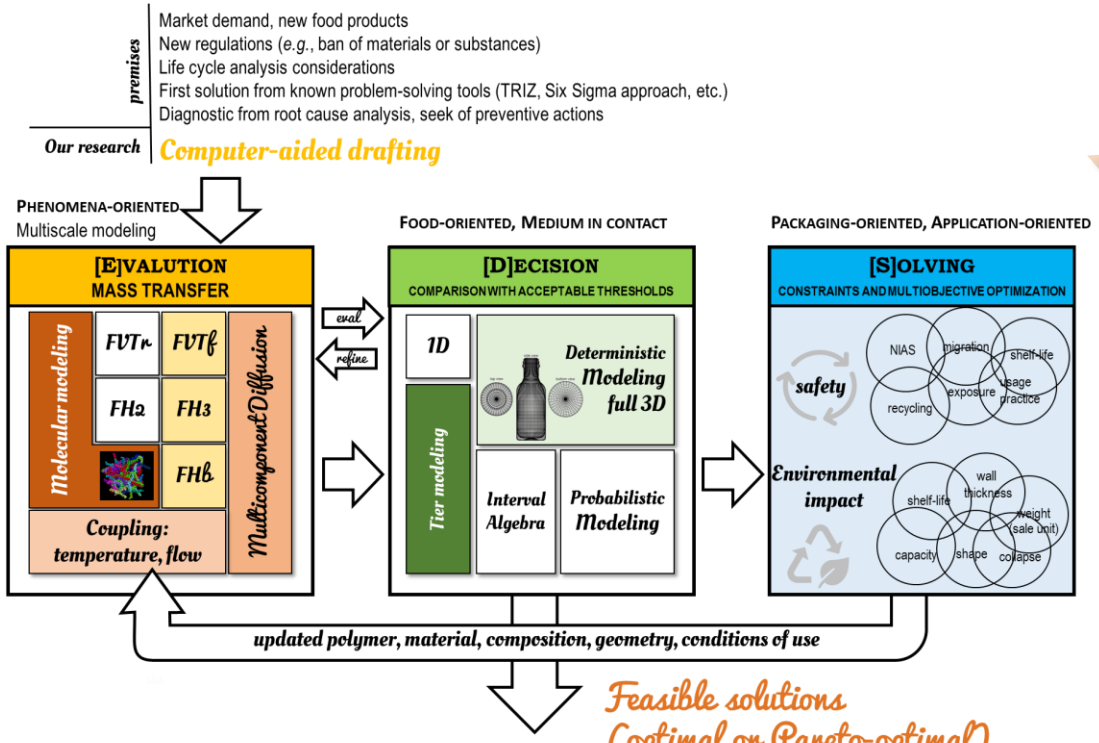


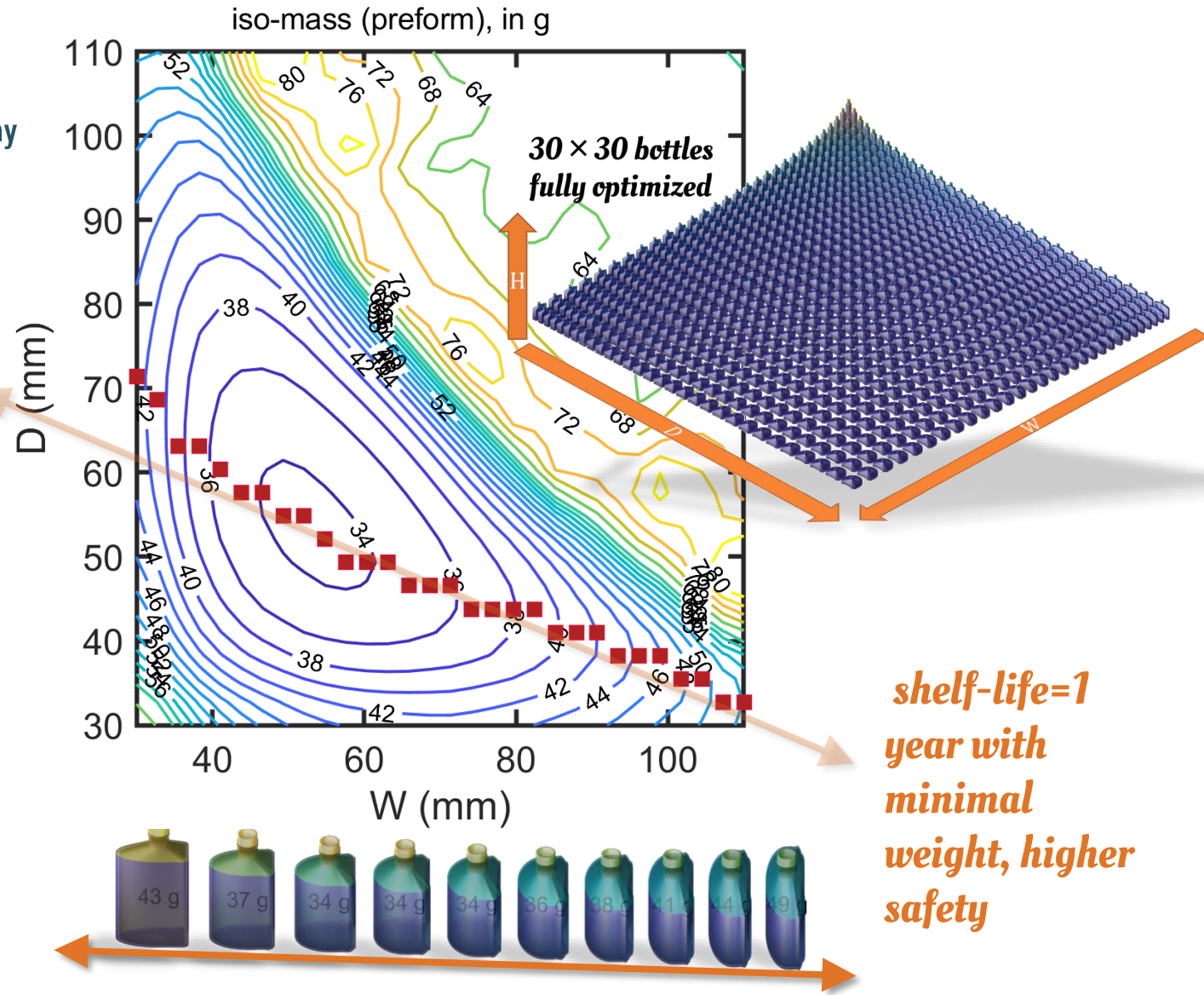
Le projet FMECAengine 3D



Example: redesign of PET bottle for alcoholic beverages (optimized shape, recycled content, reduced weight, improved shell-life)

3D prototype printed the same day

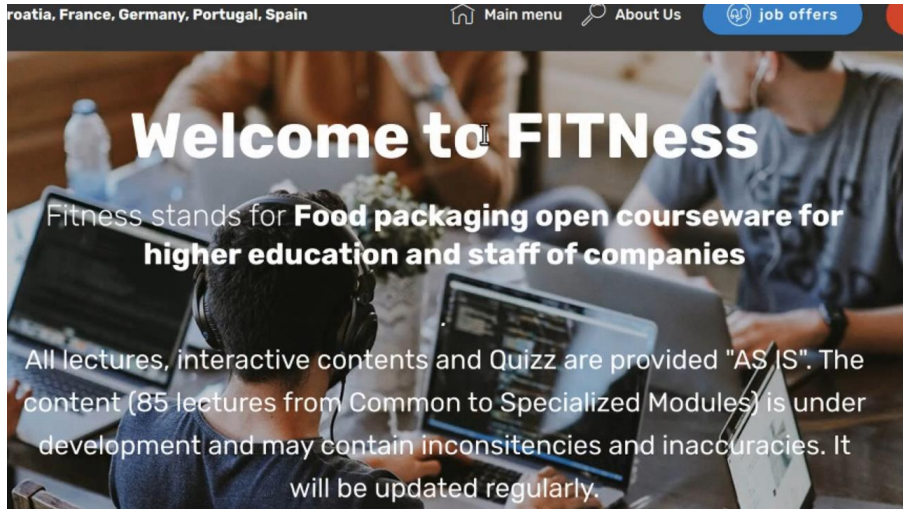


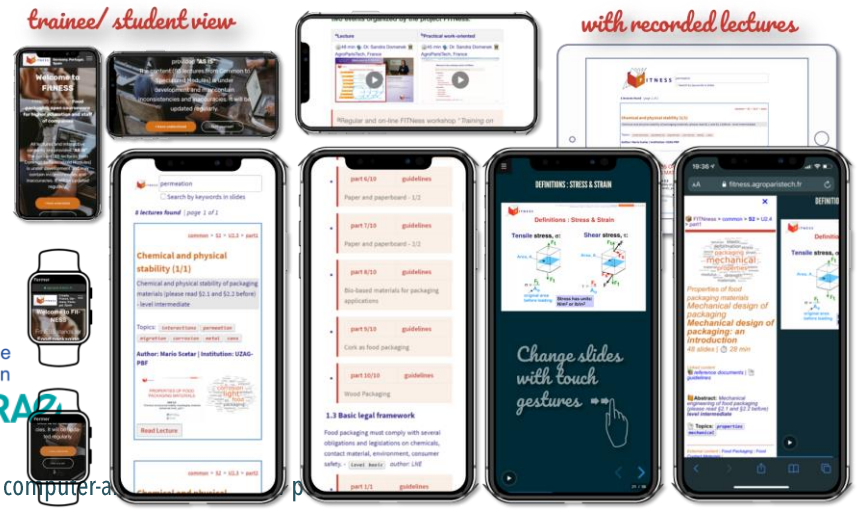


Train yourself to become green

Three months online curriculum on packaging design

https://fitness.agroparistech.fr/





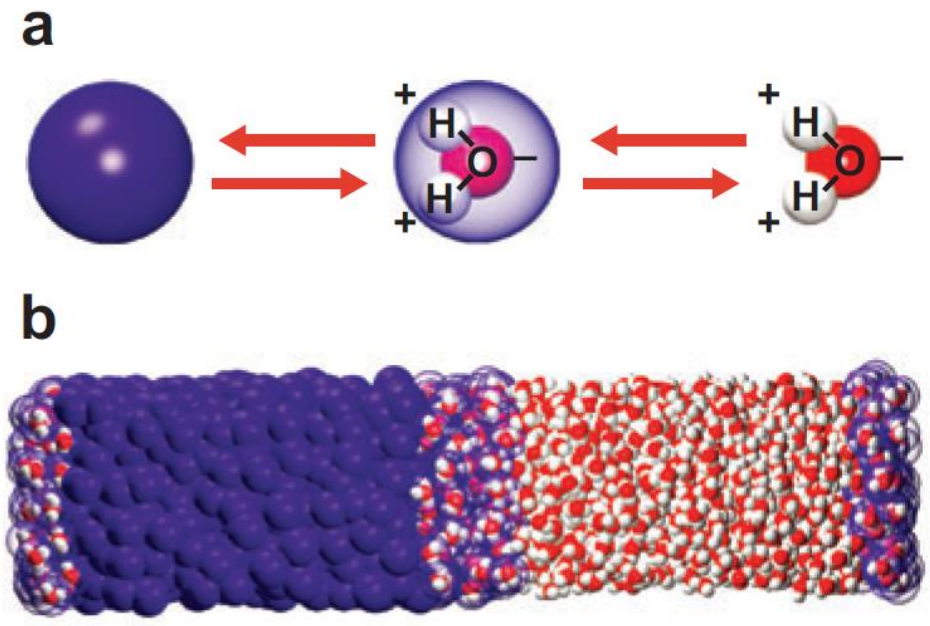
BONNE PRATIQUE

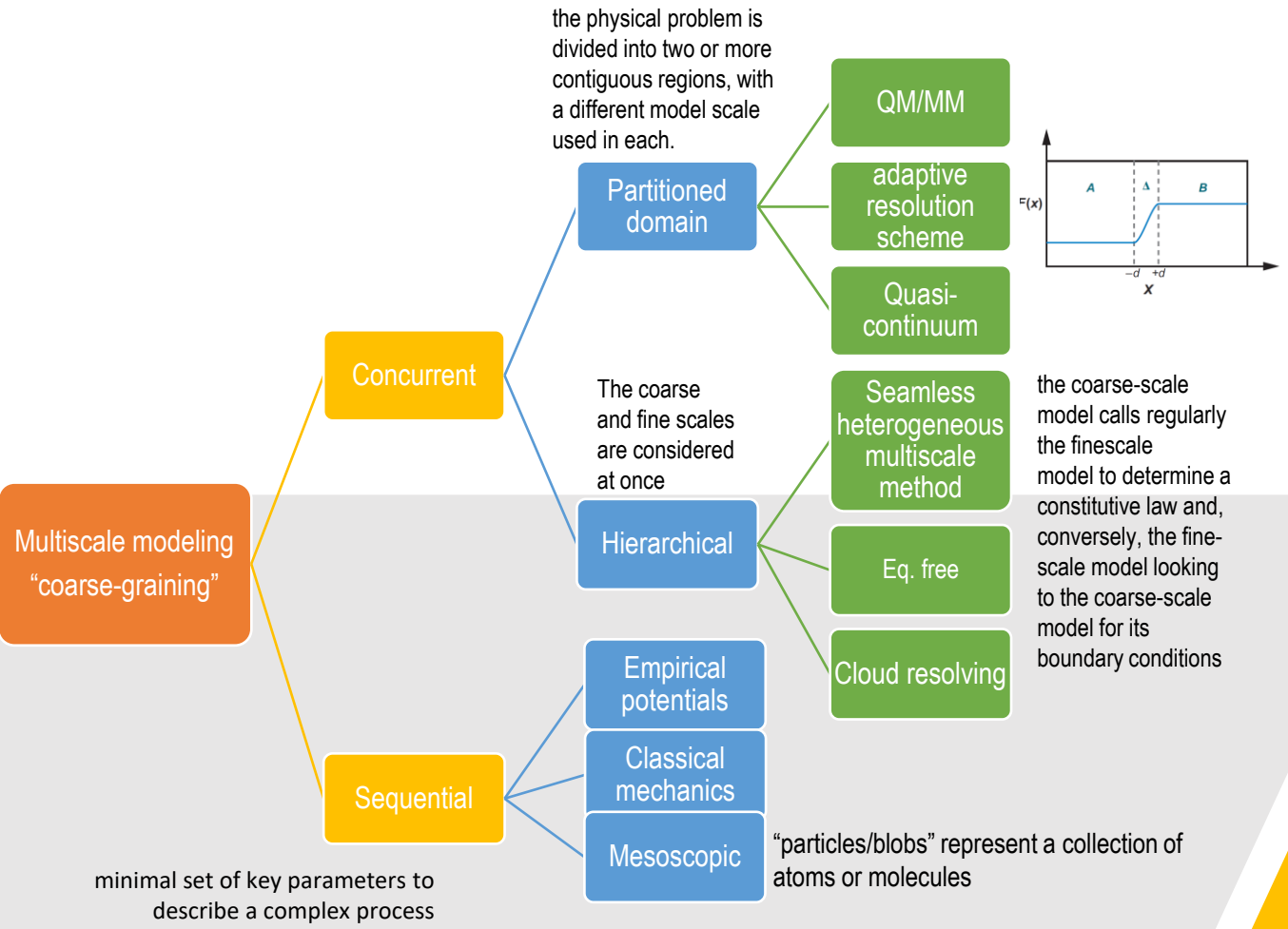
Co-funded by the Erasmus+ Programme of the European Union

INRAE

Food computer-a p

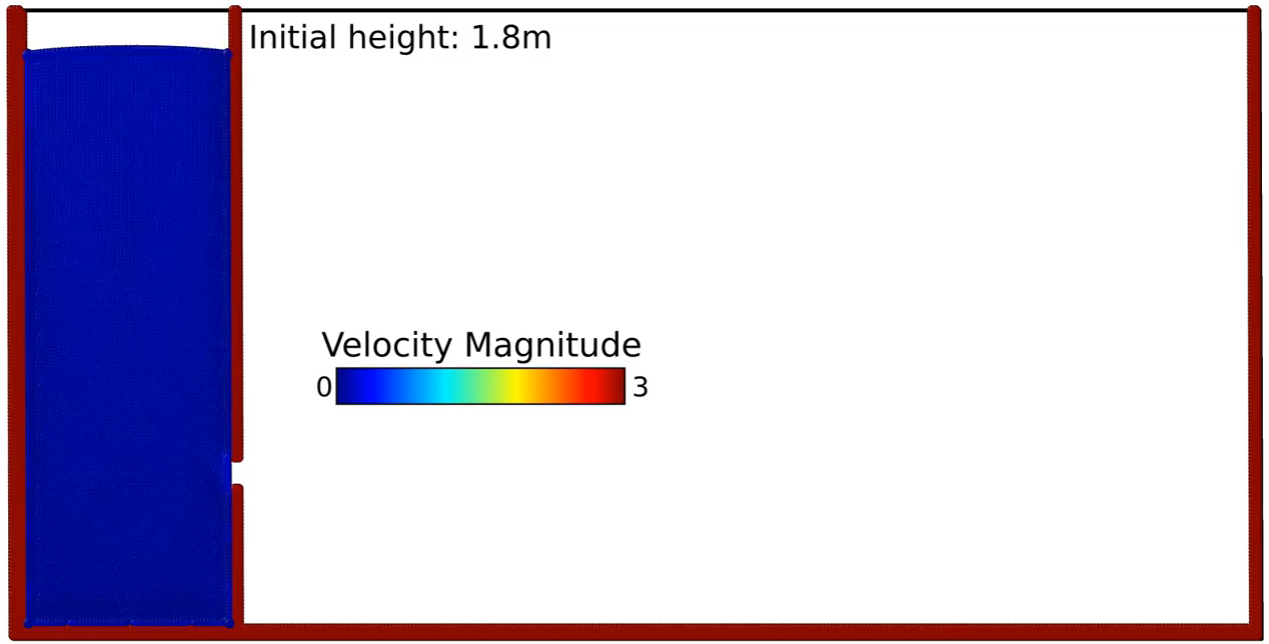
MULTI-SCALE MODELING

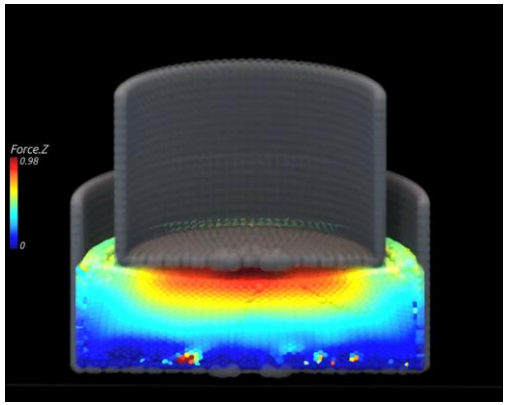


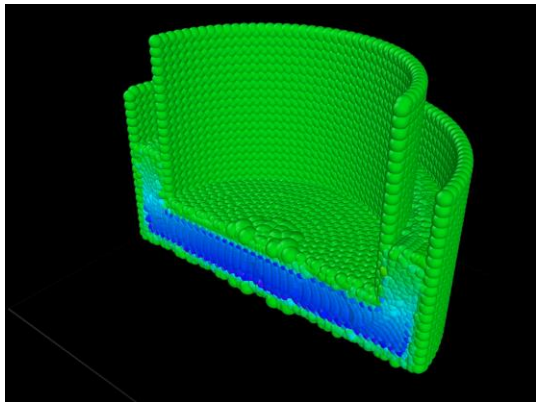


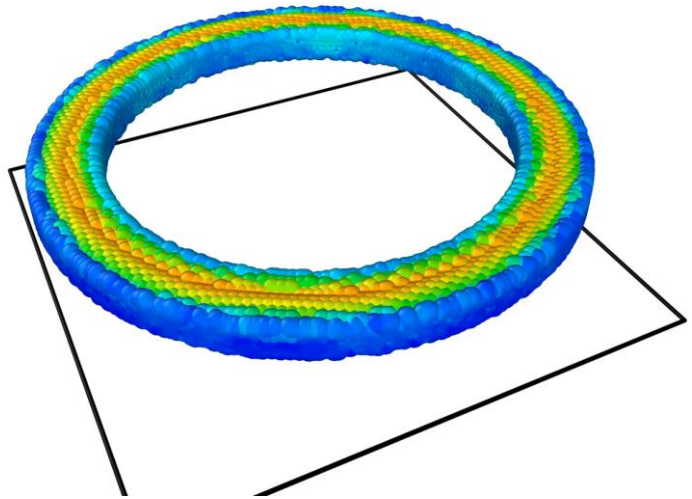
"multiscale modeling"[3] was coined in the early 1980s for modeling the transfer of energy between flow eddies at many different length scales in turbulent flows.

Overview : free surfaces

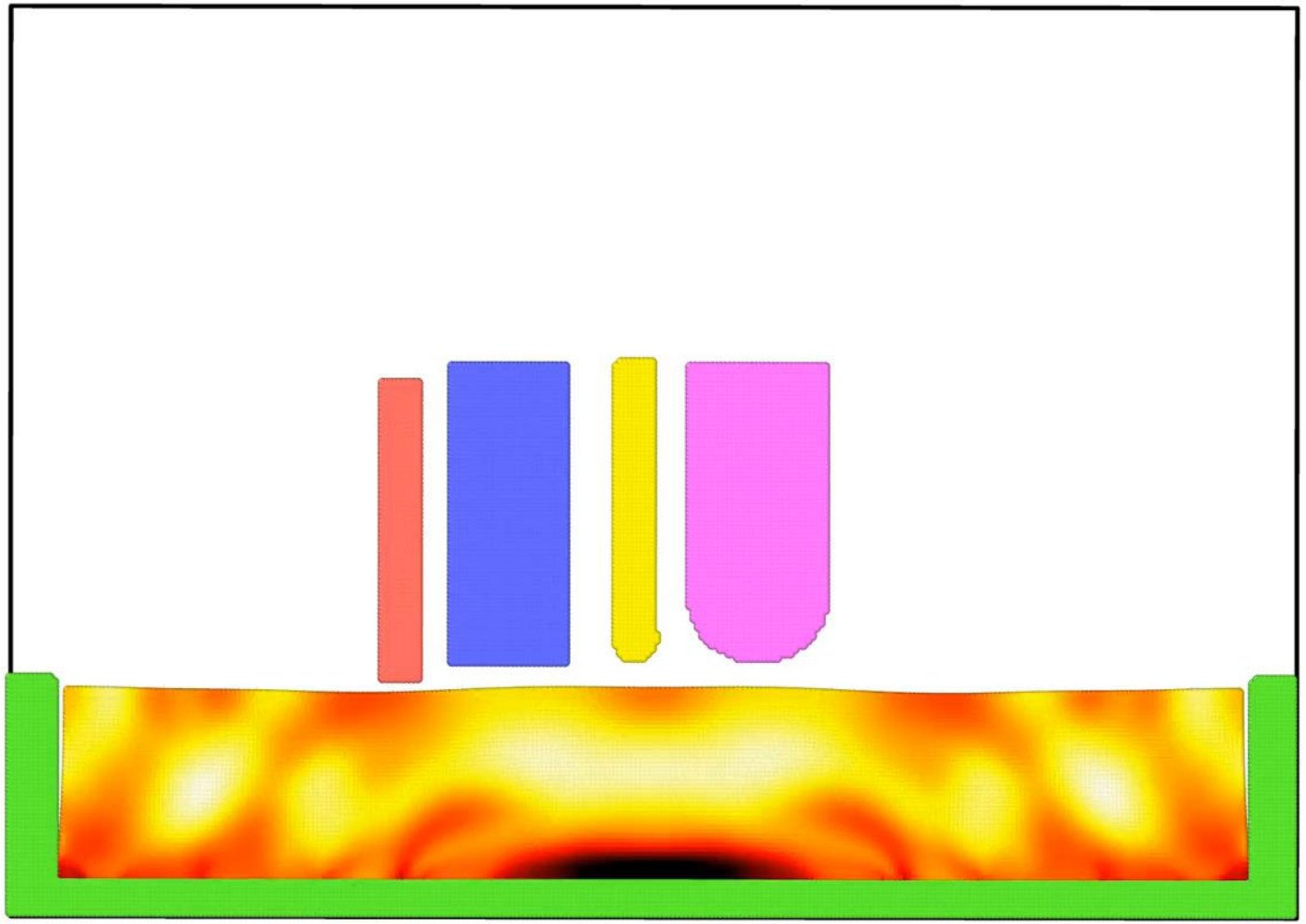


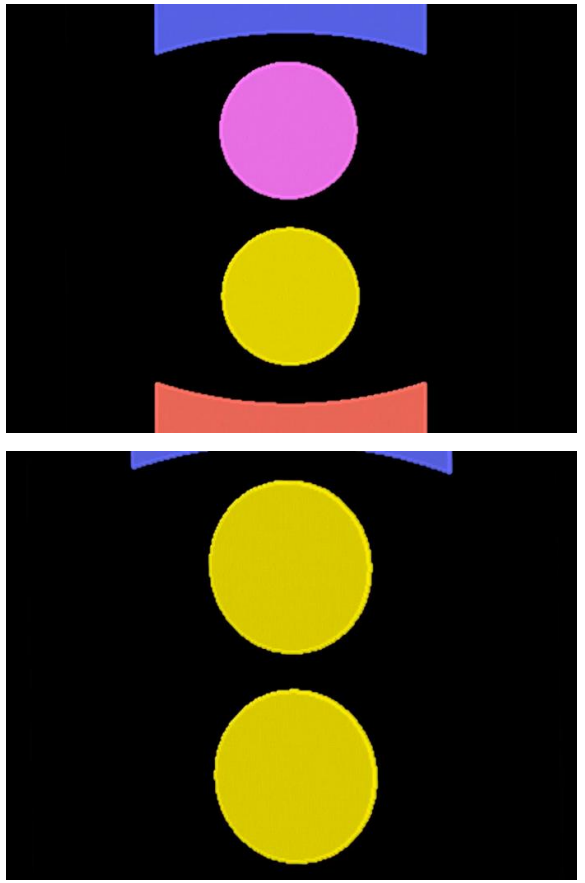


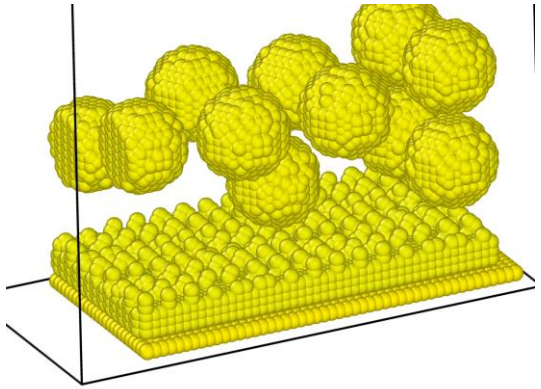




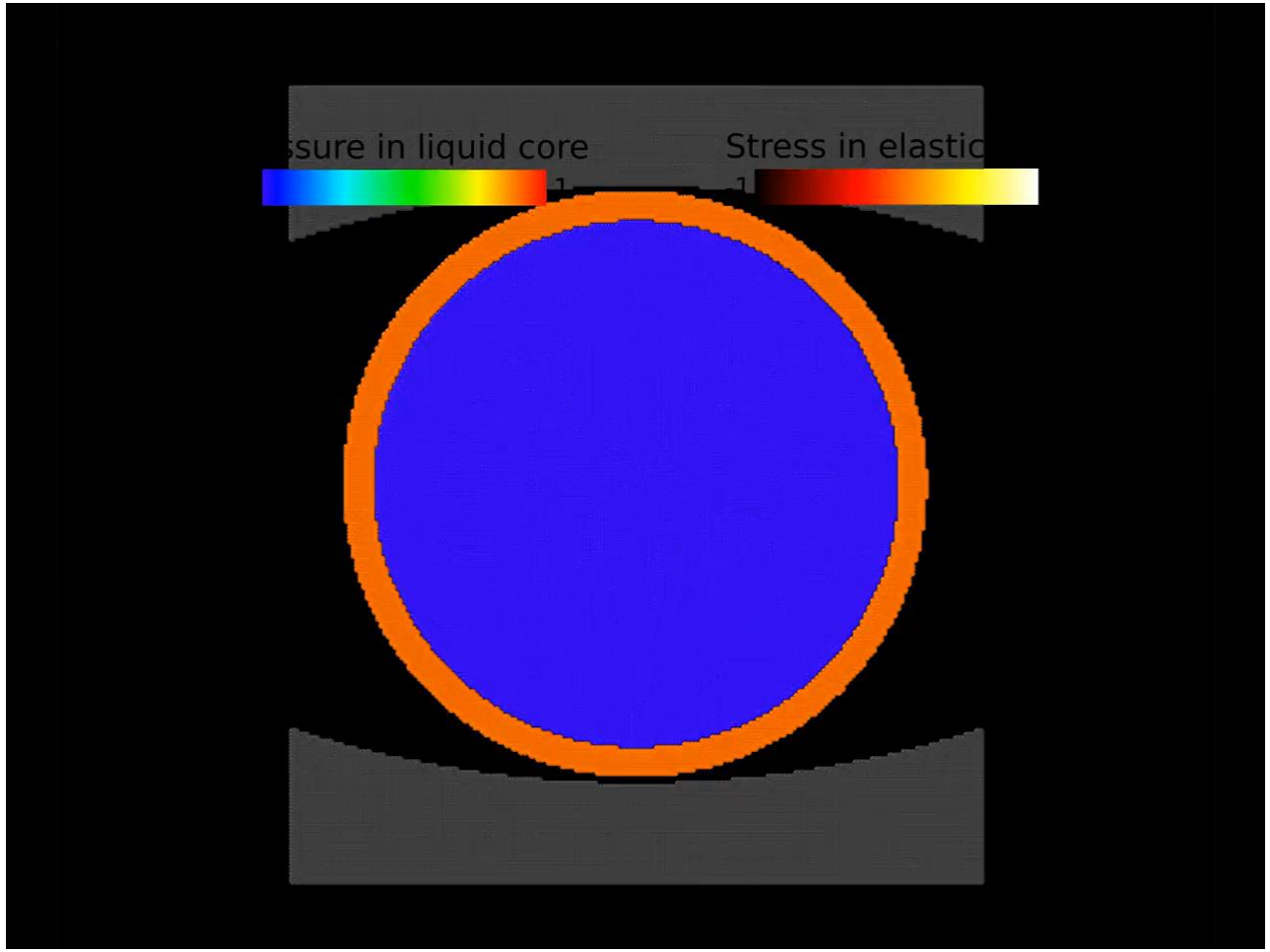
Solid interactions

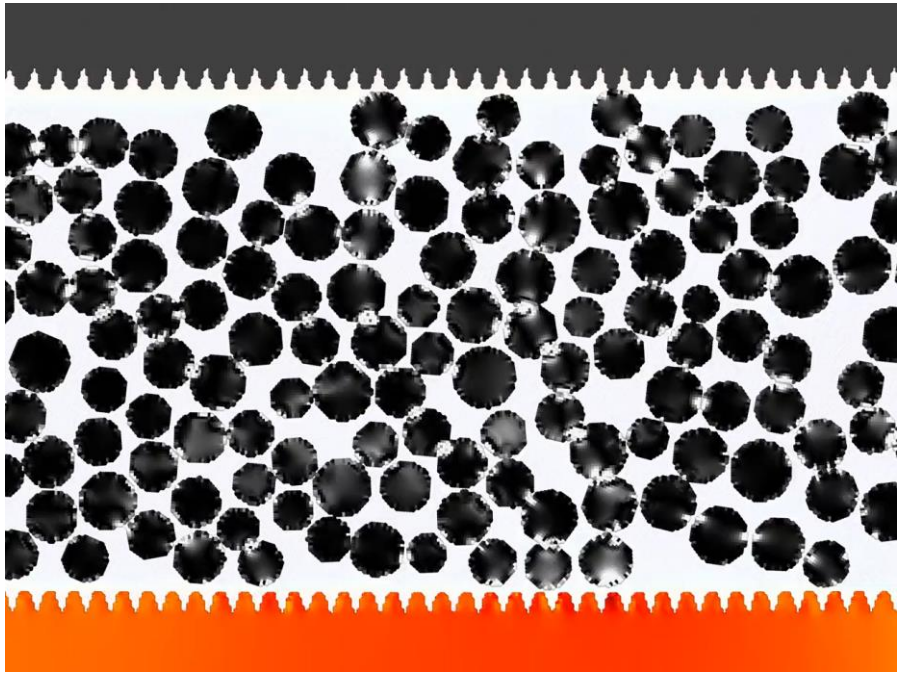


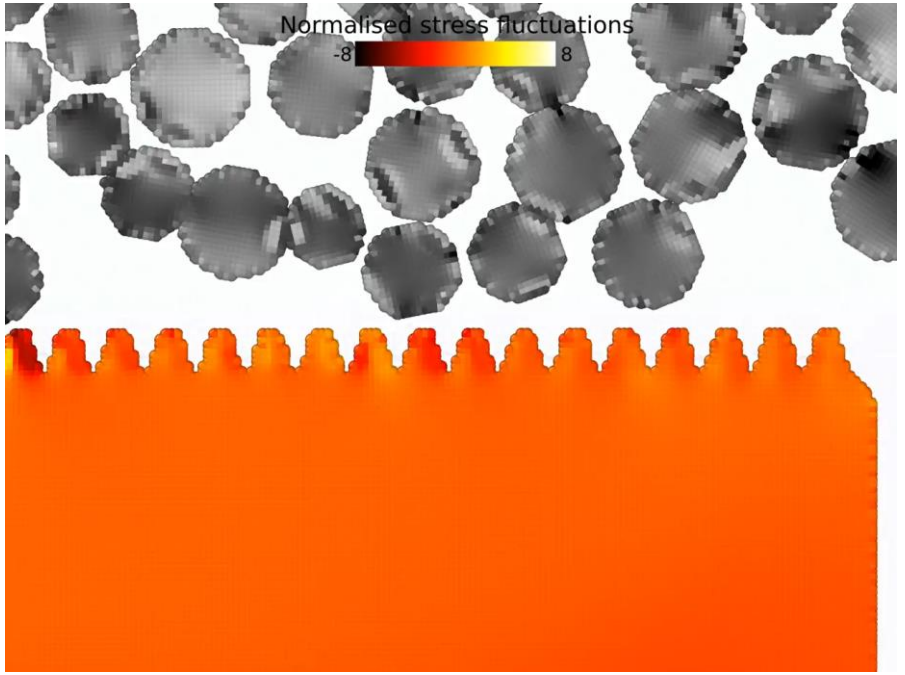




Solid-fluid interactions

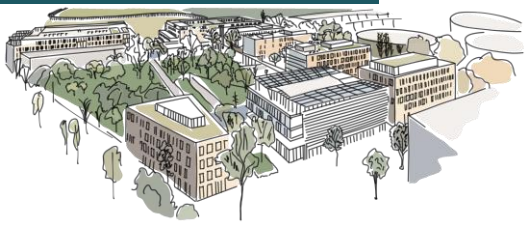




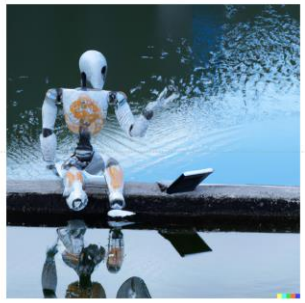


université PARIS-SACLAY

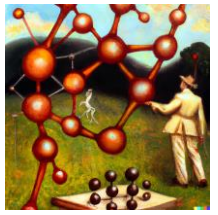
AgroParisTech
Talents for a sustainable planet

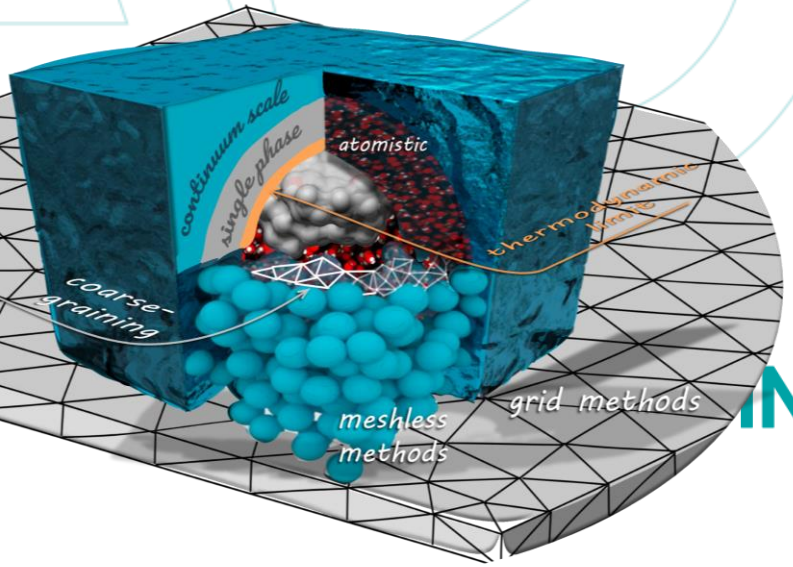


Credits: DALL-E



DIGITAL-TWIN
FROM SMALL (SCALES, LAB) TO BIG (SCALES, INDUSTRY)



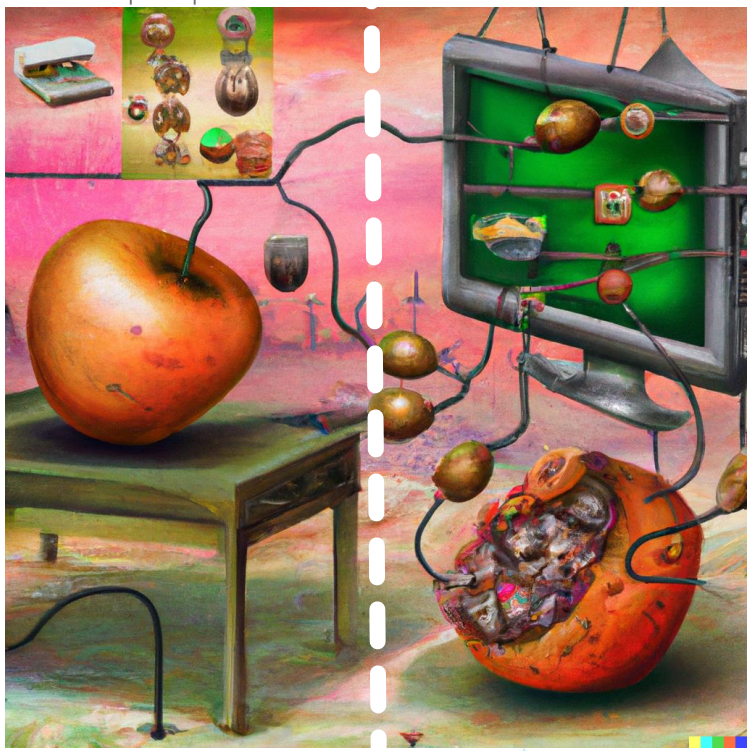


Olivier Vitrac, olivier.vitrac@agroparistech.fr

French National Institute of Agricultural and Environmental Research (INRAE)
University of Paris-Saclay – UMR 0782 SayFood – group *Modeling and Computational Engineering*
22 place de l'Agronomie, 91120 Palaiseau, FRANCE

EQUIVALENCE PRINCIPLES.
OUR EXAMPLE: THE CONCEPT OF FOOD-ATOMS

Credits: https://openai.com/dall-e-2/



information

information

actions

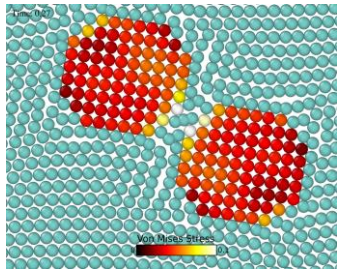
innovations

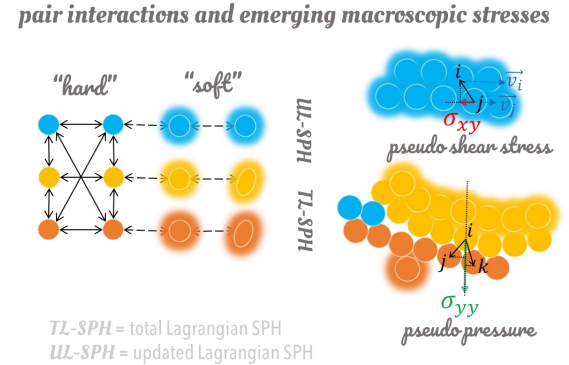
"A digital twin is a virtual representation of a physical object or system that aims to simulate its real-world characteristics and behavior

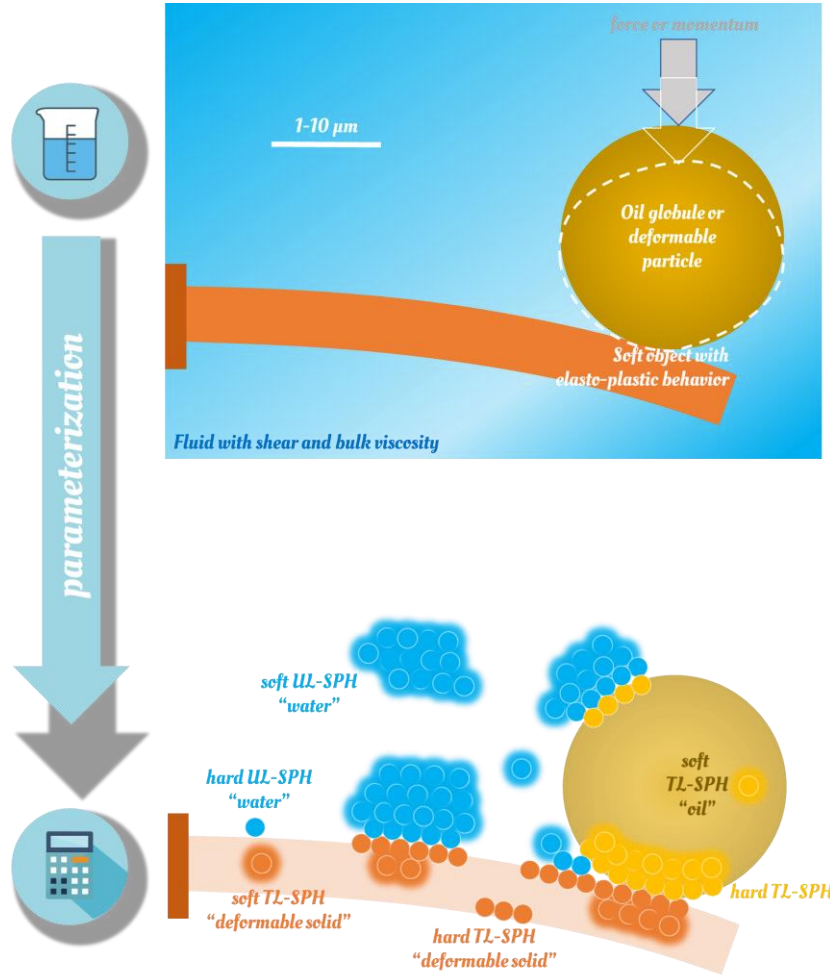
While it is meant to be as close to reality as possible, it is still a digital model and does not perfectly reflect the reality.

The digital twin is a dynamic simulation that can be updated with real-time data from the physical object, but it is not the reality itself"

Credits:https://chat.openai.com/chat

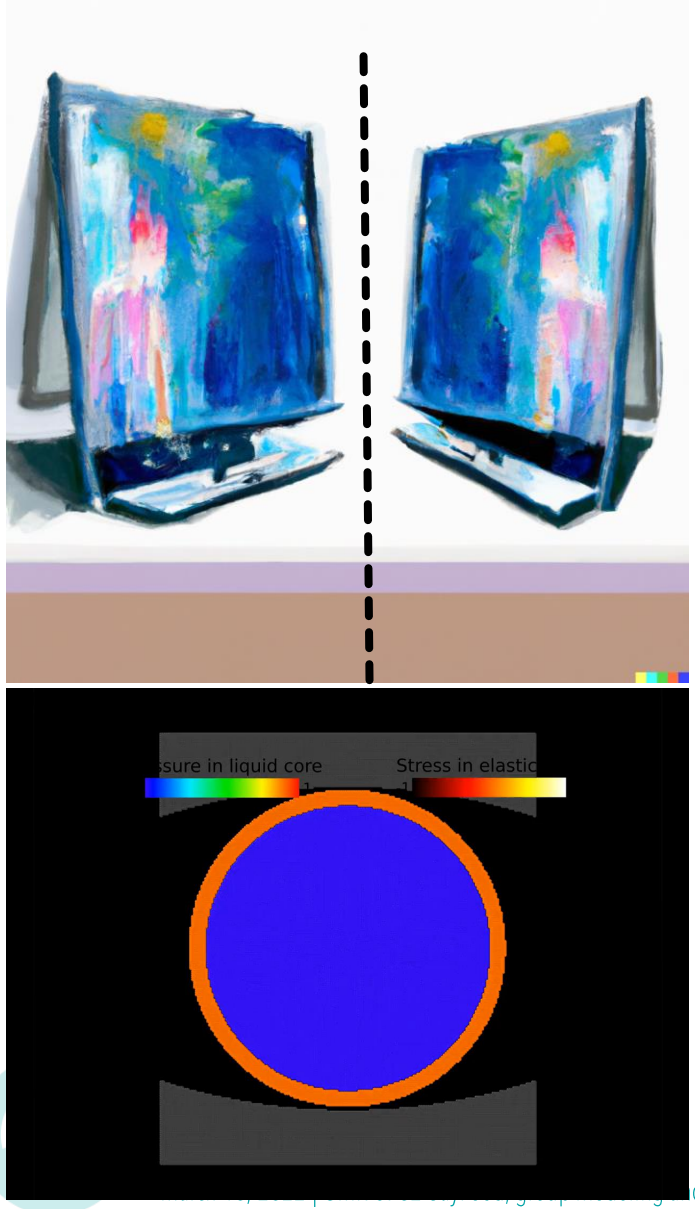


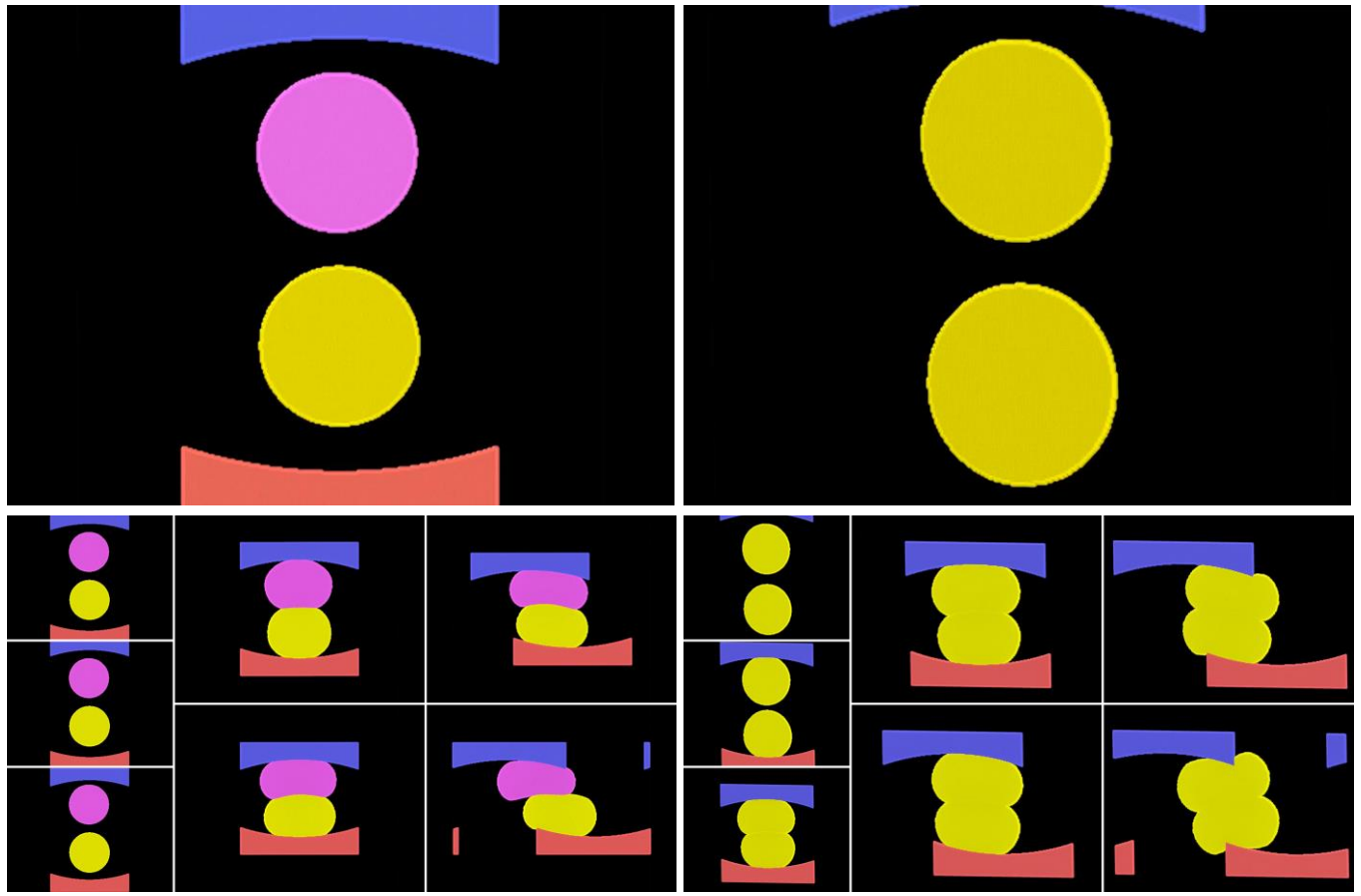




Credits: PhD William Jenkinson, Han Chen

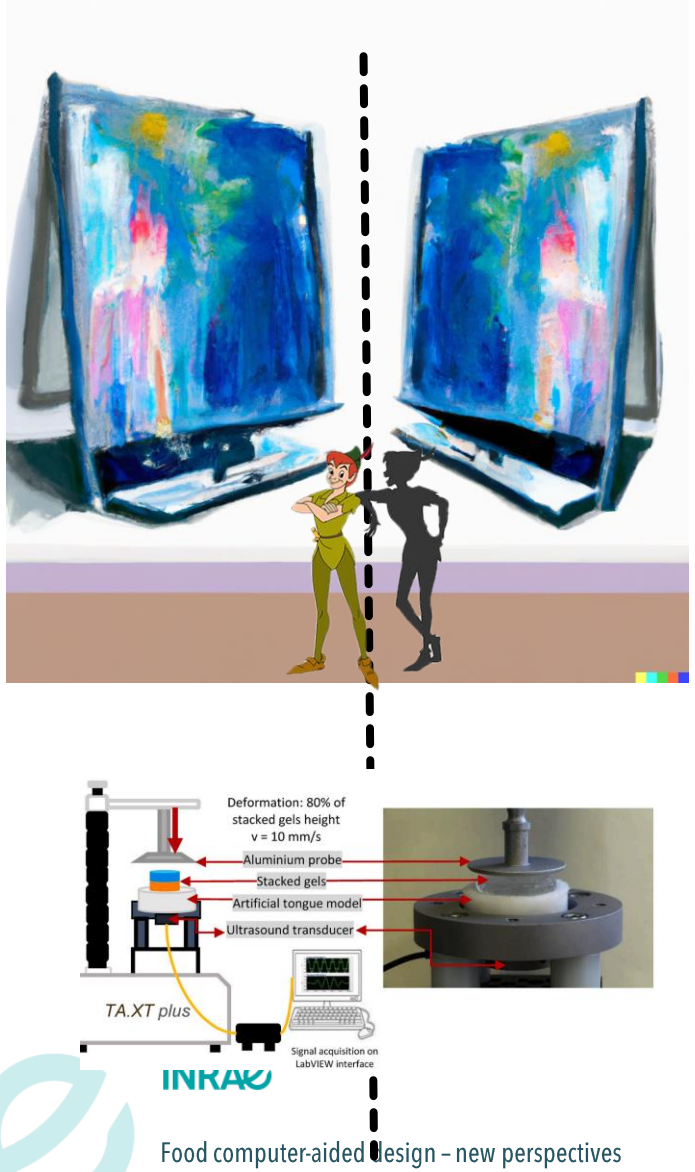
FOOD MADE WITH FOOD-ATOMS: COMPLEX PHYSICS, DIFFERENT BEHAVIORS

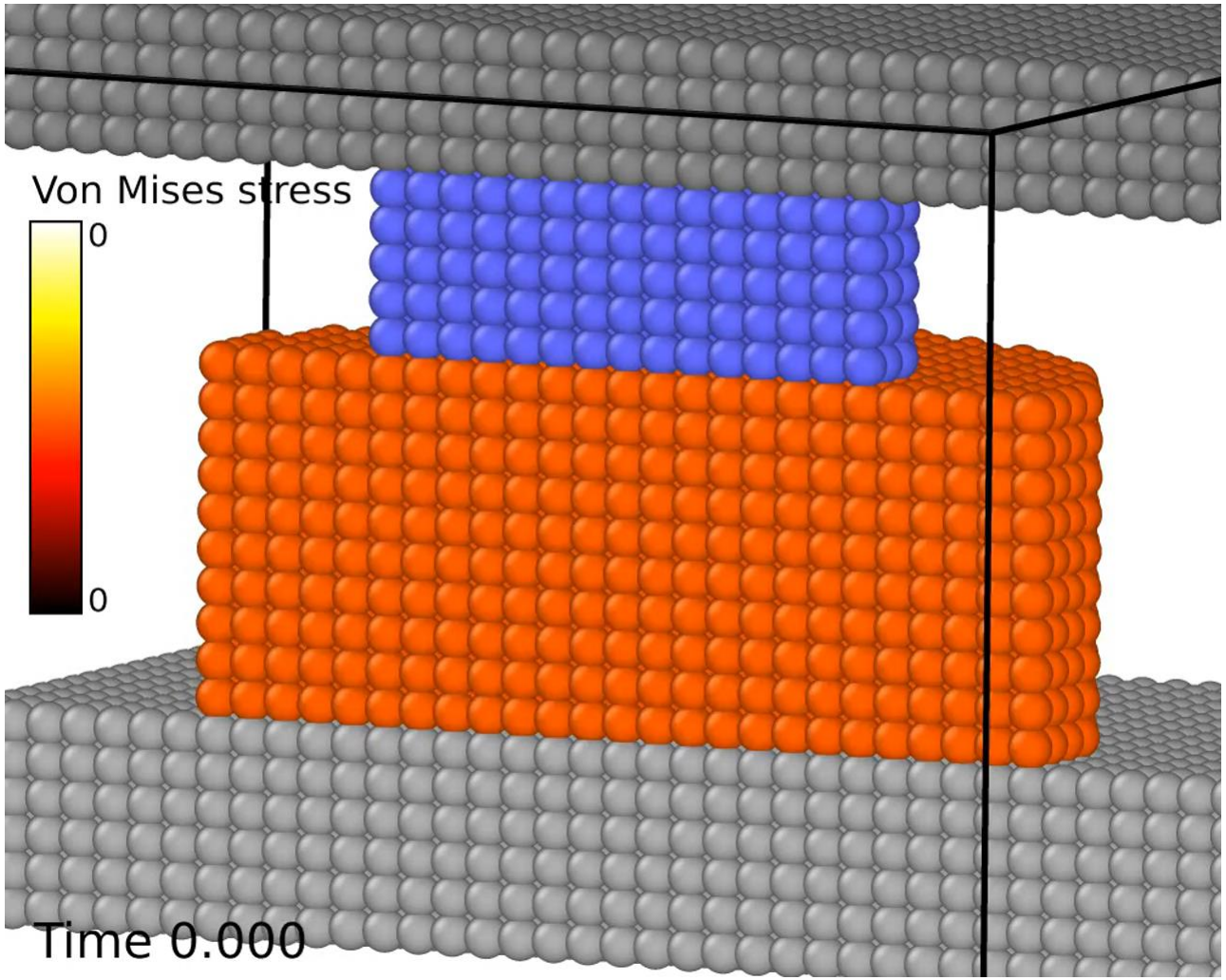




Credits: PhD William Jenkinson

EQUIVALENCE PRINCIPLES



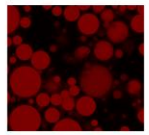
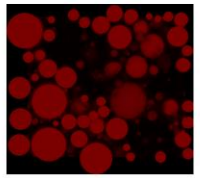
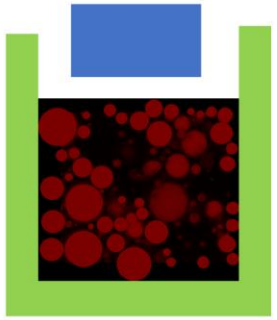
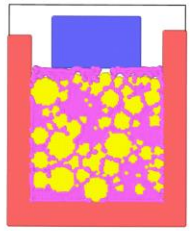


MORE THAN A SHADOW

A TWIN CAPABLE TO MOVE BY ITSELF

Shadows do not have any physical properties and cannot be manipulated directly.

Table 1. *Original and modified images corresponding to steps 1-3.*

Step1 Initial image	Step 2 Image with extended objects	Step 3 image with "movable" piston and container	RESULT with "food-atoms"
			

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Add section [Atoms] - file="default raster(raster)"
        > Add "id" (10208 values) to [Atoms]
        > Add "type" (10208 values) to [Atoms]
        > Add "mol" (1 values) to [Atoms]
        > Add "c_vol" (1 values) to [Atoms]
        > Add "mass" (1 values) to [Atoms]
        > Add "radius" (1 values) to [Atoms]
        > Add "c_contact_radius" (1 values) to [Atoms]
        > Add "x" (10208 values) to [Atoms]
        > Add "y" (10208 values) to [Atoms]
        > Add "z" (1 values) to [Atoms]
        > Add "x0" (10208 values) to [Atoms]
        > Add "y0" (10208 values) to [Atoms]
        > Add "z0" (1 values) to [Atoms]
Add section [Velocities] - file="default raster(raster)"
        > Add "id" (10208 values) to [Velocities]
        > Add "vx" (1 values) to [Velocities]
        > Add "vy" (1 values) to [Velocities]
        > Add "vz" (1 values) to [Velocities]
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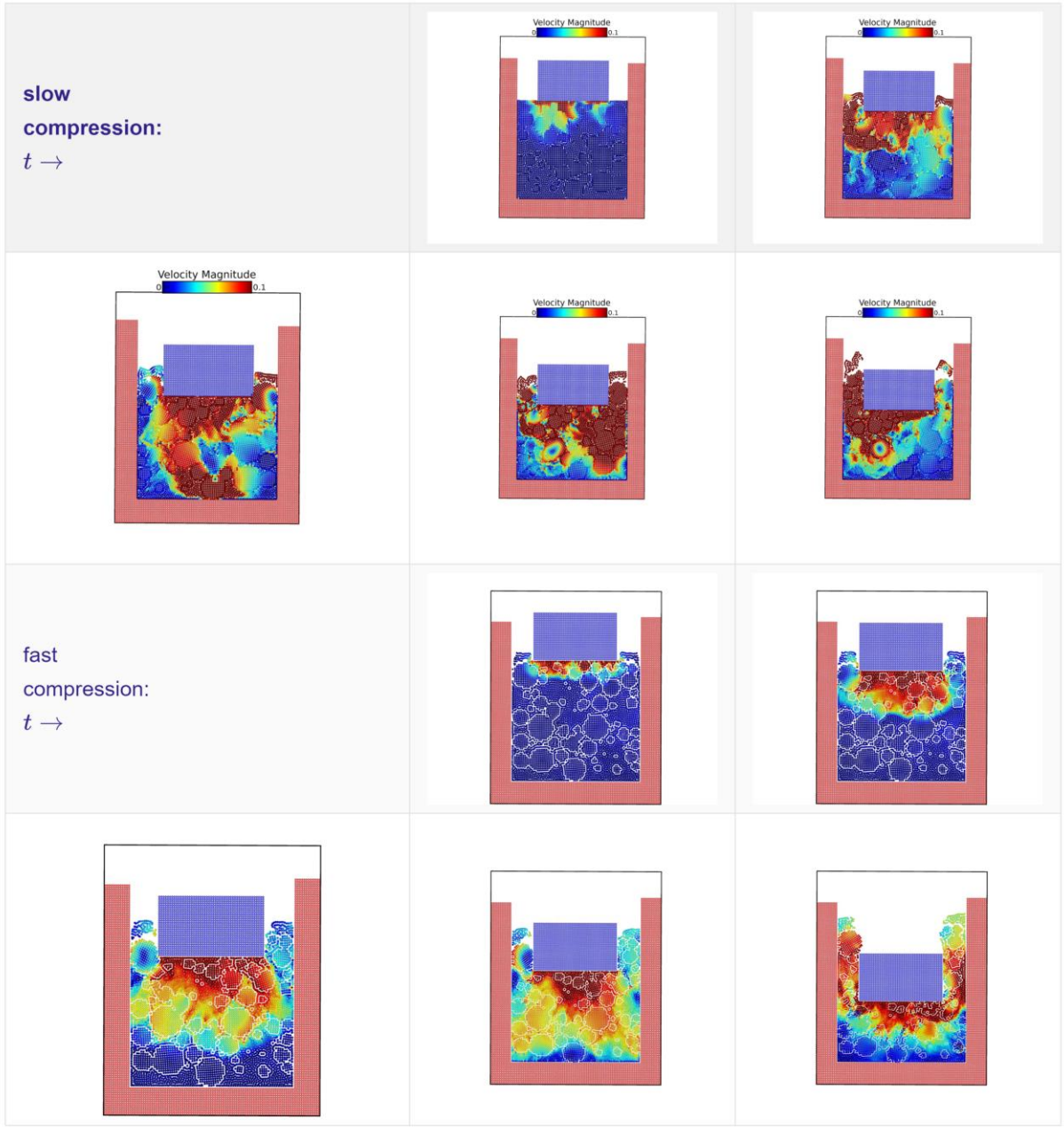
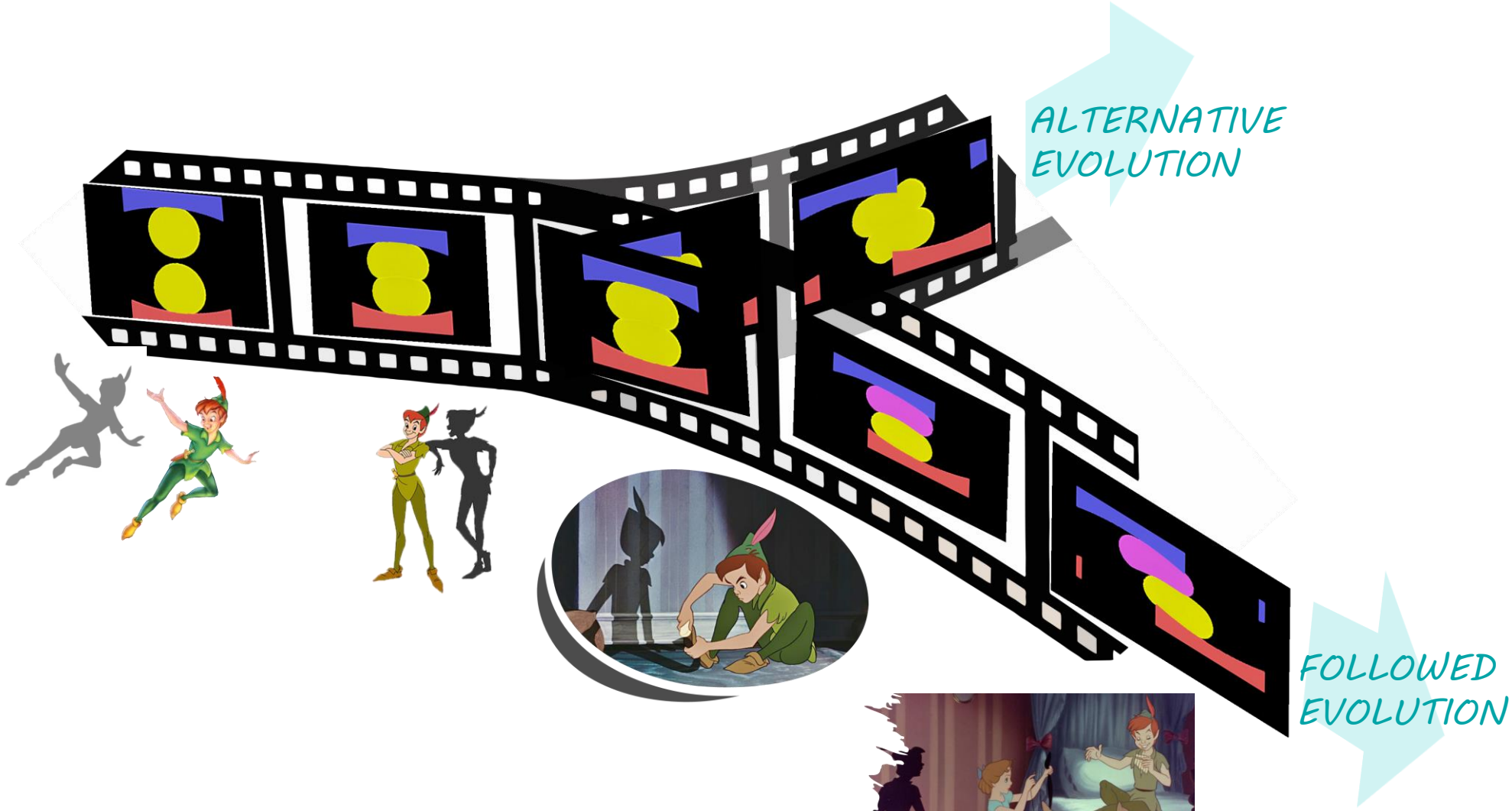


Figure 7. Step 7: Simulated evolution of the emulsion during slow and fast compression (the color represents the velocity of `food-atoms`). In the simulations, pixels (low resolution) represents food-atoms.

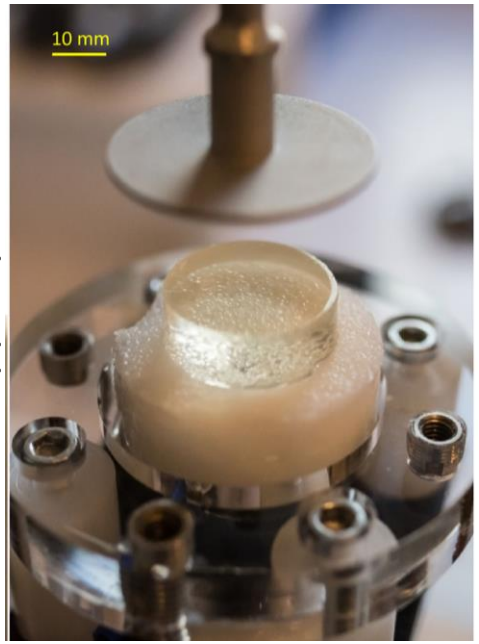
TIMELINE IN MUTITPLE SHADOWS

MANY WORLD INTERPRETATION: DIVERGING TIMELINES WHEN CRITICAL BEHAVIORS ARE OBSERVED



HOW TO TRAIN A MECHANICAL TWIN?

AS A GENERATIVE PRETRAINED TRANSFORMER (LANGUAGE PROCESSING AI), OUR MECHANICAL TWIN CAN PROCESS A LARGE CORPUS OF PHYSICS



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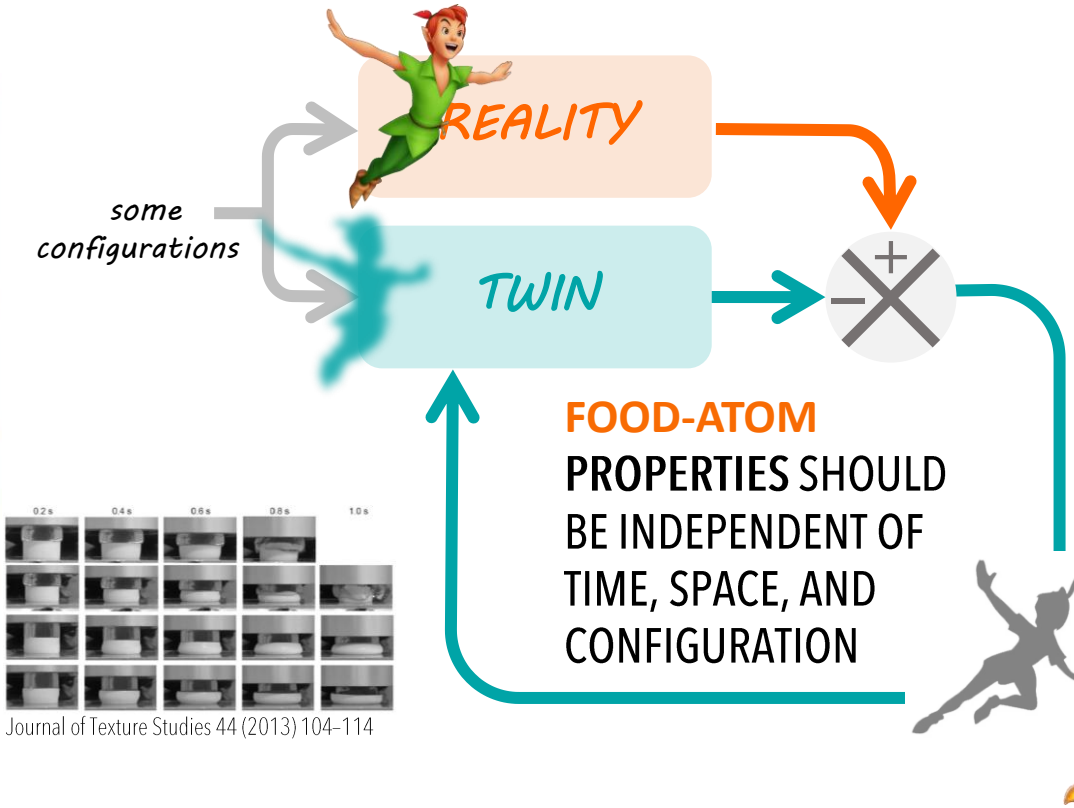
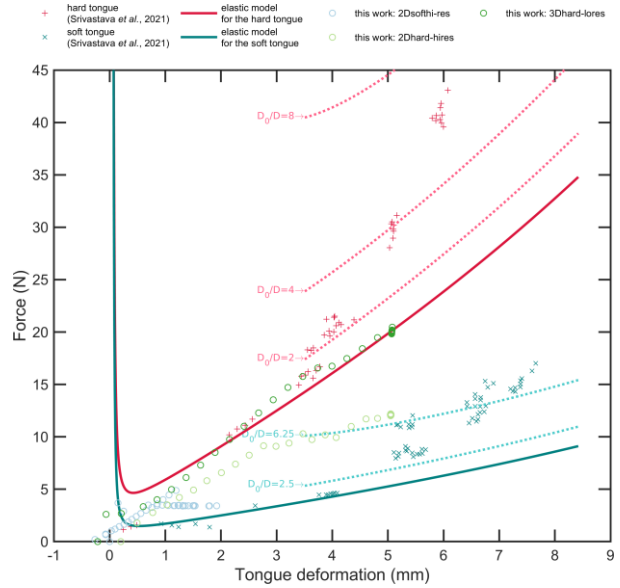
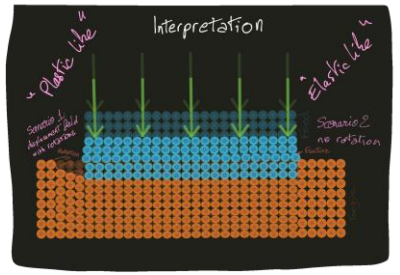
Journal of Texture Studies 44 (2013) 104–114



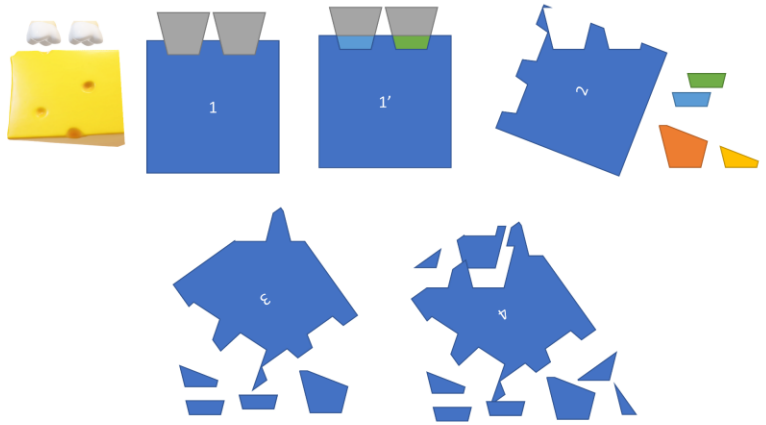




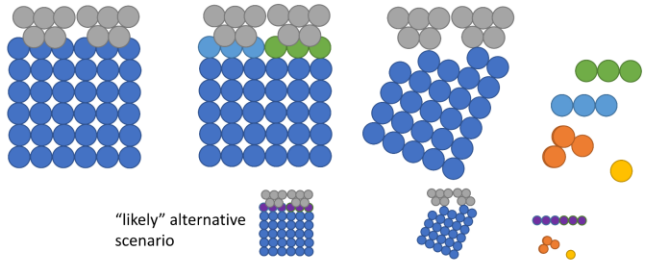
A MECHANICAL TWIN PROVIDES MORE DETAILS THAN PUNCTUAL MEASUREMENTS: RADIAL EXPANSION, COUPLING WITH WATER TRANSPORT, EXSUDATION, SLIPPING

DIGITAL TWIN: complications at microscopic scale

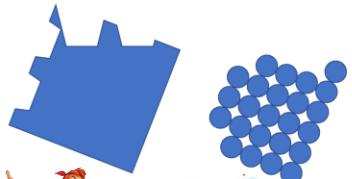
a. REAL-CASE (from an observation/experiment)

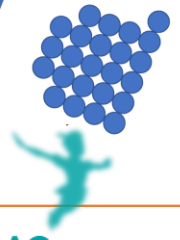


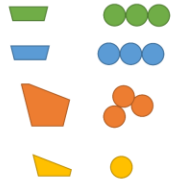
b. Real-case back-mapped onto beads (digital-shadow)



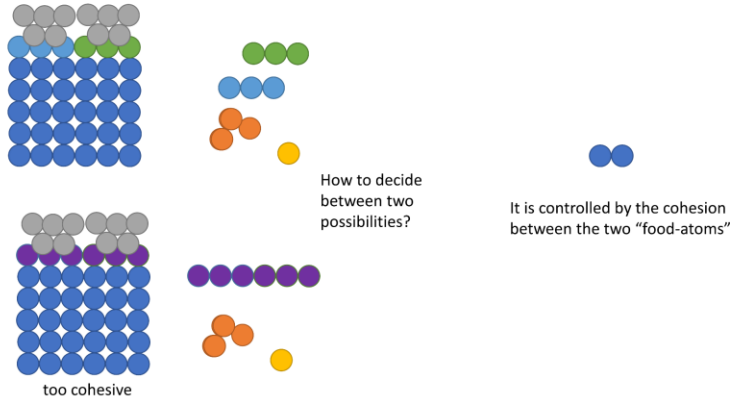
c. Comparison between the "real" and "shadowed" conditions

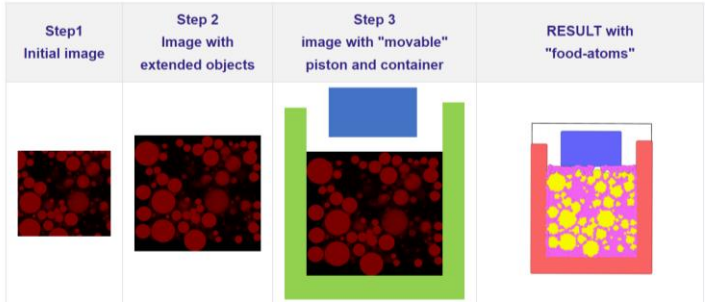






d. How an apparent adhesion property could help to recover the proper behavior without using a representation at a lower scale





Typical issues:

- Location of the observer
- No continuous observation
- 2D vs 3D
- Microscopic defect not visible

Thermodynamical analogy:
Two systems are equivalent if they are equivalent in size, in mass and at thermodynamical /mechanical equivalence

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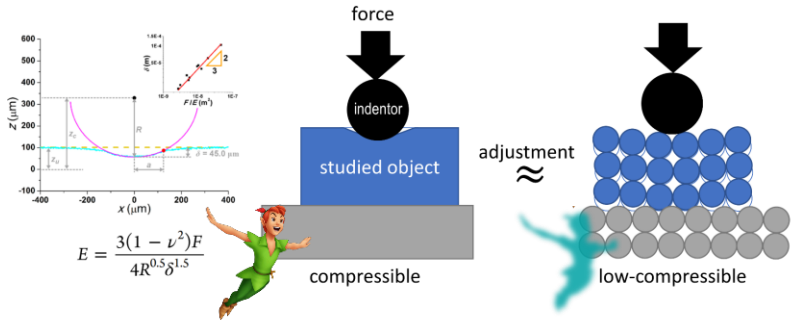
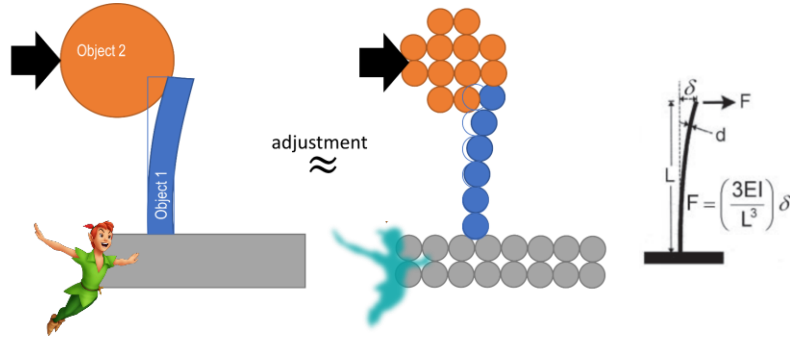
EXPERIMENTAL STRATEGY FOR THE PARAMETERIZATION OF DIAGONAL AND OFF-DIAGONAL TERMS

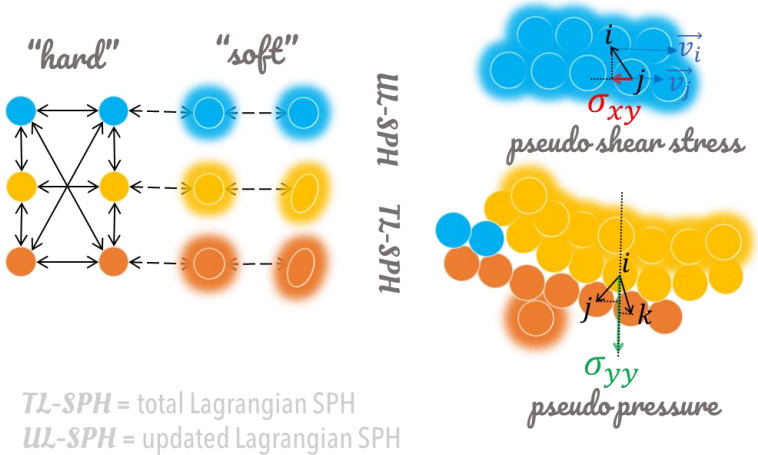


a. Parameterization of solid objects (diagonal terms): ●●

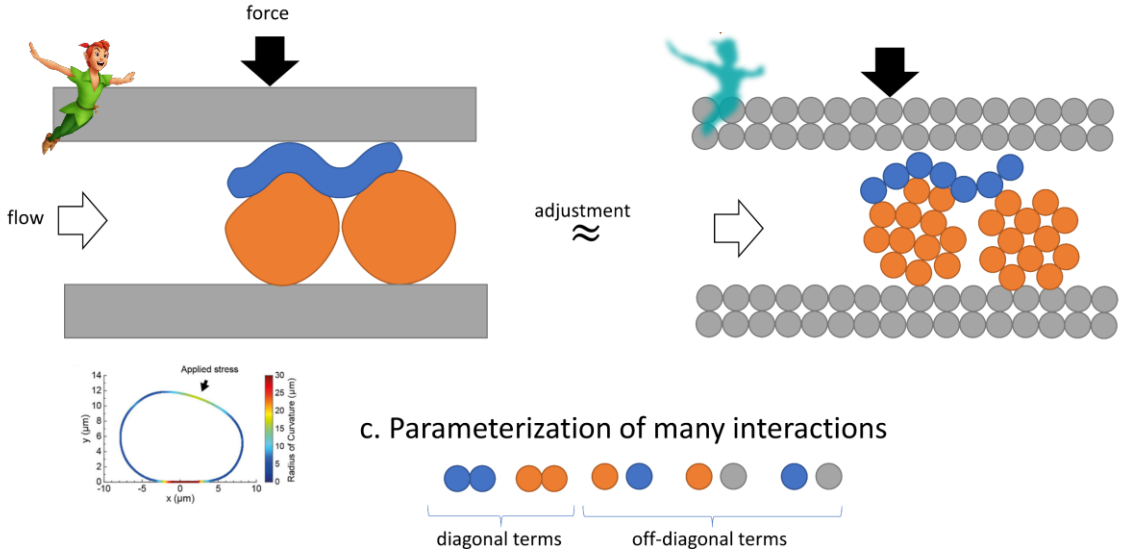


b. Parameterization of interactions between objects (off-diagonal terms): ●●

pair interactions and emerging macroscopic stresses



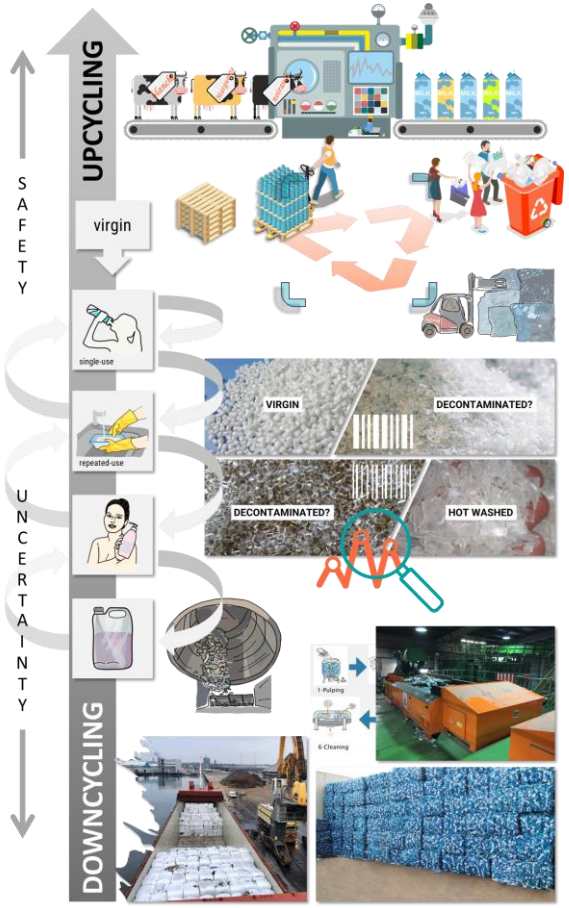
TL-SPH = total Lagrangian SPH
UL-SPH = updated Lagrangian SPH

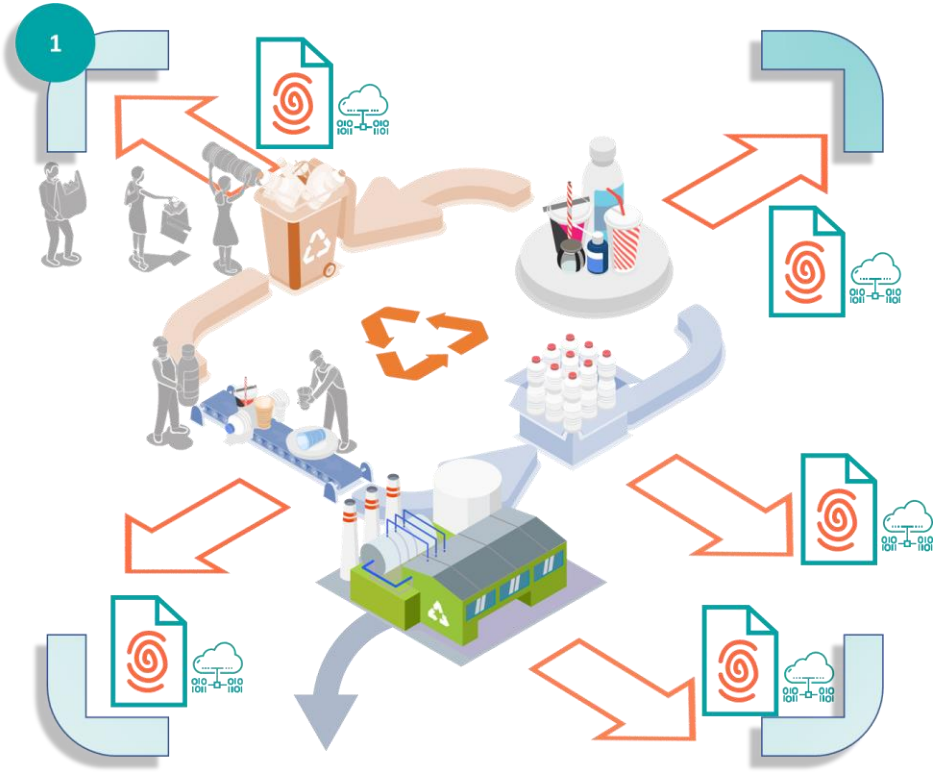


c. Parameterization of many interactions

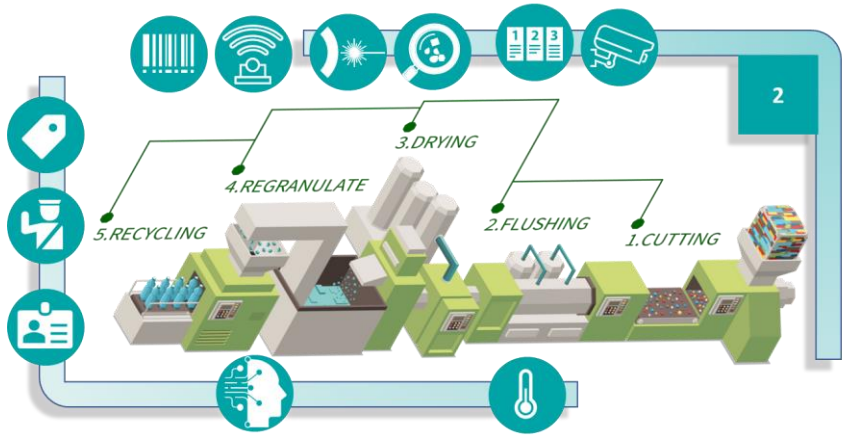
DIGITAL-TWIN FOR THE FOOD PACKAGING SUPPLY CHAIN

OVERVIEW





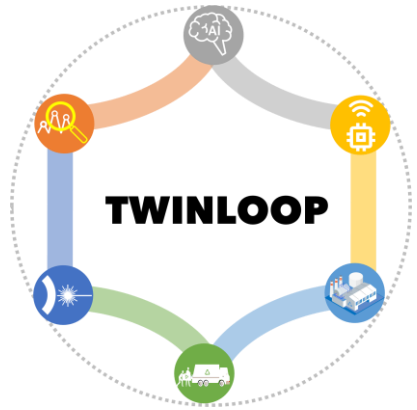
CHEMICAL-INSTRUMENTATION OF RECYCLING PLANTS



AI-RECOGNITION OF WASTE FINGERPRINTS

DIGITAL-TWIN FOR THE FOOD PACKAGING SUPPLY CHAIN

OVERVIEW OF THE PROJECT TWINLOOP (AMI ALIMENTARITE, ANR2023)



NEW SENSORS (2, 3)
- electronic noses
- spectroscopic measurements (Raman, NIR, FTIR, Fluo)
- multispectral and hyperspectral (UV/VIS/NIR) imaging
- reflectance, fast thermodesorption, microplastics detection

SAMPLE LIBRARY & REFERENCE MEASUREMENTS (3, 4)
(low- and high-resolution GC-MS)

ARTIFICIAL INTELLIGENCE (4, 5)
machine learning, chemiometrics

BLOCKCHAIN, RFID/NFC (5, 6)
traceability, decision making, modeling

ON-SITE INDUSTRIAL DEMONSTRATOR (5, 6)

RECYCLED STREAMS (7, 8)

TRL level

DECISION

RISK BALANCING, COMPLIANCE WITH EU, FR REGULATIONS

INFORMATION MANAGEMENT FOR THE CIRCULAR ECONOMY

INRAE