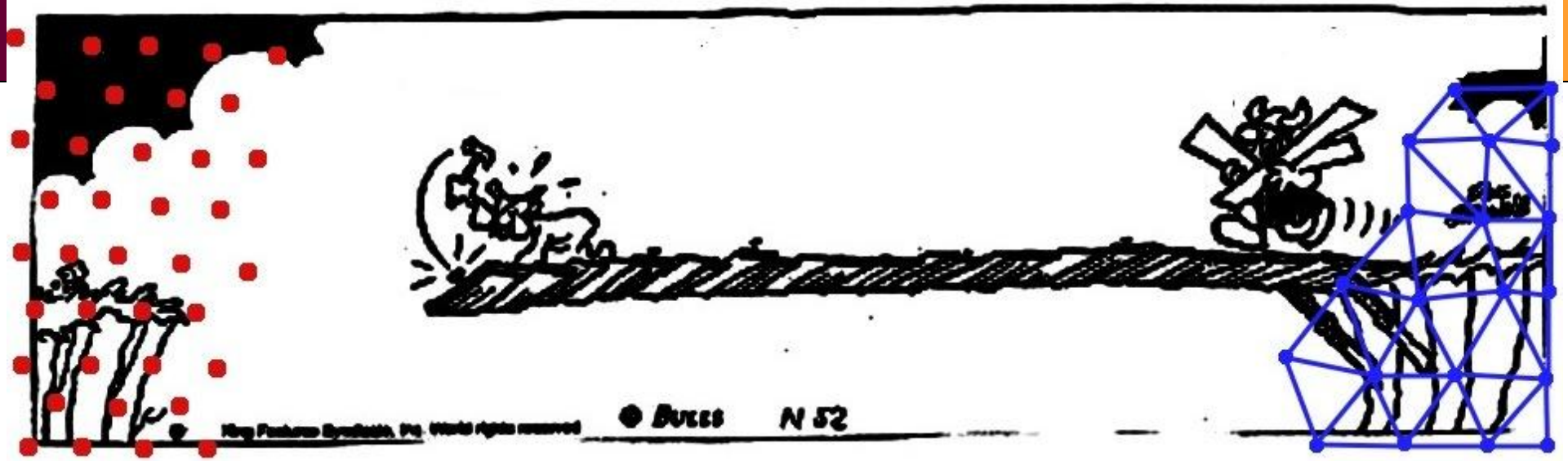

Atomistic-to-Continuum Coupling Methods for Crystalline Solids

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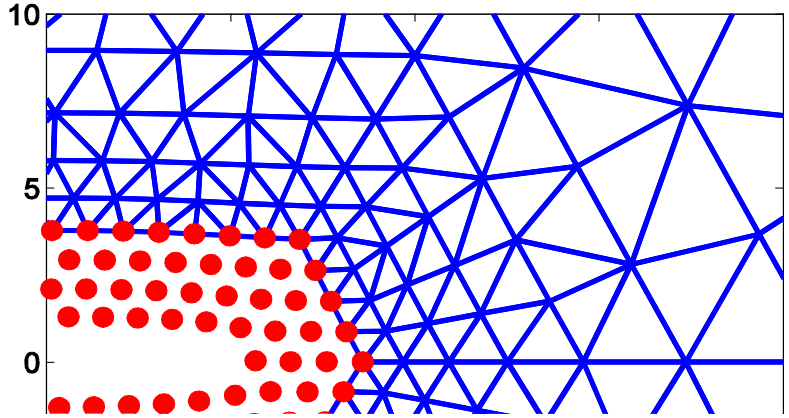
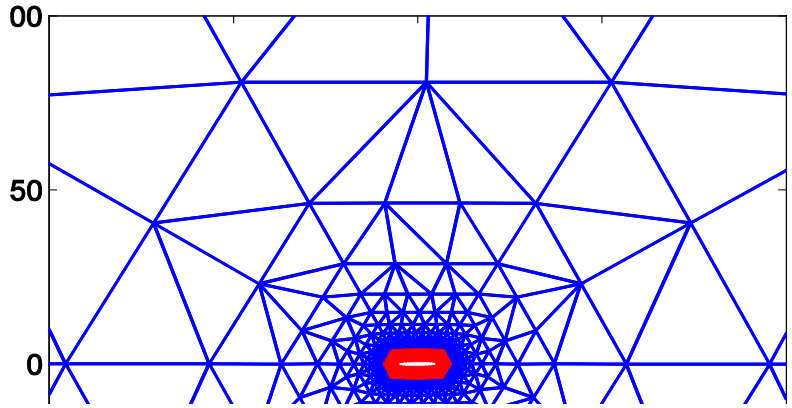




Approximation $\mathcal{E}^a(\mathbf{y})$ of the QM potential,
Continuum approximation of atomistic model,
Atomistic-to-continuum model coupling,
Coarse-graining in the continuum region,
Far-field and surface boundary conditions, and
Accelerated dynamics are required for problems with defects and long-range elastic interactions.

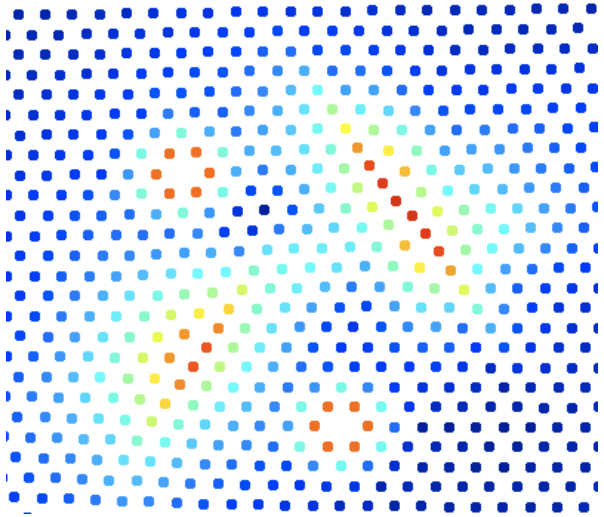
Low energy local mimina (or dynamically metastable states) of $\mathcal{E}^a(\mathbf{y})$ have a lattice structure deformed by highly localized defects:

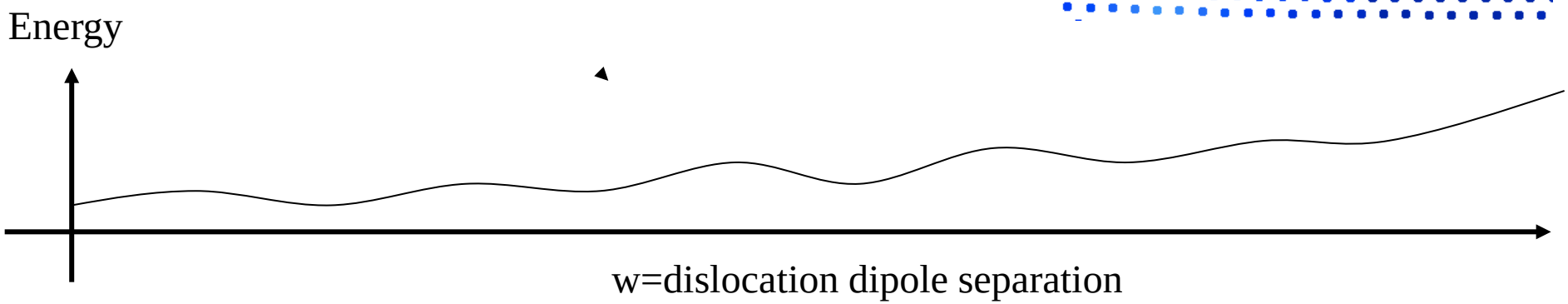
Point defects (vacancies, interstitials)

Line defects (dislocations)

Surface defects (grain boundaries).

Mathematical challenge to describe, analyze, and compute the *multiscale energy landscape.*





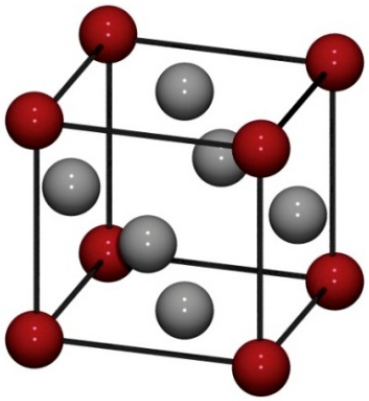
Consider interaction potentials $\mathcal{E}^a(\mathbf{y})$ whose energy-minimizing state is a (Bravais) lattice

$$A\mathbb{Z}^3 = \left\{ \sum_{i=1}^{3} m_i \mathbf{A_i} \in \mathbb{R}^3 \quad \text{for } \mathbf{m} \in \mathbb{Z}^3 \right\}$$

where $\mathbf{A} = (\,\mathbf{A_1}, \mathbf{A_2}, \mathbf{A_3}\,)$ for $\mathbf{A_i} \in \mathbb{R}^3$ are reference lattice basis vectors.

Face-Centered Cubic Lattice:

$$\mathbf{A_1} = \mathbf{a_0}\,(1,\,1,\,0), \quad \mathbf{A_2} = \mathbf{a_0}\,(1,\,0,\,1),$$
$$\mathbf{A_3} = \mathbf{a_0}\,(0,\,1,\,1).$$



The atomistic reference domain is a subset of the lattice points satisfying

$$\Omega := \{\, \xi_1, \ldots, \xi_M \,\} \subset A\mathbb{Z}^3.$$

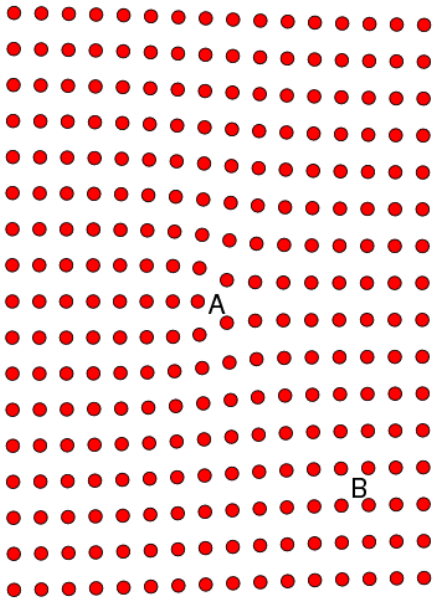
Define the space of admissible deformations $\mathbf{y}(\xi) : \Omega \to \mathbb{R}^3$ by

$$\mathcal{V} := \{\mathbf{y}(\xi) : \text{boundary conditions on } \partial\Omega\}$$

and compute local minima of

$$\underset{\mathbf{y}\in\mathcal{V}}{\text{arg local min}}\, \mathcal{E}^a(\mathbf{y}).$$

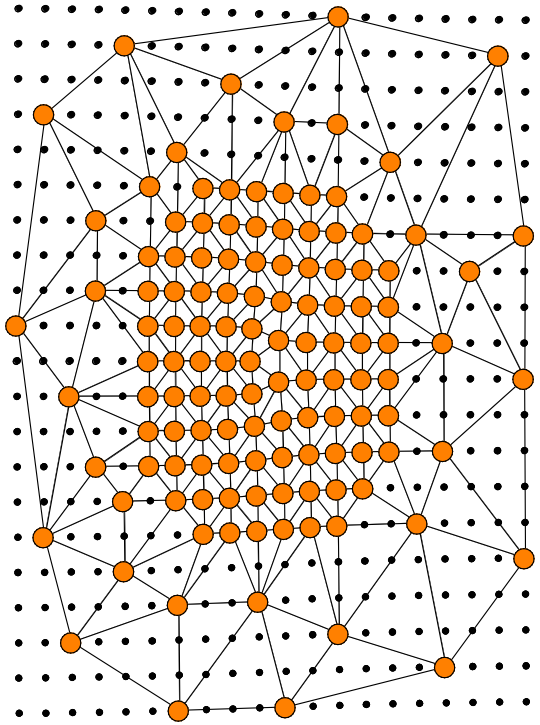
Dislocations are admissible deformations for atomistic models, but have infinite energy for continuum models.



Choose a subset of Ω to be representative atoms with reference positions

$$\Omega^{rep} := \{\xi_{j_1}, \ldots, \xi_{j_N}\} \subset \Omega$$

where $N << M$ and construct a triangular finite element mesh $T \in \mathcal{T}$ with vertices, ξ_{j_ℓ} for $j = 1, \ldots, N$.



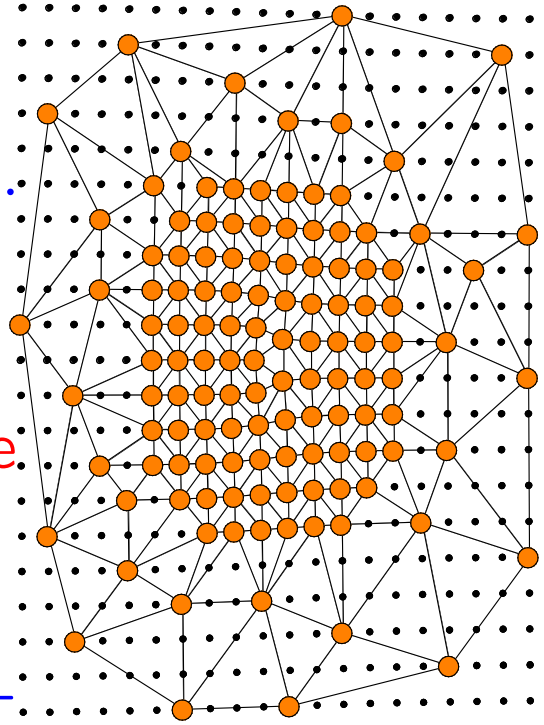
Denote the continuous, piecewise linear functions with respect to the mesh $\mathcal{T}$ by $P^1(\mathcal{T})$ and the corresponding piecewise linear approximation space by

$$\tilde{\mathcal{V}} := \mathcal{V} \cap P^1(\mathcal{T}).$$

The degrees of freedom of $\mathbf{Y} \in \tilde{\mathcal{V}}$ are ξ_{j_ℓ} for $j = 1, \ldots, N$.

Approximate

$\arg \operatorname{local\,min}_{\mathbf{y}\in\mathcal{V}} \mathcal{E}^a(\mathbf{y})$ by $\arg \operatorname{local\,min}_{\mathbf{Y}\in\tilde{\mathcal{V}}} \mathcal{E}^a(\mathbf{Y})$.



Identical to continuum piecewise linear finite element approximation except:

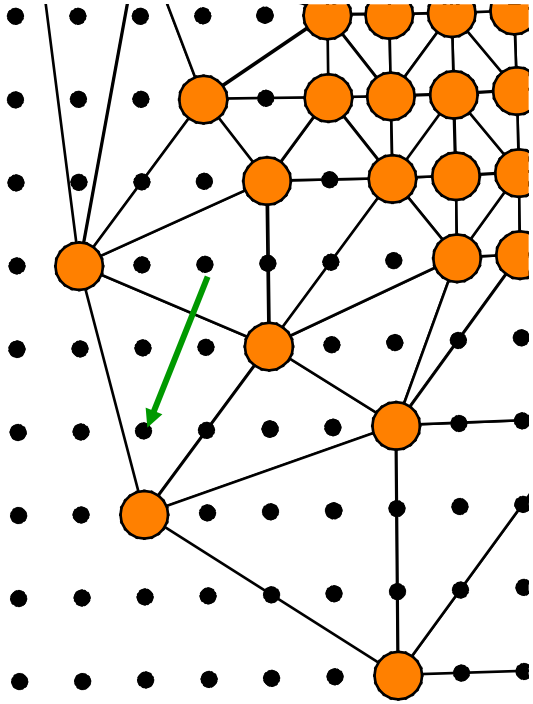
Reference domain is a lattice instead of a continuum.

Defects have finite energy and can be directly computed (they have infinite energy for continuum models such as the Volterra solutions).

Error: Displacement field constrained to be linear within each element.

Approximate

$\arg \operatorname{local\,min}_{\mathbf{y}\in\mathcal{V}} \mathcal{E}^a(\mathbf{y})$ by $\arg \operatorname{local\,min}_{\mathbf{Y}\in\tilde{\mathcal{V}}} \mathcal{E}^a(\mathbf{Y})$.



Degrees of freedom reduced to $N << M$.

Must still compute $O(M)$ atomistic interactions because of nonlocal interactions.

Still need further approximation. Remedies:

Approximate by Strain Energy Density derived from Cauchy-Born. Solve by continuum linear finite elements. Modeling error introduced.

or

Approximate by quadrature (sampling) of atomistic energy.

The Cauchy-Born continuum strain energy density is equal to the atomistic energy density for uniform strain $\mathbf{y}^F(\xi) := F\xi$:

$$W(\mathbf{F}) := \frac{1}{\det A}\mathcal{E}_\ell^a\left(\mathbf{y}^F\right)$$
$$= \frac{1}{\det A}\left\{\frac{1}{2}\sum_{\mathbf{m}\in\mathbb{Z}^3}\phi\left(|m_i\mathbf{F}\mathbf{A_i}|\right) + G\left(\sum_{\mathbf{m}\in\mathbb{Z}^3}\rho\left(|m_i\mathbf{F}\mathbf{A_i}|\right)\right)\right\},$$

where $\det A$ is the volume of the reference unit cell and the sum is restricted by $|m_i\mathbf{F}\mathbf{A_i}| \leq r_{\text{cut}}$.

Approximate FEM-A, $\mathcal{E}^{\mathsf{a}}(\mathbf{Y})$, by FEM-C:

$$\mathcal{E}^{\mathsf{c}}(\mathbf{Y}) = \sum_{T \in \mathcal{T}} \nu_T W\left(\nabla \mathbf{Y}|_T\right) = \int_\Omega W\left(\nabla \mathbf{Y}(x)\right)\, dx$$

where ν_T is the volume of element T and $W(\nabla \mathbf{Y}|_T)$ is the continuum strain energy density.

The work to compute the energy or forces has now been reduced to $\dim(\tilde{V}) = N$.

Modeling error introduced.

Motivation for Atomistic Modeling Near Defects

$$\mathcal{E}^{\mathrm{a}}(\mathbf{y}) - \mathcal{E}^{\mathrm{c}}(\mathbf{y}) = \mathrm{O}\left(\varepsilon^2 \int_\Omega \left|D^2 y(x)\right|^2 + \left|D^3 y(x)\right| \, dx\right)$$

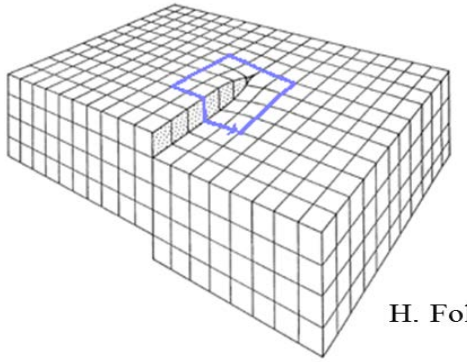
where ϵ is the scaled lattice spacing (Blanc, Le Bris, & Lions). Second-order Cauchy-Born for multilattices: Van Koten & Ortner.

Deformation near a dislocation has singularity

$$D^2 y(x_1, x_2, x_3) = \mathrm{O}\left(\frac{1}{r^2}\right)$$

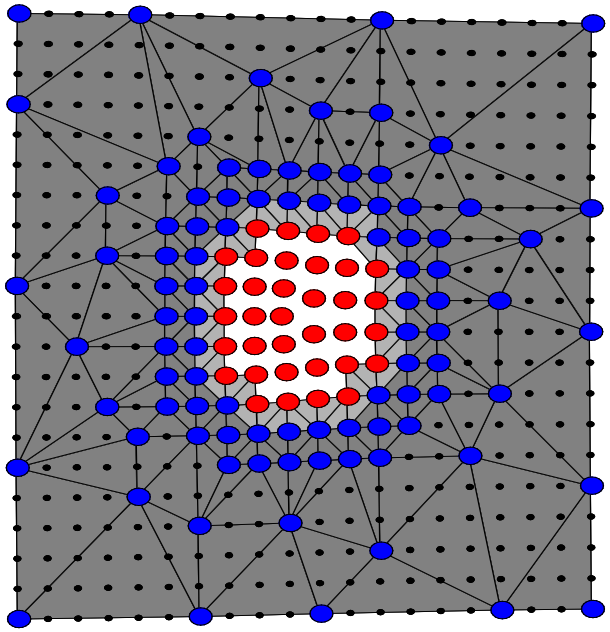
where r is the distance to the dislocation. The singularity is cut-off at $r = \mathrm{O}(\varepsilon)$, so

$$\mathcal{E}^{\mathrm{a}}(\mathbf{y}) - \mathcal{E}^{\mathrm{c}}(\mathbf{y}) = \mathrm{O}(1)!$$



For accuracy, keep atomistic interactions where the strain varies on the atomistic scale.

Energy-based Quasicontinuum Approximation (QCE)



For accuracy, use atomistic interactions for repatoms where the deformation gradient varies on the atomistic scale.

For efficiency, use strain energy density where the deformation gradient is sufficiently uniform.

$$\mathcal{E}^{\mathrm{QCE}}(\mathbf{Y}) = \sum_{\text{atomistic}} \mathcal{E}_j^a(\mathbf{Y}) + \sum_{T\in\mathcal{T}} \nu_T W\left(\nabla\mathbf{Y}|_{\mathbf{T}}\right)$$

$$= \sum_{\text{atomistic}} \mathcal{E}_j^a(\mathbf{Y}) + \int_{\Omega_c} W\left(\nabla\mathbf{Y}(x)\right) dx.$$

QCE energy of Tadmor, Ortiz, and Phillips conserves energy for uniform strain and has direct implementation with no special interfacial calculations by modifying ν_T for triangles that border the interface.

Coupling Error for Uniform Deformaton: The Patch Test

$$\mathcal{E}^{\mathrm{QCE}}(\mathbf{Y}) = \sum_{\text{atomistic}} \mathcal{E}_j^a(\mathbf{Y}) + \sum_{T\in\mathcal{T}} \nu_T W\left(\nabla \mathbf{Y}|_{\mathbf{T}}\right)$$
$$= \sum_{\text{atomistic}} \mathcal{E}_j^a(\mathbf{Y}) + \int_{\Omega_c} W\left(\nabla \mathbf{Y}(x)\right) dx.$$

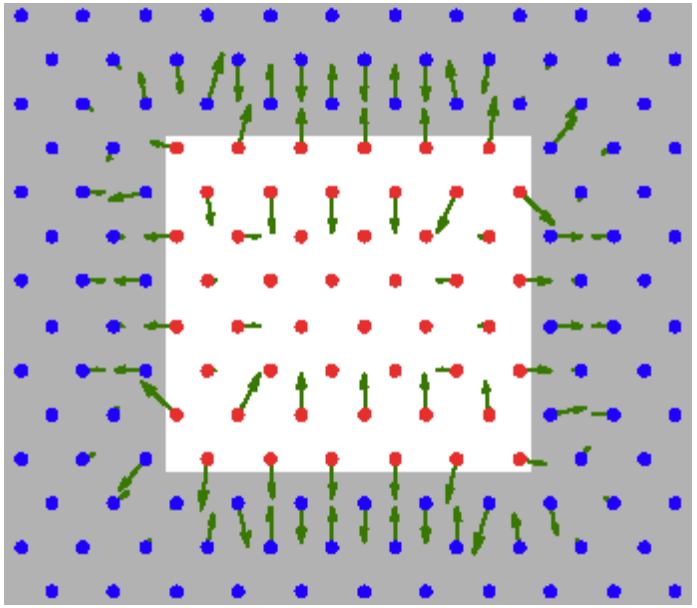
Uniformly strained deformation $\mathbf{y}^F(\xi) := F\xi$.

By symmetry, $\delta\mathcal{E}^{\mathrm{a}}\left(y^F\right) = \delta\mathcal{E}^{\mathrm{c}}\left(y^F\right) = 0.$

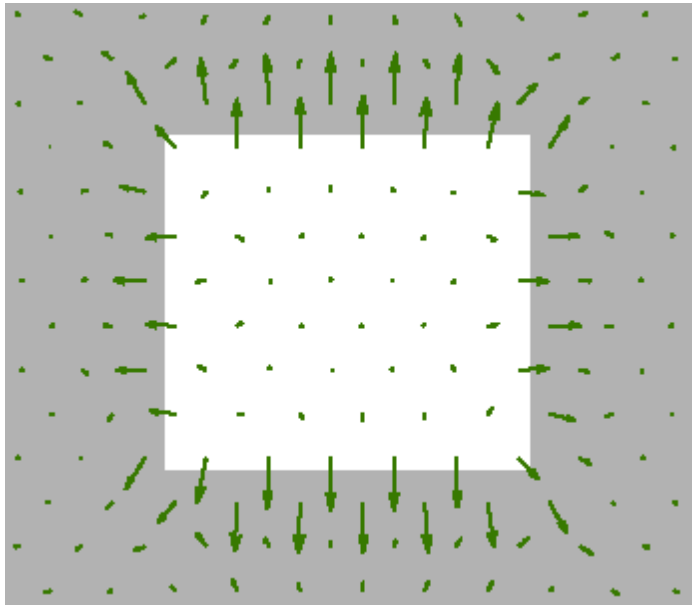
QCE energy does not satisfy the *patch test:* there are nonzero "ghost" forces in the a/c interface under uniform strain (Tadmor, et. al.)

$$\frac{\partial \mathcal{E}^{\mathrm{QCE}}}{\partial y_m}\left(\mathbf{y}^F\right) \neq 0$$

for $\mathbf{y}_m \in r_{\mathrm{cut}}$-width neighborhood of the a/c interface.



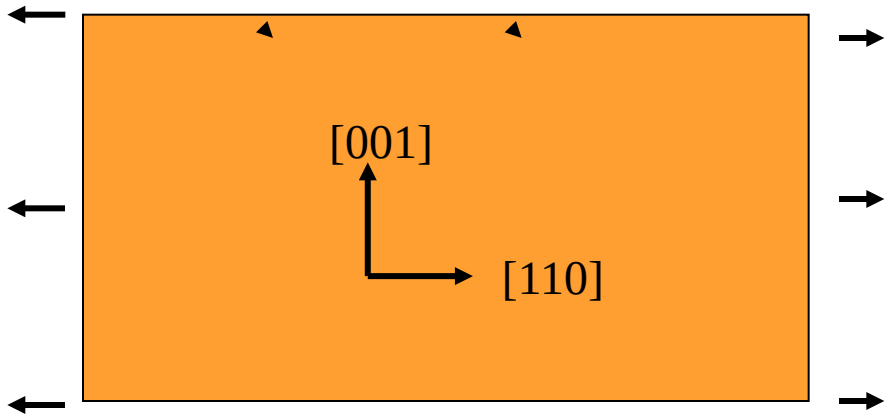
Ghost Forces

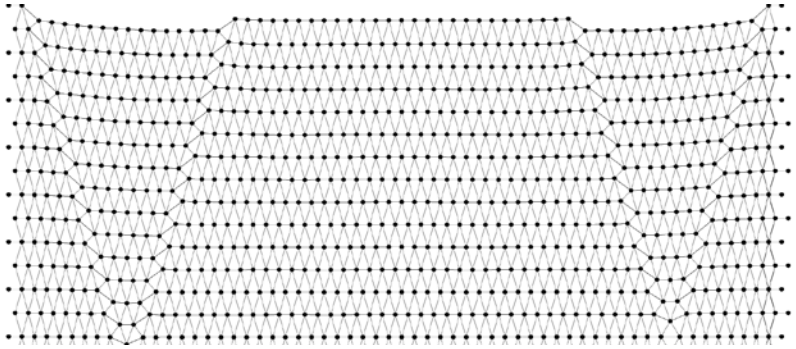


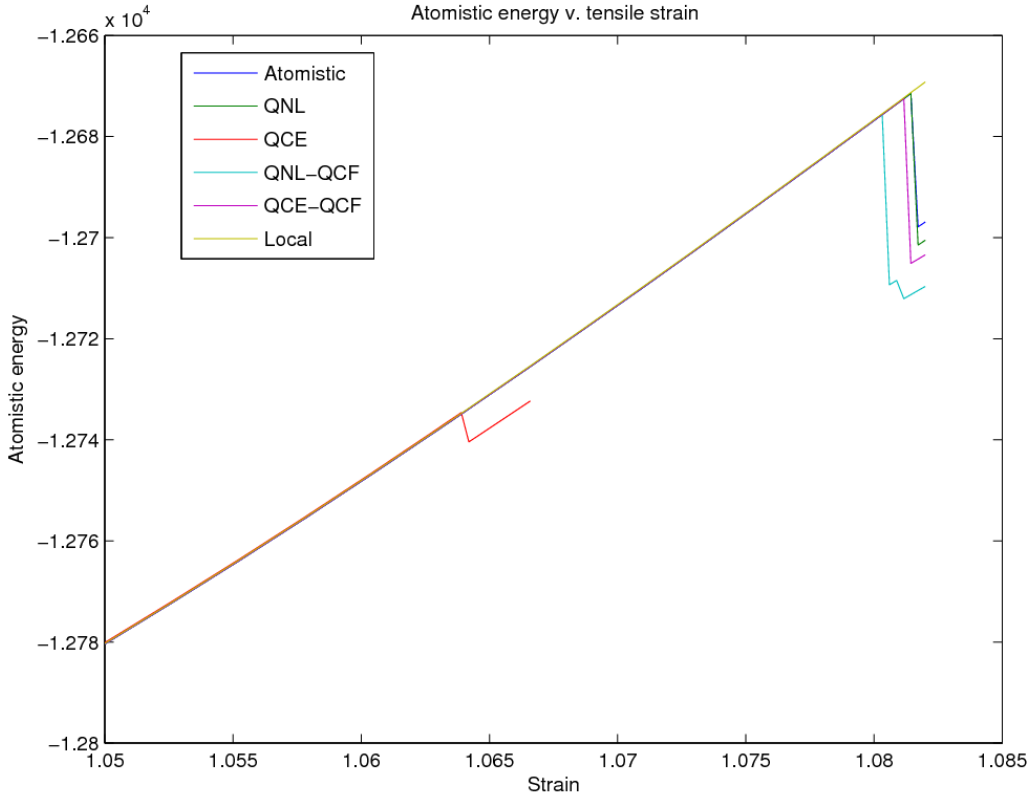
Displacement Error

Approximation of Lattice Stability for Tensile Loading

Accuracy near lattice instabilities requires that $\delta^2\mathcal{E}^{QC}(y^{qc})$ is positive definite iff (to first order error) $\delta^2\mathcal{E}^{a}(y^{qc})$ is positive definite. $\mathcal{E}^{QCE}(y)$ has O(1) critical strain error (Dobson, Luskin & Ortner).







Van Koten, Li, Luskin & Ortner

Comparison of BQCE and Other Coupled Energies

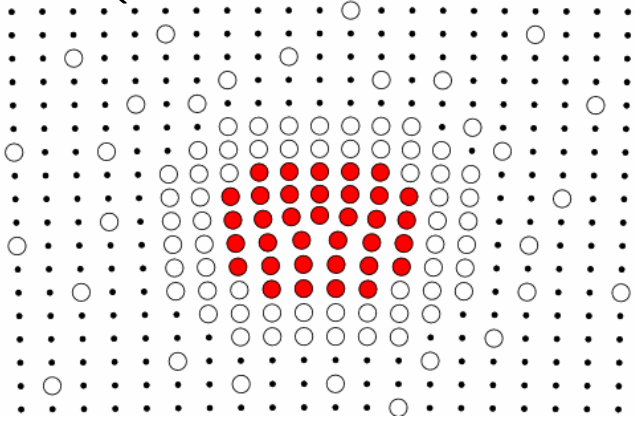
Method	Ghost Force	Implementation	Model
QCE Tadmor, Ortiz, & Phillips	Yes	Medium	Multi-body, 3D
BQCE Van Koten, Luskin & Ortner	Controllable	Medium +	Multi-body, 3D
Quasinonlocal Shimokawa, et al.	Corners & Coarsening	Hard	Multi-body, 3D short-range
Geom Reconstr E, Lu & Yang	Corners & Coarsening	Not yet	Planar interface
GR-AC Ortner & Zhang	No	Very Hard	2D Many-body NN
Shapeev Shapeev, Li & Luskin in 1D	No	Hard	Pair interaction 2D, finite range

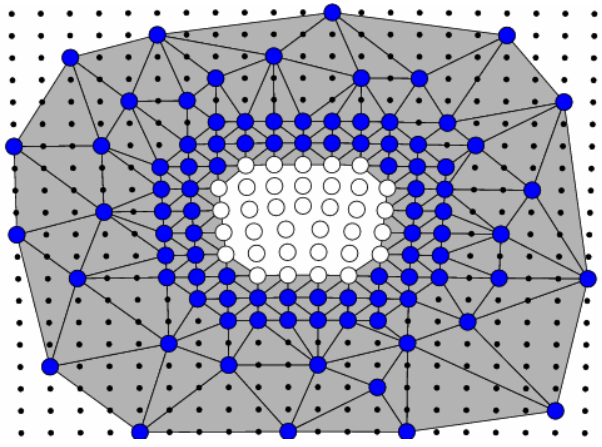
Force-Based Quasicontinuum Method (QCF):

$$\mathcal{F}_j^{QCF}(\mathbf{Y}) = \begin{cases} \mathcal{F}_j^a(\mathbf{Y}) = -\dfrac{\partial \mathcal{E}^{\mathrm{a}}(\mathbf{Y})}{\partial Y_j} & \text{if } Y_j \text{ is atomistic,} \\ \mathcal{F}_j^c(\mathbf{Y}) = -\dfrac{\partial \mathcal{E}^{\mathrm{c}}(\mathbf{Y})}{\partial Y_j} & \text{if } Y_j \text{ is continuum.} \end{cases}$$

Most popular method to couple multiphysics models generally, such as molecular mechanics to quantum mechanics.

QCF is the only known patch test consistent scheme with $O(N)$ work to evaluate all of the forces, but is nonconservative and INDEFINITE (Dobson, Luskin & Ortner).





Blended Force-Based Methods

QCF is patch test consistent for many-body potentials, multilattices, 3D, but is not conservative and not positive definite. Blended QCF needs small interface width to be efficient.

Blended QCF is positive definite if and only if the atomistic model is positive definite and the blending width $K \gg N^{1/5}$ in atomistic scale or ($O(\epsilon^{4/5})$ blending width in the continuum scale) (Xingjie Helen Li, Luskin, & Ortner).

Lu & Ming have proven that a blended force-based method is stable in $w^{2,2}$ if the blending width $K = O(N)$ (or $O(1)$ blending width in the continuum scale).

References

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