#25 Predictive Simulation of Materials by QC and Accelerated Dynamics Methods

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Motivation & Objectives

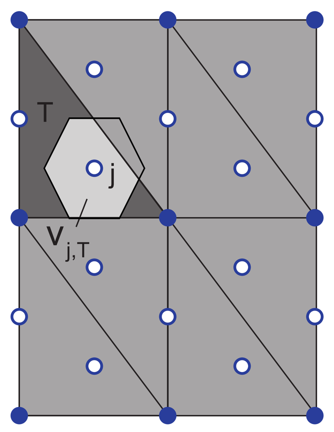
The QC method increases the computational system size by modeling the region surrounding localized defects by an atomistic model and regions with smoothly varying deformation by a coarse-grained continuum model. Hyperdynamics accelerates time by modifying the energy landscape of a system in a controlled 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 structure and multiscale temporal phenomena coexist, such as thermally-activated defect nucleation in the vicinity of a crack tip during crack corrosion.

Atomistic Energy per Atom

- Reference domain: $\Omega \subset \mathcal{L}$, a Bravais lattice, Deformation: $y : \Omega \to \mathbb{R}^d$
- We define an **atomistic energy per atom** $\mathcal{E}^a_j(y)$ and a **total atomistic energy** $\mathcal{E}^a(y)$ of the deformation y by (for EAM)

$$\mathcal{E}^a(y) := \sum_{j\in\Omega} \mathcal{E}^a_j(y) \text{ where } \mathcal{E}^a_j(y) := \frac{1}{2}\sum_{i\neq j}\phi(r_{ij}) + G\left(\sum_{i\neq j}\rho(r_{ij})\right).$$

Continuum Energy per Atom (Volume-Based)



- $\Omega^{rep} \subset \Omega$: representative atoms with triangulation $\mathcal{T}$.
- For piecewise affine deformations y

$$\mathcal{E}^c_j(y) := \int_{Vor(j)} W(\nabla y)dx = \sum_{T\in\mathcal{T}} v_{j,T} W(\nabla y|_T).$$

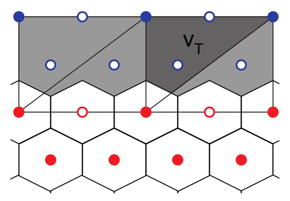
  - $v_{j,T}$:= volume of Voronoi(j)$\cap T$
  - W(F):= Cauchy-Born strain energy density
- For $y^F = Fx$, $\mathcal{E}^a_j(y^F) = \mathcal{E}^c_j(y^F)$.

Quasicontinuum Energy [Tadmor, Ortiz, Phillips]

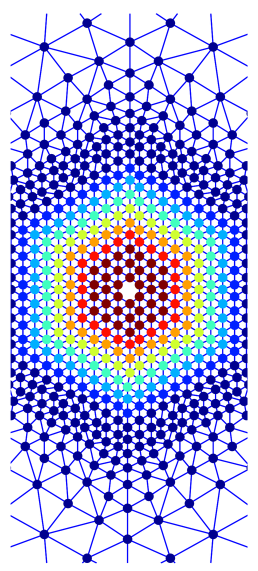
- The **Quasicontinuum Energy (QCE)** is defined by

$$\mathcal{E}^{QCE}(y) := \sum_{j\in A}\mathcal{E}^a_j(y) + \sum_{j\in C}\mathcal{E}^c_j(y) = \sum_{j\in A}\mathcal{E}^a_j(y) + \sum_{T\in\mathcal{T}} v_T W(\nabla y|_T).$$

- C consists of atoms whose Voronoi cells are contained in the triangulated region.
- $A := \Omega \setminus C$. $\quad v_T := \sum_{j\in C} v_{j,T}$.



Blended Quasicontinuum Energy (BQCE) [Van Koten, Luskin, Ortner]



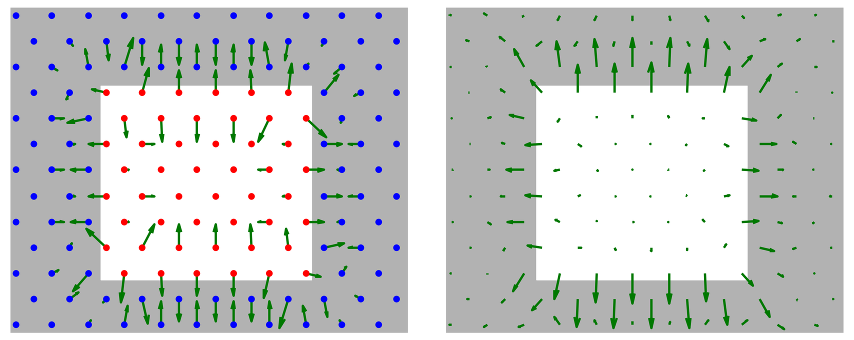
- Choose $\beta : \Omega \to [0,1]$ a **blending function**.
- Define the **Blended Quasicontinuum Energy**

$$\begin{aligned}\mathcal{E}^\beta(y) :&= \sum_{j\in\Omega}\beta_j\mathcal{E}^a_j(y) + (1-\beta_j)\mathcal{E}^c_j(y)\\ &= \sum_{j\in\Omega}\beta_j\mathcal{E}^a_j(y) + \sum_{T\in\mathcal{T}} v^\beta_T W(\nabla y|_T),\end{aligned}$$

  where $v^\beta_T := \sum_{j\in C}(1-\beta_j)v_{j,T}$.
- v^β_T is computed explicitly from β and $\mathcal{T}$.

The Patch Test

A *patch test consistent energy* has no forces (*ghost forces*) under uniform strain. GR-AC [Ortner, Zhang] is a patch test consistent 2D coupling energy for many-body nearest-neighbor interactions in a hexagonal lattice. A general 2D many-body patch test consistent coupling energy has not yet been constructed, but the BQCE 3D energy for general many-body interactions can be efficiently implemented. **BQCE optimally and controllably reduces the QCE ghost force errors.**

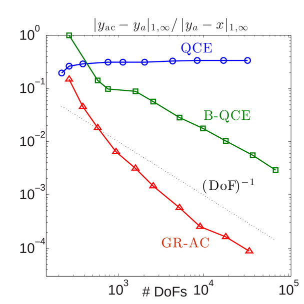


(a) Ghost Forces for QCE (b) Displacement Error

BQCE for 2D Defects: Complexity Estimates [Van Koten, Luskin, Ortner]

- Suppose y_a **is a local minimum of** $\mathcal{E}^a$ **with** $|D^2 y_a| \simeq r^{-\alpha}$.
- For a dislocation: $\alpha = 2$.

Method	$w^{1,\infty}$ Error	Complexity
GR-AC	$\Vert hD^2 y_a\Vert_\infty + \ldots$	DoF^{-1}
BQCE	$\Vert hD^2 y_a\Vert_\infty + \Vert D^2\beta\Vert_\infty + \ldots$	DoF^{-1}



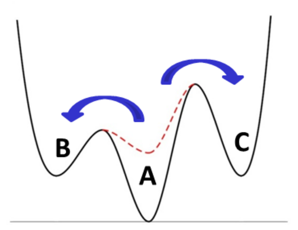
- **GR-AC and BQCE both have O(DoF^{-1}) error in $w^{1,\infty}$ for a dislocation.**
- Figure left: Error for the approximation of a vacancy ($\alpha = 3$) in a hexagonal lattice.

Hot-QC [Dupuy, Tadmor, Legoll, Miller, Kim]

- The **Potential of Mean Force** $\mathcal{E}^{PMF}(y^{\mathcal{A}}, \theta)$ reproduces the equilibrium properties of observables $O(y^{\mathcal{A}}, m^{\mathcal{A}})$ at temperature θ that depend only on the positions $y^{\mathcal{A}}$ and momenta $m^{\mathcal{A}}$ in $\mathcal{A}$.
- The **Hot-QC Energy** approximates $\mathcal{E}^{PMF}(y^{\mathcal{A}}, \theta)$ by using the local harmonic approximation and Cauchy-Born coarse-graining in $\mathcal{C}$:

$$\tilde{\mathcal{E}}^{QC}(y, \theta) := \sum_{j\in A}\mathcal{E}^a_j(y) + \sum_{T\in\mathcal{T}} v_T \tilde{W}(\nabla y|_T, \theta).$$

Accelerated Dynamics [Voter]

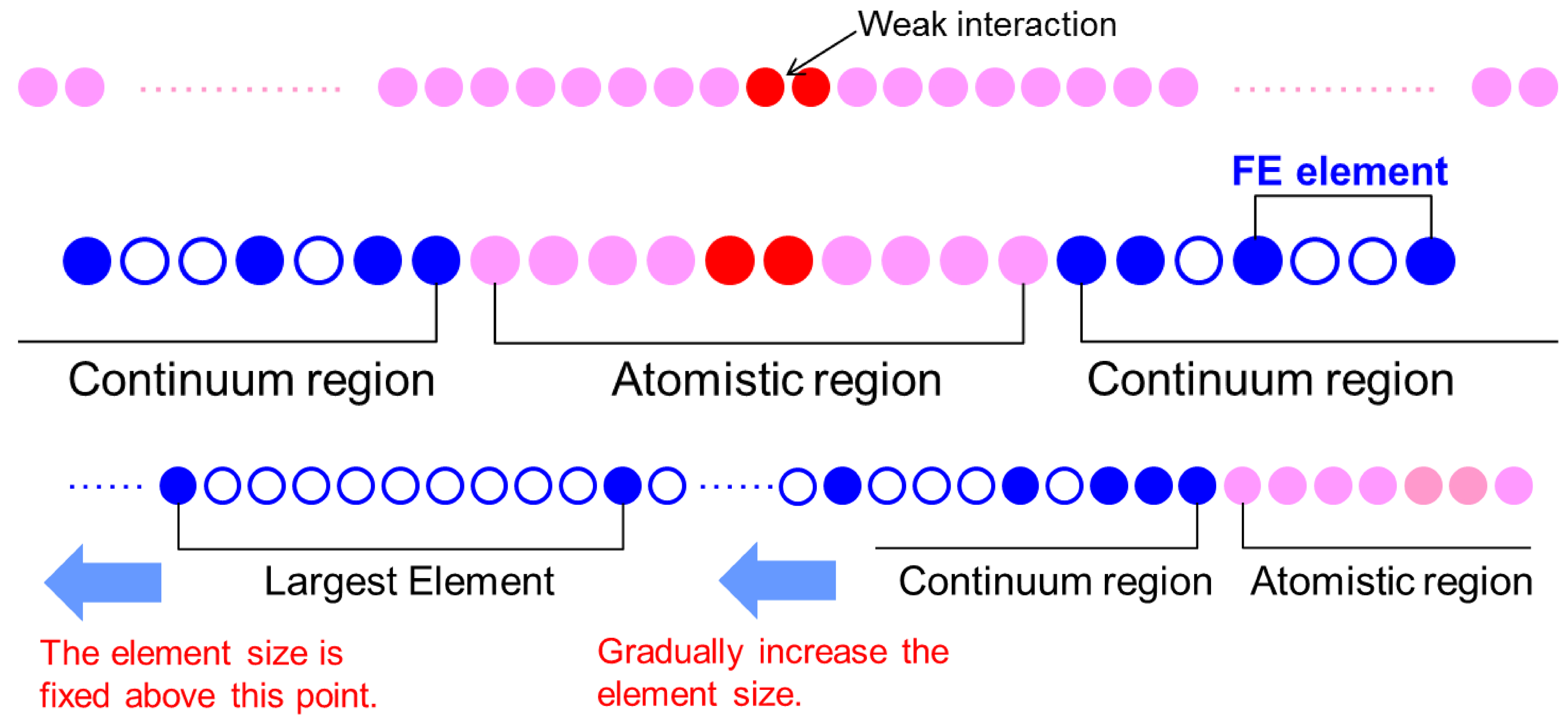


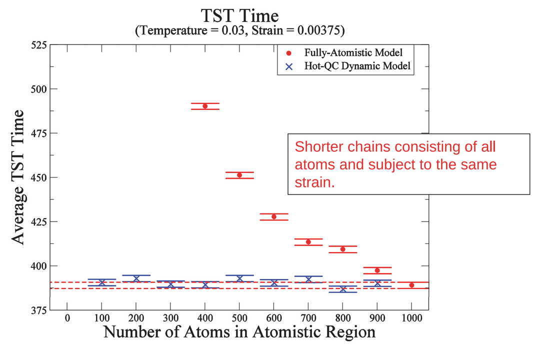
- Hyperdynamics utilizes a bias potential to accurately accelerate the state-to-state dynamics of rare events.
- The ratio of any two escape rates out of A depends only on the dividing surfaces for these paths, where the bias potential is required to be zero; thus hyperdynamics correctly accelerates escapes in Hot-QC.

See Poster 71 by Danny Perez for research on Parallel Replica Dynamics.

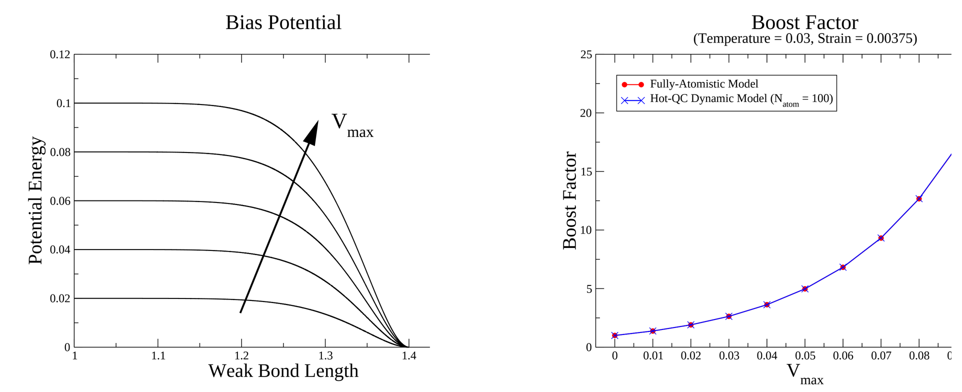
HyperQC Model Problem [Kim, Tadmor, Luskin, Perez, Voter]

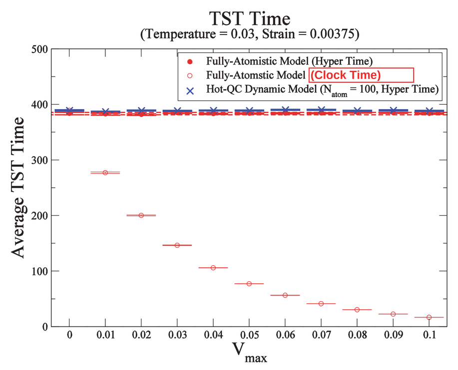
Lennard-Jones potential with one weak bond, Langevin thermostat (θ=0.03), NN interaction, strain=0.00375, # of atoms=1000.





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!





Hyper-QC method can reproduce the original TST time with both a smaller number of atoms and shorter simulation times.

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