# Motivation & Objectives

The QC method increases the computational system size by modeling the region surrounding localized defects by an atomistic model and regions with smoothly varying deformation by a coarse-grained continuum model. Hyperdynamics accelerates time by modifying the energy landscape of a system in a controlled way so that rare events like material failure occur at a higher rate. The development of hyper-QC has the potential to enable the study of realistic materials systems where multiscale spatial structures and multiscale temporal phenomena coexist, such as thermally-activated defect nucleation in the vicinity of a crack tip during crack corrosion.

## Atomic Energy per Atom

- \( \Omega \subset \mathcal{L} \) is a Bravais lattice, Deformation: \( \mathbf{y} : \Omega \to \mathbb{R}^d \)

We define an atomistic energy per atom \( \epsilon_{\mathcal{A}}^{\mathcal{V}}(y) \) and a total atomic energy \( \epsilon_{\mathcal{A}}(y) \) of the deformation \( y \) for (EAM)

\[
\epsilon_{\mathcal{A}}(y) := \sum_{j \in \Omega} \epsilon_{\mathcal{A}}^{\mathcal{V}}(y) \quad \text{where} \quad \epsilon_{\mathcal{A}}^{\mathcal{V}}(y) := \frac{1}{2} \sum_{i \neq j} \rho(r_{ij}) + G \left( \sum_{i \neq j} \rho(r_{ij}) \right).
\]

## Continuum Energy per Atom (Volume-Based)

\( \Omega^{\mathcal{V}} \subset \Omega \) represents atomic sites with triangulation \( \mathcal{T} \).

For piecewise affine deformations \( y \)

\[
\epsilon_{\mathcal{T}}^{\mathcal{V}}(y) := \int_{\Omega^{\mathcal{V}}} W(\nabla y) dx = \sum_{T \in \mathcal{T}} v_T W(\nabla y|_T).
\]

- \( v_T := \text{volume of Voronoi}(y)\nabla y|_T \)
- \( W(F) := \text{Cauchy-Born strain energy density} \)
- For \( y_T = F x \), \( \epsilon_{\mathcal{T}}^{\mathcal{V}}(y_T) = \epsilon_{\mathcal{T}}^{\mathcal{V}}(y) \).

## References


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Lennard-Jones potential with one weak bond, Langevin thermostat (\( T = 0.03 \)), NN interaction, strain = 0.00375, \# of atoms = 1000.

Hot-QC models even with only 100 atoms can reproduce the TST time of the original system (1000 atoms), but all-atom models with a smaller number of atoms do not!