Multi-scale approaches in Material Science

III-ème école d'été "Modélisation des Matériaux" - Banyuls-sur-Mer 19-23 Août 2024

Michel Perez

Université de Lyon - INSA Lyon - MATEIS - UMR CNRS 5512

Merci!

Modeling

Modeling... what for?

Aim of this “lecture”

What it is and what it is not

✓ A warm up for this summer school

Aim of this “lecture”

What it is and what it is not

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- × A complete panorama on modelling scales

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- ✓ (Naive?) Examples to illustrate the multi-scale approach

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- × A review of state-of-the-art techniques

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What it is and what it is not

- ✓ A warm up for this summer school
- × A complete panorama on modelling scales
- ✓ (Naive?) Examples to illustrate the multi-scale approach
- × A review of state-of-the-art techniques
- ✓ A climbing up of the modelling scales (to the top?)

Aim of this “lecture”

What it is and what it is not

- ✓ A warm up for this summer school
- × A complete panorama on modelling scales
- ✓ (Naive?) Examples to illustrate the multi-scale approach
- × A review of state-of-the-art techniques
- ✓ A climbing up of the modelling scales (to the top?)
- × An ad-free presentation

Who am I?

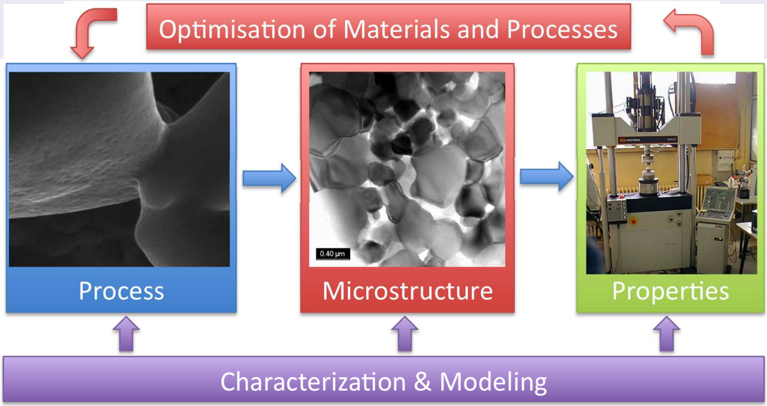
Michel Perez: CV in 5 lignes

Michel.Perez@insa-lyon.fr

- INSA: 1996
- PhD at INP Grenoble on levitation
- Assistant professor (2001)
- Teaching Physics, Thermodynamics and Material Science
- Research in material science: multi-scale modelling
  http://michel.perez.net.free.fr/

INSA Lyon: MATEIS
MATerials Engineering and Sciences

Strategy of the group

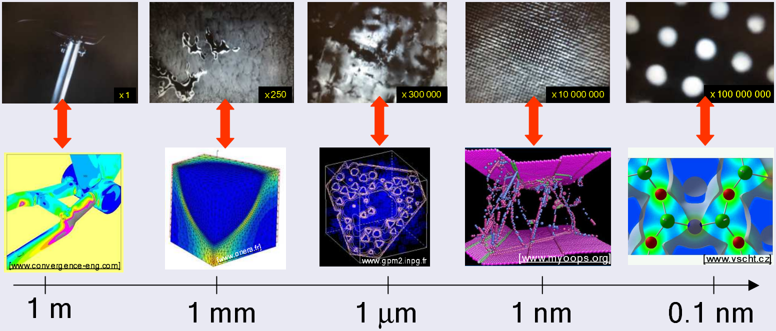


Multi-scale approach

A video to warm up

Multi-scale approach

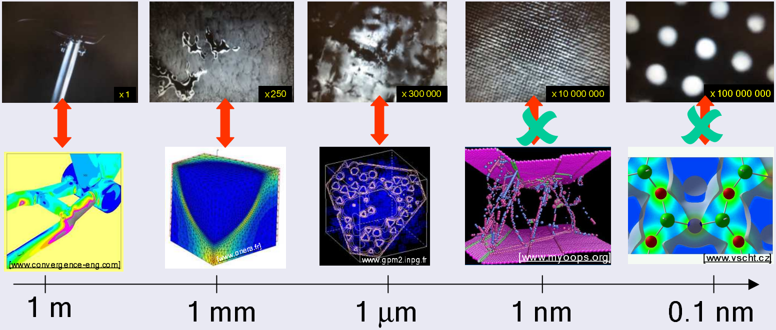
Different scales in material science



- Classical scheme: experiment ↔ modelling

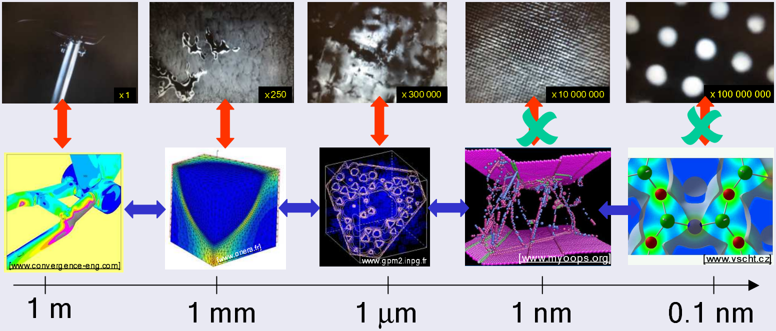
Multi-scale approach

Different scales in material science



- Not always possible!

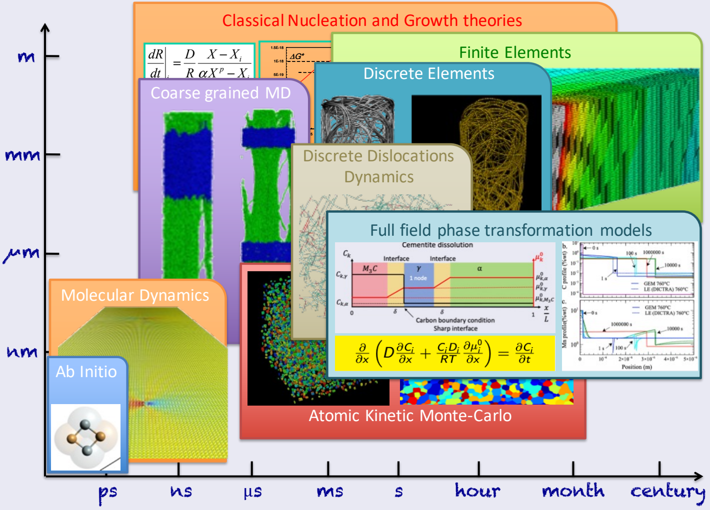
Different scales in material science



- Aim connect modelling at different scales

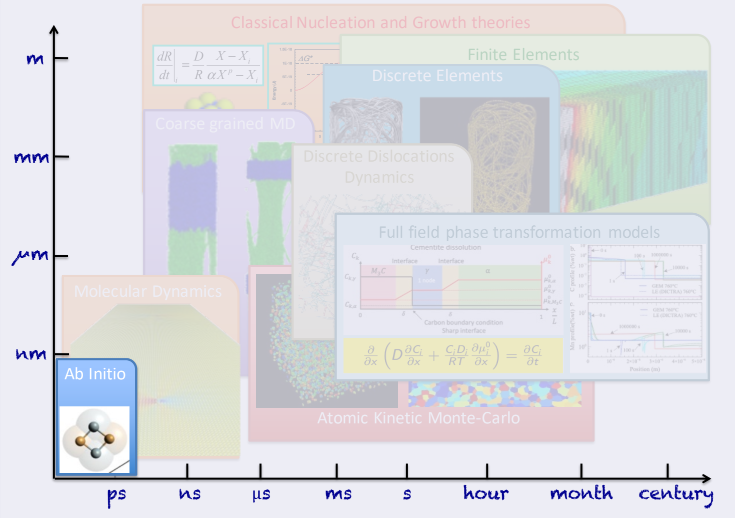
Multi-scale approach

Different scales in material science



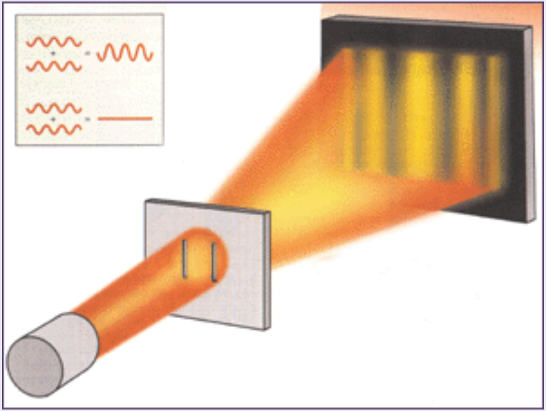
Multi-scale approach

Different scales in material science



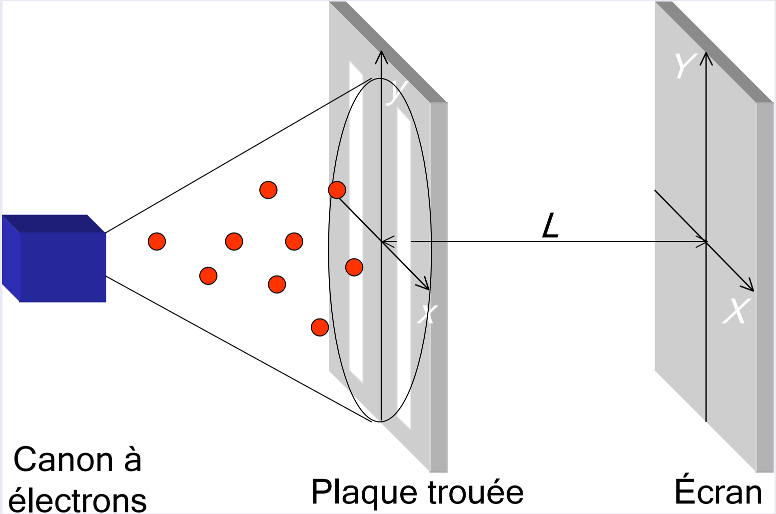
A journey into the quantum world

Back to a very simple experiment: Young's double slit (1801)



- Light = waves
- What about matter?

More complex: with electrons (1961)



More complex: with electrons (1961)

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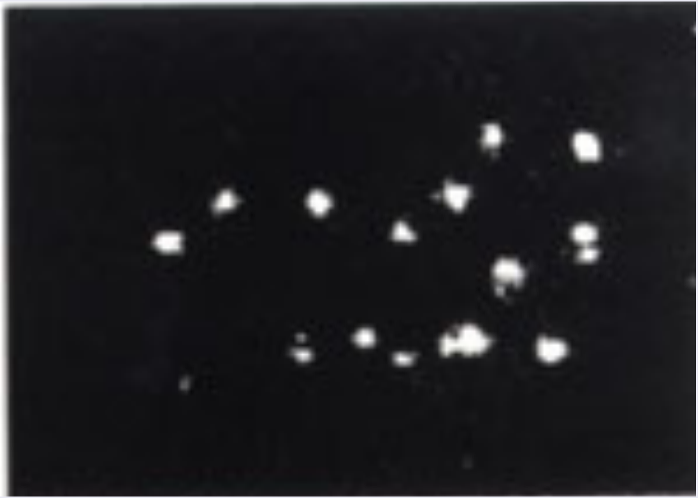

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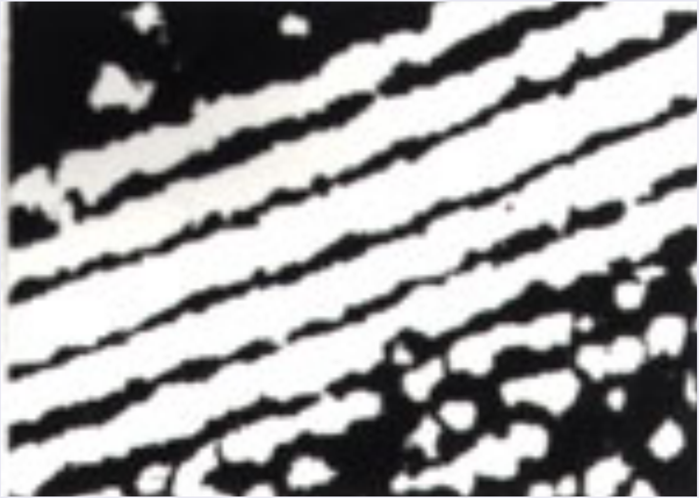
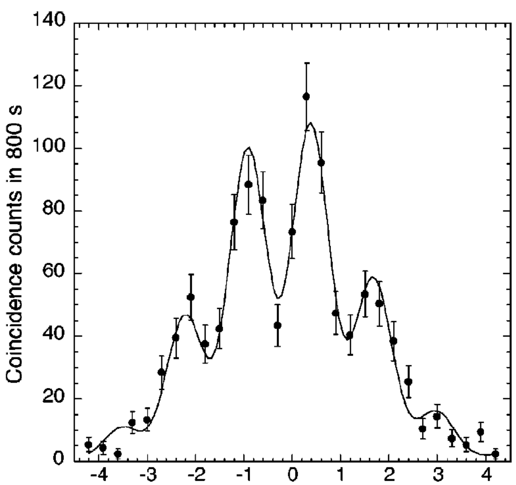
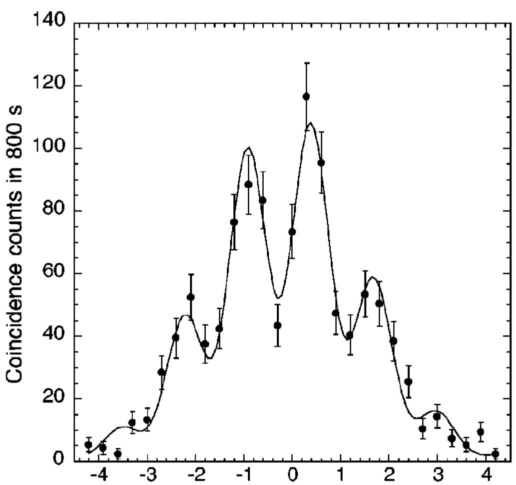


More complex: with electrons (1961)



Double-slit quantum eraser, S. P. Walborn, M. O. Terra Cunha, S. Padua,1 and C. H. Monken, *PHYS. REV. A* **65**(2002)

Even more complex: with a detector (2002)



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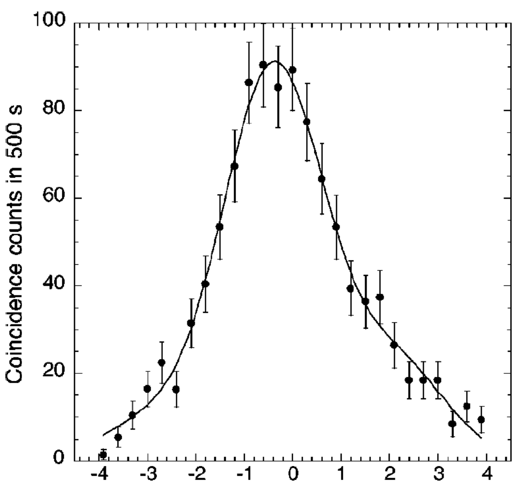
A journey into the quantum world

Even more complex: with a detector (2002)



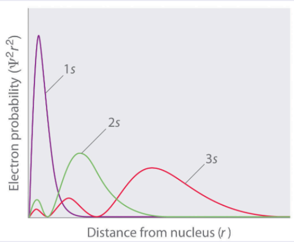
Double-slit quantum eraser, S. P. Walborn, M. O. Terra Cunha, S. Padua,1 and C. H. Monken, *PHYS. REV. A* **65**(2002)

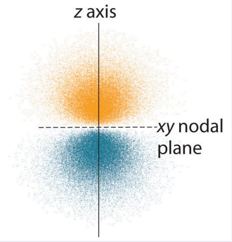
Hydrogen atom

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{r}) + V(|\mathbf{r}|)\psi(\mathbf{r}) = E\psi(\mathbf{r})$$

- $V(|\mathbf{r}|) = e^2/|\mathbf{r}|$
- Laplacian in spherical coordinates (r, θ, ϕ)
- $\psi(\mathbf{r}) = R(r)P(\theta)u(\phi)$

$\Rightarrow$ 3 set of eq. and 3 quantum numbers: n, l, m





A journey into the quantum world

General case

$$\left[-\frac{\hbar^2}{2m}\sum_i \nabla^2 + \sum_i V(\mathbf{r}_i) + \sum_i \sum_j U(\mathbf{r}_i, \mathbf{r}_j)\right]\psi(\mathbf{r}) = E\psi(\mathbf{r})$$

$\Rightarrow$ hopeless !

DFT: a path towards simplification

- Find a simpler problem with same solution !
- $E_{\mathrm{exact}}(\mathbf{R}_i, \mathbf{r}_n) \rightarrow E_{\mathrm{approx}}(\mathbf{R}_i, \rho(\mathbf{r}))$

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r}) + \int \frac{e^2\rho(\mathbf{r}')d\mathbf{r}'}{|\mathbf{r}-\mathbf{r}'|} + V_{\mathrm{XC}}(\mathbf{r})\right]\psi_i(\mathbf{r}) = \epsilon_i\psi_i(\mathbf{r})$$

Local Density Approximation (exchange correlation energy)

- $V_{XC}(\mathbf{r}) = V_{XC}^{\mathrm{electron\ gas}}(\rho(\mathbf{r}))$

DFT: practical Implementation

1 Guess initial value of $\rho(\mathbf{r})$

$\Downarrow$

2 $\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r}) + \int \frac{e^2\rho(\mathbf{r}')d\mathbf{r}'}{|\mathbf{r}-\mathbf{r}'|} + V_{\mathrm{XC}}(\mathbf{r})\right]\psi_i(\mathbf{r}) = \epsilon_i\psi_i(\mathbf{r})$

$\Downarrow$

3 $\psi_i(\mathbf{r})$

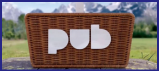
$\Downarrow$

4 $\rho(\mathbf{r}) = \sum_i |\psi_i(\mathbf{r})|^2$

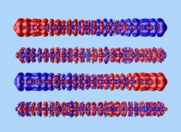
$\Downarrow$

5 loop to 1 until convergence

A journey into the quantum world



Andrés Saúl
Département Théorie et Simulation Numérique
CINaM/CNRS (Marseille, FRANCE)



It will be a slow discussion about
concepts that one must understand and methods that one must manage
when one is interested on the electronic properties of
systems composed of atomic nuclei and electrons (molecules, solids, crystals, ...)

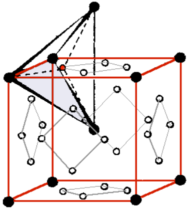
- Entrée
  - The hydrogen atom to remember atomic orbitals
  - Multi-electron atoms to discuss the formation of shells and screening
  - A systems with two atoms and two electrons to discuss bonding
- Plat
  - Many atoms and many electrons
    - Methods and approximations neglecting the electron-electron interactions
    - Methods and approximations tacking into account the electron-electron interactions
- Dessert
  - La *"surprise du chef "*

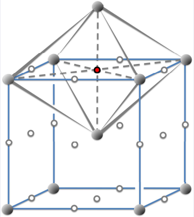
Structure électronique des matériaux
- Lundi 19 Août 11h-13h
- Mardi 20 Août: 08h00-10h00

Application

Find interatomic potential

- Goal: Fe-C interaction potential for Molecular Dynamics
- Two reference configurations: C in octa and tetra sites





- Correct energy barrier for diffusion: 0.815 eV

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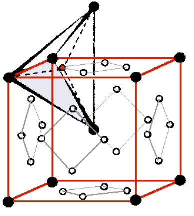
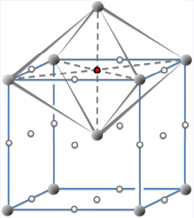
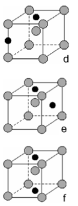
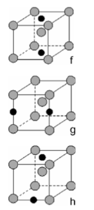






- Correct energy barrier for diffusion: 0.815 eV
- Test on many configurations (C, Fe, Va)

Tabulated potential for Molecular Dynamics

[Becquart el al, Comp. Mat. Sc. **40** (2007)]

Atomic Kinetic Monte-Carlo

Petr Grigorev, Arnaud Allera et Martin Uhrin
MATEIS, IRSN et INP-UGA

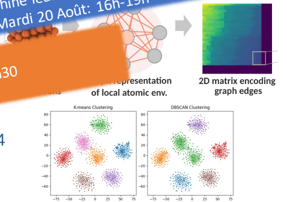
- 1.1 Python ecosystem
- 2.1 Neighbors maps
- 2.2 Structural analysis (ML)

Ecosystème python
➢ Lundi 19 Août: 16h-19h

Machine learning
➢ Mardi 20 Août: 16h-19h

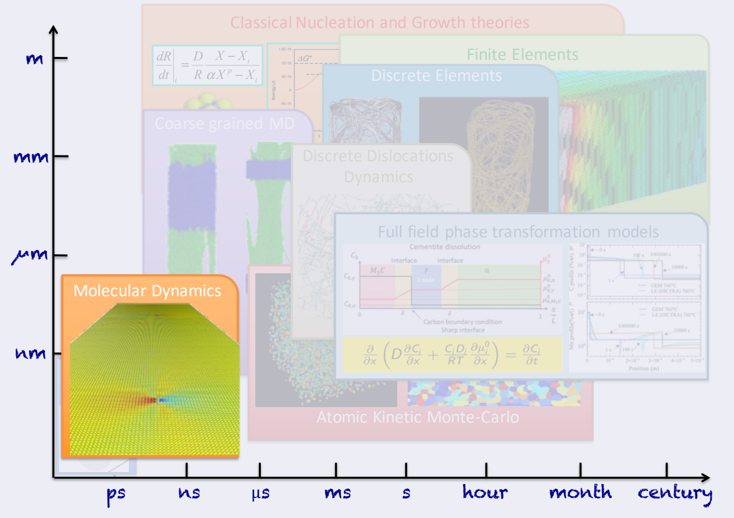
Machine Learning
➢ Mardi 20 Août: 10h30-12h30
➢ Jeudi 22 Août: 8h-10h

tinyurl.com/ModMat2024



Multi-scale approach

Different scales in material science



Molecular dynamics / Molecular statics

Principle

- Second Newton's law

$$m_i \frac{d\mathbf{v_i}}{dt} = \mathbf{f_i}$$

- Pair interactions: $\mathbf{f_i} = \sum_j \mathbf{f_{ij}} = \sum_j \mathbf{grad}\, U_{ij}$
- Integration in various "ensembles": NVE, NVT, NPT...

EAM potential (embedded atom method)

- Pair interaction energies AND electronic density

$$E_{tot} = \frac{1}{2} \sum_i \sum_{j \neq i} U_{ij}(\mathbf{r}_{ij}) + \sum_i F_i \left(\sum_{j \neq i} \rho(\mathbf{r}_{ij}) \right)$$

Integration of Newton's equations: Euler vs Verlet

Euler (order 1)

$$\mathbf{x}(t+\Delta t) =$$
$$\mathbf{v}(t+\Delta t) =$$

Verlet (order 2)

$$\mathbf{x}(t+\Delta t) =$$
$$\mathbf{x}(t-\Delta t) =$$

$$\mathbf{x}(t+\Delta t) =$$

Modified Euler (order ?)

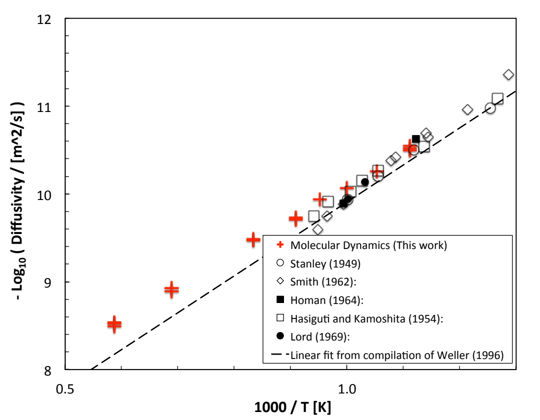
$$\mathbf{x}(t+\Delta t) =$$
$$\mathbf{v}(t+\Delta t) =$$

$$\mathbf{x}(t+\Delta t) =$$

Molecular dynamics

Results: let the carbon move!

Diffusivity (from Einstein's relation): $6DT = \langle |r(t) - r(0)|^2 \rangle$



Molecular dynamics

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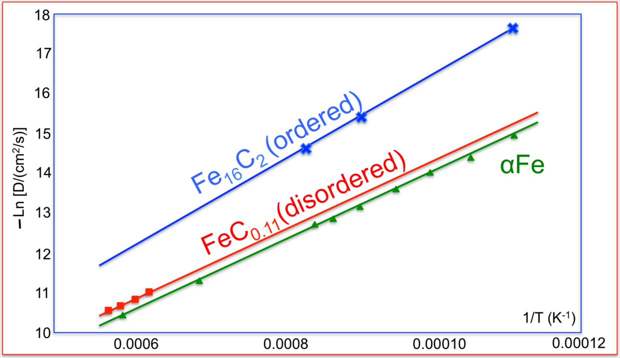
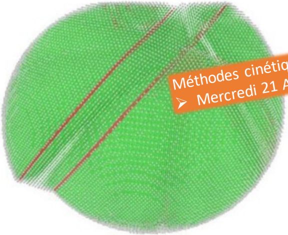


Diffusivity of C in various phases

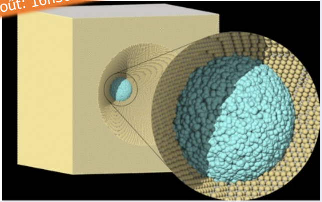
Atomic Kinetic Monte-Carlo

Laurent Pizzafalli
Institut P' (Poitier)

INSTITUT P' UPR CNRS 3346
Université de Poitiers cnrs ISAE ENSMA

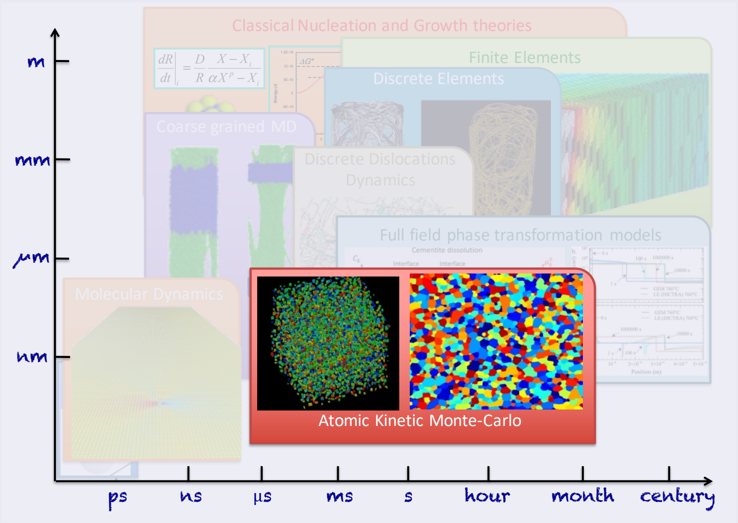


Méthodes cinétiques: dynamique moléculaire
➤ Mercredi 21 Août: 16h30-18h30



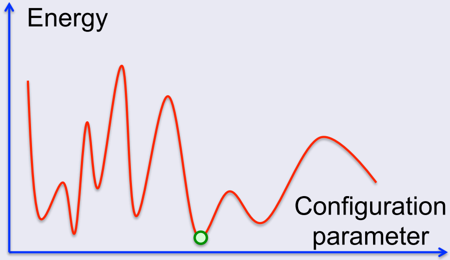
Multi-scale approach

Different scales in material science



Monte-Carlo Metropolis

What is the most stable phase?



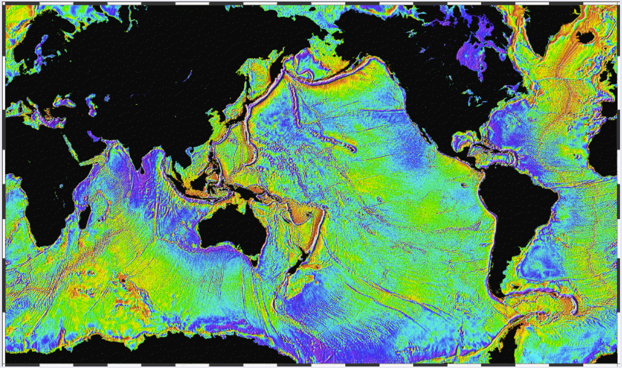
- Energy:

$$E(x, y, z, v_x, v_y, v_z)$$

- Values of x, y, z, v_x, v_y and v_z that minimize E?

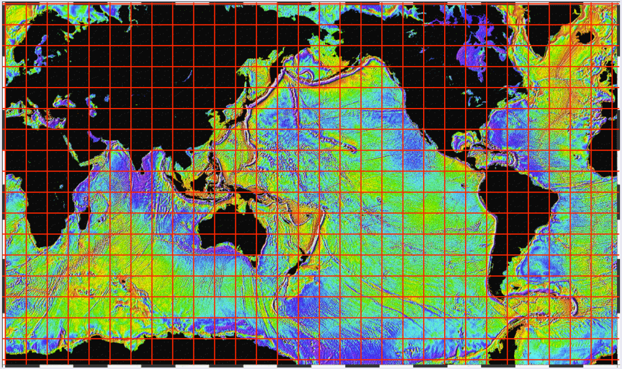
Monte-Carlo Metropolis

Example: what is the deepest point in the ocean?



Monte-Carlo Metropolis

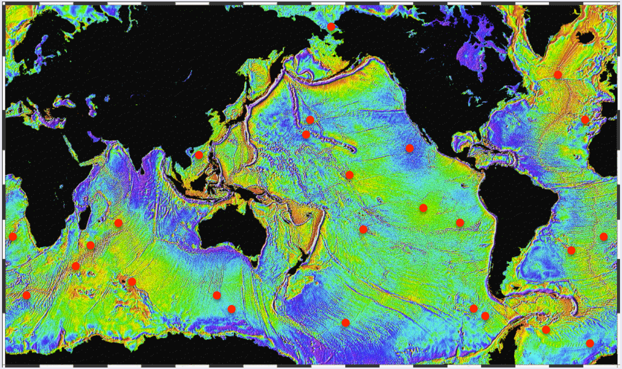
Example: what is the deepest point in the ocean?



- ☺ Sure we will find it!
- ☹ At what cost?

Monte-Carlo Metropolis

Example: what is the deepest point in the ocean?

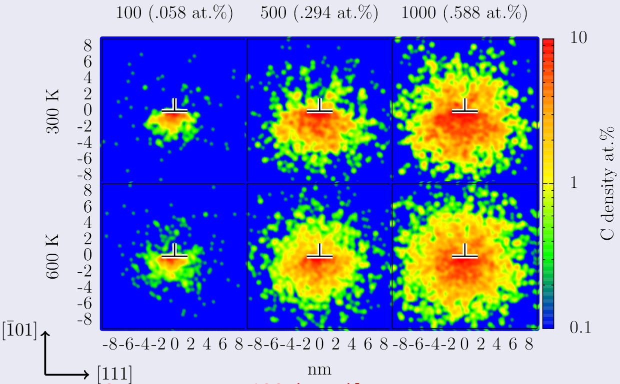


- ☺ Low probability
- ☹ Cost is controlled

$$P_{i \to j} = \min(1, \exp\left[-\Delta E_{ij}/kT\right])$$

Monte-Carlo Metropolis

Application: build up of a Cottrell atmosphere

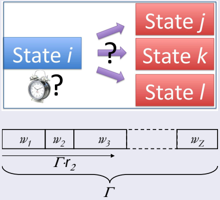


[Waseda et al, Scripta Mater. **129** (2016)]

- ≈150 C atoms per nm (same as measured with TAP)
- Max. C concentration: 8.8% (TAP: 8%)

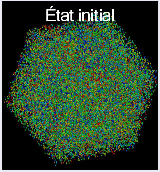
Atomic Kinetic Monte-Carlo

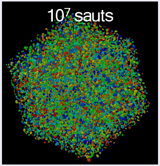
Principle

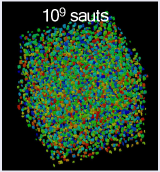


- Transition frequency from $i \rightarrow j$:
  $w_j^i = w_0 \exp\left(\frac{-\Delta E_{ij}}{kT}\right) \quad w_0 \approx 10^{14}$ Hz
- Residence time i
   $r_1 \rightarrow \tau_R = -\frac{\ln r_1}{\sum_j w_j}$
- Choice of a particular transition  r_2

Example: precipitation from a supersaturated solid solution

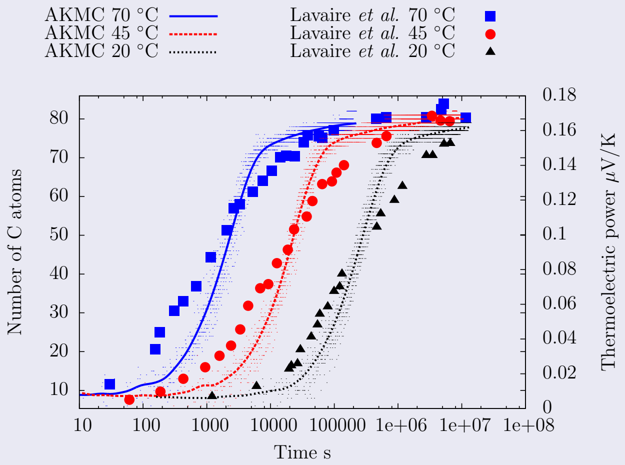






Atomic Kinetic Monte-Carlo

Formation kinetics: AKMC vs ThermoElectric Power

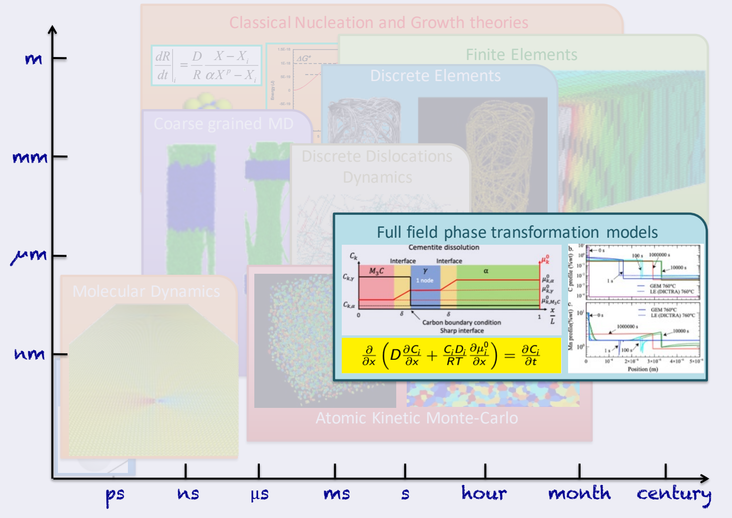


- Same kinetics **without any adjustable parameter**

Atomic Kinetic Monte-Carlo

Multi-scale approach

Different scales in material science

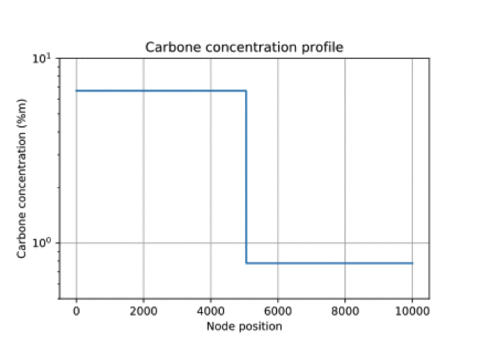


Full Field models ($\alpha \leftrightarrow \gamma$ transformation)

First ingredient: diffusion of solute elements (Fick's law)

- Classical diffusion model (implicit resolution scheme):

$$\frac{\partial C_i}{\partial t} = D_i \frac{\partial^2 C_i}{\partial x^2} \Rightarrow \frac{C_i^{t+\Delta t} - C_i^t}{\Delta t} = D_i \frac{C_{i+1}^{t+\Delta t} - 2C_{i+1}^{t+\Delta t} + C_{i-1}^{t+\Delta t}}{\Delta x^2}$$



Full Field models ($\alpha \leftrightarrow \gamma$ transformation)

Second ingredient: an interface

- Interface = chemical potential variation

$$\frac{\partial C_i}{\partial t} = \frac{\partial}{\partial x}\left(D \frac{\partial C_i}{\partial x}\right)$$

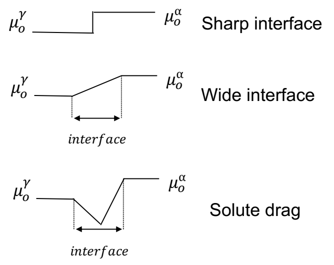
$$\Downarrow$$

$$\frac{\partial C_i}{\partial t} = \frac{\partial}{\partial x}\left(\frac{D_i C_i}{RT}\frac{\partial \mu_i}{\partial x}\right)$$

$$\mu_i = \mu_{0,i} + RT\ln(C_i)$$

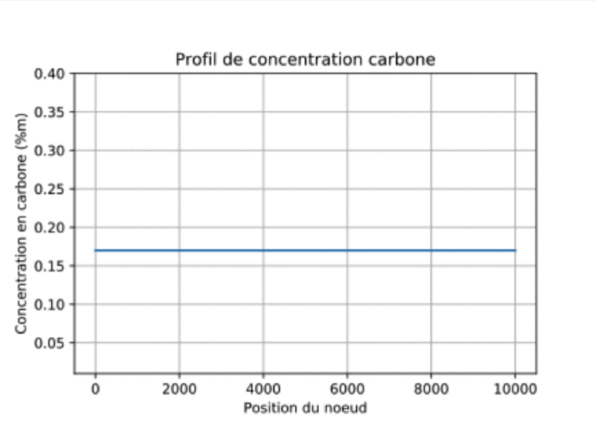
$$\Downarrow$$

$$\frac{\partial}{\partial x}\left(D\frac{\partial C_i}{\partial x} + \frac{C_i D_i}{RT}\frac{\partial \mu_i^0}{\partial x}\right) = \frac{\partial C_i}{\partial t}$$



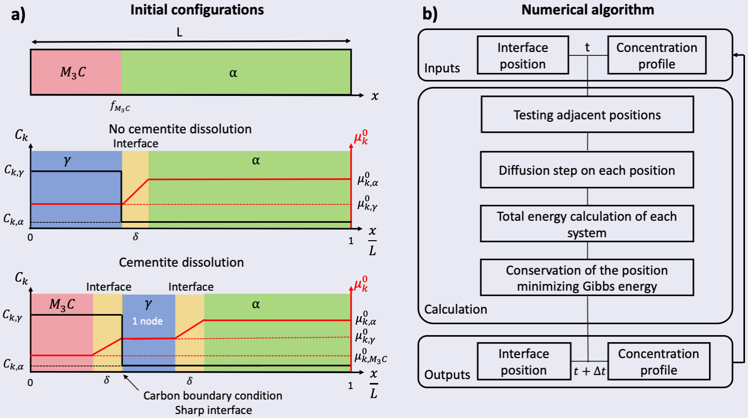
Second ingredient: an interface !

- Starting point: constant concentration



Full Field models ($\alpha \leftrightarrow \gamma$ transformation)

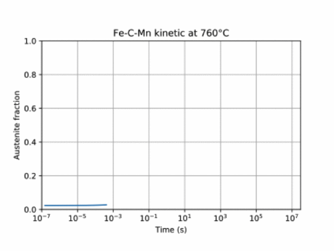
Third ingredient: moving the interface(s) !

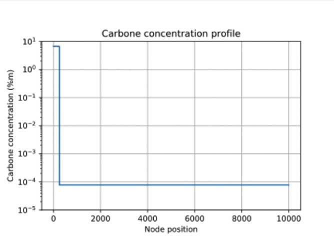


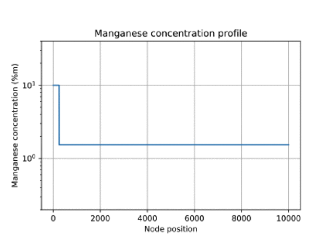
- Choice of position that minimises the Gibbs energy
- Check that interface does not move too fast

Full Field models ($\alpha \leftrightarrow \gamma$ transformation)

Results: austenite formation at 760°C (FeCMn steel)

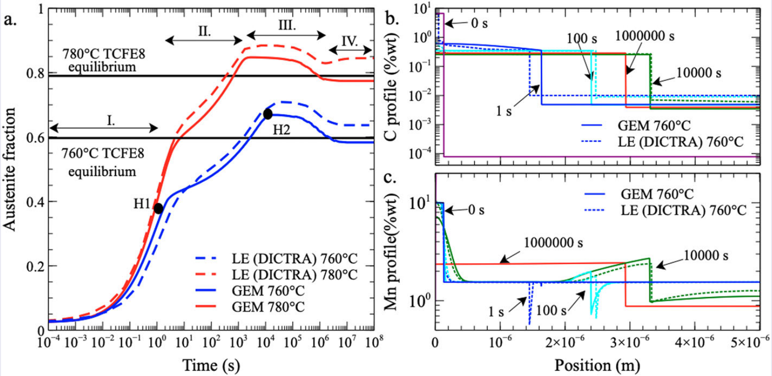






Full Field models ($\alpha \leftrightarrow \gamma$ transformation)

Austenitic transformation kinetics (DICTRA vs GEM)



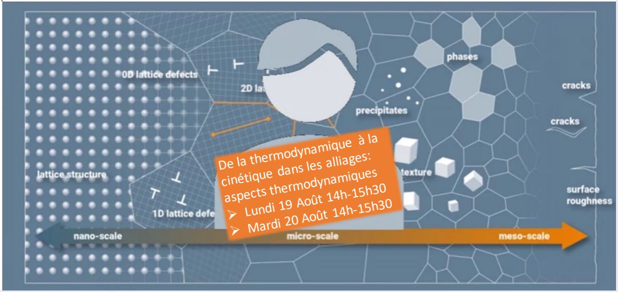
[A. Mathevons et al, Phil. Mag. Lett. **101** (2021)]

- Complex transformation kinetics due to 3 different diffusion coefficients

Full Field models

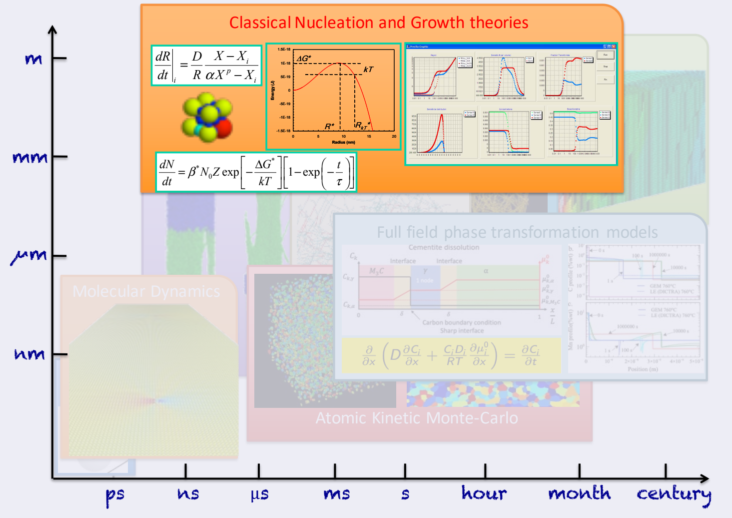
Mohamed Gouné
Institut de Chimie de la matière Condensée de Bourdeau

icmcb
institut de chimie de la matière condensée de bordeaux

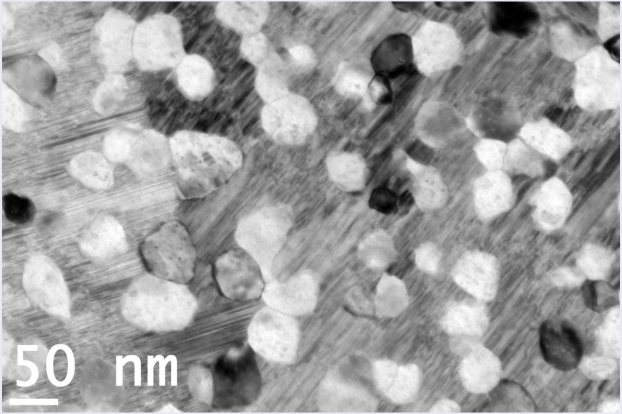


Multi-scale approach

Classical Nucleation and Growth Theories



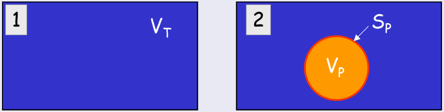
Mean field precipitation modelling

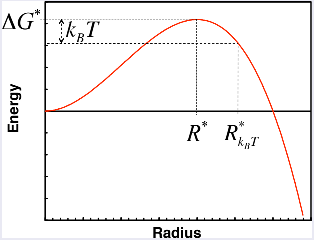


- What are these two phases?

Classical nucleation and growth theories

Nucleation rate





$$\Delta G = G_2 - G_1 = \frac{4}{3}\pi R^3 \Delta g + 4\pi R^2 \gamma$$

- Δg: driving force for nucleation (thermo. and/or Monte-Carlo)
- γ: interfacial energy

$$\frac{dN}{dt} = N_0 Z \beta^* \exp\left(-\frac{\Delta G^*}{kT}\right) \exp\left(-\frac{\tau}{t}\right)$$

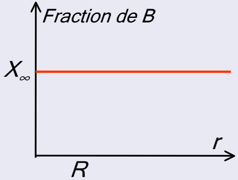
Classical nucleation and growth theories

Growth law: Linear out-of-equilibrium thermodynamics

Fick's law:

$$J = -D\frac{\partial C}{\partial r}$$

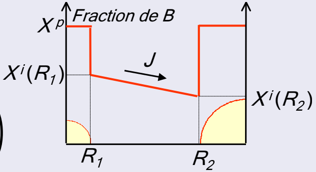
$$\frac{dR}{dt} = \frac{D}{R}\frac{X - X^i(R)}{X^p - X^i(R)}$$



Effet of precipitate size (Gibbs-Thomson)

- Precipitate composition $A_x B_y$

$$X^i(R) = X^i(\infty)\exp\left(\frac{(x+y)R_0}{yR}\right)$$



[M. Perez, Scripta Mat. **52** (2005)]

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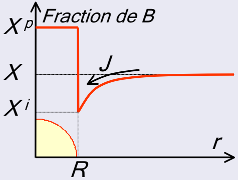

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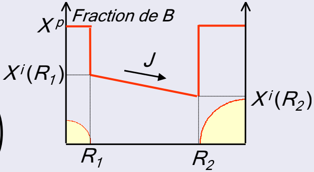

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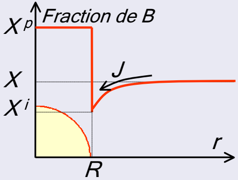

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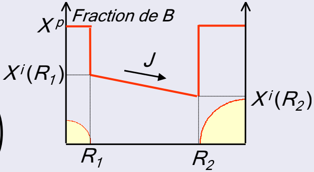

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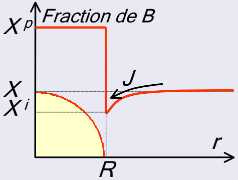

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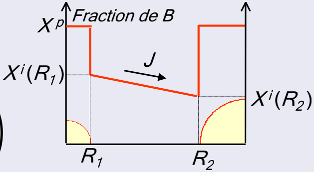

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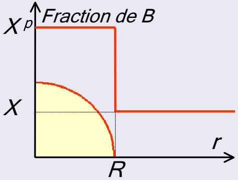

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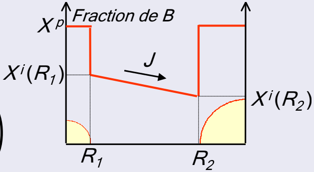

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Multi-scale approaches

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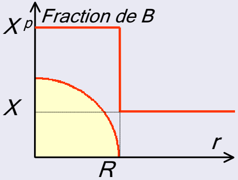

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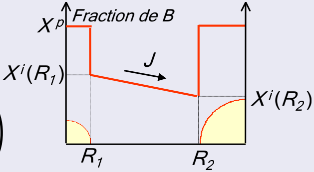

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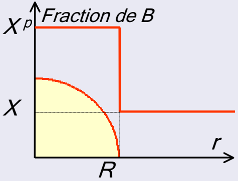

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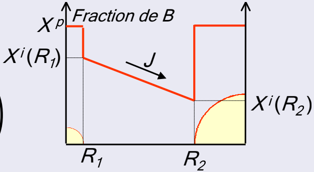

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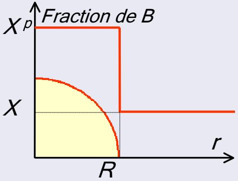

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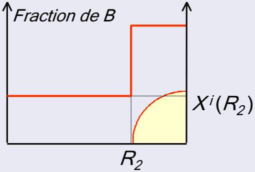
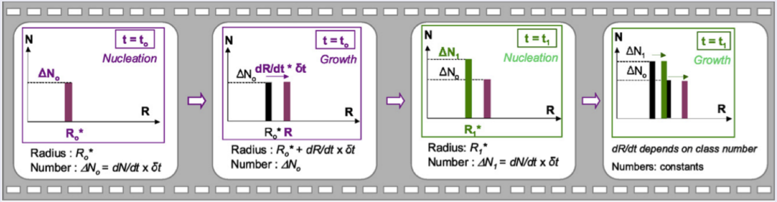


Classical nucleation and growth theories

Implementation in a home made precipitation software: PreciSo



Whole precipitate size distribution evolution

for non-isothermal treatments

[M. Perez et al, Acta Mater. **56** (2008)]

Classical nucleation and growth theories

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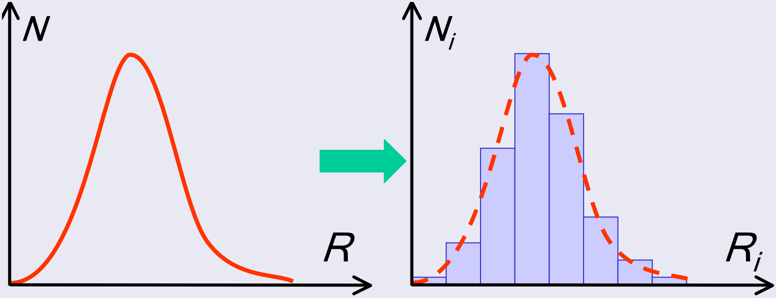
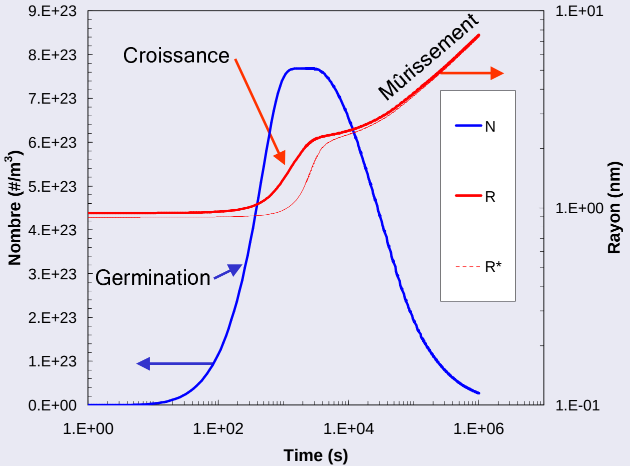


Whole precipitate size distribution evolution for non-isothermal treatments

[M. Perez et al, Acta Mater. **56** (2008)]

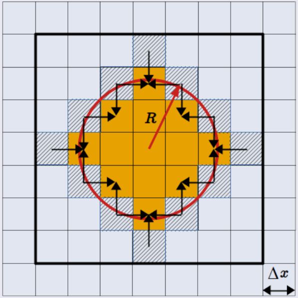
Classical nucleation and growth theories

Example of precipitation kinetics



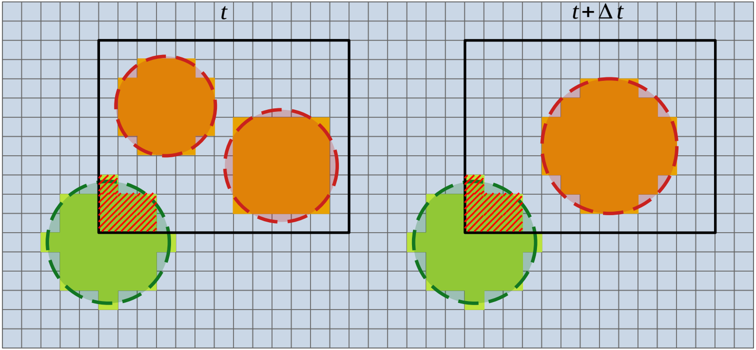
CNGTs vs Full Field

Sharp Interface Full field mModel (ShIFuMo)

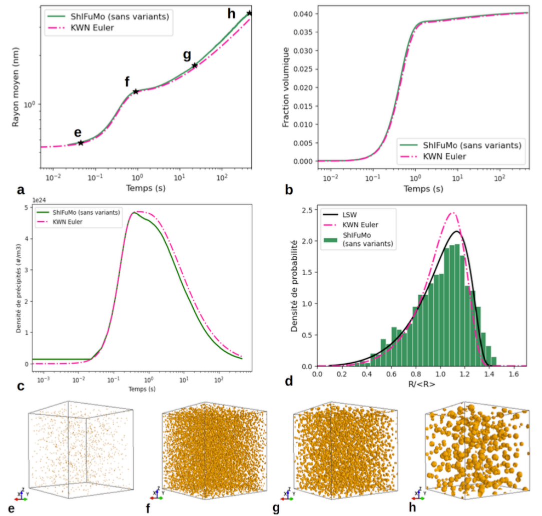


- Nucleation: Classical Nucleation Theory
- Growth: Classical Growth Theory (Zener)
- But: 3D diffusion: Full Field

Coagulation

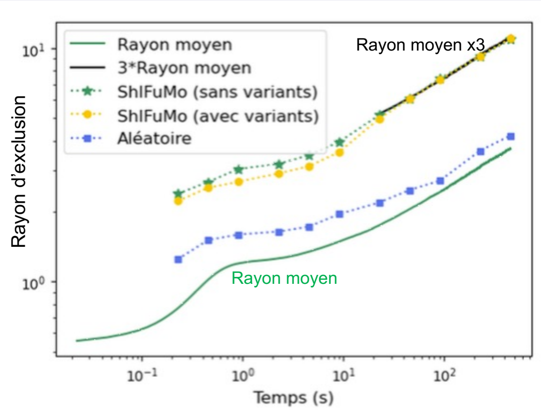


Comparison


ShIFuMo (sans variants)
KWN Euler
Rayon moyen (nm)
Temps (s)
Fraction volumique
Densité de précipités (#/m3)
1e24
LSW
ShIFuMo
(sans variants)
Densité de probabilité
R/<R>
a
b
c
d
e
f
g
h

CNGTs vs Full Field

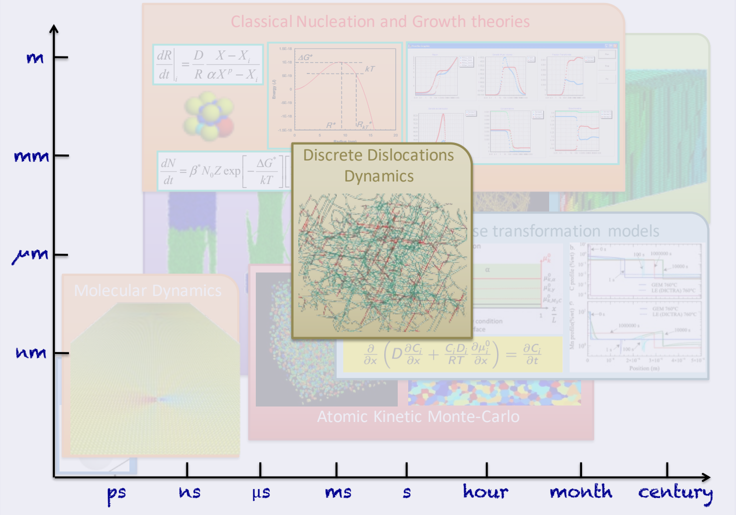
Coagulation



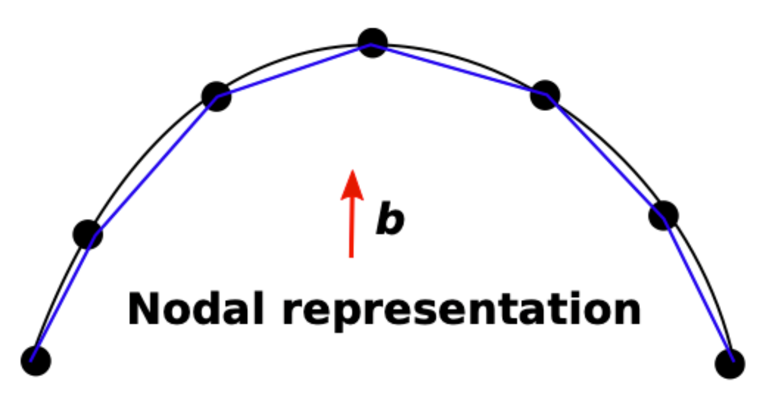
- Improve CNGTs from Sharp Interface Full Field model !

Multi-scale approach

Discrete Dislocations Dynamics



Presentation



- Dislocation: discretised into segments (mixed dislocation)

Discrete Dislocations Dynamics

Effective net force per unit lengh

$$\mathbf{F}_{\text{eff}} = \underbrace{\sigma b \times \xi}_{\text{Peach-Koehler}} + \underbrace{F_{\text{lt}}}_{\text{Line tension}} - \underbrace{\frac{\mathbf{v}}{|\mathbf{v}|} F_{\text{peierls}}}_{\text{Peierls friction}}$$

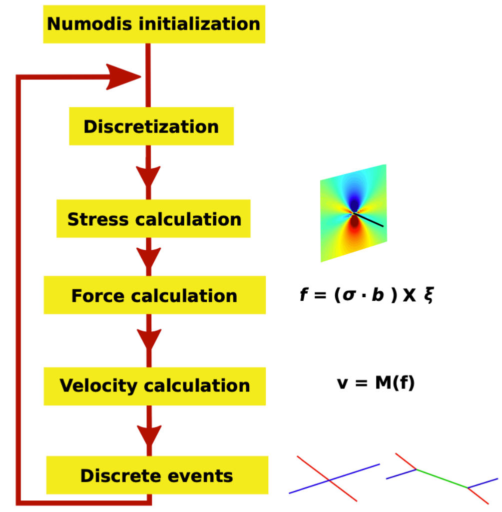
Dynamics

$$\mathbf{v} = \frac{\mathbf{F}_{\text{eff}}}{B}$$

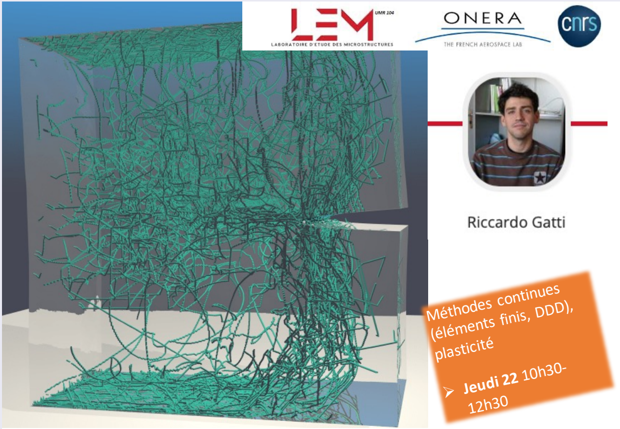
Stress and strain update

$$\sigma = \sum_{\text{nodes}} \delta\sigma_i \text{ and } \epsilon = \sum_{\text{nodes}} \delta\epsilon_i$$

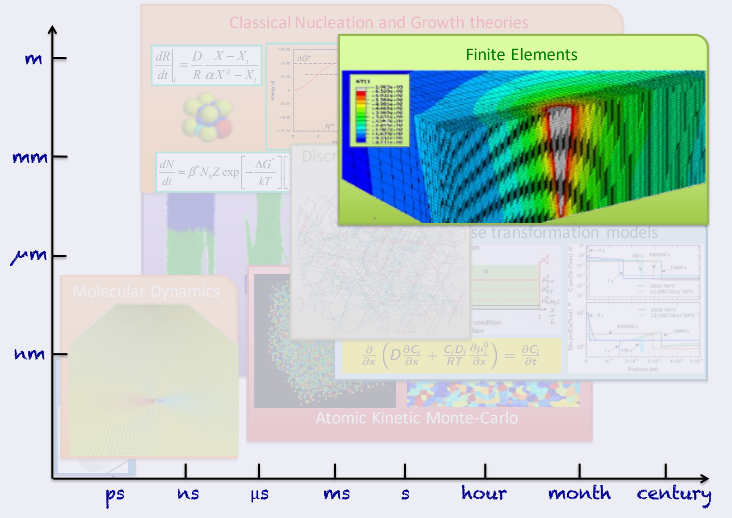
Exemple of Numodis (CEA) algorithm



Discrete Dislocations Dynamics



Different scales in material science



Finite Elements Method

Newton's second law

$$\rho \frac{\partial^2 u}{\partial t^2} - \nabla \sigma = \mathbf{f}$$

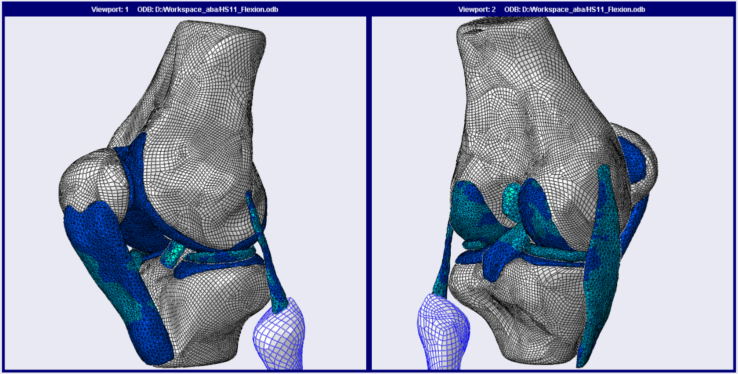
Constitutive law (e.g. thermo-elastic)

$$\sigma^{ij} = C^{ijkl} \epsilon^{kl} - \beta^{ij} (T - T_0)$$

Linearized strain

$$\epsilon = \frac{1}{2} \left(\nabla u + \nabla u^T \right)$$

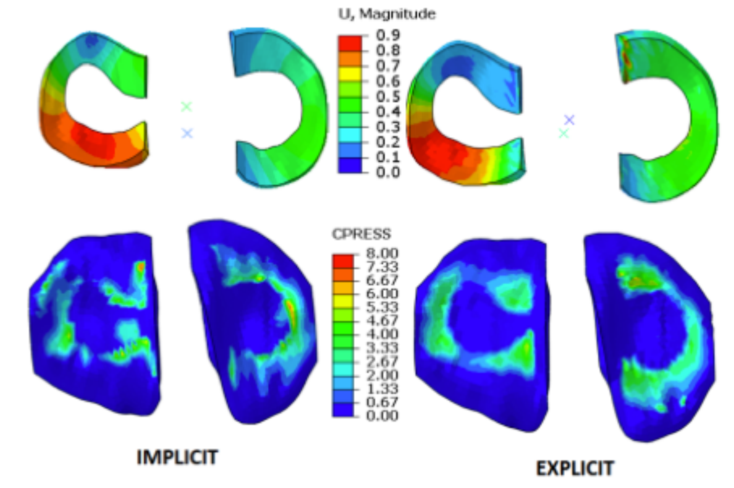
Mesh of a meniscus



[From https://ris.utwente.nl/ws/files/6153316/CMBBE2014-Hamid-Submitted.pdf]

Finite Elements Method

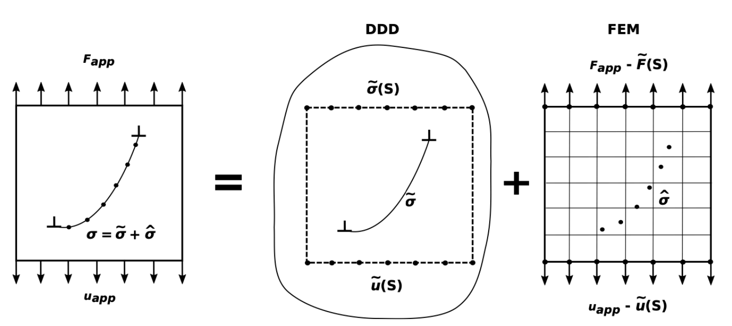
Displacements and pressure on the meniscus



[From https://ris.utwente.nl/ws/files/6153316/CMBBE2014-Hamid-Submitted.pdf]

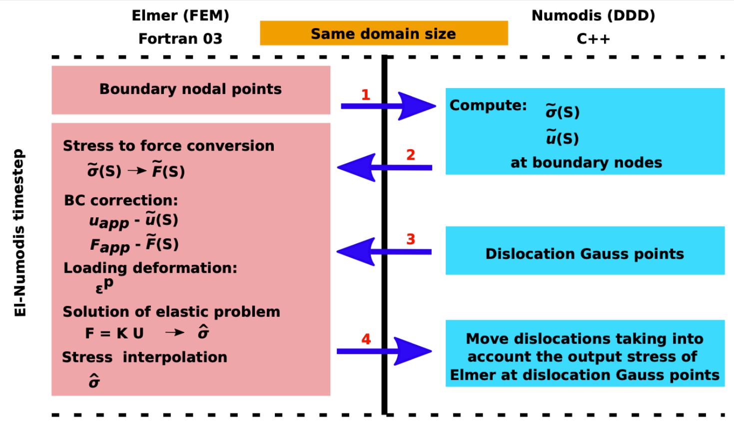
Finite Elements Method and DDD coupling

Two complementary methods

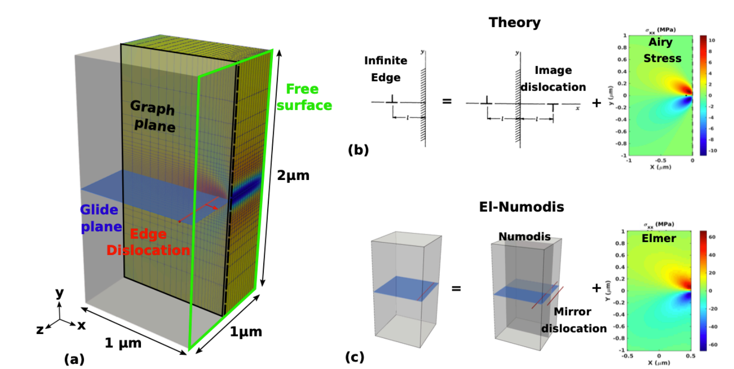


Finite Elements Method and DDD coupling

Principle

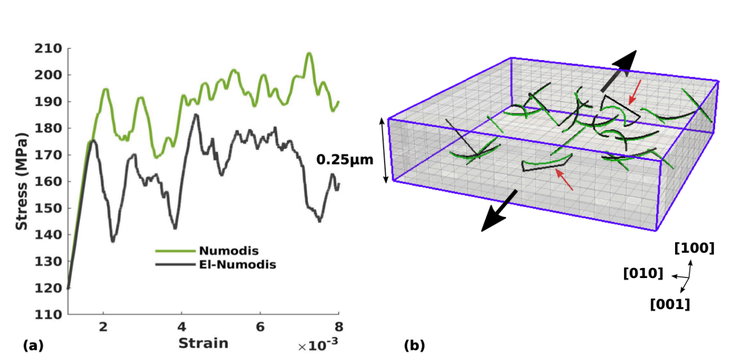


Validation


Graph plane
Free surface
2µm
Glide plane
Edge Dislocation
1 µm
1µm
(a)
Theory
Infinite Edge
Image dislocation
Airy Stress
(b)
El-Numodis
Numodis
Mirror dislocation
Elmer
(c)

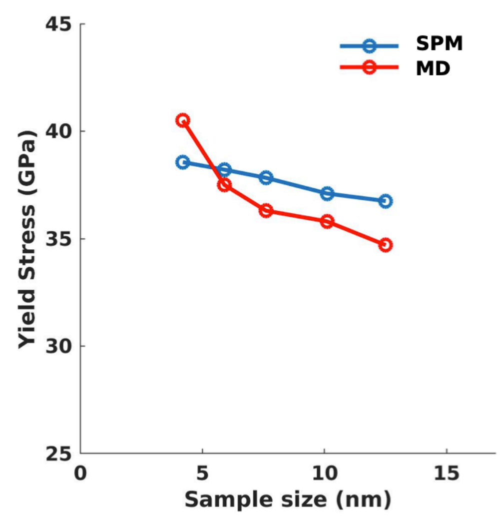
Finite Elements Method and DDD coupling

Results



The icing on the cake...

Comparison with MD



Last break !

Lucia Sargentini
Univ. Paris Saclay CEA

Statistical m… tainty
quan… erials

Lucia SA…

Universit…
Service d… …t de Mécanique des Fluides
91191, Gif…

Méthodes statistiques pour la quantification/propagation d'incertitudes dans les matériaux

➤ Vendredi 22 Août: 8h-10h

1. Calibration under uncertainty

The importance of the experimental data
The importance of the physics
The importance of the statistical model

2. Uncertainty of assessed model

The importance of sensitivity analysis
The importance of the statistical model for the quantification of uncertainty

Conclusions

Conclusions

Make your own conclusion

Thank you!

The METAL team

{Team building 2023}