Internal training session: Modelling for optimization of FreeMe processes – 11:20

16/06/2023

Thessaloniki, Greece

IDENER

Israel Bellanato

Toxic
FREE MEtallization process
for plastic surfaces

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Multi-scale modelling: Background and motivation

- The goal of multi-scale modelling is to uncover the physical behaviour and properties of a material or a process, obtaining more exhaustive results by working in several scales (different lengths and times, from atoms to continuum matter), adding value to the models implemented.
- Multi-scale modelling emerged in the 1990s in order to reduce nuclear tests in the USA. Since then, it has become a powerful ally in materials development.
- It has even been awarded with a Nobel Prize in Chemistry: M. Karplus, M. Lewitt and A. Warshel (2013), for the development of a multi-scale model using classical and quantum mechanical theory to model complex chemical systems and reactions.

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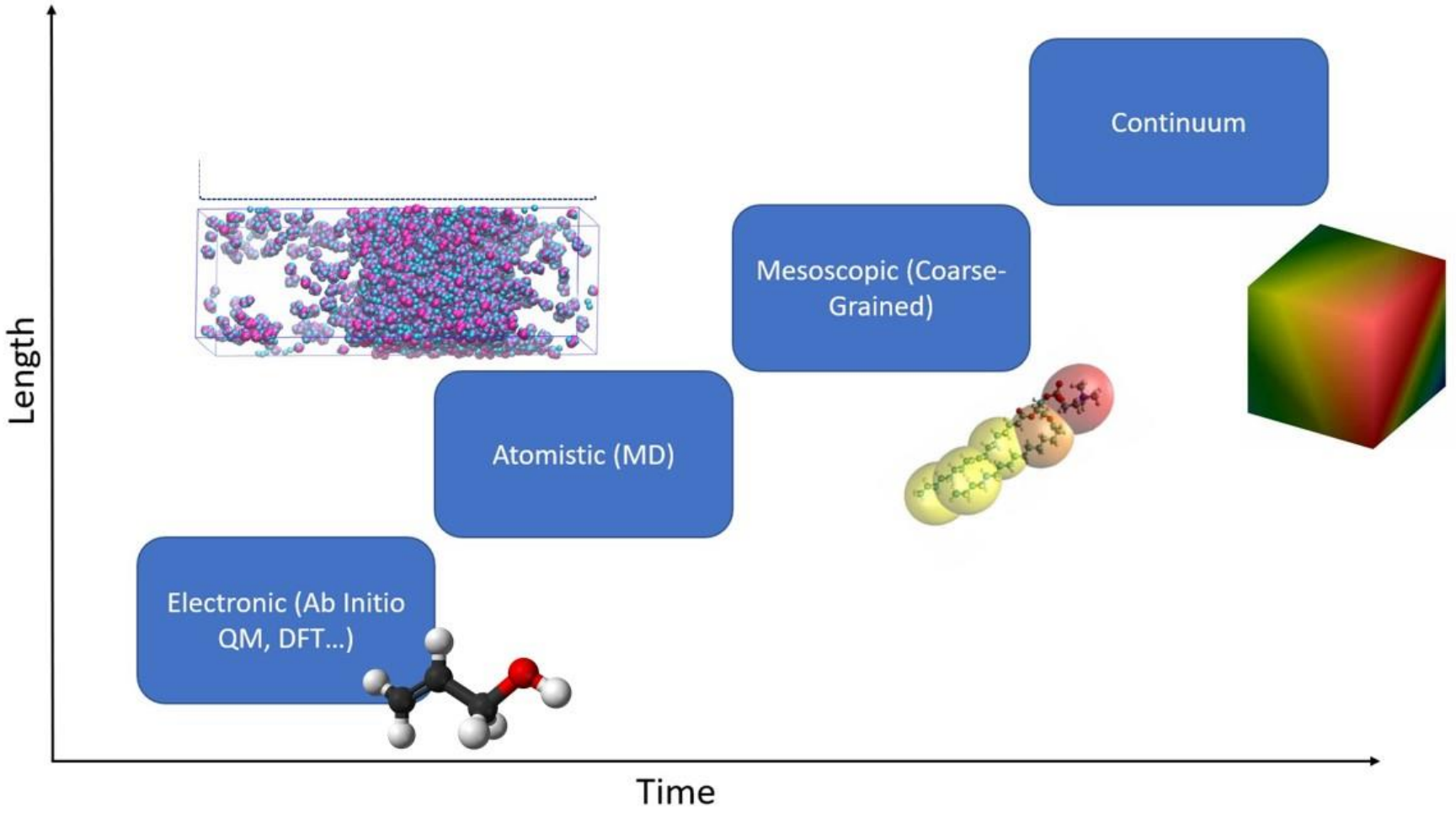
Multi-scale modelling: Background and motivation



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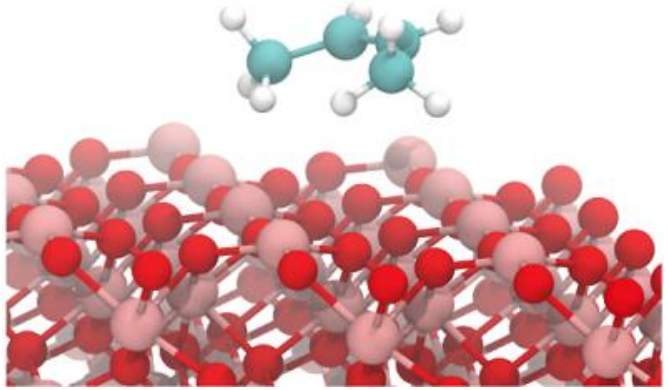
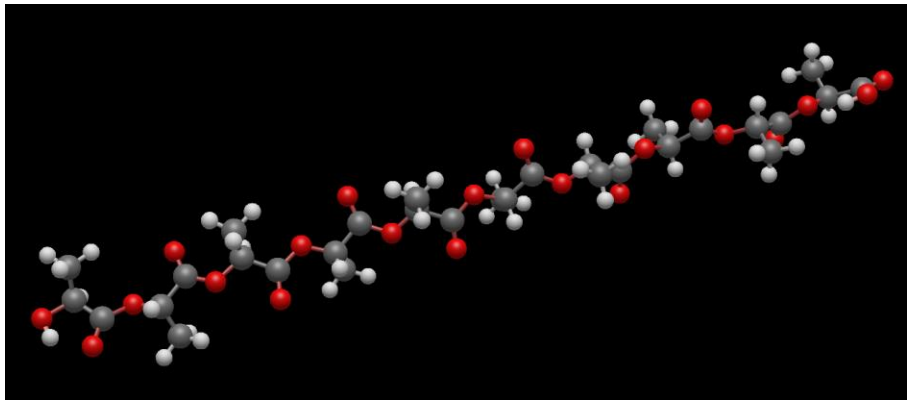
Ab-initio DFT modelling

- Ab-initio means from first principles, so the calculations are based on Quantum Mechanics (QM).
- DFT (Density Functional Theory) is the theory behind a large group of ab-initio calculations.
- We introduce the positions of the atoms we have and select pseudopotentials and other parameters to measure energies.
- Some ab-initio packages are Quantum Espresso, Gaussian, VASP and ORCA.
- Examples of ab-initio calculations are the bulk (unit cell) and surface energies of a material, or the energetic interactions between two molecules.





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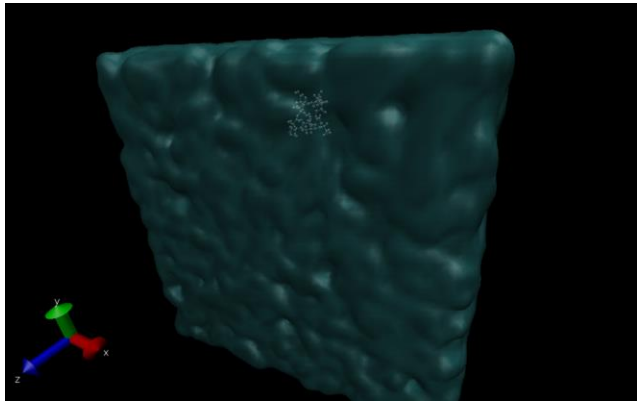
Molecular Dynamics (MD)

- Molecular Dynamics is used to perform simulations with molecular systems at the atomistic scale, that is, involving large numbers of atoms.
- We generate the topology of the molecules (e.g., with Avogadro) and set the force fields (e.g., with the LigParGen server) to account for the interactions in the simulations.
- The molecular subsystems (molecules, water boxes, etc.) are equilibrated at this stage for a better integration in the system afterwards.
- We can then construct the system generating the molecules in the simulation box (in determined or random positions) and perform another system equilibration (usually NVT + NPT).
- With the system equilibrated, we can perform the production runs (usually NPT) in order to study the trajectories of the particles and the properties of the system, often averaged over time.



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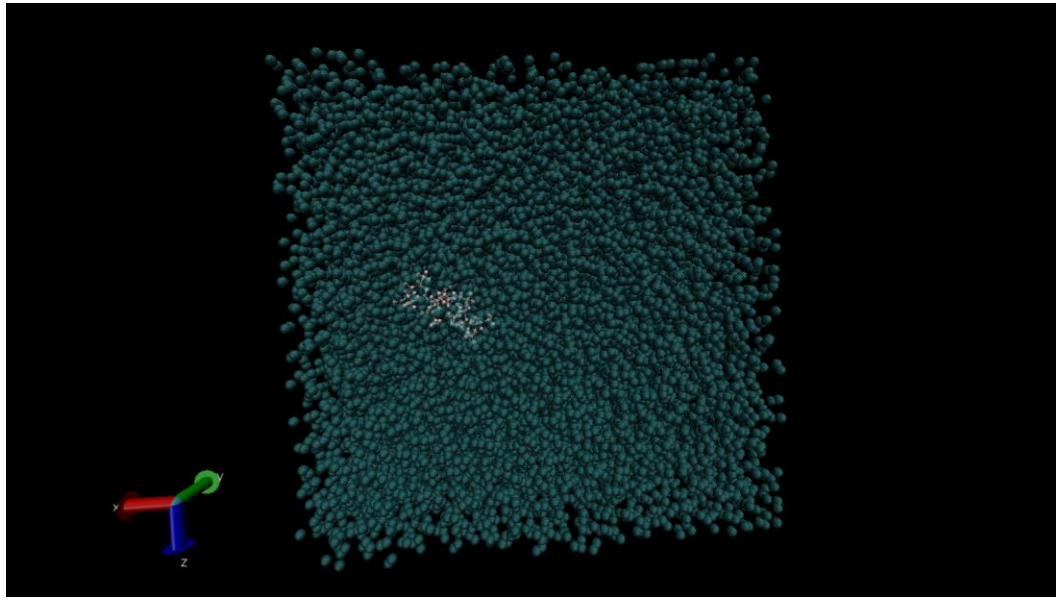
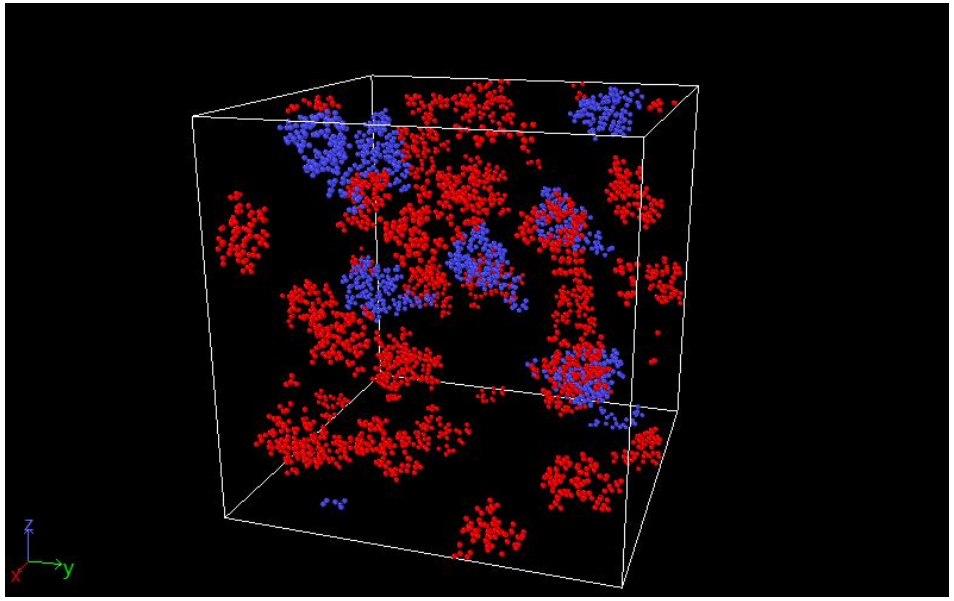
Molecular Dynamics (MD)

- Examples of programs to perform MD on are Gromacs and LAMMPS.
- Examples of MD in FreeMe are the ones given before, but many more particles can be simulated (consider that the water is composed of water molecules, but VMD lets us present it as a liquid surface).





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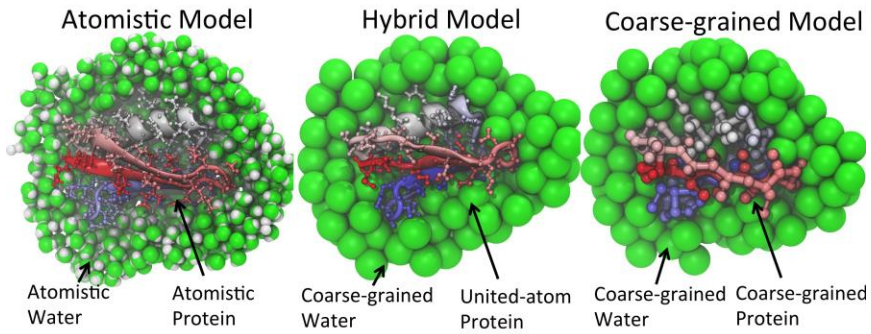
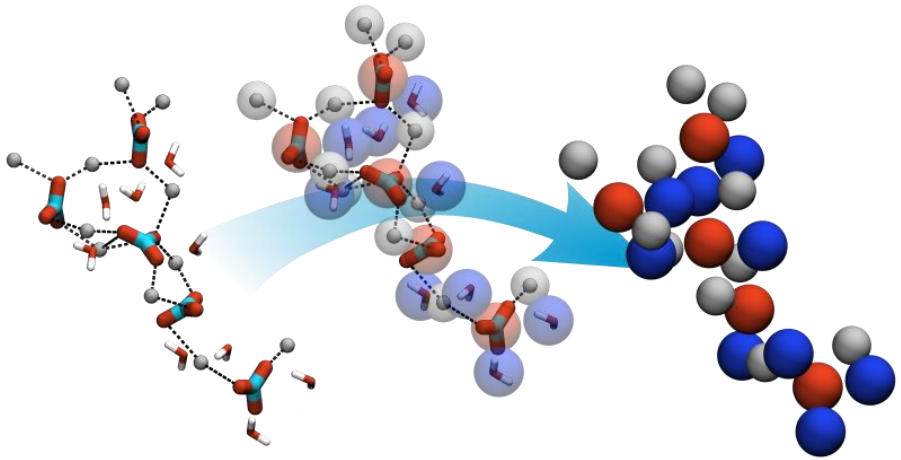
Coarse-Grained (CG) MD

- Coarse-Grained methods are specific MD implementations in which groups of atoms are considered as beads for the MD simulation. For example, we could consider water as the group of 2 H and 1 O, or as the H_2O molecule. This leads to feasible simulations of more complex systems.
- In this case, one also must configure the topology of the system and the force fields (which are different to those of atomistic MD simulations) to account for the interactions in the simulations.
- Gromacs and LAMMPS have modules for CG implementations.
- Examples of CG implementations are given below.





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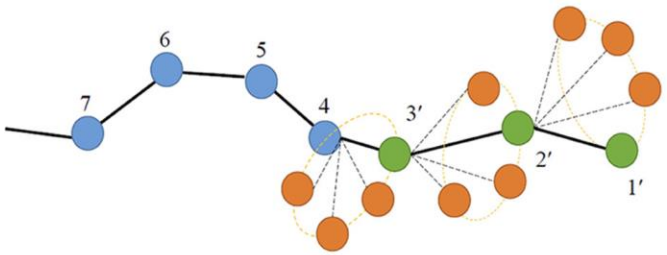
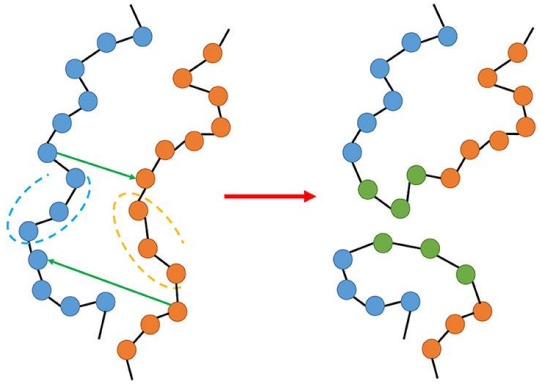
Monte Carlo (MC) methods

- Monte Carlo methods are computational algorithms based on repeated random sampling (in accordance with a certain distribution) to obtain numerical results. The main idea is to use randomness to solve problems that may be deterministic.
- There are several applications of Monte Carlo to the field of materials modelling (MC, kMC), and the basis of the method is the stochastic movement of particles (molecules, atoms, beads), transferring the system randomly over the phase-space and approximating the mean values of various properties.
- There are studies on deposition processes performed with MC and kMC (N. Cheimarios et al., Front. Phys., 2021).
- An example of a software for MC modelling would be Cassandra.





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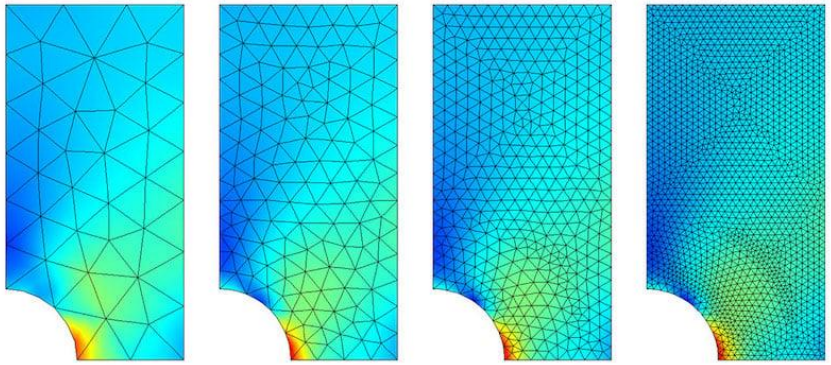
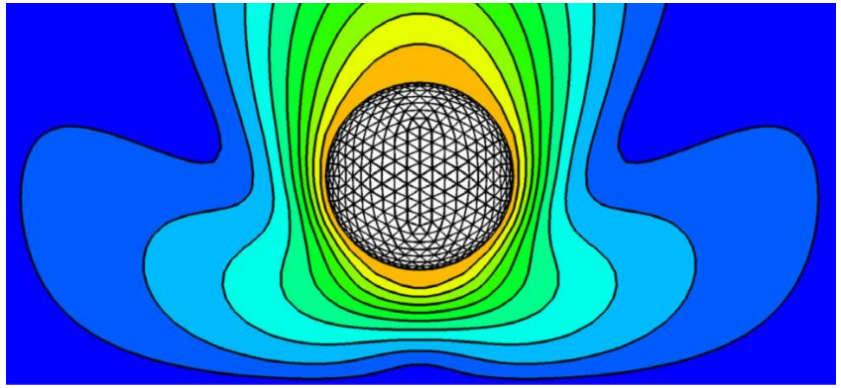
Continuum models

- Finite Element Method (FEM) and Computational Fluid Dynamics (CFD).
- In FEM, we solve PDEs in two or three space variables. In order to do that, we divide the domain in a set of "finite elements" (space discretisation). The FEM formulation of a boundary value problem finally results in the approximation of the solution over the established domain. Then, calculus of variations is applied in order to minimise the associated error function. ANSYS and COMSOL Multiphysics can be used to model FEM problems. In our study, it could be used to predict where lack of adhesion is more likely.
- CFD is used to simulate fluid flows and heat transference. It is based on the Navier-Stokes equations, and also takes into consideration boundary conditions. OpenFOAM and FLUENT can be used to perform CFD modelling.





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THANK YOU!

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