Multiscale Aspects of Materials Modelling:

A Mathematician's View

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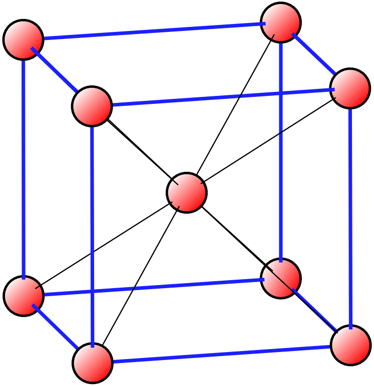
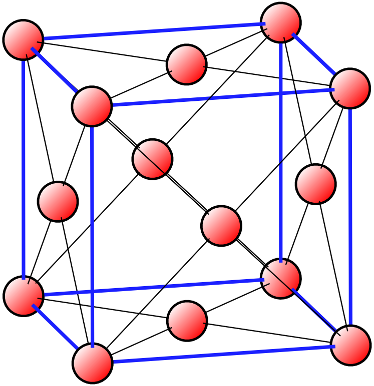
IPAM Tutorials

March 2023

A motivating multiscale system: Crystals



Body-Centred Cubic (BCC)



Face-Centred Cubic (FCC)

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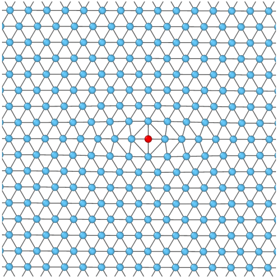
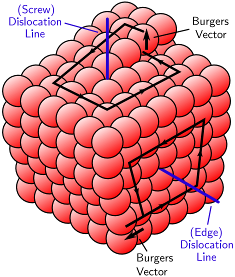
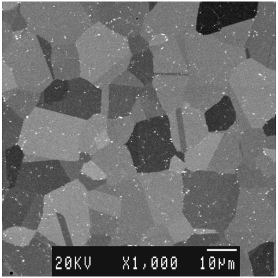


0D: Point Defects

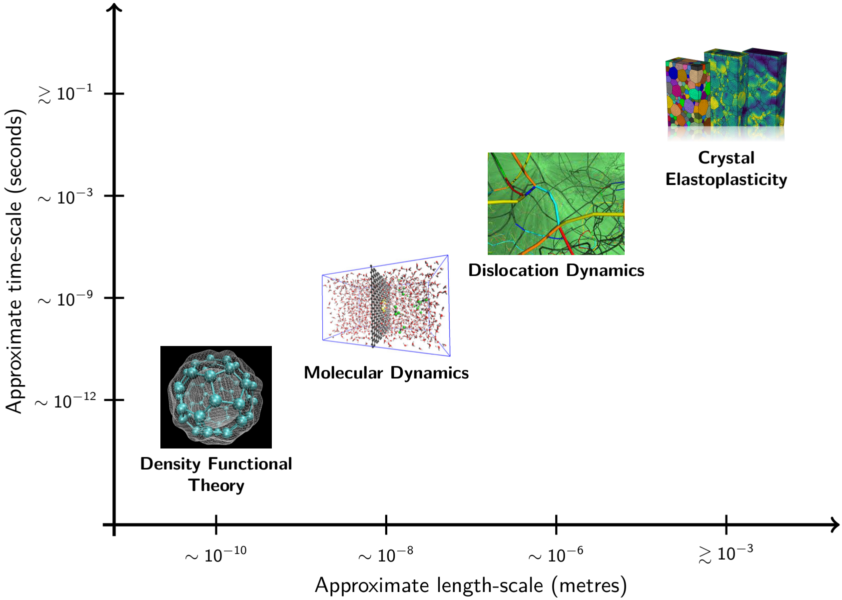


1D: Dislocations



2D: Grain boundaries

Modelling approaches



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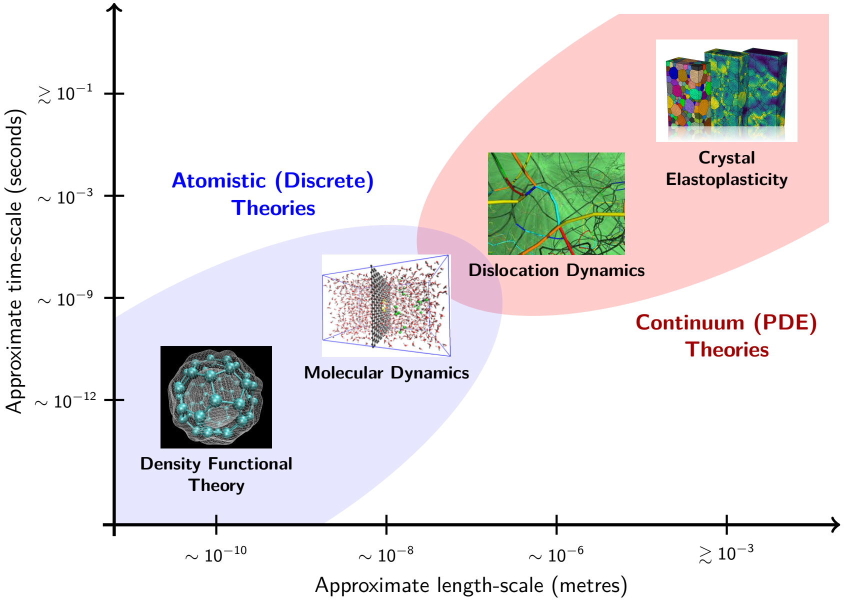

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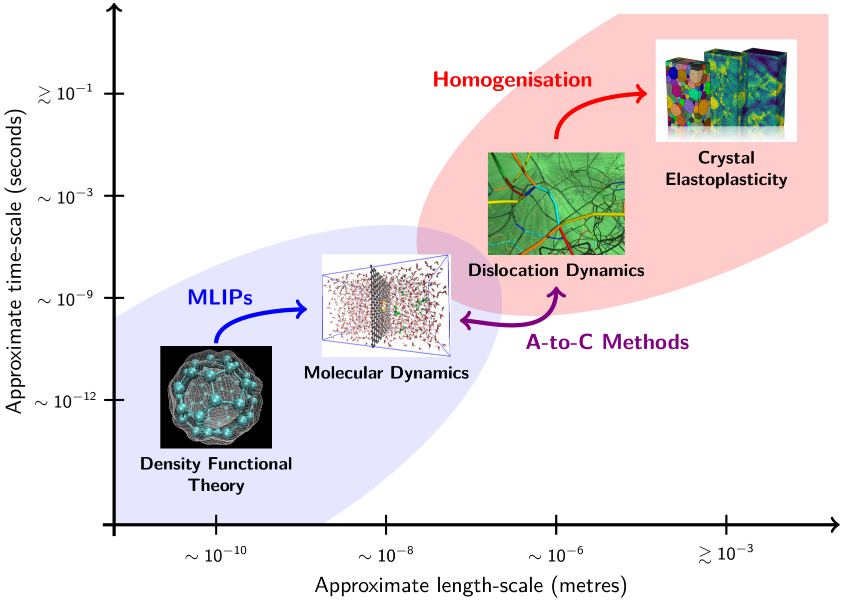
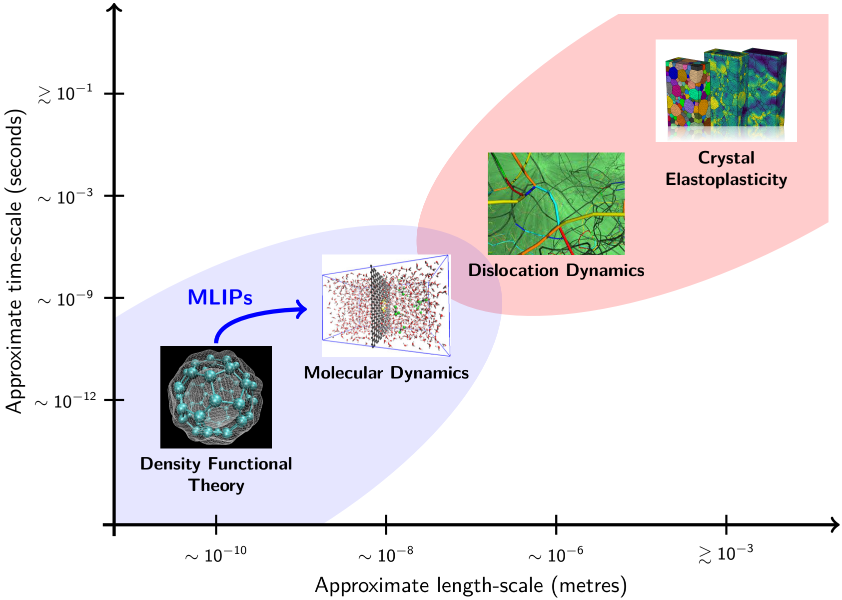
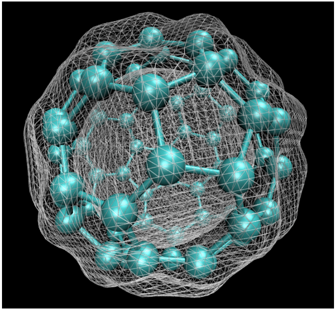


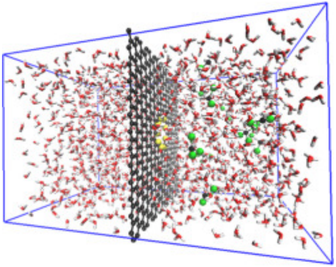
Machine-Learned Interatomic Potentials (MLIPs)



Atomistic theories

- Variables in these theories:
  - **Atomic nuclei** $\ell_i \in \mathbb{R}^3$
  - **Electron density** (in DFT).





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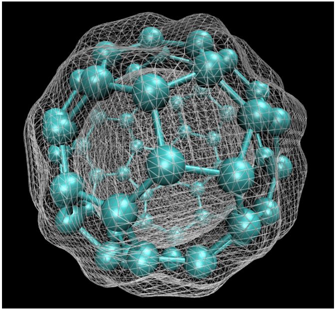

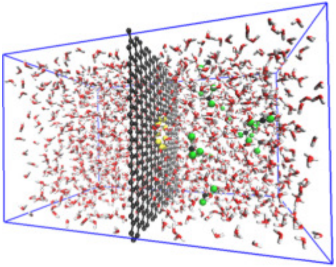

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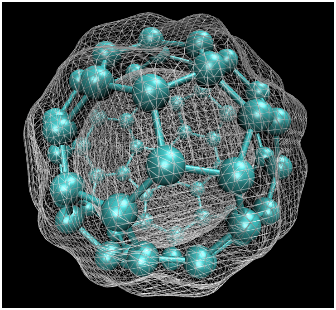

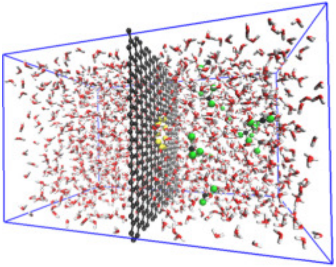

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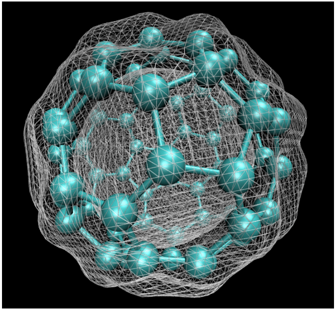
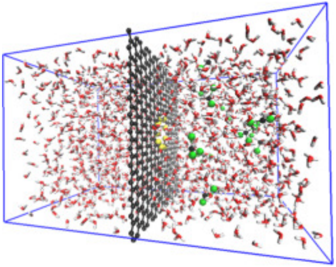
- **MD energies** are empirical and fitted: cheaper, but not uniformly accurate (c.f. Tim Germann's talk).





Machine-Learned Interatomic Potentials (MLIPs)

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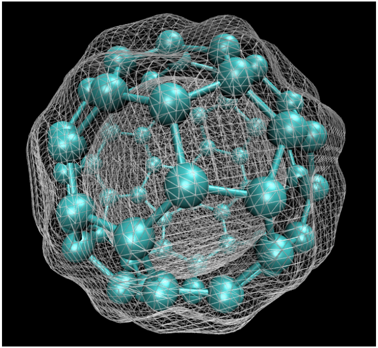
- **Compile** a database of expected environments: strained crystal, stacking fault, dimer pair, ...



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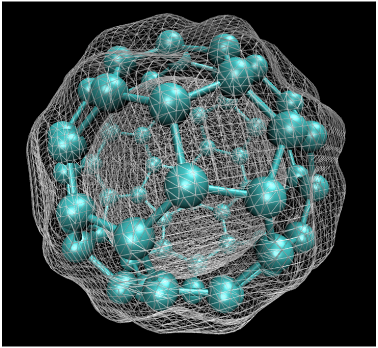

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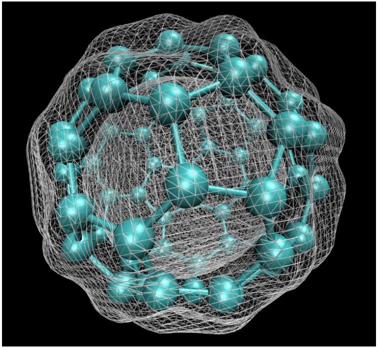

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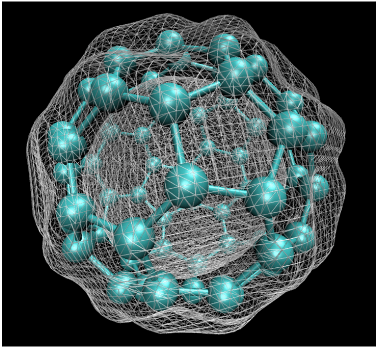
- **Fit** parametric energy (and forces) using a regression methodology.



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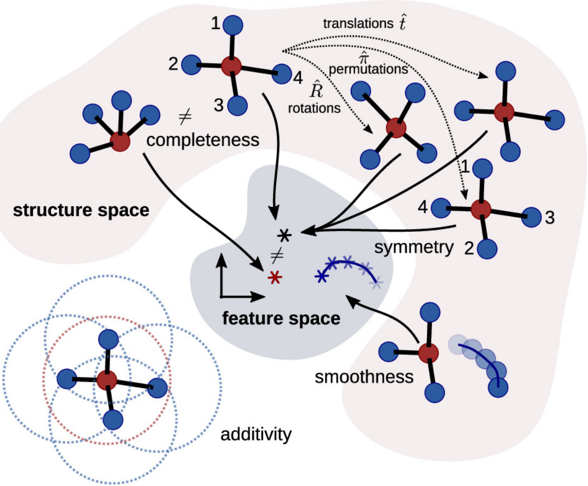
Key ingredient: **Descriptors** which compress structural information.



Musil et al, 2021

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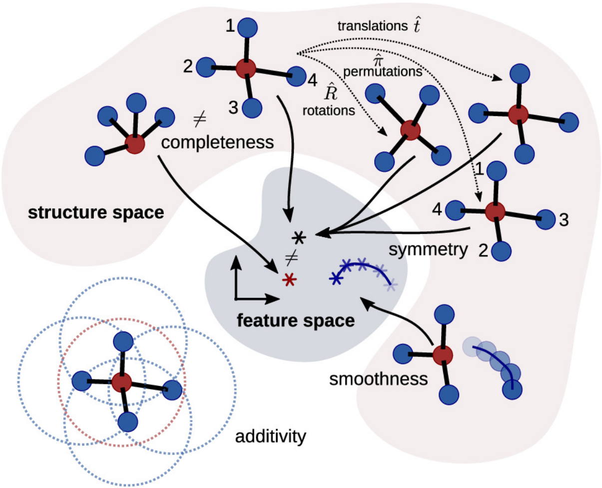

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Efficient representations 'integrate out' symmetries.

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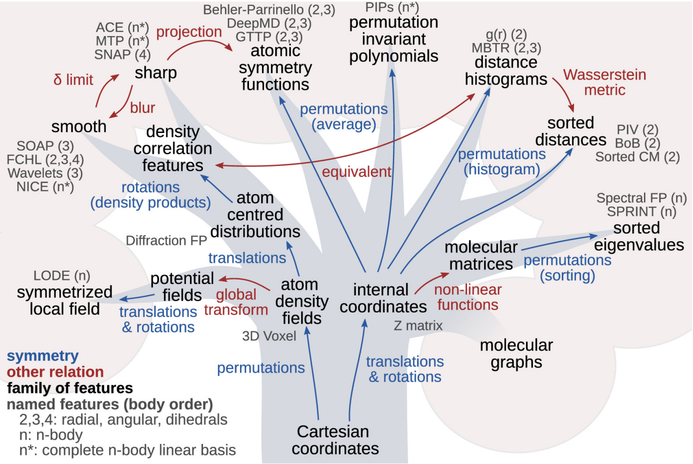

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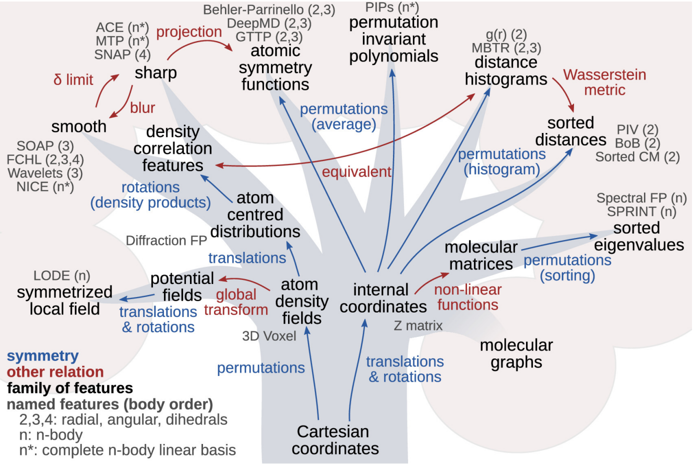

Open questions:

- Which architectures/descriptors are ‘best’? Efficiency, completeness...

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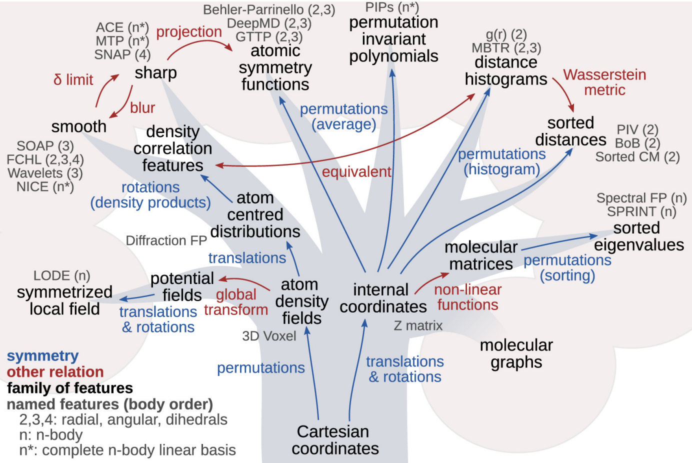
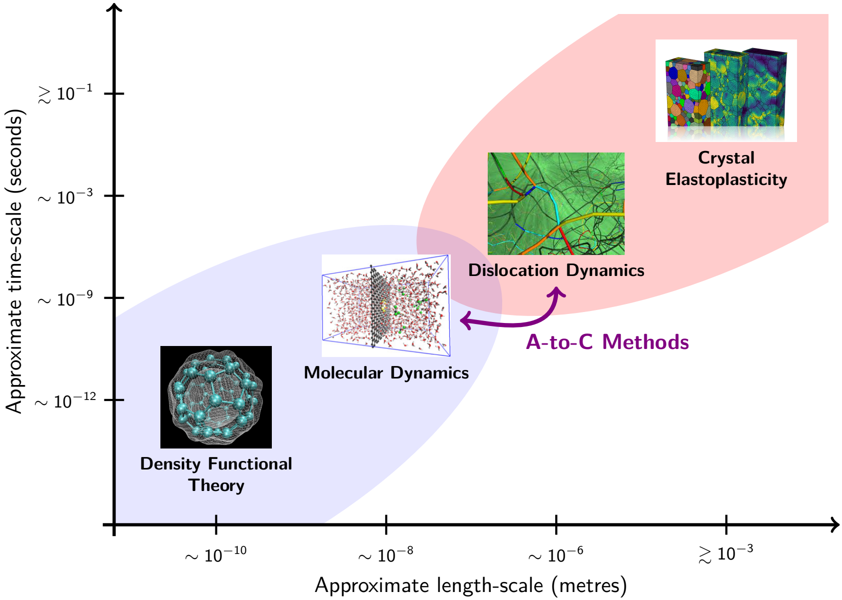


Open questions:

- Which architectures/descriptors are 'best'? Efficiency, completeness...
- How do we effectively handle many different species at the same time?

Reference: Musil et al, 2021. Chemical Reviews, 121(16), 9759–9815.

Atomistic-to-Continuum Methods



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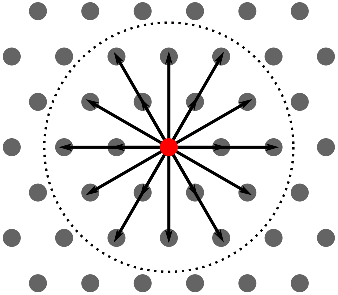
- Consider a **deformation** of atoms, $\mathbf{y} : \Lambda \to \mathbb{R}^3$, so ℓ moves to $\mathbf{y}(\ell)$.



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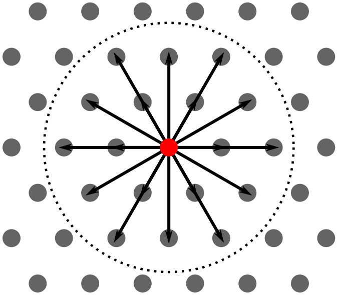

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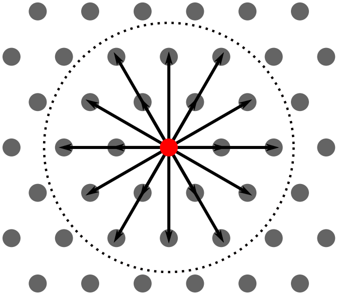
$$D\mathbf{y}(\ell) := \Big\{ \mathbf{y}(\ell + \rho) - \mathbf{y}(\ell) \Big\}_{\rho \in \mathcal{R}}.$$



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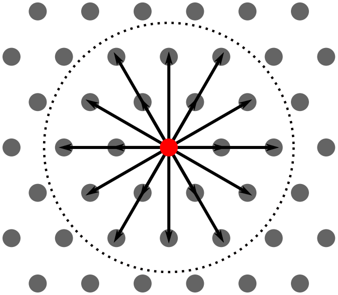

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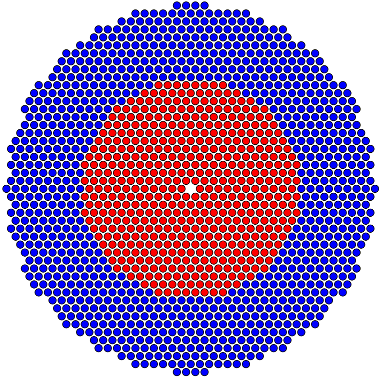
- For example, when interactions are pairwise:

$$V_\ell = \sum_{\rho \in \mathcal{R}} \varphi\Big(\mathbf{y}(\ell + \rho) - \mathbf{y}(\ell) \Big)$$

Atomistic-to-Continuum Methods

- Seek **local minima** and **saddle points** of atomistic energy $\mathcal{E}$, i.e. $\bar{\mathbf{y}}$ such that $\delta\mathcal{E}(\bar{\mathbf{y}}) = 0$.



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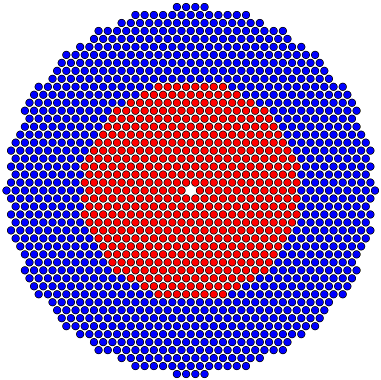

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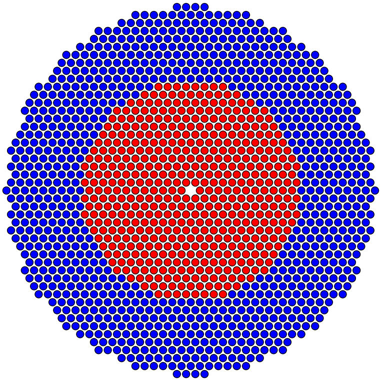

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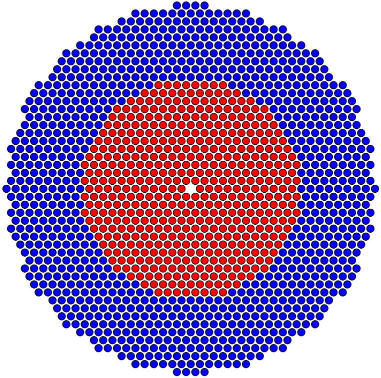
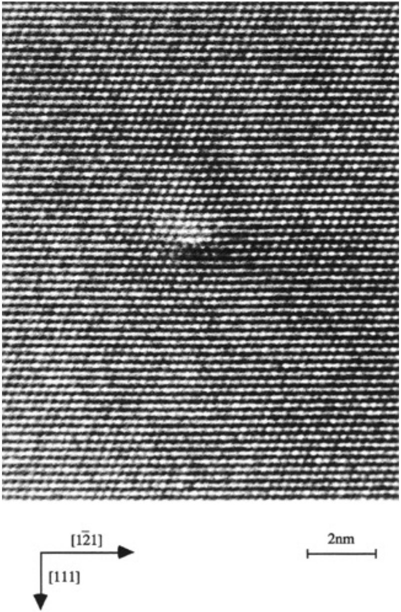


Question: How should the **boundary conditions** be set to achieve an efficient approximation?

An observation



Inkson, 1994

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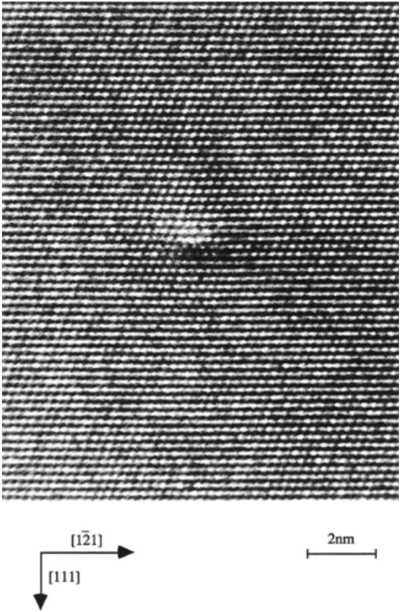

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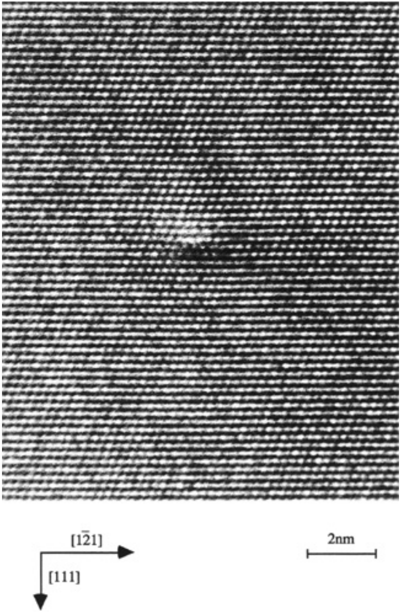

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- **Continuum Linear Elasticity (CLE)** provides singular solutions thought to predict atomic displacements away from defects.
- Use this insight to inform computational and mathematical approaches.

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In practice: Often use periodic boundary conditions.

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  - QM/MM: DFT coupled to MD.
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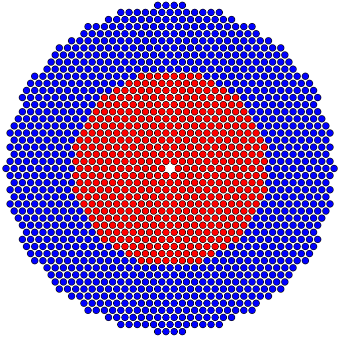

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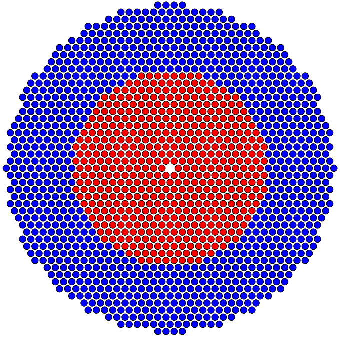
- **Challenges**:
  - Ghost forces in coupling methods due to incompatibility of models.
  - Dynamics: reducing degrees of freedom means information loss.



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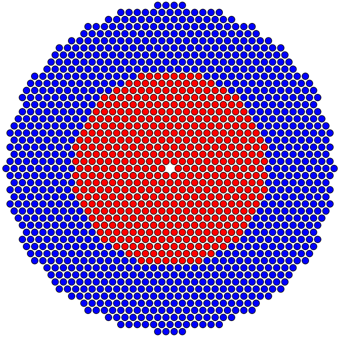
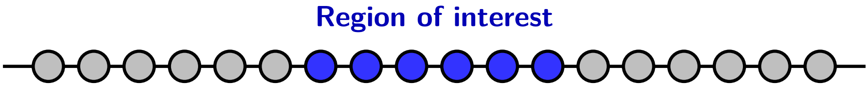


References:

– Luskin and Ortner, 2013. Acta Numerica, 22, 397-508.
– Ehrlacher et al, 2016. Arch. Rational Mech. Anal. 222, 1217–1268.

Coarse-graining



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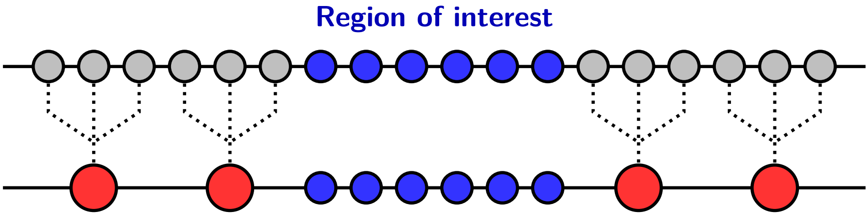

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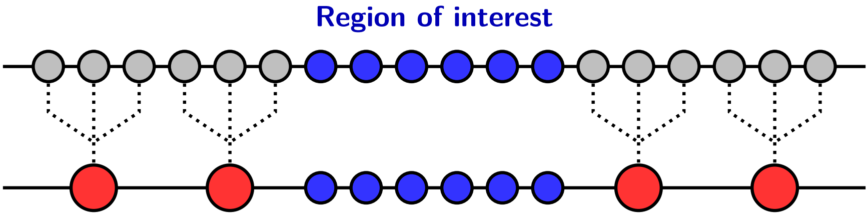

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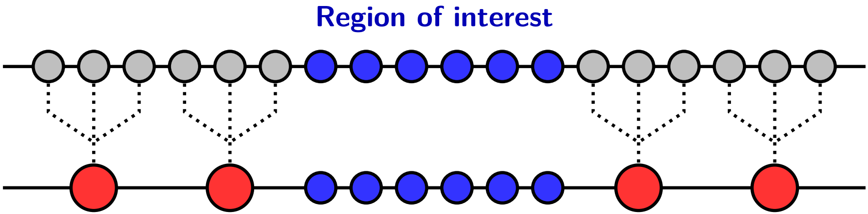

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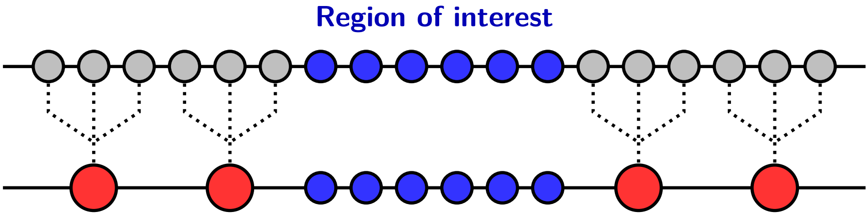

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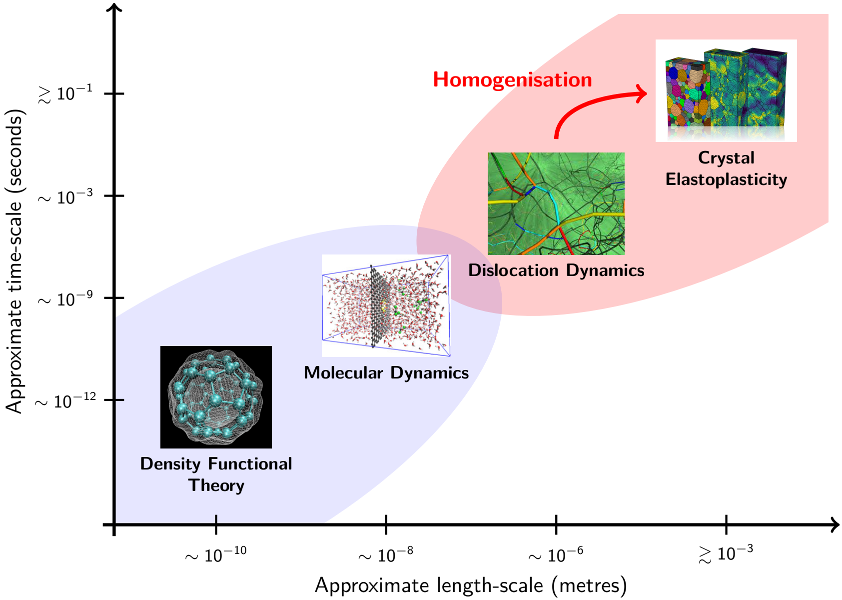
Open problem:

- Find a robust framework to fit free energy and compatible thermostat.

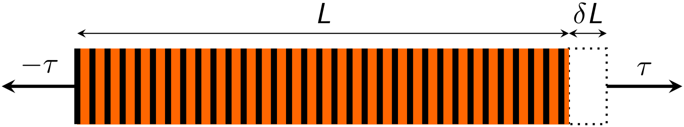
Reference:
– Lelièvre, Rousset and Stoltz, Free Energy Computations: A Mathematical Perspective.

Homogenisation



Homogenisation basics: Periodic case

Periodic layered material subject to tensile stress:



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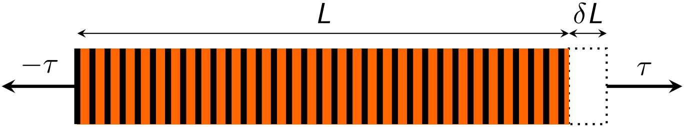

1D linear elasticity: $\displaystyle \frac{d\sigma}{dx} = 0, \qquad \sigma = k(\tfrac{x}{\varepsilon})\frac{du}{dx}$

Tensile loads: $-\sigma(0) = -\tau, \qquad \sigma(L) = \tau.$

Homogenisation basics: Periodic case

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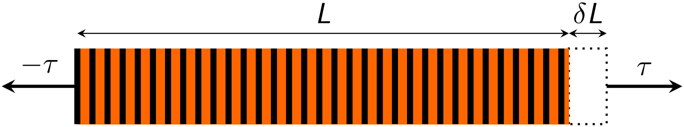

1D linear elasticity: $$\frac{d\sigma}{dx} = 0, \qquad \sigma = k(\tfrac{x}{\varepsilon})\frac{du}{dx}$$

Tensile loads: $-\sigma(0) = -\tau, \qquad \sigma(L) = \tau.$

Constant stress: $$\frac{du}{dx} = \frac{\tau}{k(\frac{x}{\varepsilon})} \quad \text{and} \quad \delta = \frac{\tau}{L}\int_0^L \frac{1}{k(\frac{x}{\varepsilon})}\,\mathrm{d}x$$

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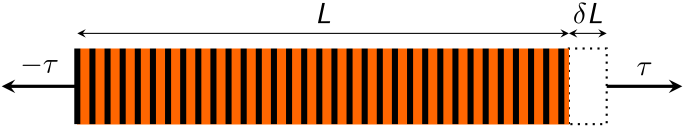

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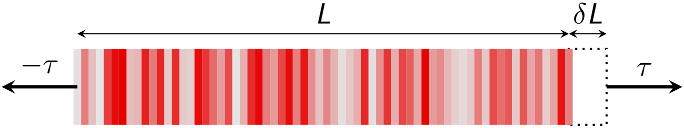
Effective stress-strain: $$\tau = K\,\delta, \quad K = \left(\frac{1}{L}\int_0^L \frac{1}{k(\frac{x}{\varepsilon})}\,\mathrm{d}x\right)^{-1}$$

$$\approx \left(\frac{\alpha_1}{k_1} + \frac{\alpha_2}{k_2}\right)^{-1}$$

Homogenisation basics: Stochastic case

Random layered material subject to tensile stress:



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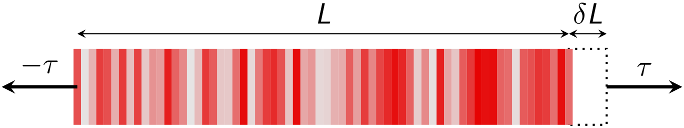

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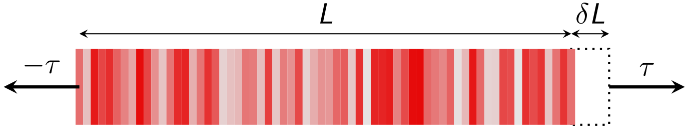

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Assuming **ergodicity**, spatial mean approximates the true mean:

$$\frac{1}{K} \approx \mathbb{E}\left[\frac{1}{k}\right].$$

Homogenisation basics

- More generally, consider the problem

$$-\nabla \cdot \left(\mathbf{C}\left(\frac{\mathbf{x}}{\varepsilon}\right) : \nabla \mathbf{u}^{\varepsilon} \right) = \mathbf{f}.$$

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  The effective $\overline{\mathbf{C}}$ may be found numerically by solving a **cell problem**.

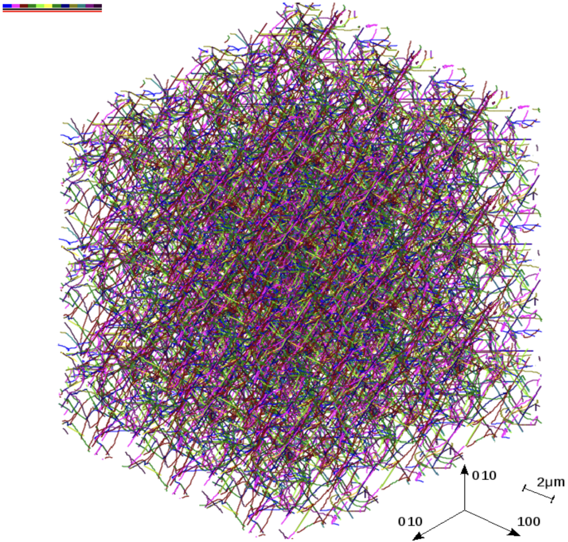
- Can treat **random** coefficients, and **nonlinear** problems: **sampling** and **fitting** then become significant challenges.

  References:

  – Pavliotis and Stuart, Multiscale Methods: Averaging and Homogenization.

  – Braides, Gamma-convergence for Beginners

An open problem: Predicting plasticity



Micromegas Manual

Job advert...

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Assistant Professor in Predictive Modelling and Scientific Computing (107274-0323)

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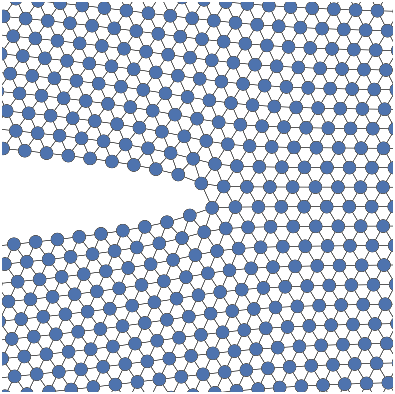
Vacancy Type/Job category	Academic
Department	School of Engineering
Sub Department	Mechanical, Materials and Process
Salary	£44,414 - £52,841 per annum
Location	University of Warwick, Coventry
Vacancy Overview	Full time, permanent position. The School of Engineering is seeking to recruit a talented and enthusiastic Assistant Professor in Predictive Modelling on the traditional research and teaching pathway. We are looking for someone who can help us strengthen and broaden our research activities, while also contributing to teaching of the newly established MSc in Predictive Modelling and Scientific Computing to start in the 2023-2024 academic year. We are open to appointments in any aspect of predictive modelling and scientific computing research consistent with the activities of the Warwick Centre for Predictive Modelling and the facilities available in the School and the University. Those with backgrounds in mathematical and statistical foundations of predictive modelling, or in in its application to physics-based uncertainty quantification (for example aligned with existing WCPM strength areas such as continuum solid or fluid mechanics, environmental sustainability, energy, materials science) are particularly encouraged to apply. The appointee will complement existing activity in the School or establish new activity, and it is expected the research will have

Summary

- **Multiscale methods** continue to develop in computational Materials Science, connecting and improving models, but mature tools are available.



Summary

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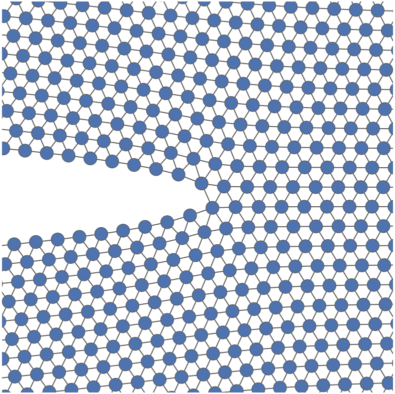
- Both **theory development** and **numerical implementation** in robust, scaleable code have important roles to play for the future of Materials modelling.



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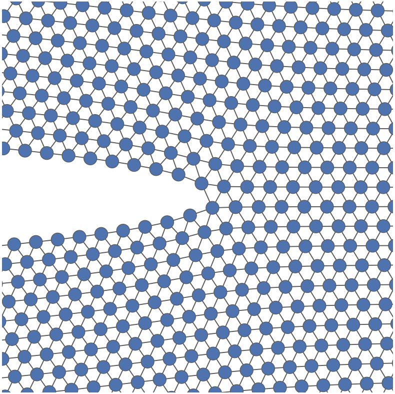

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– Pavliotis and Stuart, *Multiscale Methods*, Springer, 2008.
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