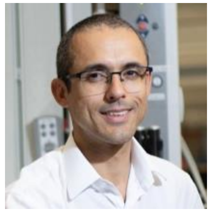
Trends and challenges in Molecular and Particle-based Mechanics

Andrea Giuntoli – University of Groningen

Igor Ostanin – University of Twente

Saullo Giovani Pereira Castro – Delft University of Technology



Azahara Luna Triguero – Eindhoven University of Technology

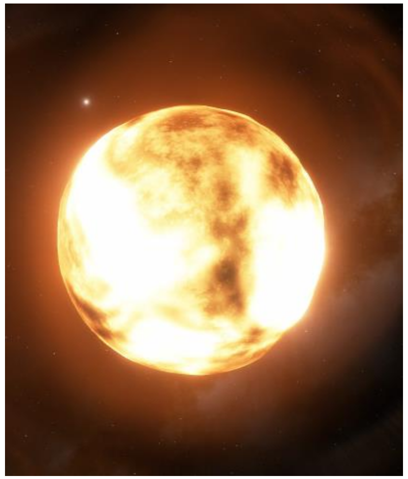
What is a particle?

Hydrogen atom ~10^{-11} m

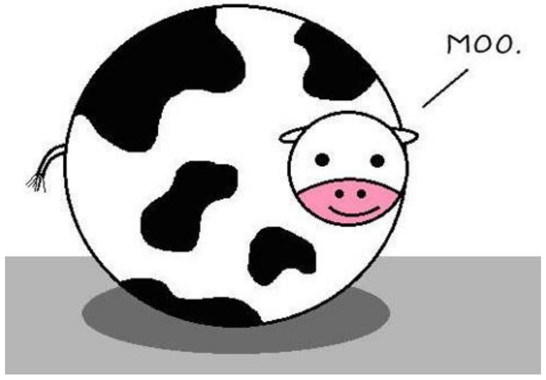
άτομος: indivisible

Atomos: basic unit of any material

-Democritus ~400BC



Star ~ 10^9 m

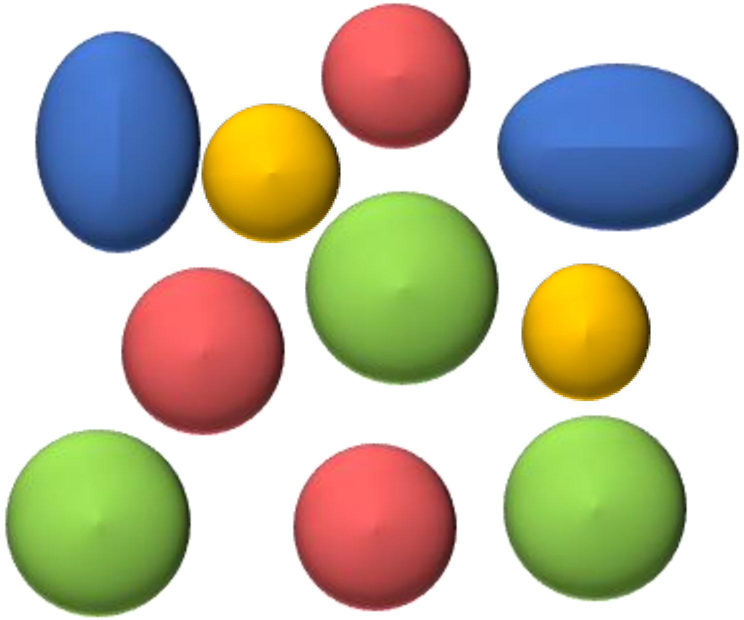


Cow ~ 1m

> *"All models are wrong.*
> *But some models are useful."*
> -George Box

Length and time scales associated to particles

Length scale **σ** and mass **M** associated to the particle size



The interactions between particles determine the equation of motion, thus the timescale **τ**

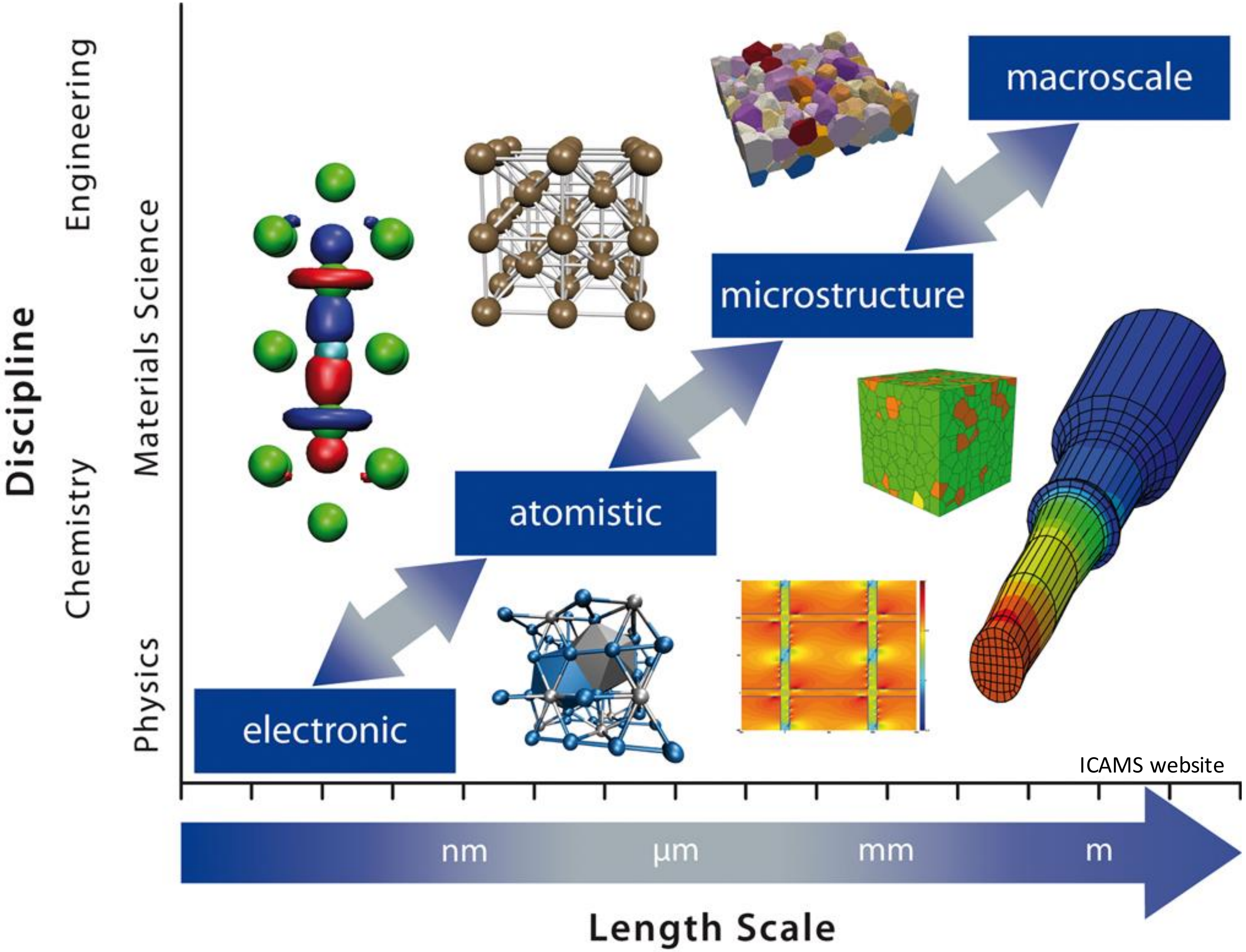
$$\boxed{\tau \sim \sqrt{\frac{m\sigma^2}{\varepsilon}}}$$

Constraints and limitations: how to bridge the scales?

Time resolution: $\sim 10^{-3}\tau$
Timescale limit: $\sim 10^{6}\tau$

Size resolution: σ
Size limit: $\sim 10^{3}$σ ($\sim 10^{9}\sigma^{3}$)

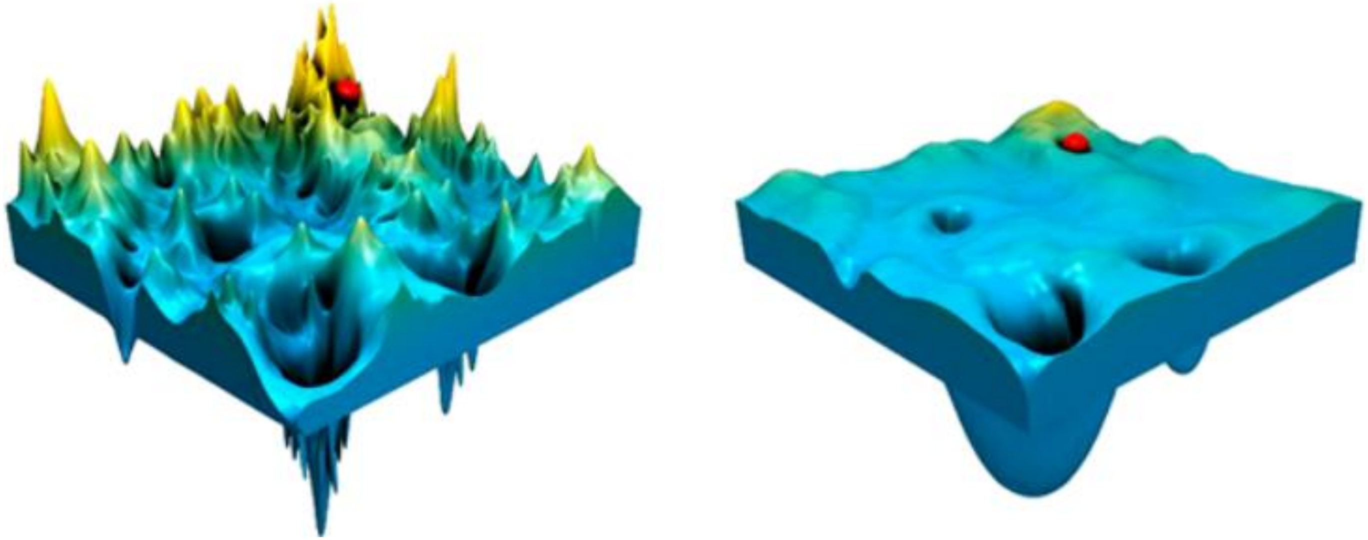
The first is harder to overcome
(no parallelization)



ICAMS website

Multiscale modeling challenges: *proper* coarse-graining

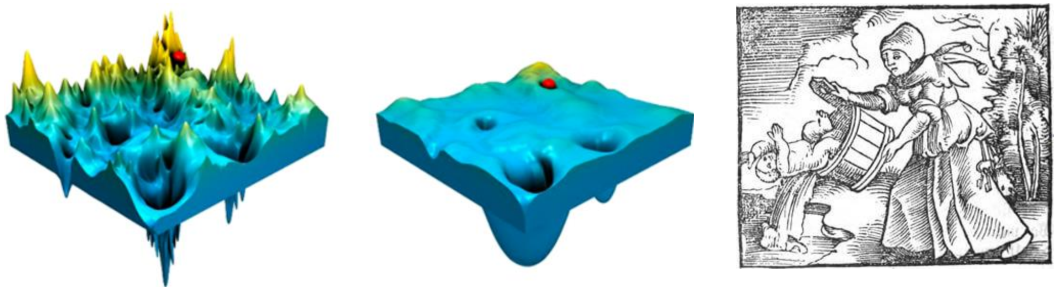
Coarse-graining = loss of information

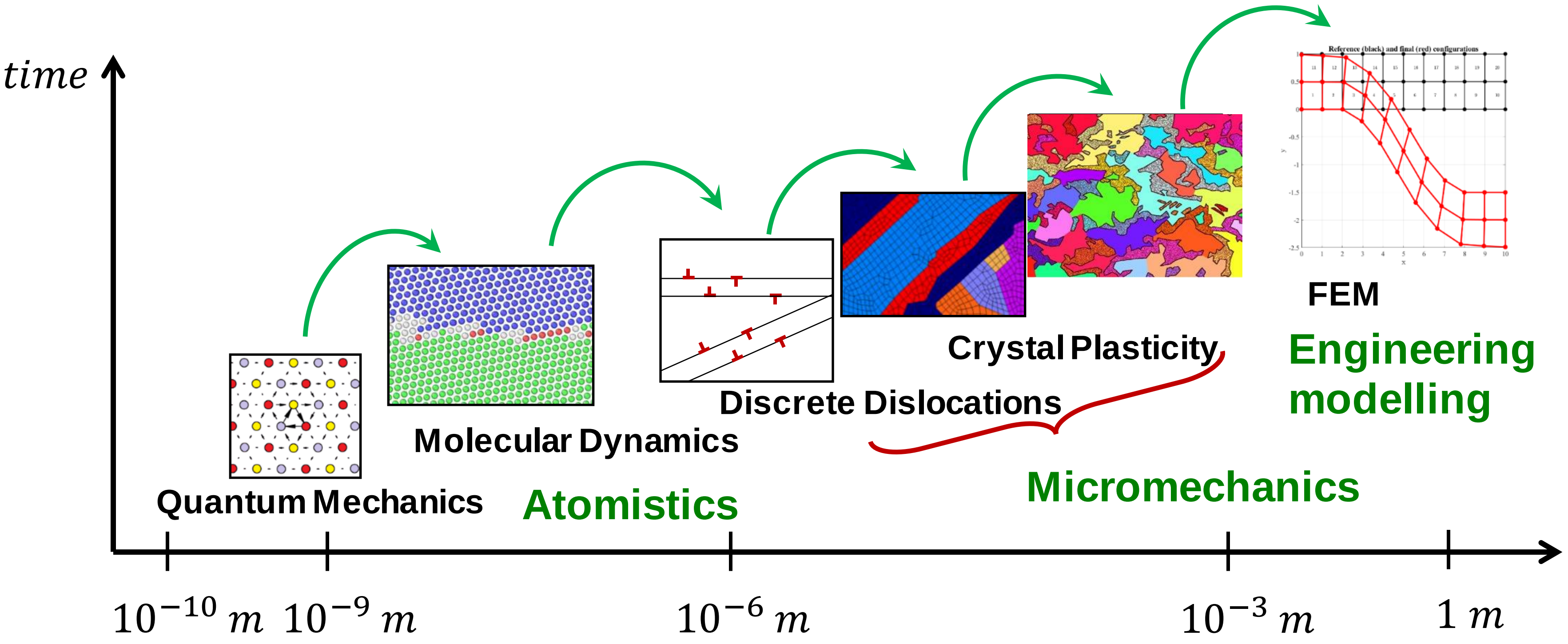


Kmiecik et al., Chemical Reviews 2016

Don't throw the baby out with the bathwater!

Multiscale modeling challenges: *proper* coarse-graining





time

FEM

Engineering modelling

Crystal Plasticity

Discrete Dislocations

Micromechanics

Molecular Dynamics

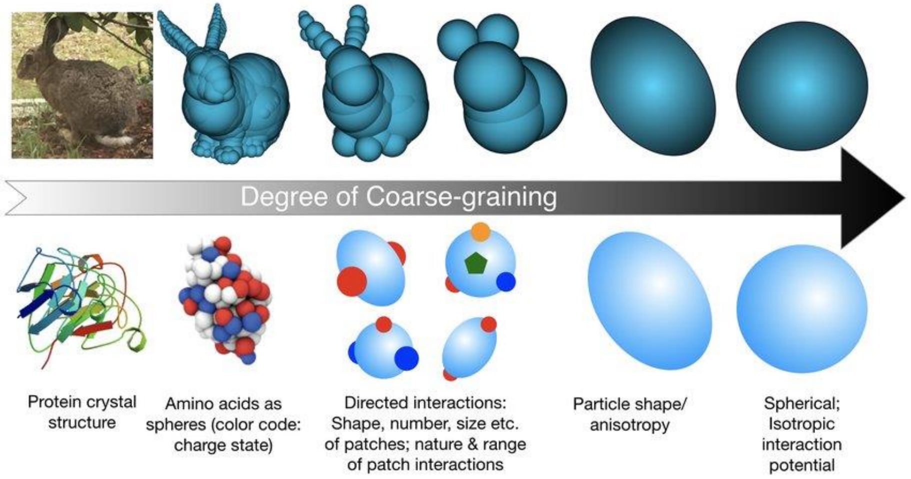
Quantum Mechanics

Atomistics

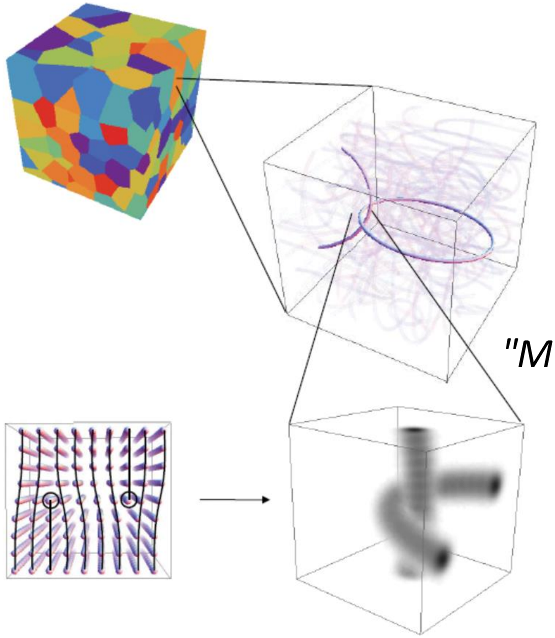
$10^{-10}\ m$ $10^{-9}\ m$ $10^{-6}\ m$ $10^{-3}\ m$ $1\ m$

From Maresca MSM group (RuG)

Coarse-graining vs homogeneization: the role of emergence



Stradner & Schurtenberger, Soft Matter 2020

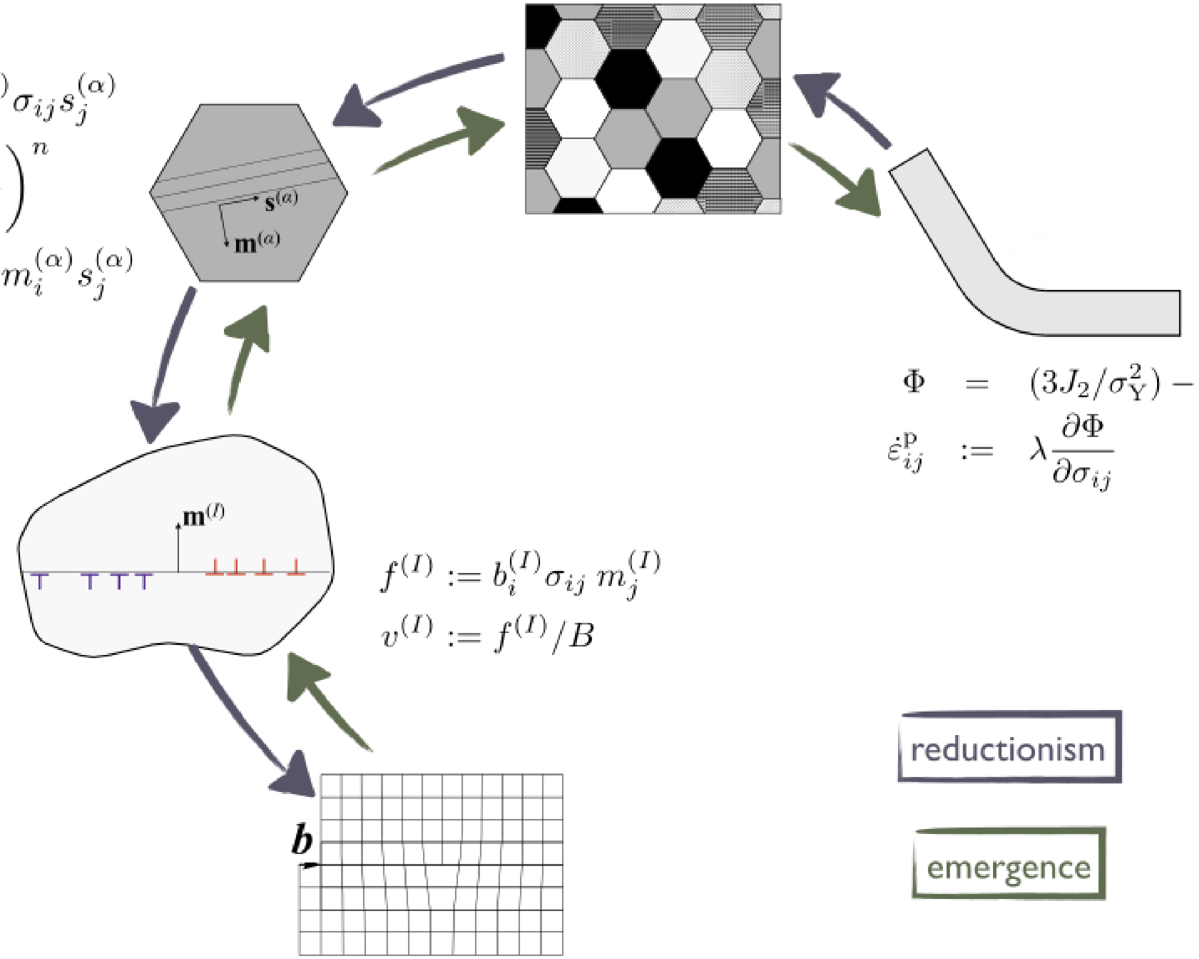


Schieber & Hütter
"Multiscale Modeling beyond Equilibrium"
Physics Today 2020

$$\tau^{(\alpha)} := m_i^{(\alpha)} \sigma_{ij} s_j^{(\alpha)}$$

$$\frac{\dot{\gamma}^{(\alpha)}}{\dot{\gamma}_0} := \left(\frac{\tau}{\tau_0}\right)^n$$

$$\dot{\varepsilon}_{ij}^{\mathrm{p}} := \dot{\gamma}^{(\alpha)} m_i^{(\alpha)} s_j^{(\alpha)}$$



$$\Phi = (3J_2/\sigma_{\mathrm{Y}}^2) - 1$$

$$\dot{\varepsilon}_{ij}^{\mathrm{p}} := \lambda \frac{\partial \Phi}{\partial \sigma_{ij}}$$

$$f^{(I)} := b_i^{(I)} \sigma_{ij}\, m_j^{(I)}$$

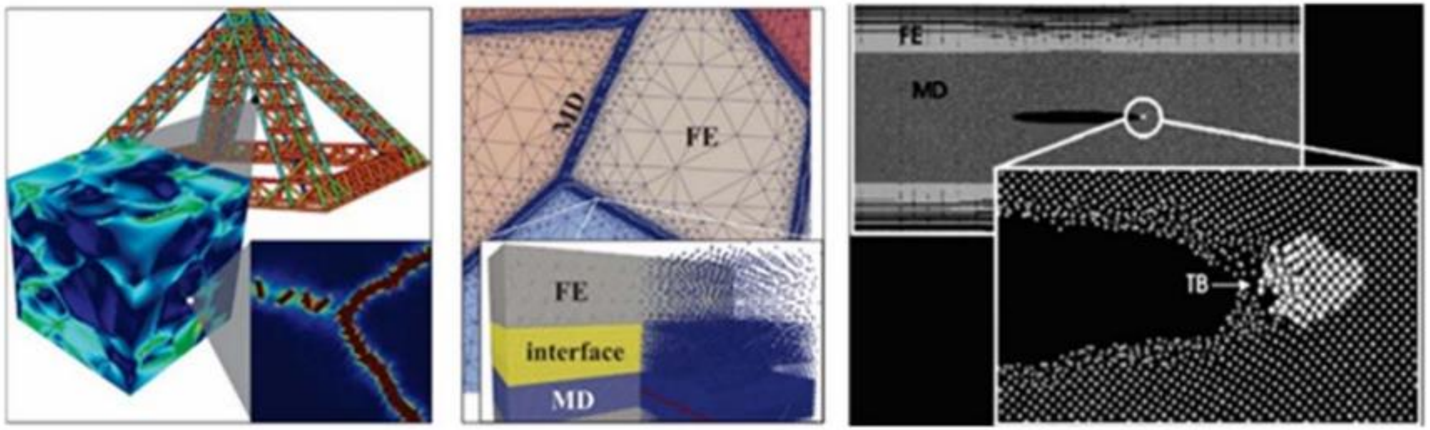
$$v^{(I)} := f^{(I)}/B$$

reductionism

emergence

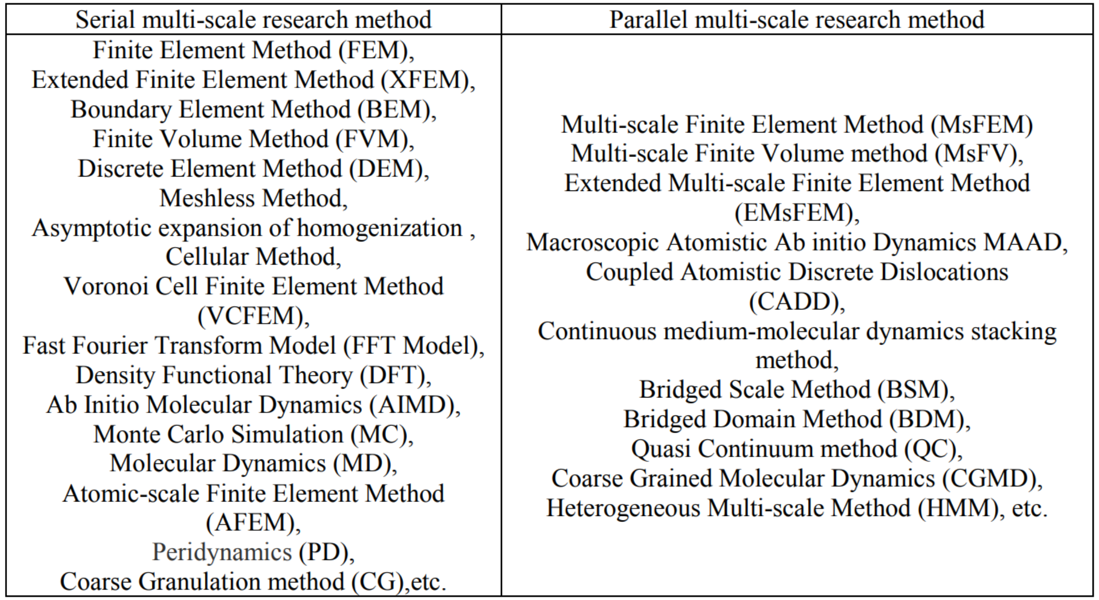
Van der Giessen,
"Micromechanics & emergence in time"
Eur. J. Mech. A Solids 2019

Multiscale modeling challenges:
hierarchical vs concurrent scale-bridging simulations



Van der Giessen, Kochmann, et al.,
"Roadmap on Multiscale Materials Modeling"
Modelling Simul. Mater. Sci. Eng. 2020

Table 1. Main methods of multi-scale analysis



Serial multi-scale research method	Parallel multi-scale research method
Finite Element Method (FEM), Extended Finite Element Method (XFEM), Boundary Element Method (BEM), Finite Volume Method (FVM), Discrete Element Method (DEM), Meshless Method, Asymptotic expansion of homogenization , Cellular Method, Voronoi Cell Finite Element Method (VCFEM), Fast Fourier Transform Model (FFT Model), Density Functional Theory (DFT), Ab Initio Molecular Dynamics (AIMD), Monte Carlo Simulation (MC), Molecular Dynamics (MD), Atomic-scale Finite Element Method (AFEM), Peridynamics (PD), Coarse Granulation method (CG),etc.	Multi-scale Finite Element Method (MsFEM) Multi-scale Finite Volume method (MsFV), Extended Multi-scale Finite Element Method (EMsFEM), Macroscopic Atomistic Ab initio Dynamics MAAD, Coupled Atomistic Discrete Dislocations (CADD), Continuous medium-molecular dynamics stacking method, Bridged Scale Method (BSM), Bridged Domain Method (BDM), Quasi Continuum method (QC), Coarse Grained Molecular Dynamics (CGMD), Heterogeneous Multi-scale Method (HMM), etc.

Zhou & Chen,
"Review on Multi-scale Simulation Methods"
IOP Conf. Ser.: Mater. Sci. Eng. 2018

Fracture as a typical multiscale problem: hierarchical vs concurrent

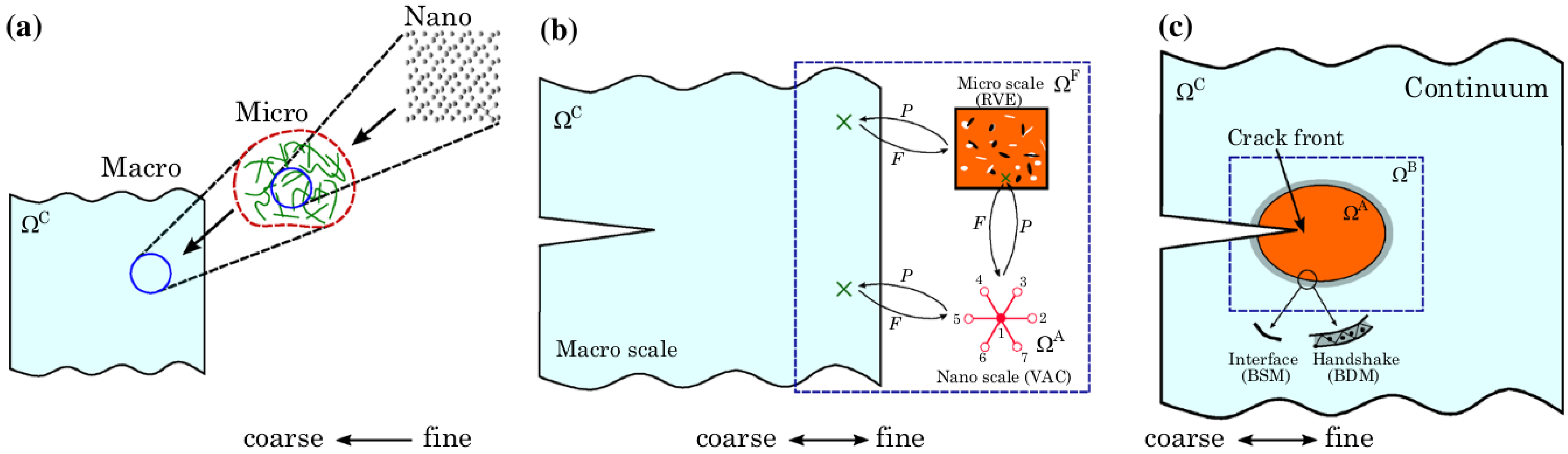
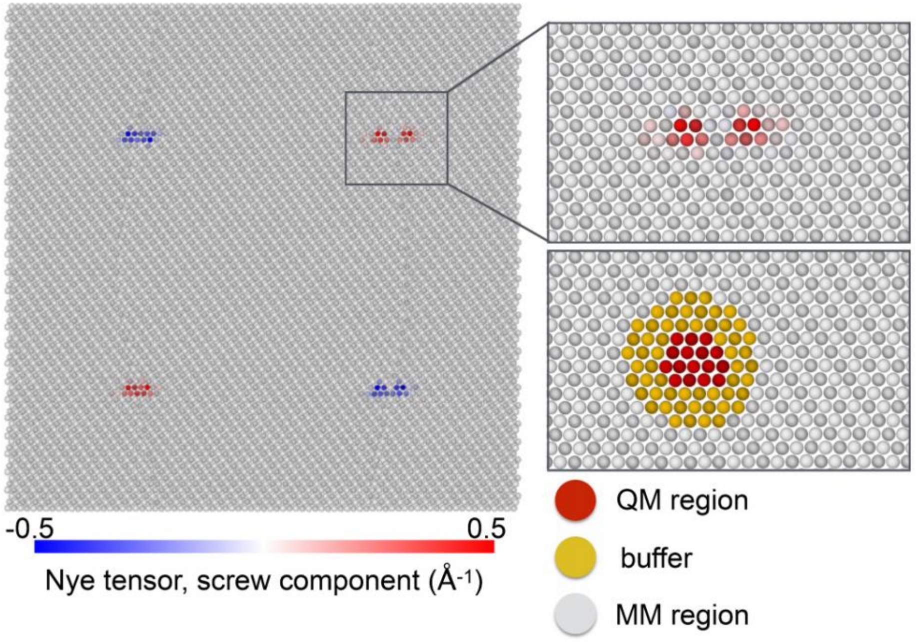


Figure 1: Schematics of **a** hierarchical, **b** semi-concurrent, and **c** concurrent multiscale methods. In the hierarchical methods the information exchange happens only from fine scale to coarse scale, whereas the interaction is two way in case of semi-concurrent and concurrent multiscale methods. Note a definite region of coupling in the concurrent multiscale methods, which does not exist in the semi-concurrent multiscale methods.

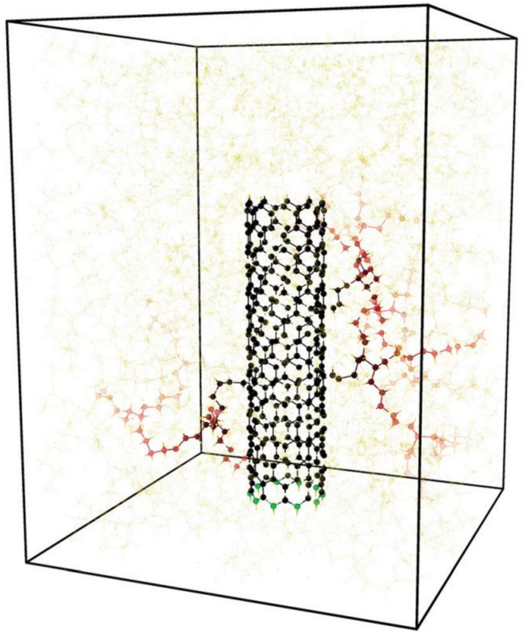
Budarapu & Rabczuk
"Multiscale Methods for Fracture: a Review"
J. Indian Inst. Sci. 2017

From quantum to all-atoms



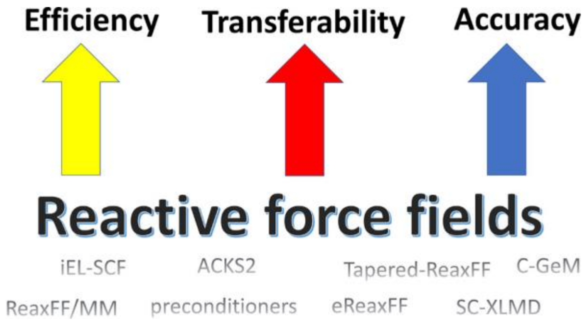
Bianchini et al., Phys. Rev. Mat. 2019

LOTF method to track moving defects with QM precision



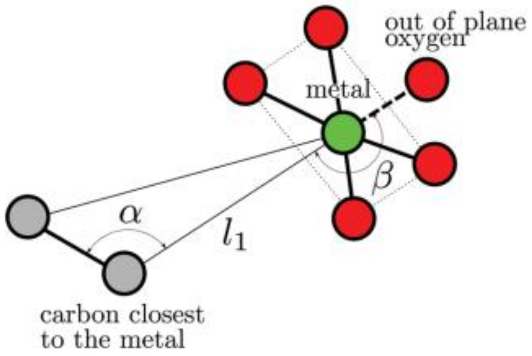
Gołebiowski, Kermode et al., *Phys. Chem. Chem. Phys. 2020*

QM precision for reactive bonds at the CNT-polymer interface



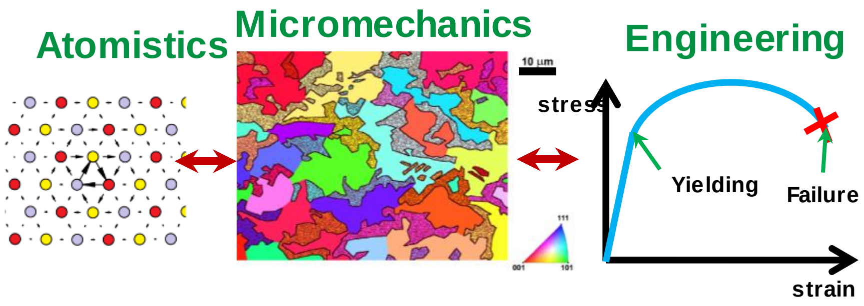
Leven et al., J. Chem. Theory Comput. 2021

All-atoms simulations: trends and challenges



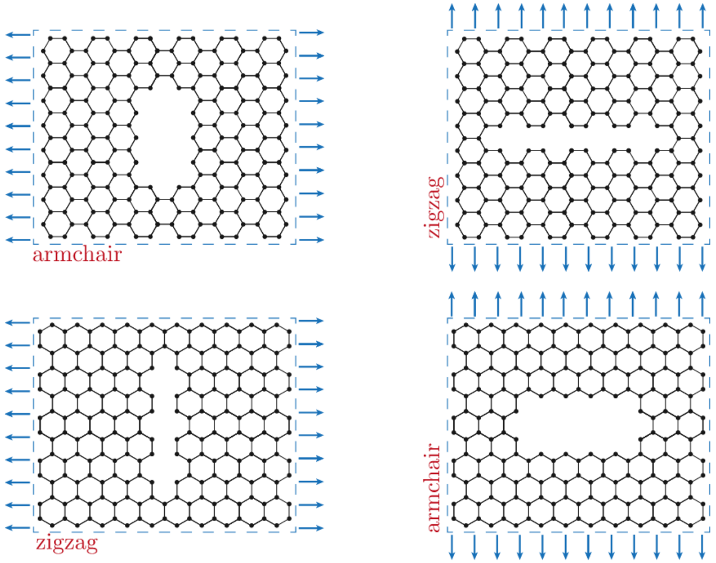
Becker, Luna-Triguero et al., Phys. Chem. Chem. Phys. 2018

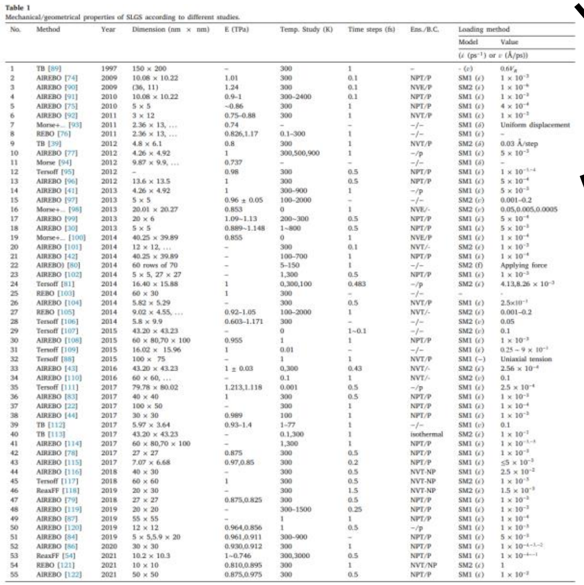
Polarizable force fields for organic-metal frameworks



Maresca et al., Nat. Commun. 2021

Analytical models from simulations to predict macroscale behavior





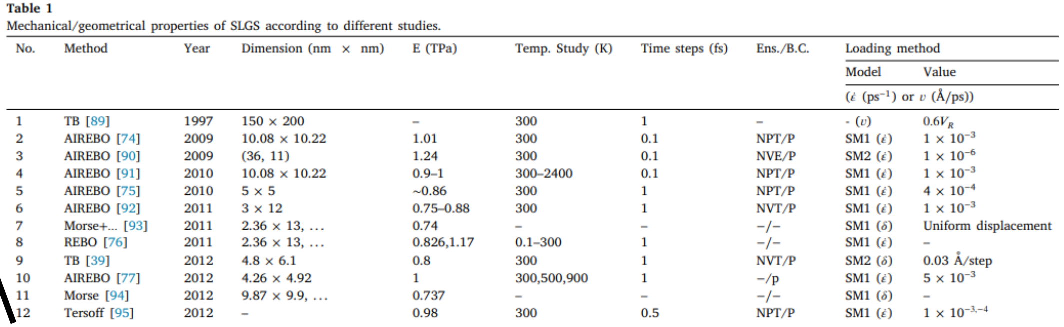


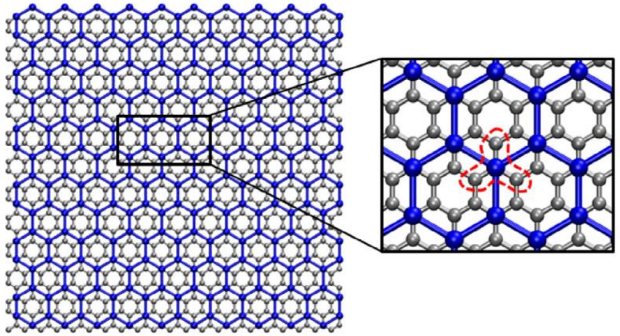
Table 1
Mechanical/geometrical properties of SLGS according to different studies.

No.	Method	Year	Dimension (nm × nm)	E (TPa)	Temp. Study (K)	Time steps (fs)	Ens./B.C.	Loading method	
								Model	Value
								($\dot{\varepsilon}$ (ps^{-1}) or υ (Å/ps))	
1	TB [89]	1997	150 × 200	–	300	1	–	- (υ)	$0.6V_R$
2	AIREBO [74]	2009	10.08 × 10.22	1.01	300	0.1	NPT/P	SM1 ($\dot{\varepsilon}$)	1×10^{-3}
3	AIREBO [90]	2009	(36, 11)	1.24	300	0.1	NVE/P	SM2 ($\dot{\varepsilon}$)	1×10^{-6}
4	AIREBO [91]	2010	10.08 × 10.22	0.9–1	300–2400	0.1	NPT/P	SM1 ($\dot{\varepsilon}$)	1×10^{-3}
5	AIREBO [75]	2010	5 × 5	~0.86	300	1	NPT/P	SM1 ($\dot{\varepsilon}$)	4×10^{-4}
6	AIREBO [92]	2011	3 × 12	0.75–0.88	300	1	NVT/P	SM1 ($\dot{\varepsilon}$)	1×10^{-3}
7	Morse+... [93]	2011	2.36 × 13, ...	0.74	–	–	–/–	SM1 (δ)	Uniform displacement
8	REBO [76]	2011	2.36 × 13, ...	0.826,1.17	0.1–300	1	–/–	SM1 ($\dot{\varepsilon}$)	–
9	TB [39]	2012	4.8 × 6.1	0.8	300	1	NVT/P	SM2 (δ)	0.03 Å/step
10	AIREBO [77]	2012	4.26 × 4.92	1	300,500,900	1	–/p	SM1 ($\dot{\varepsilon}$)	5×10^{-3}
11	Morse [94]	2012	9.87 × 9.9, ...	0.737	–	–	–/–	SM1 (δ)	–
12	Tersoff [95]	2012	–	0.98	300	0.5	NPT/P	SM1 ($\dot{\varepsilon}$)	$1 \times 10^{-3,-4}$

Torkaman-Asadi & Kouchakzadeh, Comput. Mat. Sci. 2022

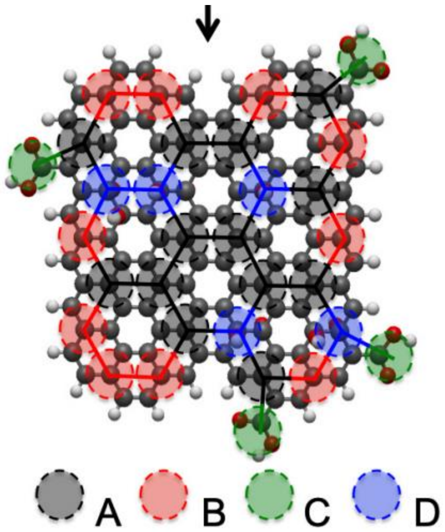
Consistency and transferability needed for force fields (e.g. for graphene)

From all-atoms to CG

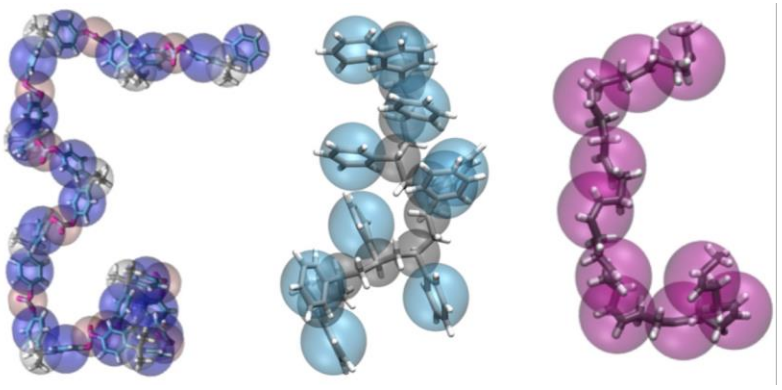


Ruiz et al., Carbon 2015

CG models for (functionalized) graphene

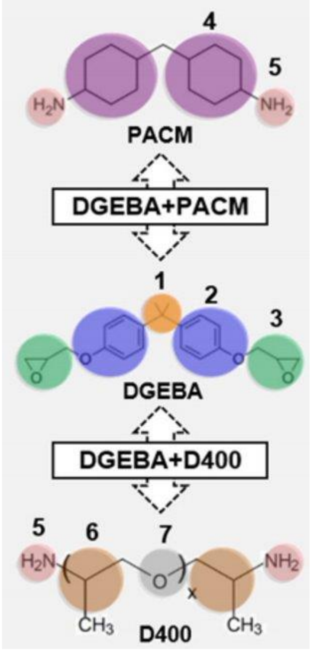


William & Lisal, 2D Mater. 2020

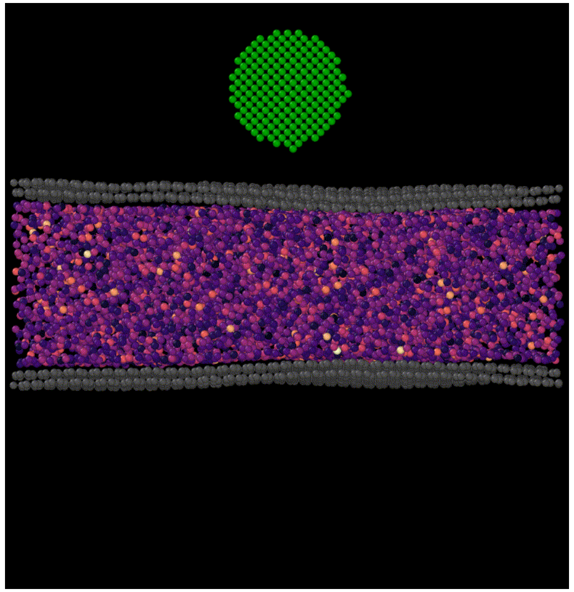


Xia et al., Science Advances 2019

Chemistry-specific, dynamically accurate polymer models



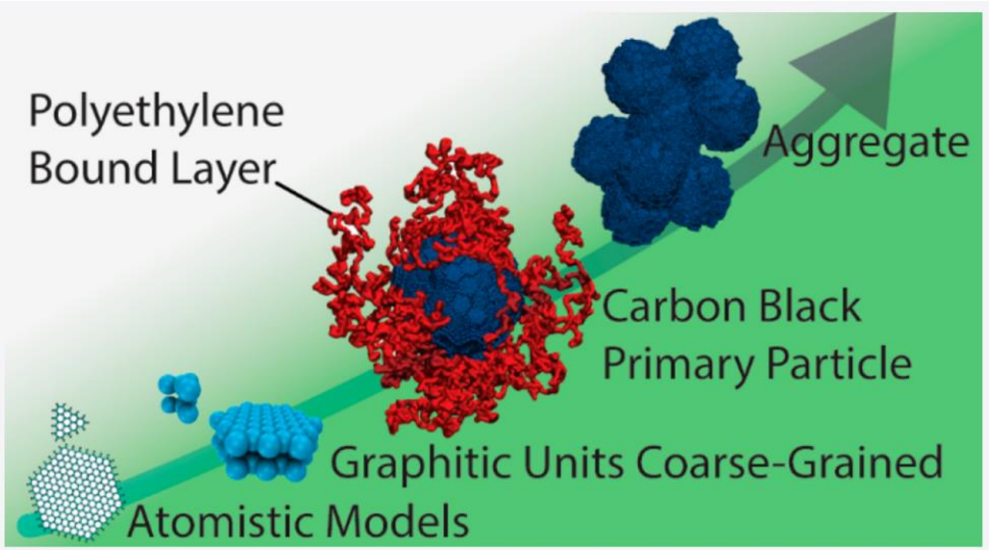
Giuntoli et al.,
npj Comput. Mat. 2021



Impact on nanocomposites with quantitative accuracy

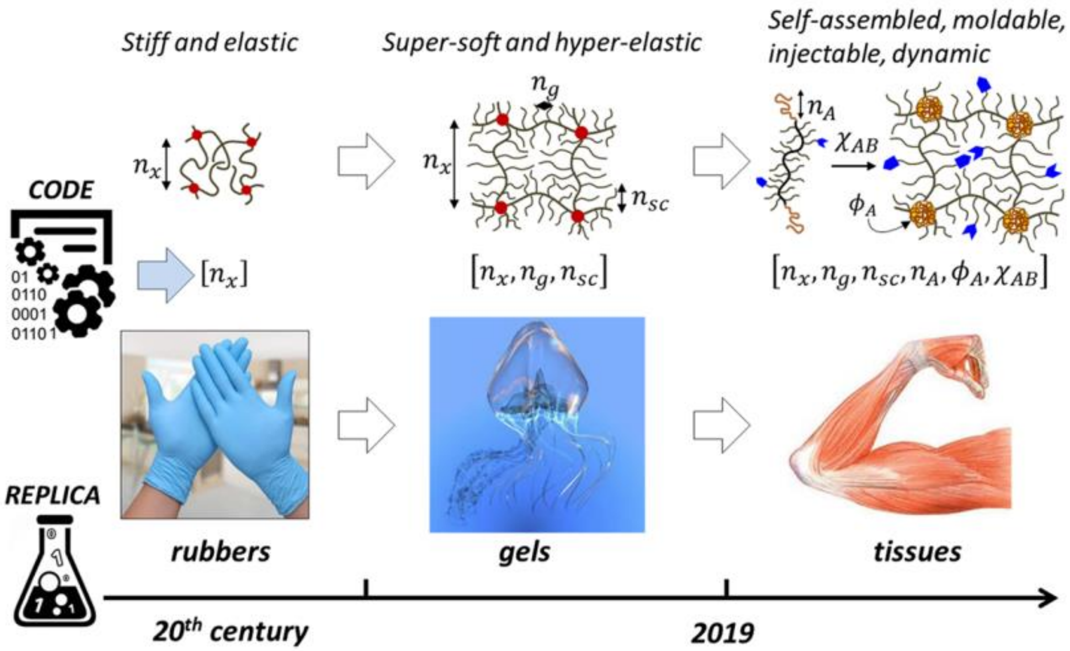
White et al., in preparation

CG simulations: trends and challenges



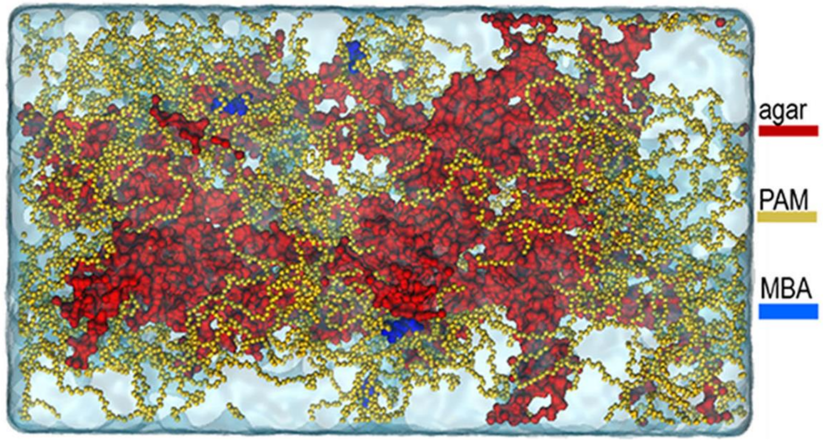
Caputo et al., J. Chem. Theory Comp. 2021

Hybrid particle-field model for polymer nanocomposites



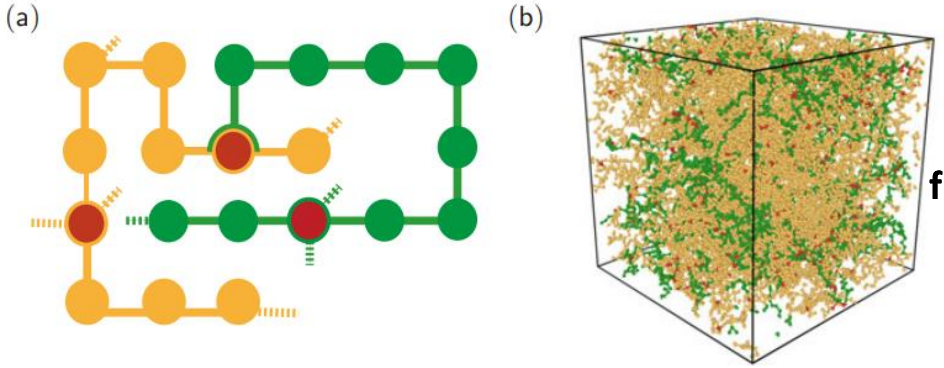
Sheiko & Dobrynin, Macromolecules 2019

Ultrasoft elastomers design



Zhang et al., npj Comput. Mat. 2021

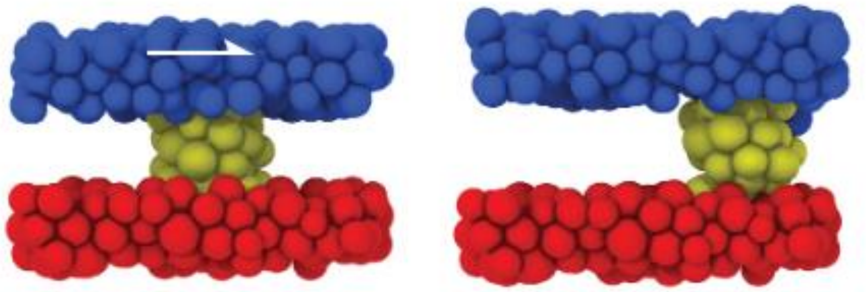
Multiscale polymerization for double-networks

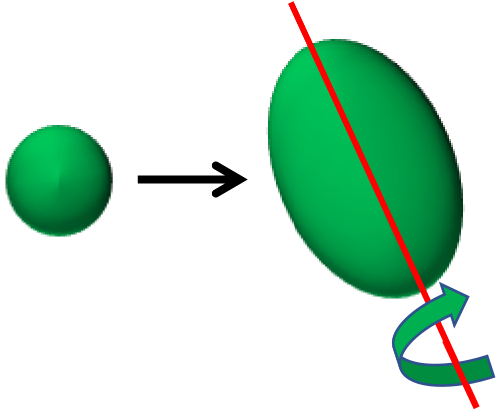


Efficient network formation algorithms for reversible networks

Raffaelli et al. (2020), Rheology, Rupture, Reinforcement and Reversibility: Computational Approaches for Dynamic Network Materials

From CG to DEM

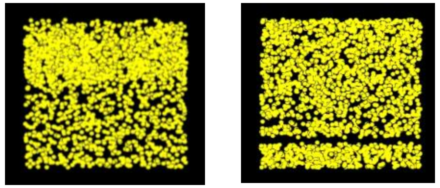




Pham-Ba & Molinari, Comput. Methods Appl. Mech. Engrg. 2022

MD-like top-down force field with reversible fracture for adhesion

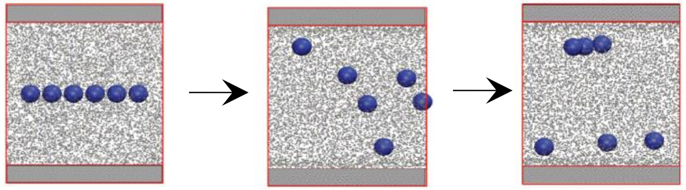
→ shear banding, shear fracture



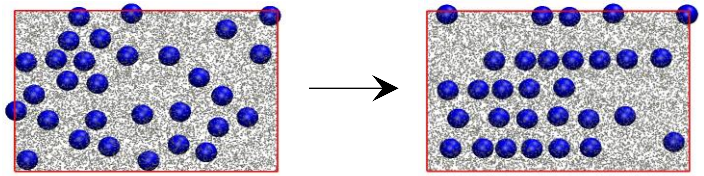
Polymers as single particles:

- **conservative forces for thermodynamics**
- **non-conservative transient forces for entanglements.**

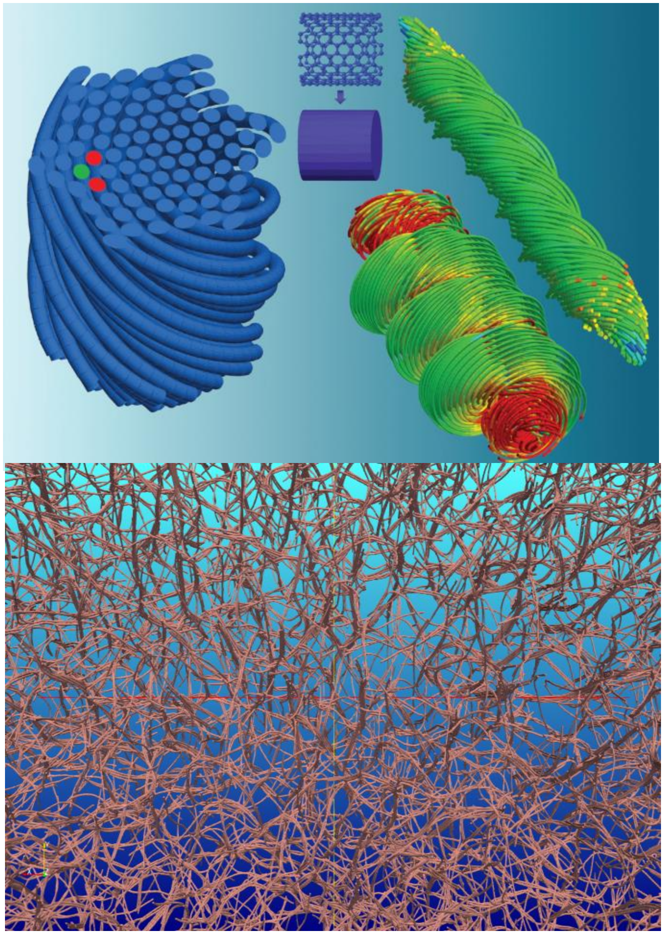
→ shear migration



→ shear alignment



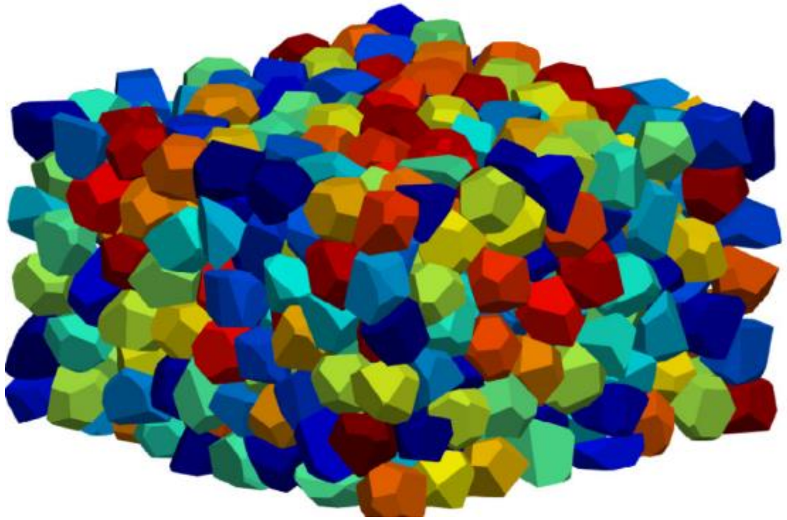
den Otter & Briels, RaPiD (Responsive Particle Dynamics)



Ostanin et al., JMPS 2013
Grebenko et al., Carbon 2022

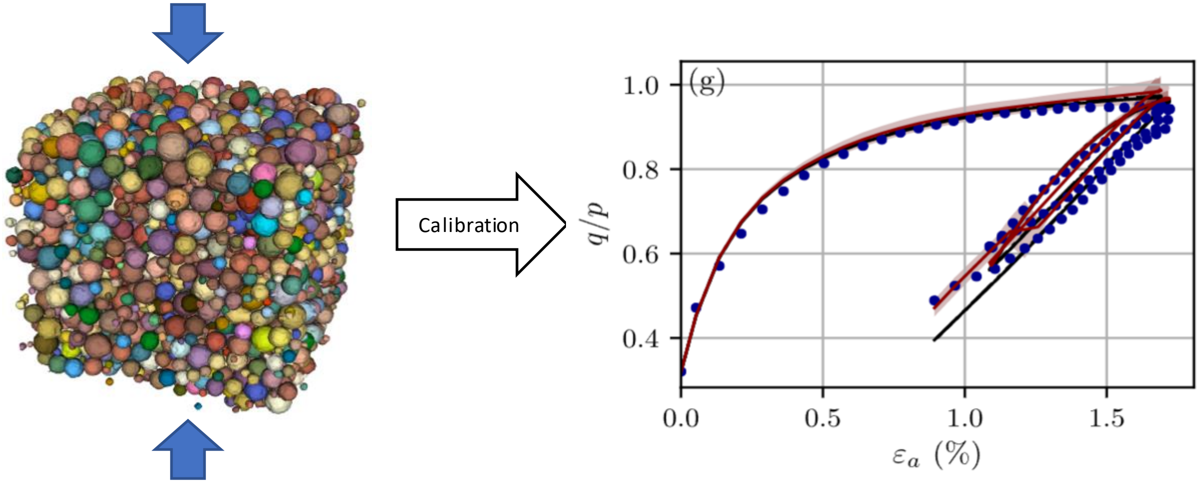
MD-informed DEM model for carbon nanotube materials

DEM simulations: trends and challenges



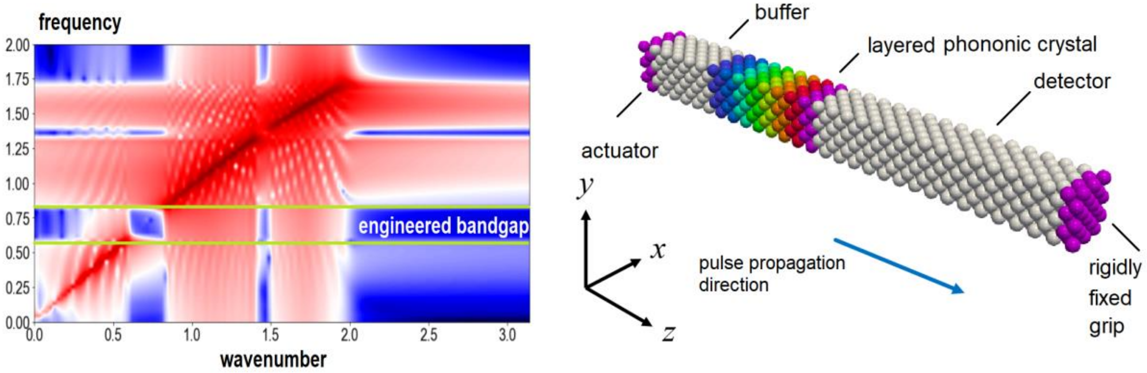
Neto et al., Comput. Methods Appl. Mech. Engrg. 2021

Virtual Element Method for flexible DEM polyhedra



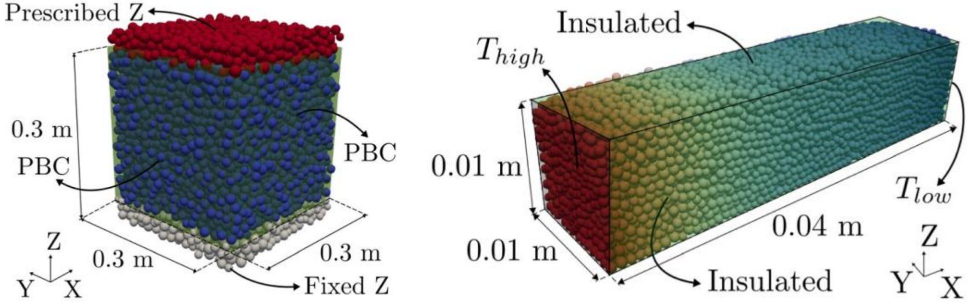
Cheng et al., CMAME 2019

Automatic ML calibration of DEM parameters



Ostanin et. al, EML 2022

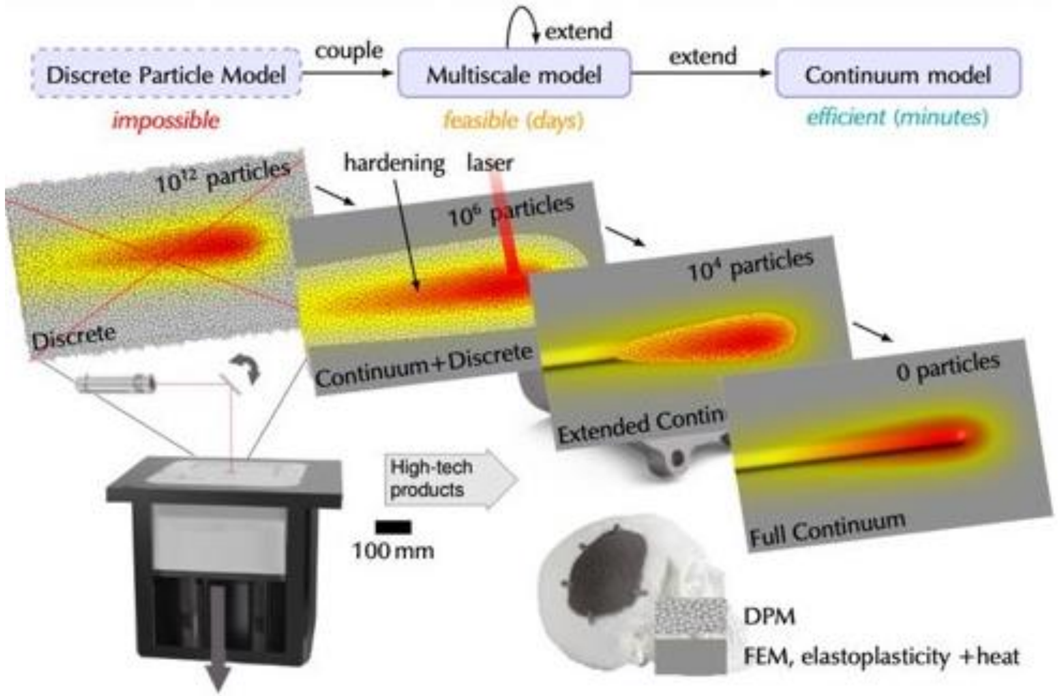
DEM to engineer the acoustic behavior of phononic cystals…



Dorussen, Geers, Remmers, Eng. Comput. 2022

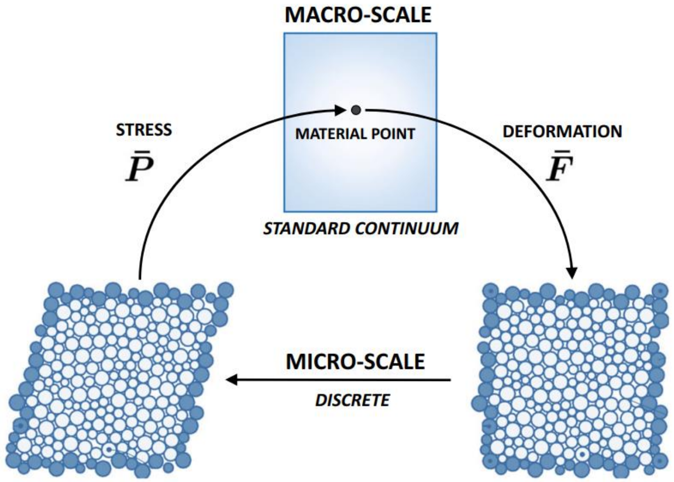
… and thermo-mechanical coupling for AM of powders

DEM-continuum coupling



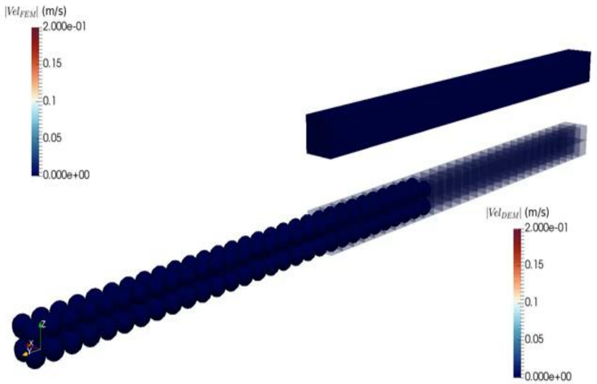
Weinhart et al., ongoing VIDI project

Virtual prototyping of particulate processes from DEM to continuum



Liu, Bosco, Suiker, Comput. Mech. 2022

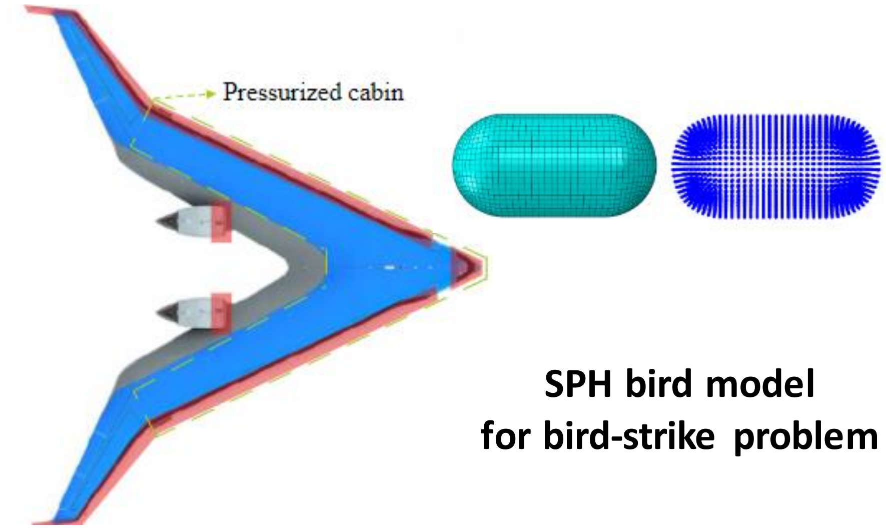
FEM-DEM framework with servo-control algorithm for boundary conditions



Coupling of fluid/solid continuum behavior to DEM

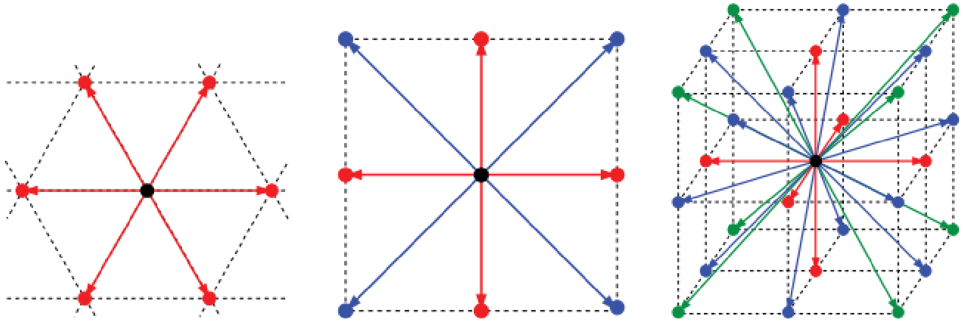
Cheng et al., CMAME 2022, in Press

Trends in mesoscopic simulations: SPH-LBM-Peridynamics-MPM



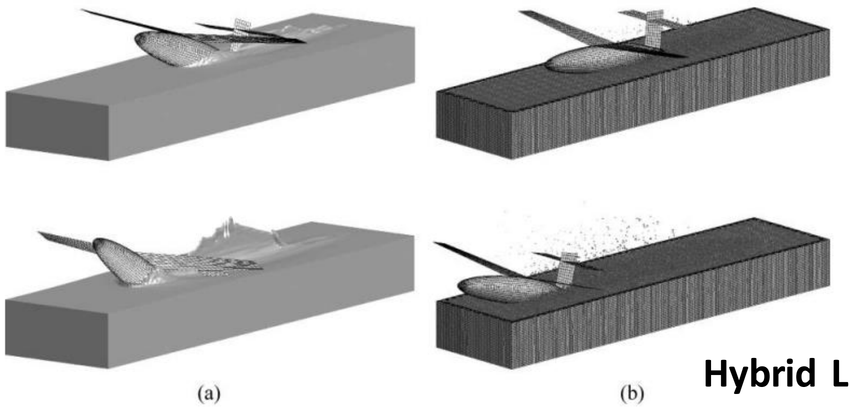
SPH bird model for bird-strike problem

Chen, Waerdt & Castro, engrxiv 2022



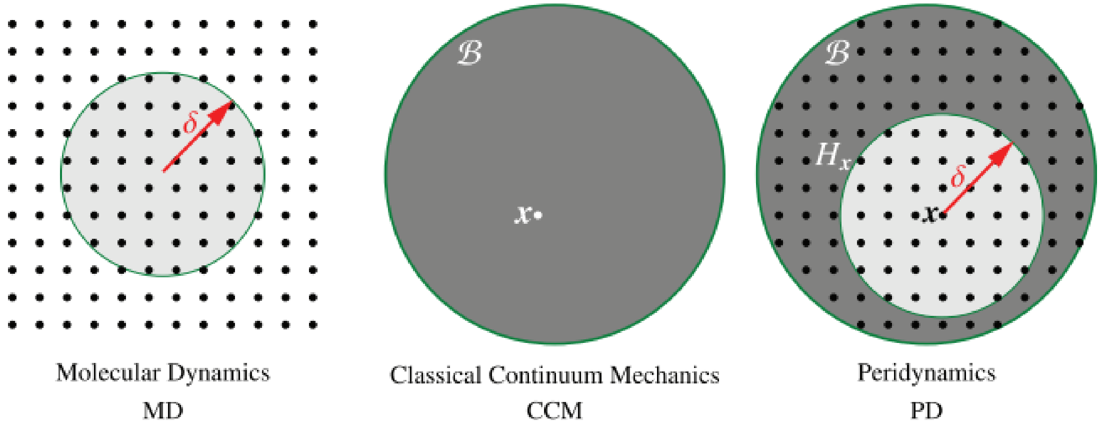
Lallemand et al., J. Comp. Phys. 2021

LBM for near incompressible fluids, complex fluids, complex boundaries



Hybrid Lagrangian-SPH water model for ditching

Bisagni & Pigazzini, Int. J. Crashworthiness 2018



Javili et al., MMS 2018

PD as a discretized formulation of the continuum for fracture more

Overview of Delft University of Technology

Scopus search based on articles from 2022 and 2023, particle, meshfree and meshless methods:

Bird strike, Smoothed Particle Hydrodynamics (SPH) (Castro SGP)

Ditching, SPH (Bisagni C, Castro SGP)

Micro-air vehicles, Lattice Boltzmann Method (LBM) (Castro SGP, van Zuilen A)

Aeroelasticity and drone deployment, LBM (de Breuker R):

Aeroacoustics for aircraft-level noise prediction, LBM (Ragni D, Avallone F, Casalino D)

Simulation of manufacturing, Floating isogeometric analysis (Siddhant K)

Delft Institute of Applied Mathematics:

- SPH (Lipari G now in Twente, Vuik C)
- Material Point Method (MPM) (Muller, M)

Soil modelling, MPM (Galavi V)

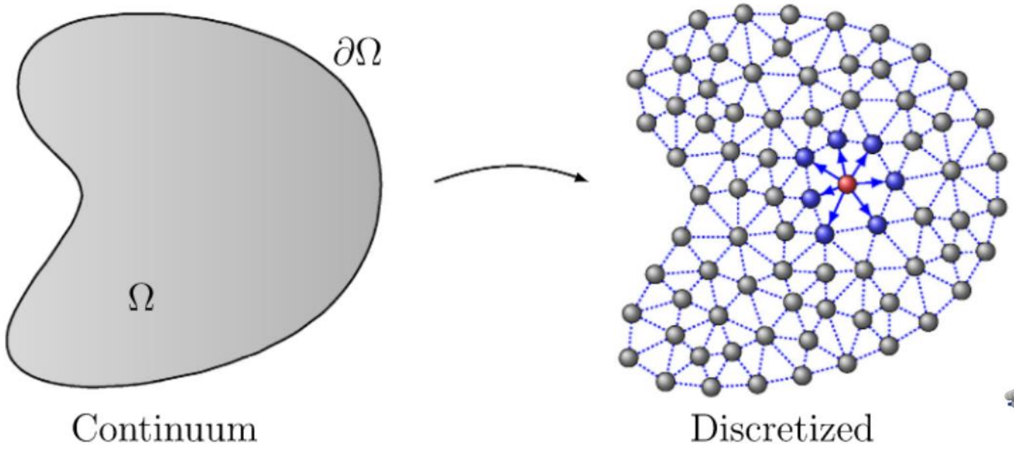
Geotechnical engineering, MPM and CTM-RPIM (Vardon PJ, Hicks MA, Pisano F)

Wave fluid dynamics, SPH (Bremer TS, Tomohiro S)

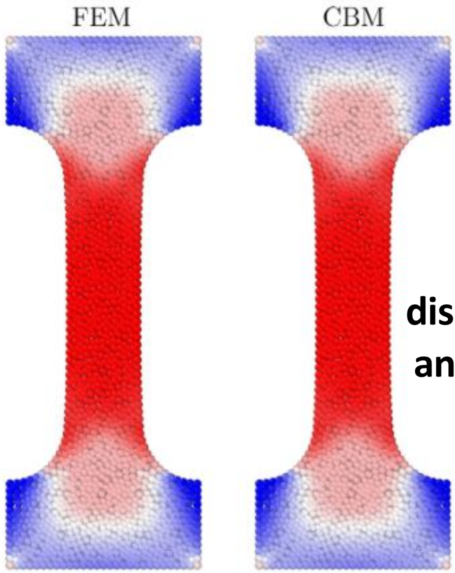
Fracture mechanics, Peridynamics (Karpenko O)

Debris flow impact, MPM (Martinelli M)

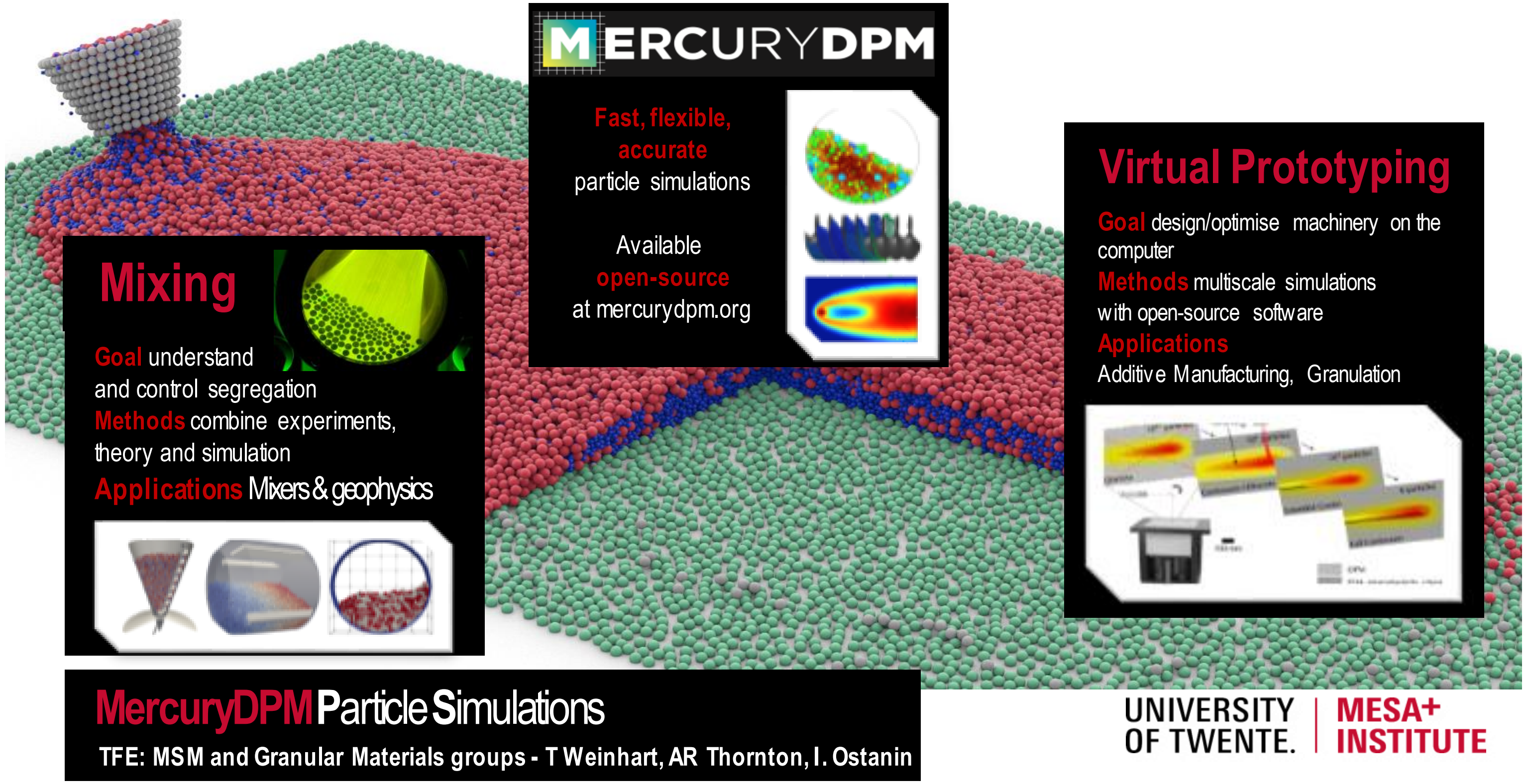
Emerging methods and tools



Sperling et al., Comput. Methods Appl. Mech. Engrg. 2022



Continuum Bond Method: stable and FEM-accurate discrete formulation for fracture and discontinuous phenomena.



Mixing

Goal understand and control segregation
Methods combine experiments, theory and simulation
Applications Mixers & geophysics

MERCURYDPM

Fast, flexible, accurate particle simulations

Available **open-source** at mercurydpm.org

Virtual Prototyping

Goal design/optimise machinery on the computer
Methods multiscale simulations with open-source software
Applications Additive Manufacturing, Granulation

MercuryDPM Particle Simulations

TFE: MSM and Granular Materials groups - T Weinhart, AR Thornton, I. Ostanin

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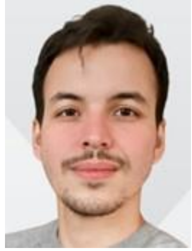
Overview and conclusions

- From great power comes great responsibility: given the flexibility of particle-based approaches, **the choice of the right model is critical**.
- Coarse-graining is **more than a tool**: success **or** failure of a CG model has conceptual implications for our understanding of the phenomenon studied.
- Hierarchical and multiscale approaches are needed, especially in view of **emergent multiscale phenomena**.
- To maximize impact models should be **general, transferable, open access, and easy to implement**.

The workshop speakers' line-up!

Juan E. Alvarez – University of Twente

Multi-scale thermo-viscoelastic modelling of powder-based processes



Leon Thijs – Eindhoven University of Technology

Investigation of single iron particle combustion in the Knudsen transition regime

Sam van Elsloo – Delft University of Technology

Application of the Immersed Interface Method to the Lattice Boltzmann Method

Varun Shah – University of Groningen

Unravelling the atomic scale interaction of H with dislocations in iron