Atomistic-continuum coupling method in 3D

- Atomistic model, Λ : reference lattice with point defect.

$$\mathcal{E}^{\mathrm{a}}(u) = \sum_{x\in\Lambda} V_x^{\mathrm{a}}(\mathrm{D}u(x)), \quad u^{\mathrm{a}} \in \arg\min_{u\in W^{1,2}} \mathcal{E}^{\mathrm{a}}(u).$$

- Atomistic / continuum coupling,

$$\mathcal{E}^{\mathrm{ac}}(u) = \sum_{x\in\Lambda^{\mathrm{a}}} V_x^{\mathrm{a}}(\mathrm{D}u(x)) + \sum_{x\in\Lambda^{\mathrm{i}}} V_x^{\mathrm{i}}(\mathrm{D}u(x)) + \sum_{T\in\mathcal{T}_h} v_T^{\mathrm{eff}} W(\nabla u).$$

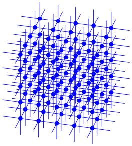
  Cauchy-Born energy density, $W(\mathrm{F}) = \frac{V(\mathrm{F}x)}{\mathrm{VOR}}$, $u^{\mathrm{ac}} \in \arg\min_u \mathcal{E}^{\mathrm{ac}}(u)$.
- Patch test consistency (ghost force removal), for uniform deformation, $\forall v : \langle \delta\mathcal{E}^{\mathrm{ac}}(u), v\rangle = 0$.
- Far field decay for point defect, $\left|\mathrm{D}^j u^{\mathrm{a}}(x)\right| \leq c\,|x|^{1-d-j}$.
- A priori analysis (degrees of freedom $N \sim R_a^d$),

$$\left\|\nabla u^{\mathrm{ac}} - \nabla u^{\mathrm{a}}\right\| \lesssim \left\|h\,\mathrm{D}^2 u^a\right\|_{\ell^2(\mathcal{T}_h/B_{R_a})} + \left\|\mathrm{D}u^a\right\|_{\ell^2(\mathbb{R}^d/B_{R_c/2})}$$

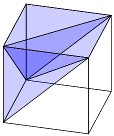
$$\lesssim R_a^{-\frac{d}{2}-1} \lesssim \begin{cases} N^{-1}, & d = 2, \\ N^{-5/6}, & d = 3. \end{cases}$$

- Reference: [Luskin, Ortner, 2013] [Ortner, Zhang, 2012, 2014] [Ehrlacher, Ortner, Shapeev, 2013]

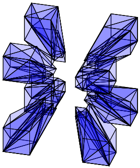
Atomistic-continuum coupling method in 3D



Atomistic lattice.



Subdivision of cube into tetrahedra.



Part of the graded mesh.

Two approaches,

- Consistent method based on geometric reconstruction, $V^{\mathrm{i}}\left(\{\mathrm{D}_i u(x)\}\right) = V\left(\left\{\sum C_{x,i,j}\,\mathrm{D}_j u(x)\right\}\right)$.
  - Force consistency, for uniform deformation, $\delta\mathcal{E}^{\mathrm{ac}}(u) = 0$.
  - Energy consistency, for uniform deformation, $V^{\mathrm{i}} = V^{\mathrm{a}}$.
  - Use symmetry to reduce the degrees of freedom of C.
- Blended Ghost Force Correction (BGFC).

Use graded mesh in the continuum region.