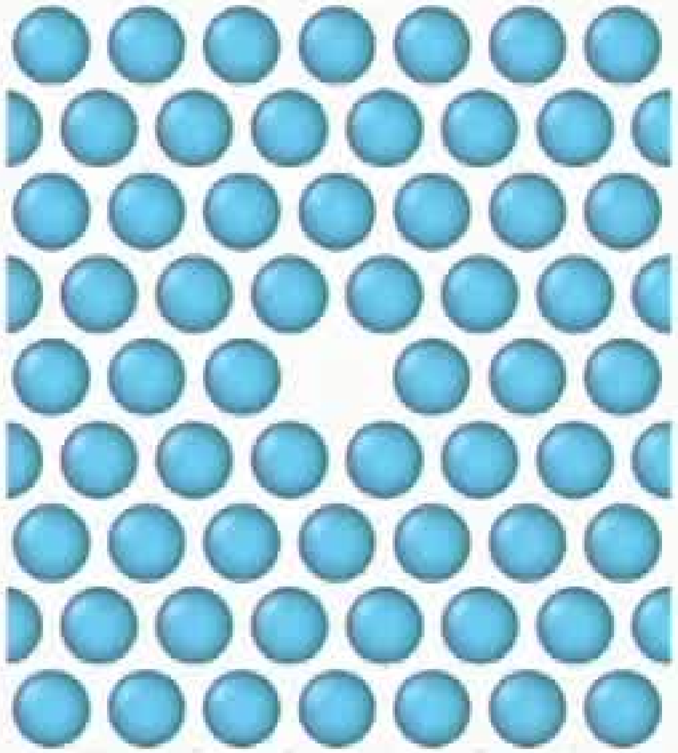
Atomistic Simulation of Crystalline Defects
[A Numerical Analysis Perspective]

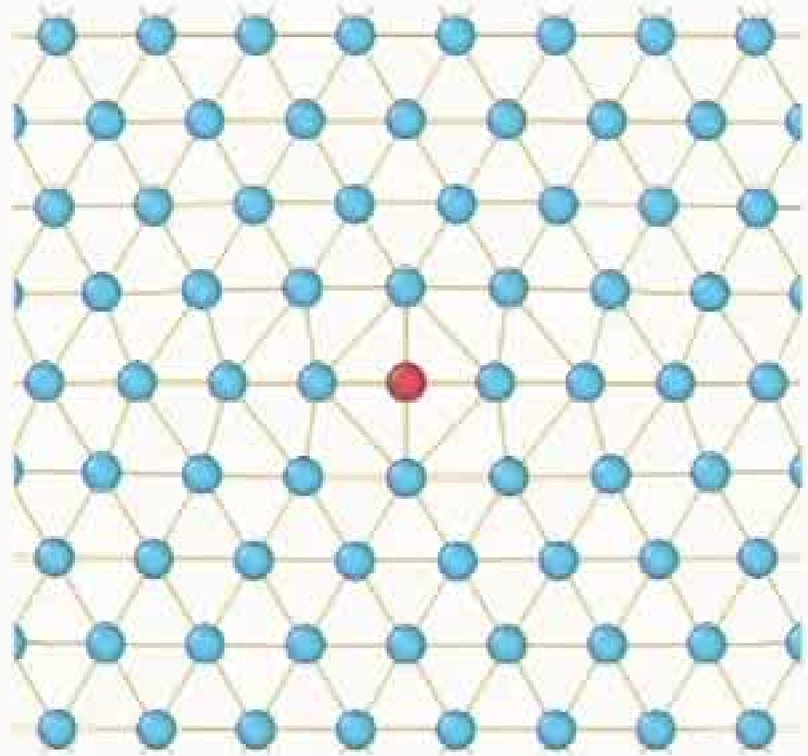
Christoph Ortner

joint work with too many people to list here

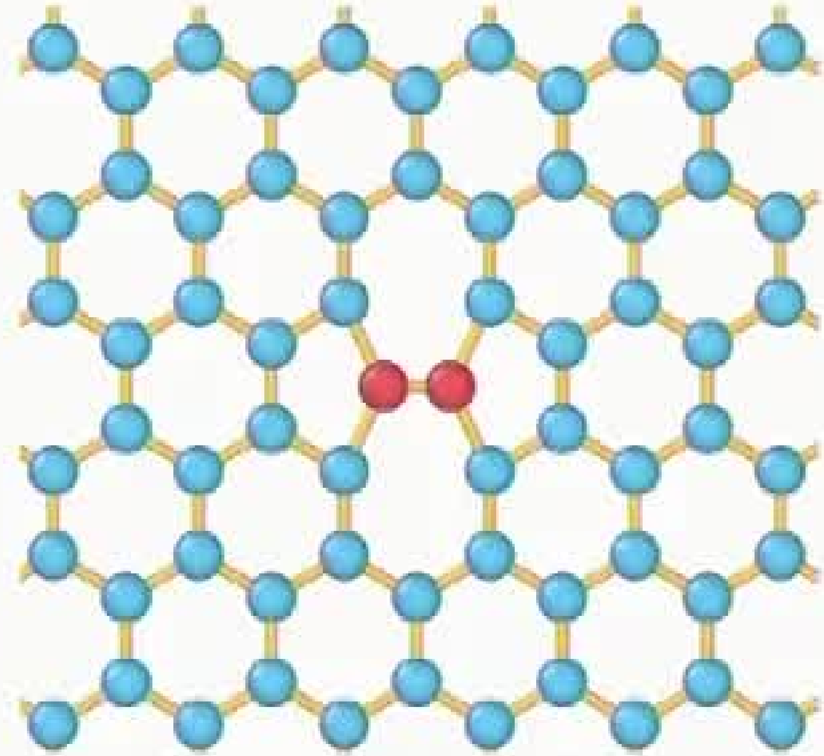
SIAM Conference on Mathematical Aspects of Materials Science
Portland, July 9–13, 2018



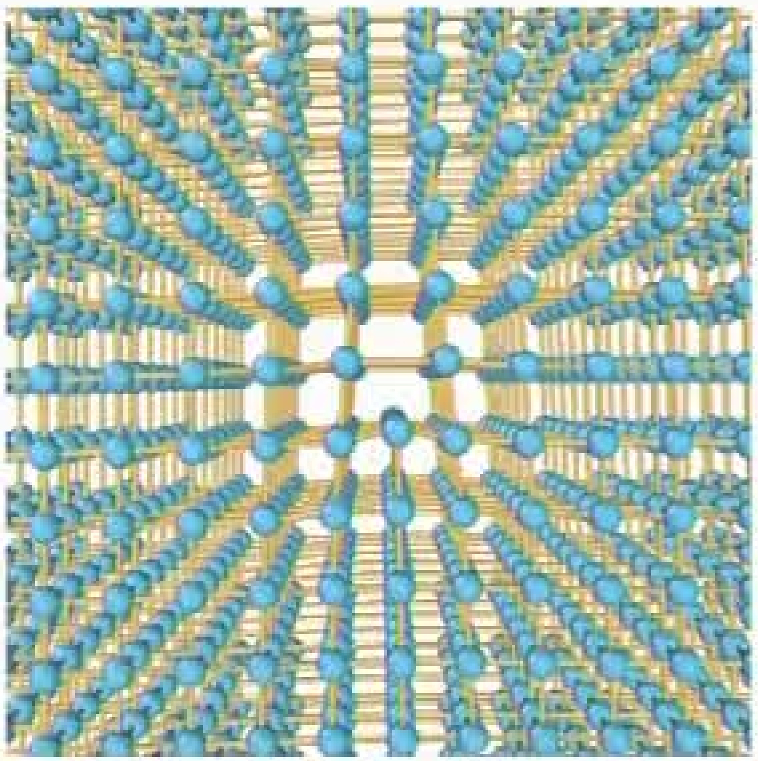
vacancy



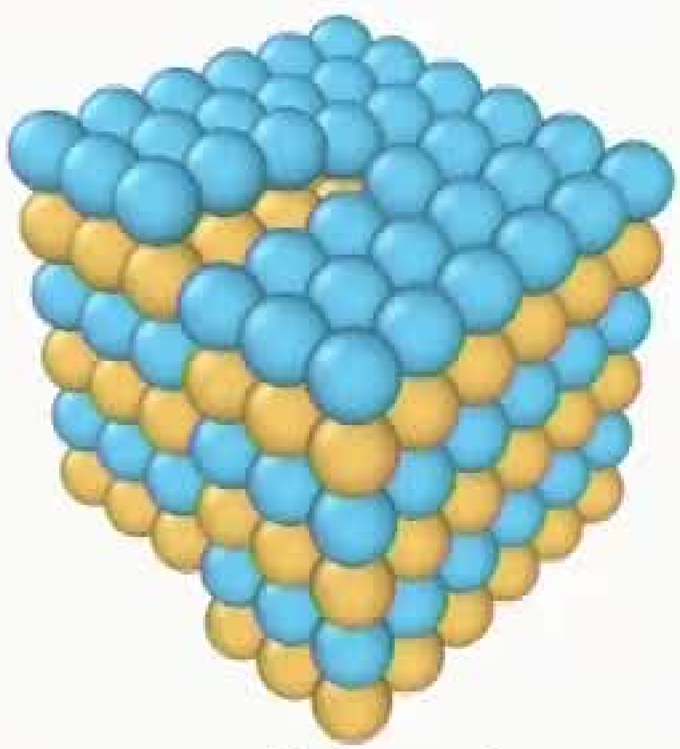
interstitial



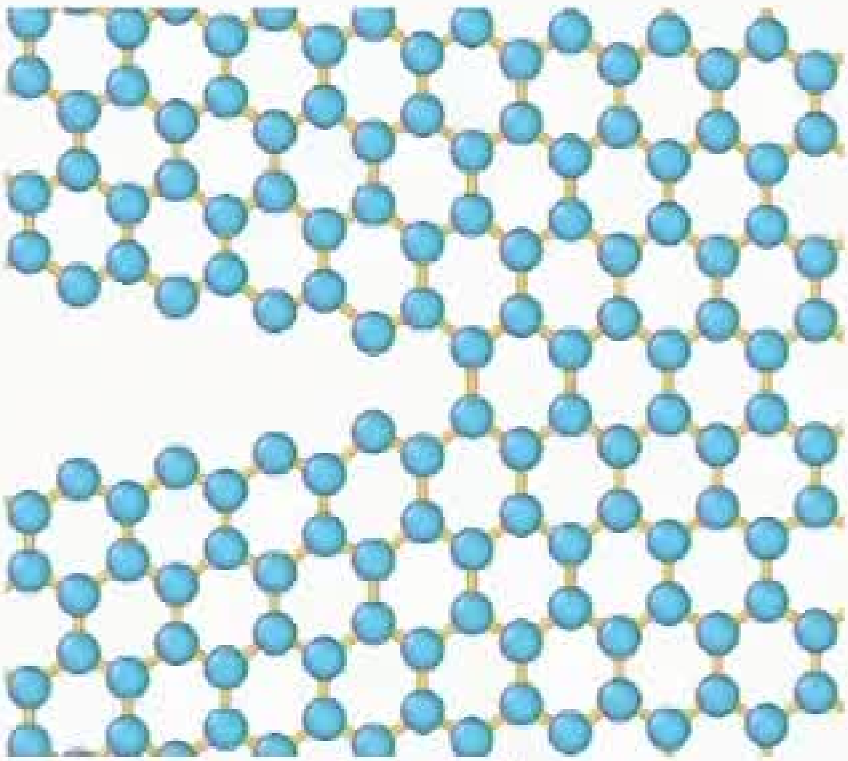
Stone-Wales defect



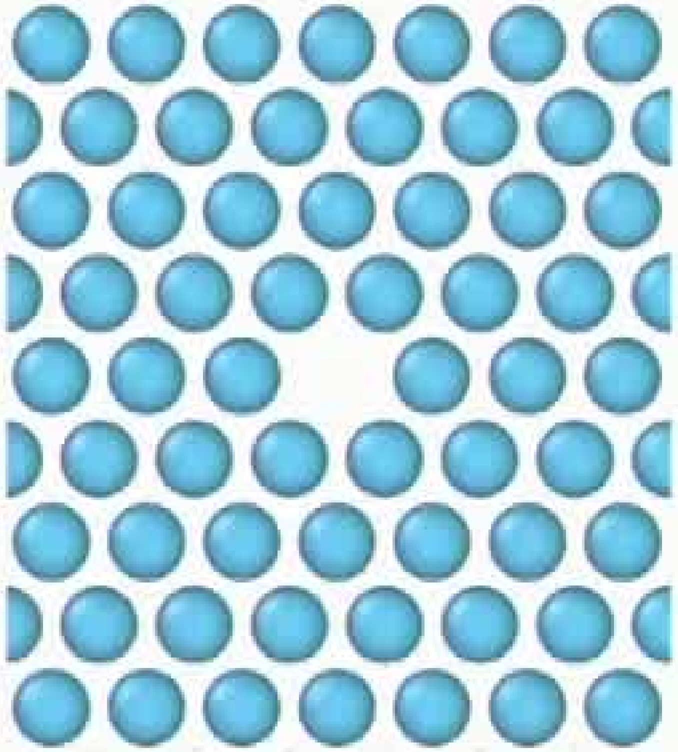
edge dislocation

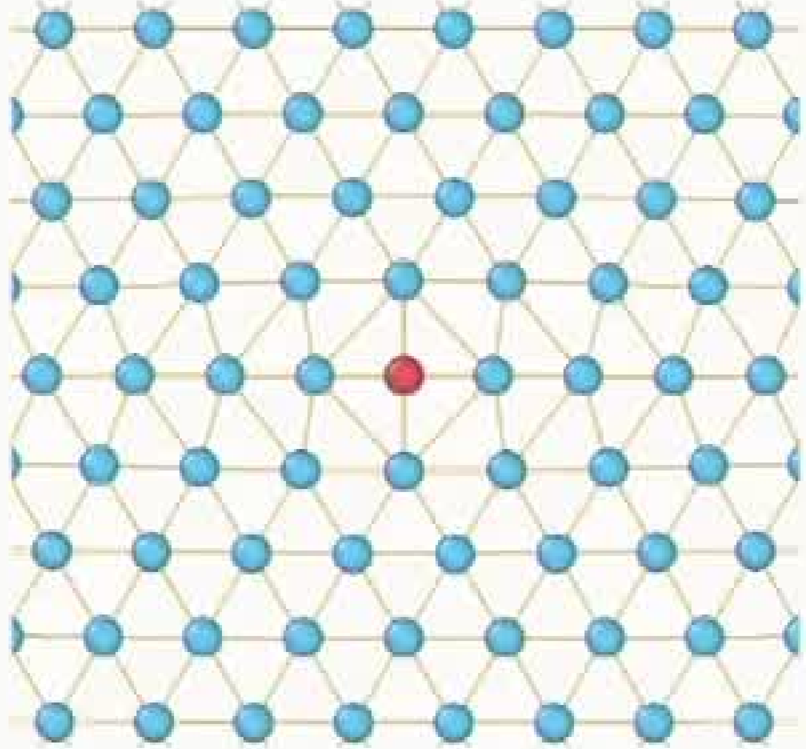


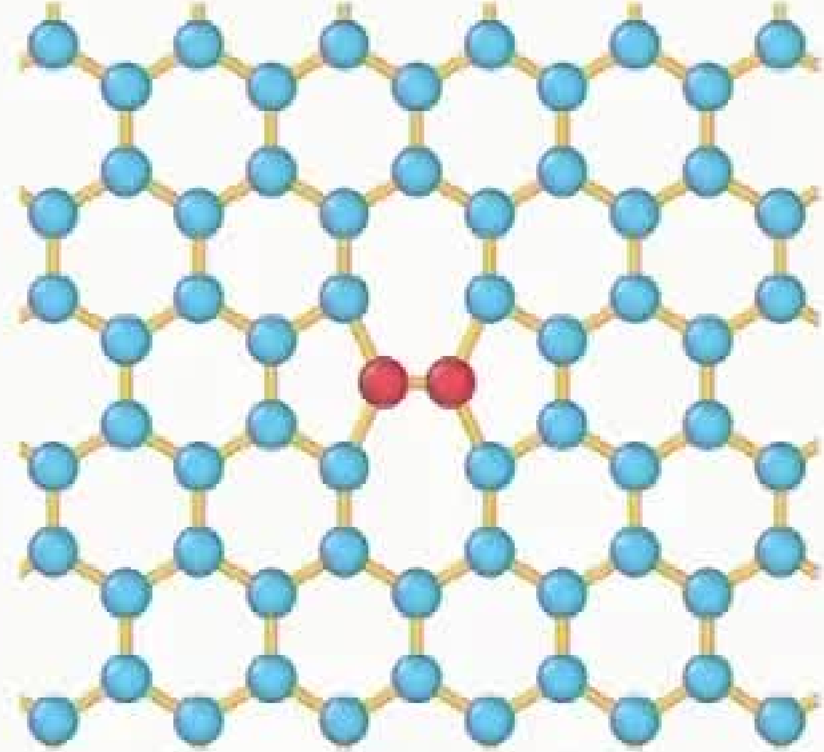
screw dislocation

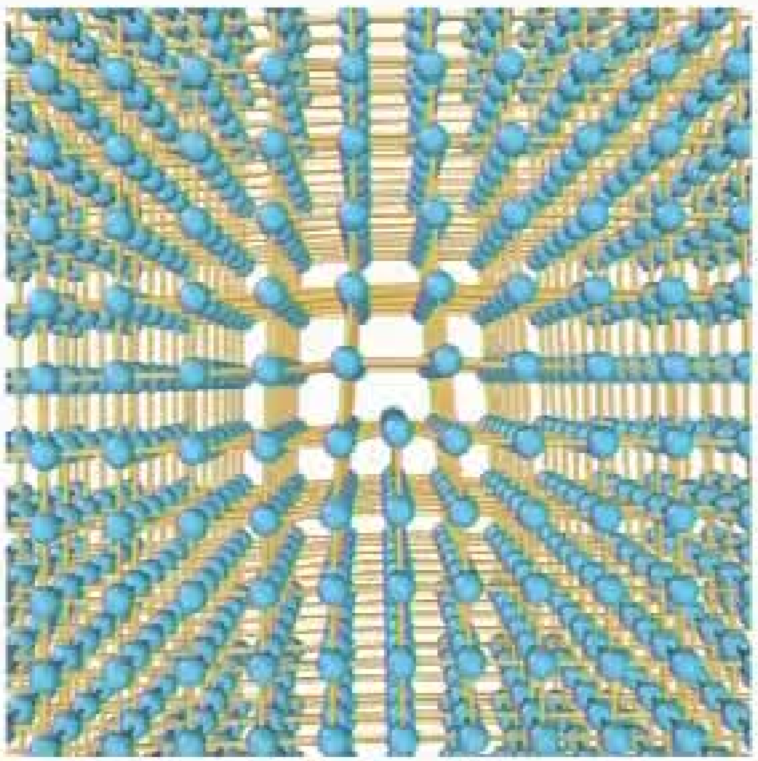


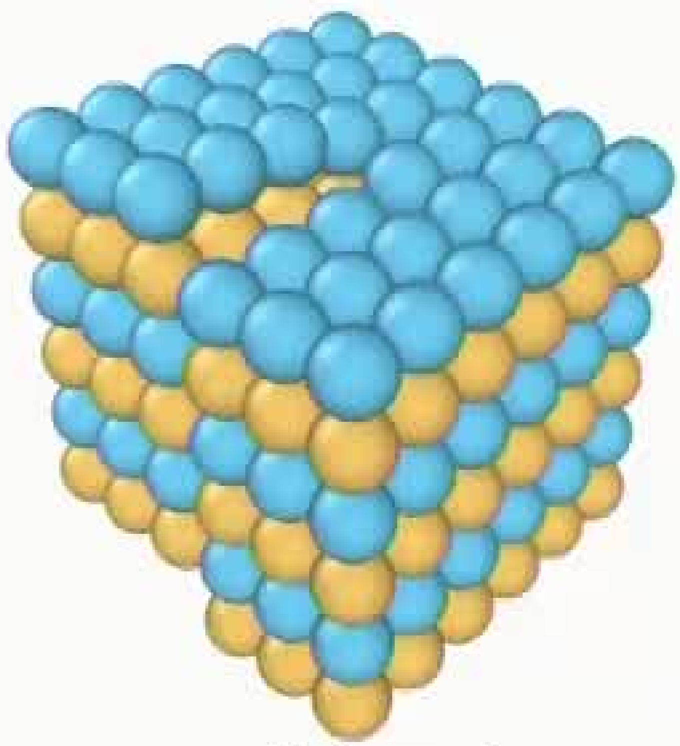
crack

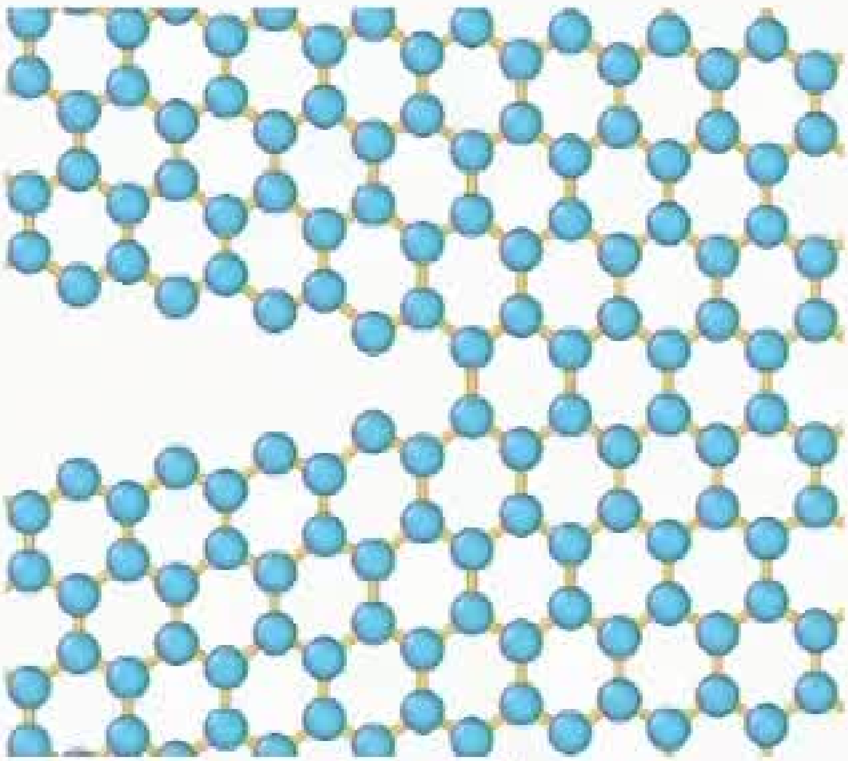

vacancy

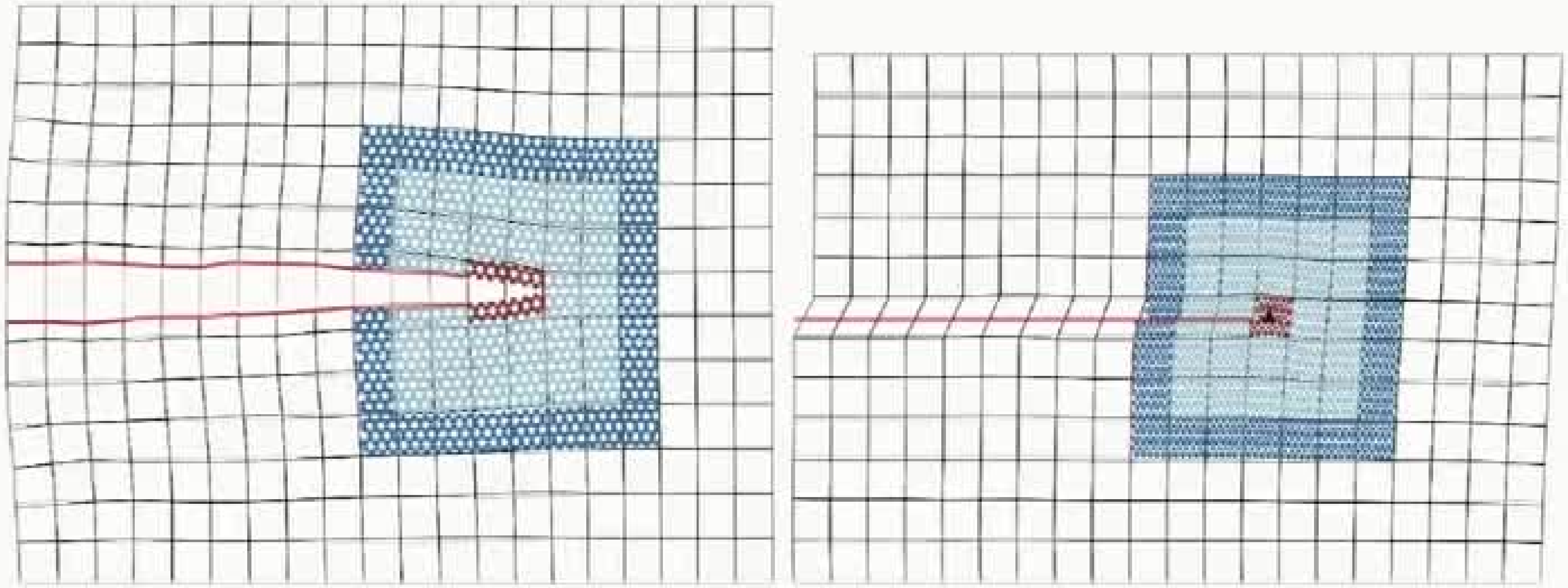

interstitial


Stone-Wales defect


edge dislocation


screw dislocation

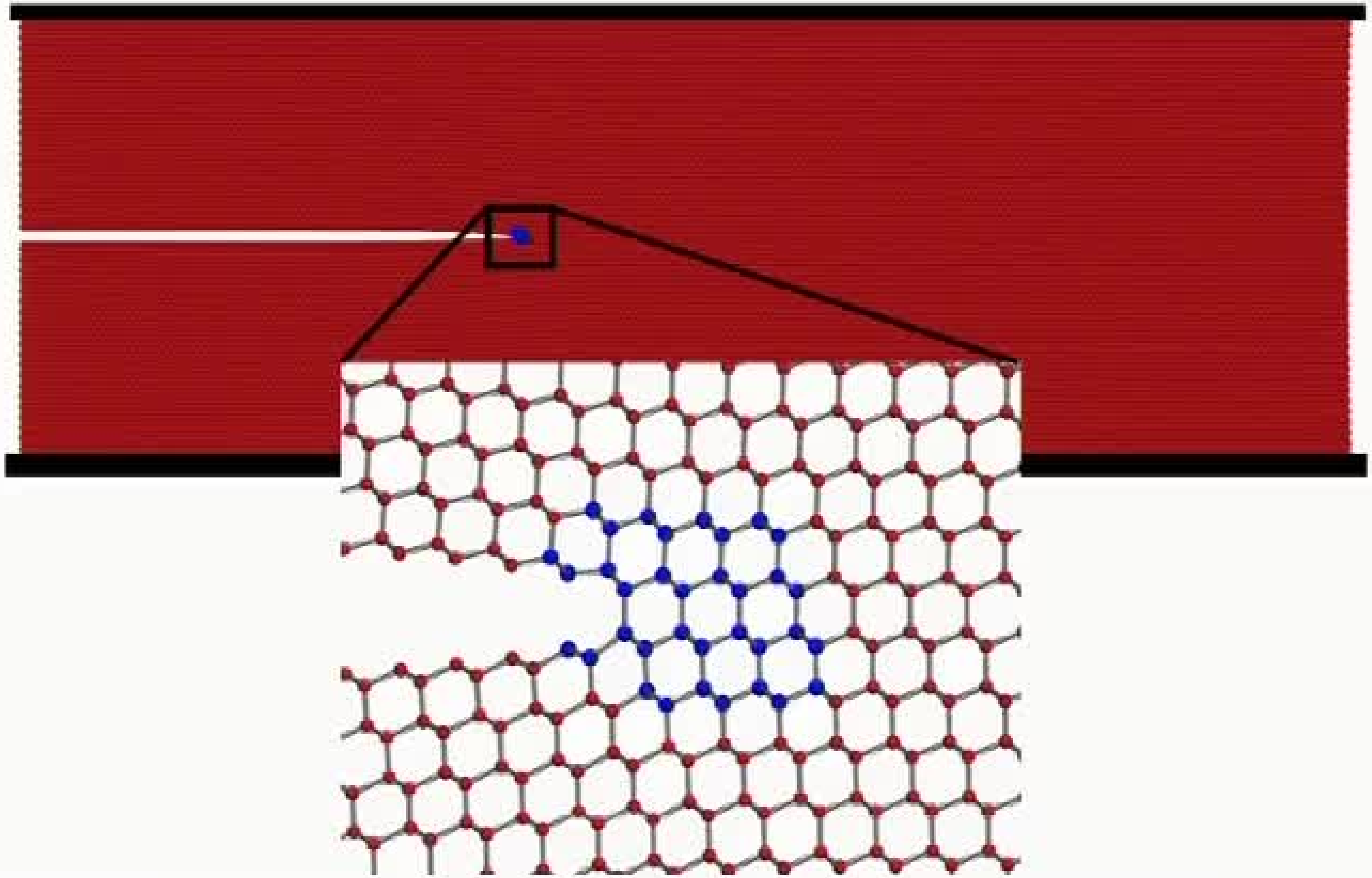

crack



(1) A crack in graphene (2) A dislocation in a hexagonal lattice

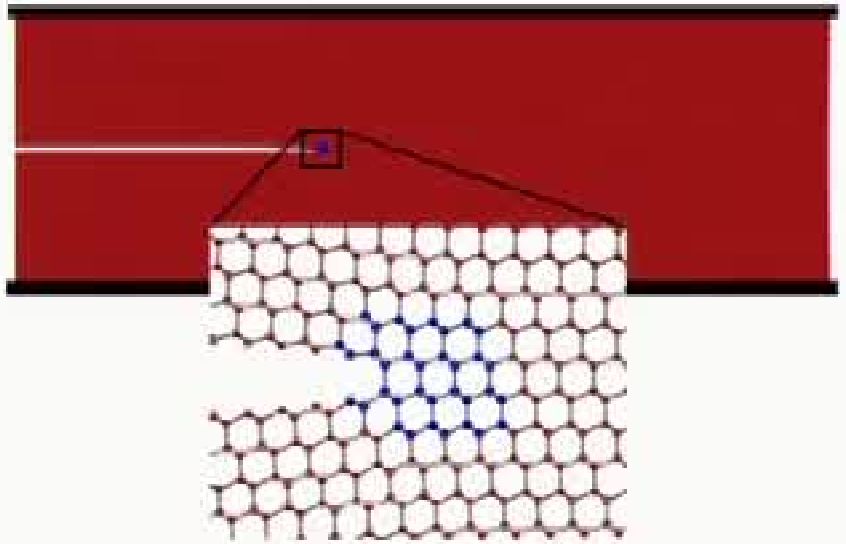
A/C Coupling
(quasi-continuum)

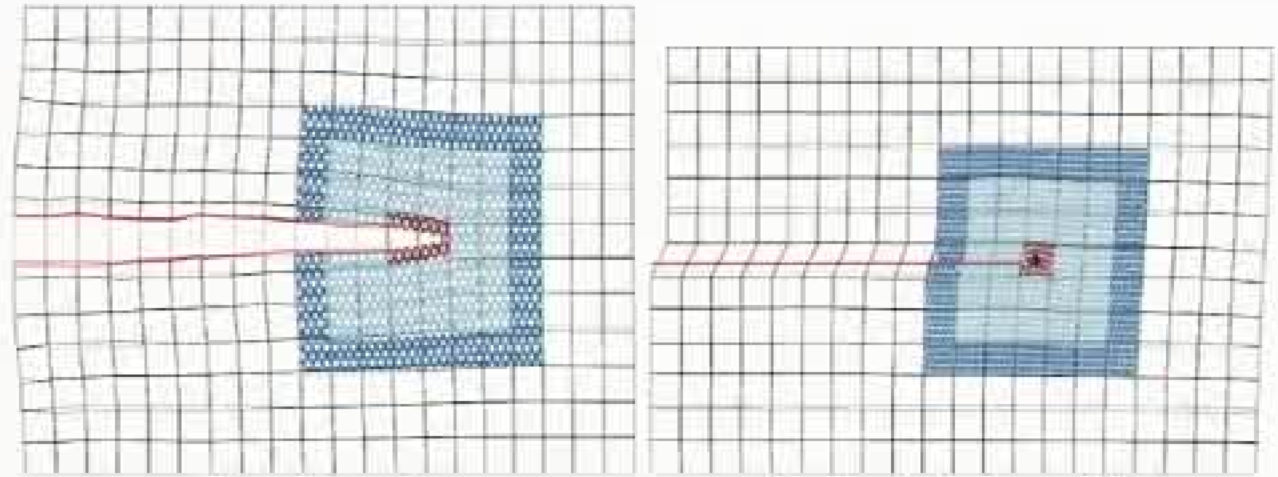
[Moseley, Oswald & Belytschko, 2013]



QM/MM Coupling

[Kermode, Albaret, Sherman, Bernstein, Gumbsch, Payne, Csanyi, de Vita; Nature, 2008]





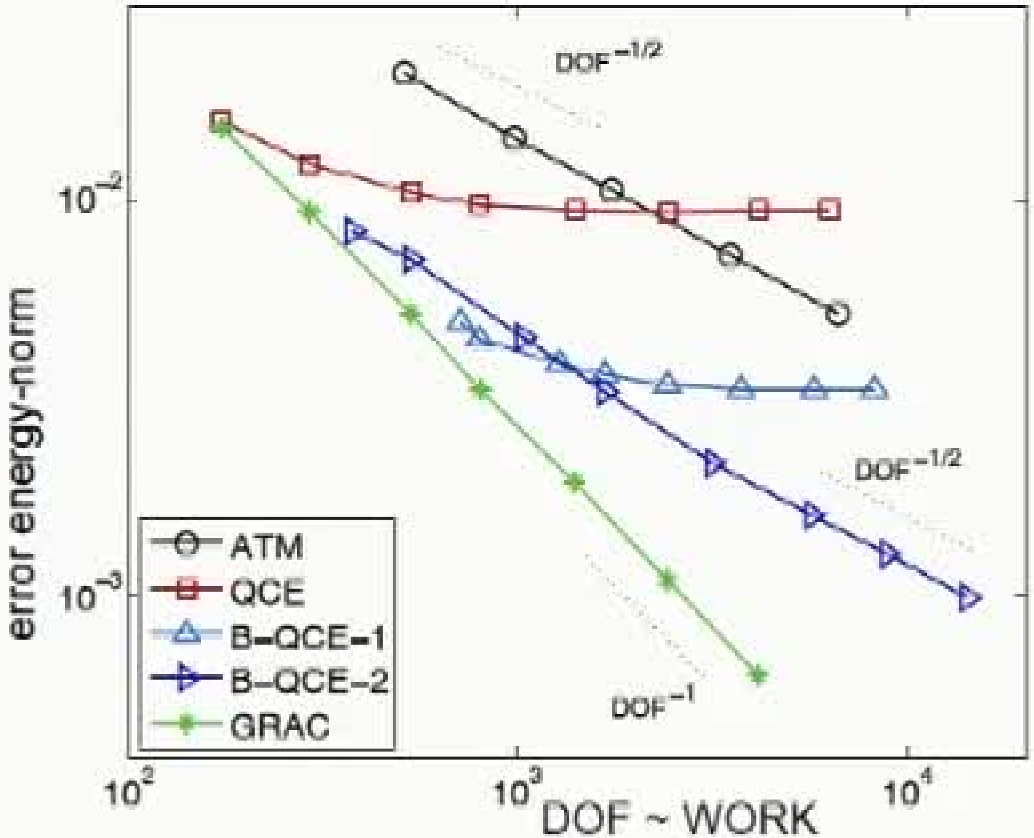
(1) A crack in graphene (2) A dislocation in a hexagonal lattice

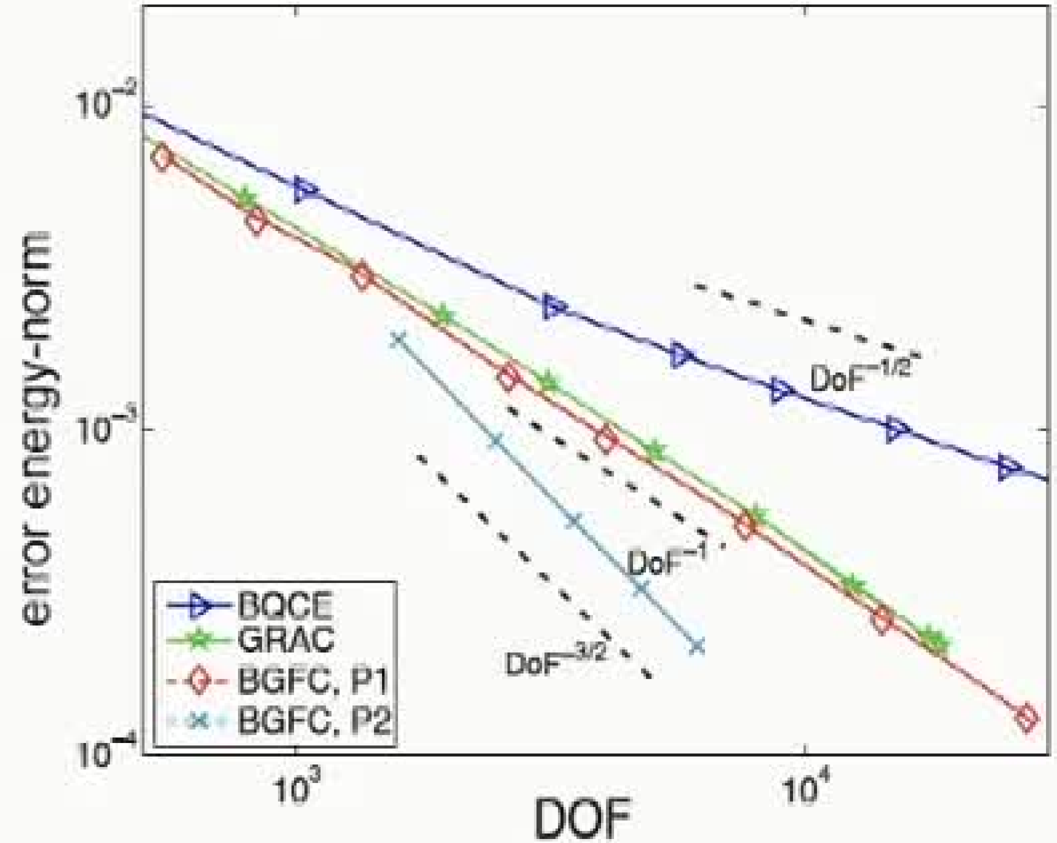
- **Concurrent multi-scale schemes** come in many, many variants:
  - **A/C, Quasicontinuum** [Tadmor, Ortiz, Kochmann, Geers, Belytschko, ...]
  - **QM/MM** [Kaxiras, Bernstein, Csanyi, Kermode, Sherwood, Catlow, ...]
  - Flexible boundary conditions [Sinclair, Woodward, Rao, Trinkle, Li, ...]
  - CADD = Coupl. Atomistic and Discr. Disloc. Dyn. [Curtin, Miller, ...]
  - QM-to-Continuum Coupling [Gavini, Bhattacharya, Suryanarayana, ...]
  - ...

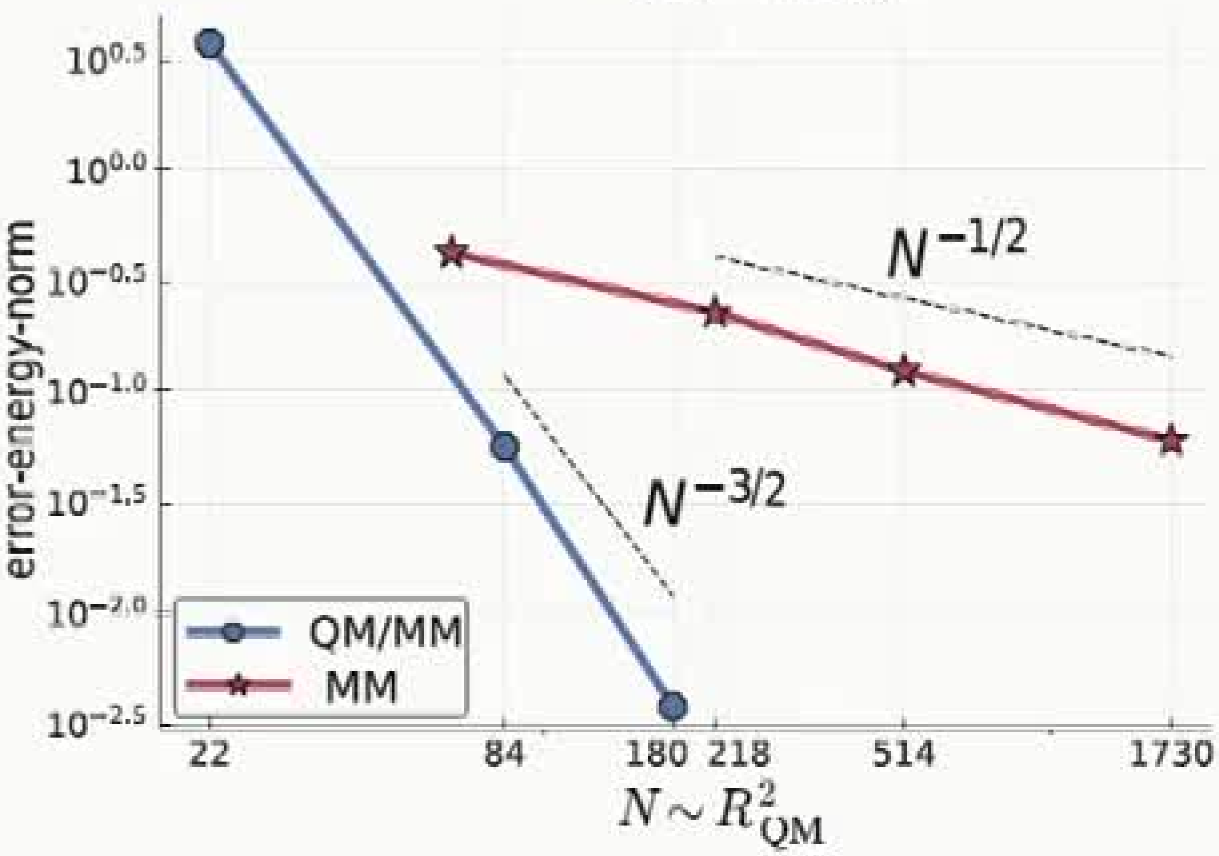
- **Central Challenge: interface coupling mechanism**

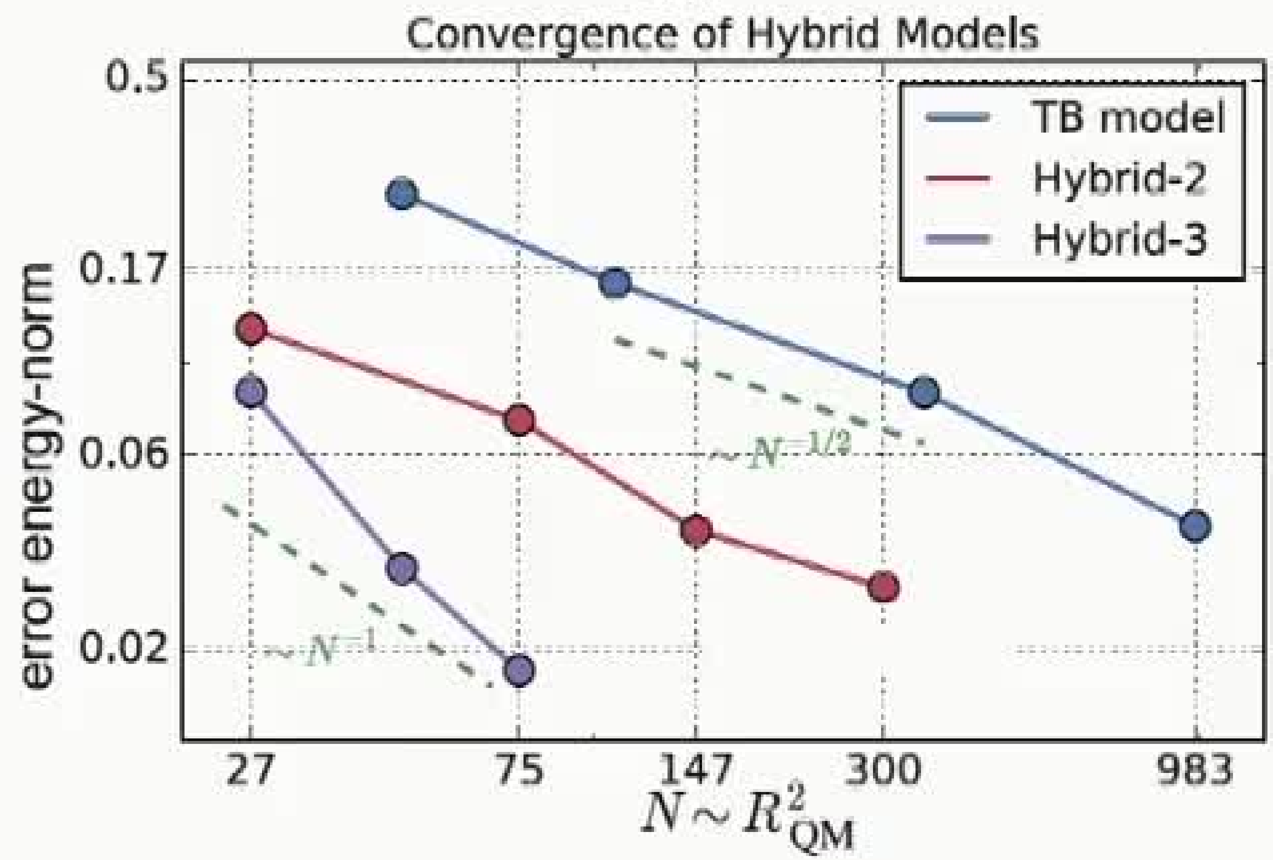
- **Today's Talk:** evaluate from a numerical analysis perspective
  - separate code, model, approximations
  - estimate approximation error
  - identify and remove bottlenecks
  - balance approximation parameters ⇒ optimise!

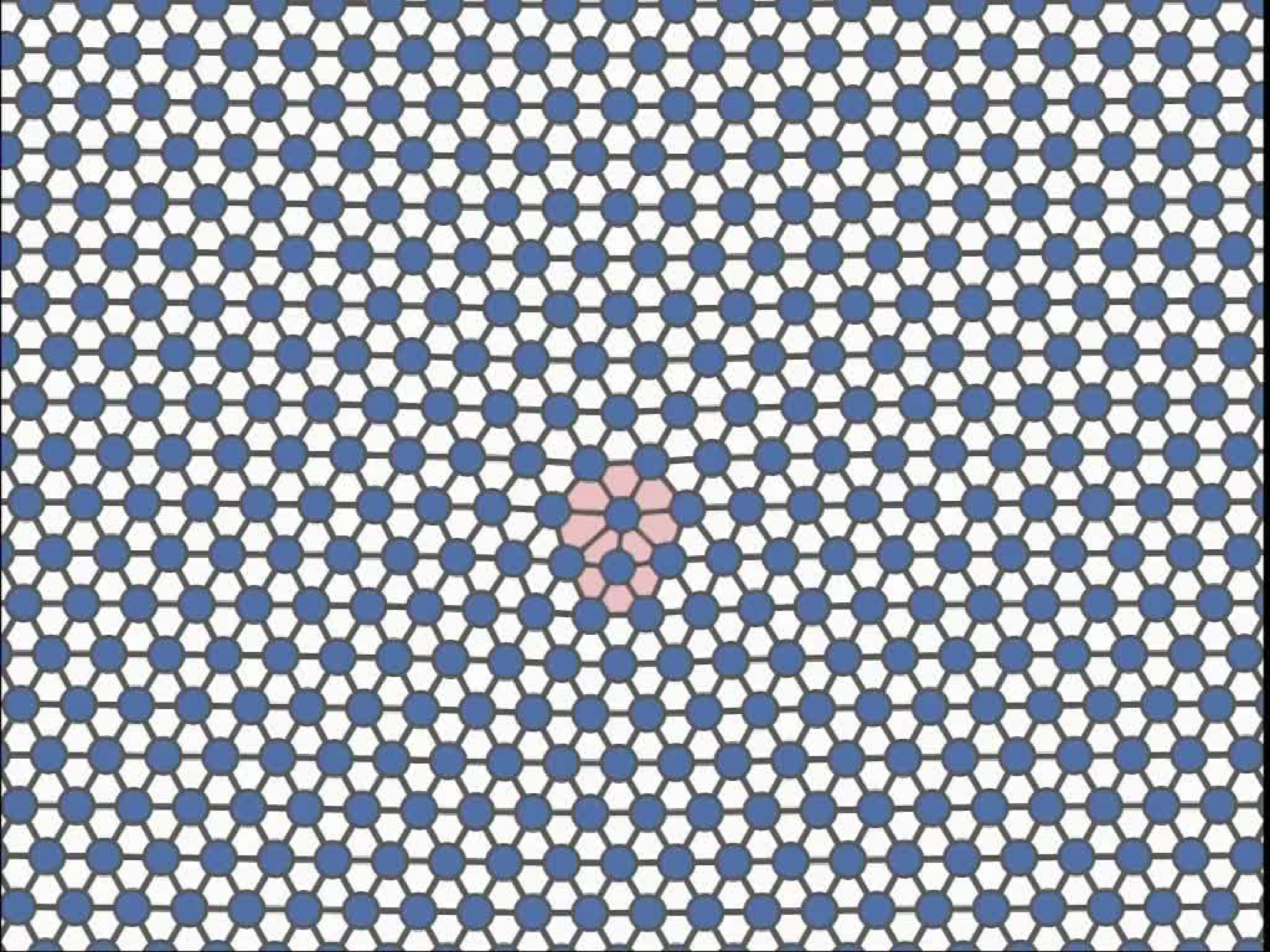
The Goal of Numerical Analysis

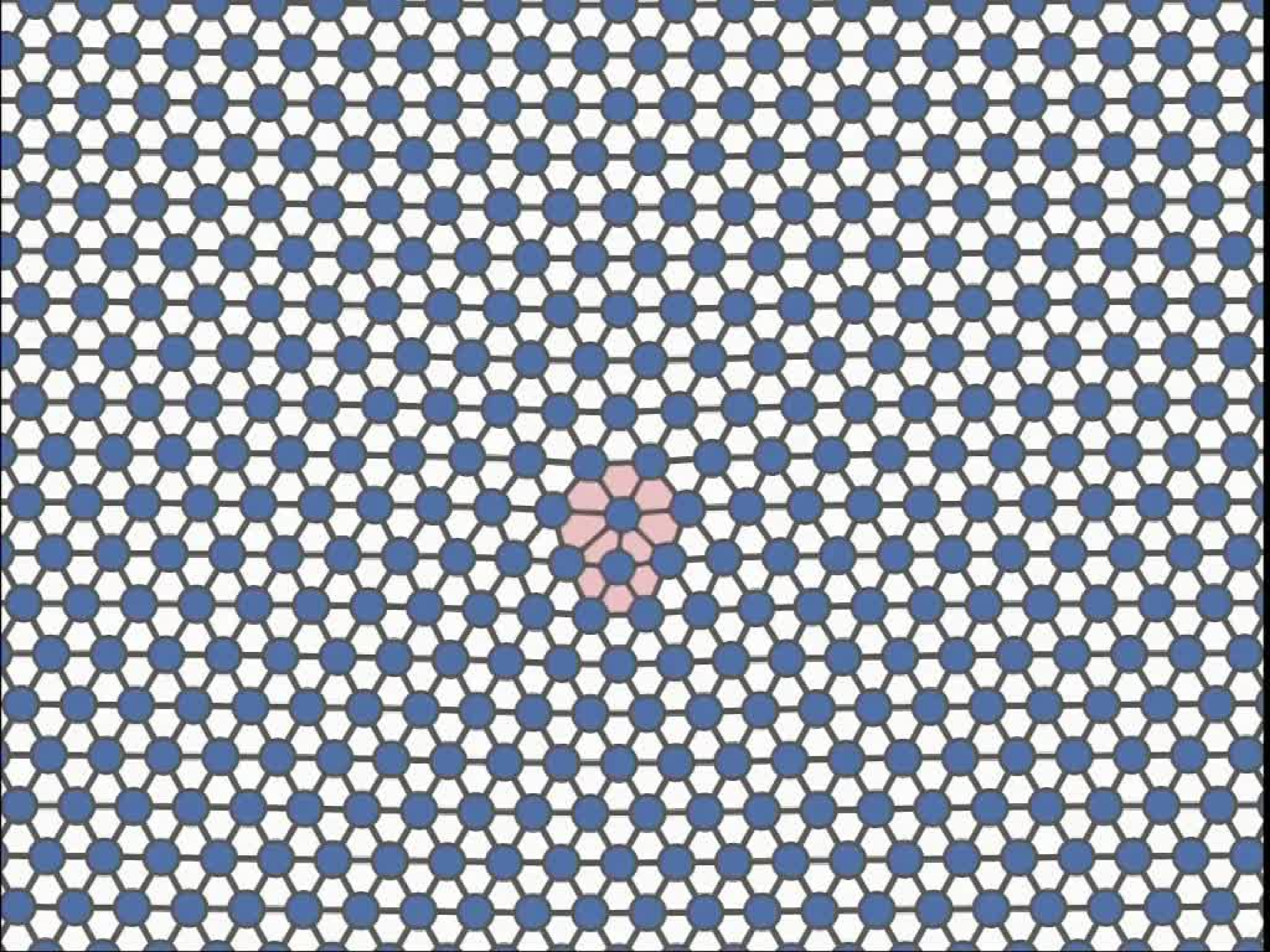












Lennard-Jones Cluster Model for Edge Dislocation

Positions: $y = (y_\ell)_{\ell \in \Omega_R} \subset \mathbb{R}^d$

Energy: $E(y) := \sum_{i \neq j} \phi_{\mathrm{LJ}}(r_{ij}) = \sum_\ell E_\ell(y)$

$$\bar{y}_R \in \arg\min E(y) \quad \text{subj.to} \quad y_\ell = y_\ell^{\mathrm{FF}} \text{ for } \ell \in \partial\Omega_R$$

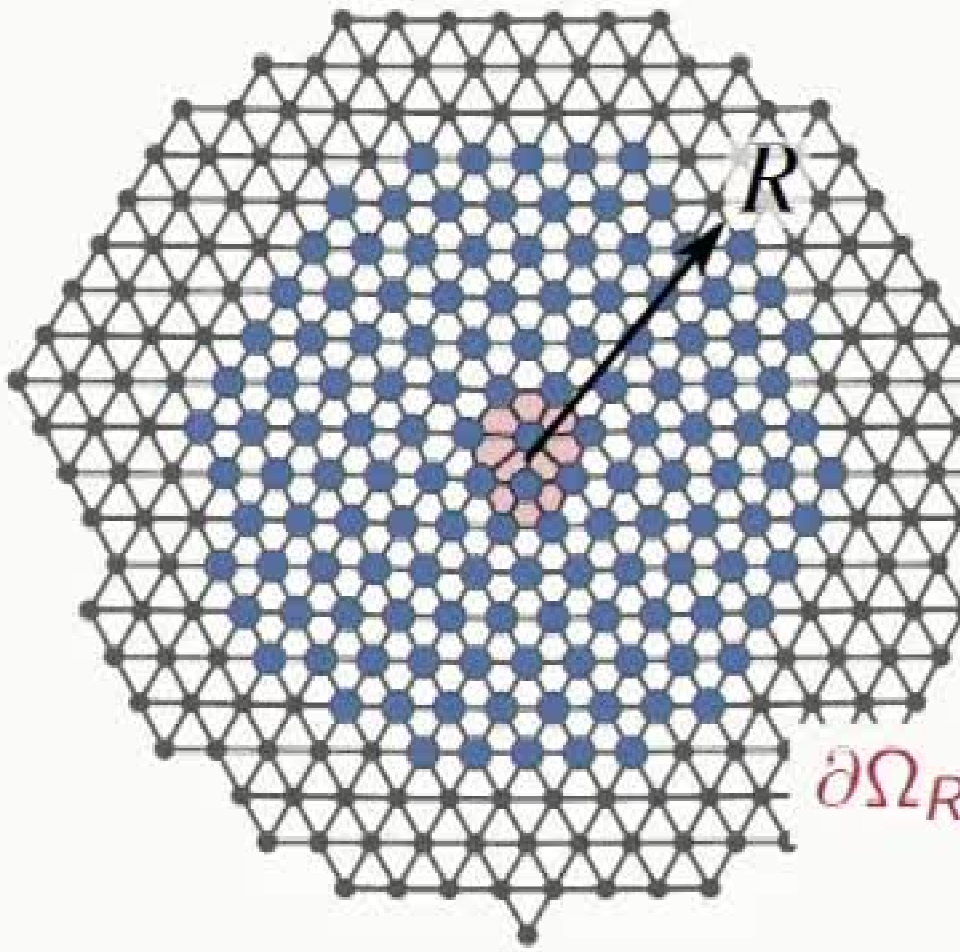
$$y_\ell^{\mathrm{FF}} := x_\ell + w(x_\ell)$$

$$\operatorname{div} \mathbb{C} : \nabla w = 0$$

$$(w^+ - w^-)|_\Gamma = b$$

$$(\nabla w^+ - \nabla w^-)|_\Gamma = 0$$

$$\text{net-force} = 0$$



Convergence as $R \to \infty$?

Limit Model $R \to \infty$

Hudson/CO/2015; Ehrlacher, Shapeev, CO/2016

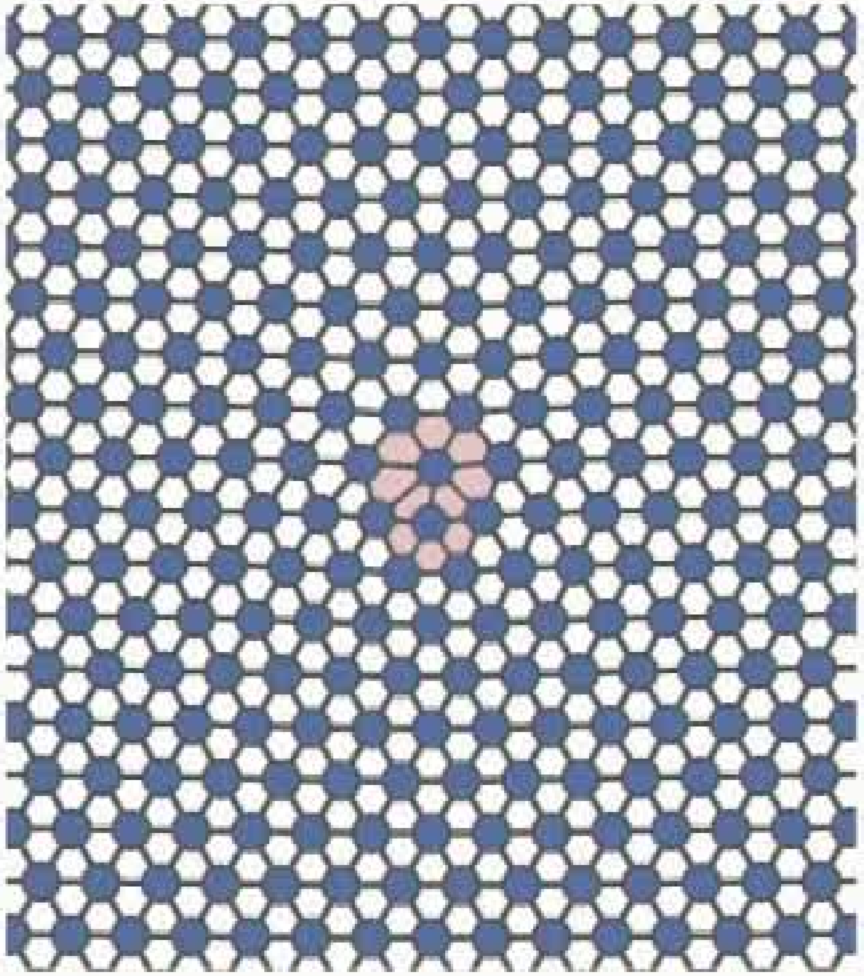
$$\bar{u} \in \arg\min \{ \mathcal{E}(u) \mid u \in \mathcal{H}_E \}$$

$$\mathcal{E}(u) := \sum_\ell E_\ell(y^{\mathrm{FF}} + u) - E_\ell(y^{\mathrm{FF}})$$

$$\mathcal{H}_E := \{ \text{ finite-}\mathcal{E} \text{ displacements} \}$$

$$\|u\|_E \approx \|\nabla u\|_{L^2}$$

Far-field b.c. encoded in $\boxed{y = y^{\mathrm{FF}} + u}$



Theorem 1: $\mathcal{E} \in C^k(\mathcal{H}_E)$ for some k, i.e., "$\mathcal{E}(u)$ is well-defined and well-behaved"

Theorem 2: $|\nabla^j \bar{u}(x)| \lesssim |x|^{-1-j}$

Proof: $$\mathcal{E}(u) = \sum_\ell \underbrace{\Big(E_\ell(y^{\mathrm{FF}} + u) - E_\ell(y^{\mathrm{FF}}) - \langle \delta E_\ell(y^{\mathrm{FF}}), u \rangle \Big)}_{\sim |Du_b|^2 \sim |\nabla u|^2} + \langle f, u \rangle$$

Conceptual key point: $\boxed{|f_\ell| \lesssim |\ell|^{-3} \quad \Rightarrow \quad \langle f, u \rangle \le C\|u\|_E}$

Atomistic Cell Problem as a Galerkin Approximation

1. **Exact Model:**

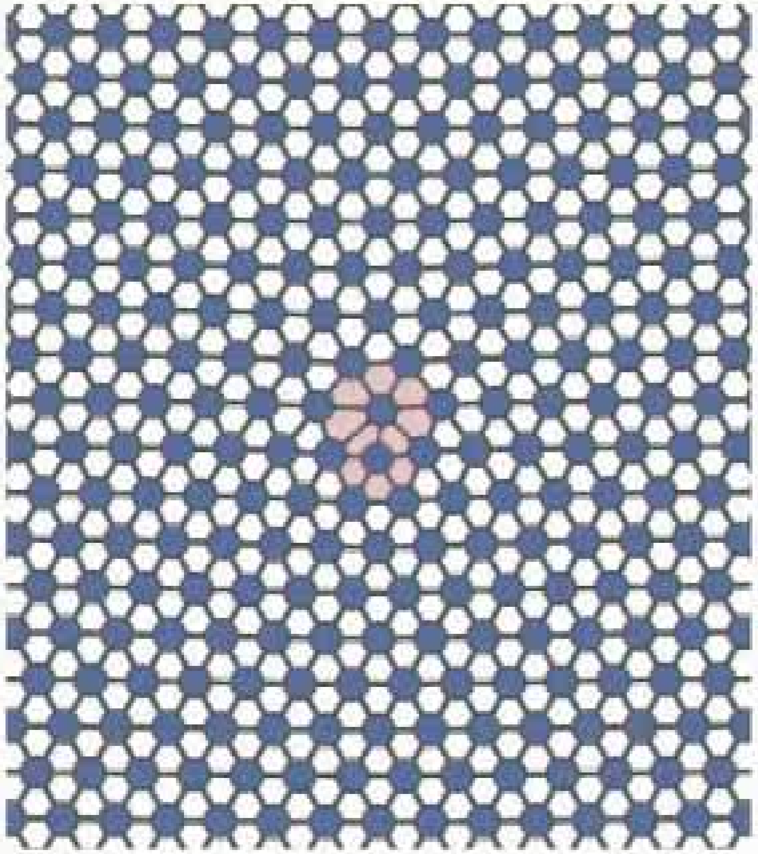
$$\bar{u} \in \arg\min \{ \mathcal{E}(u) \,|\, u \in \mathcal{H}_E \}$$

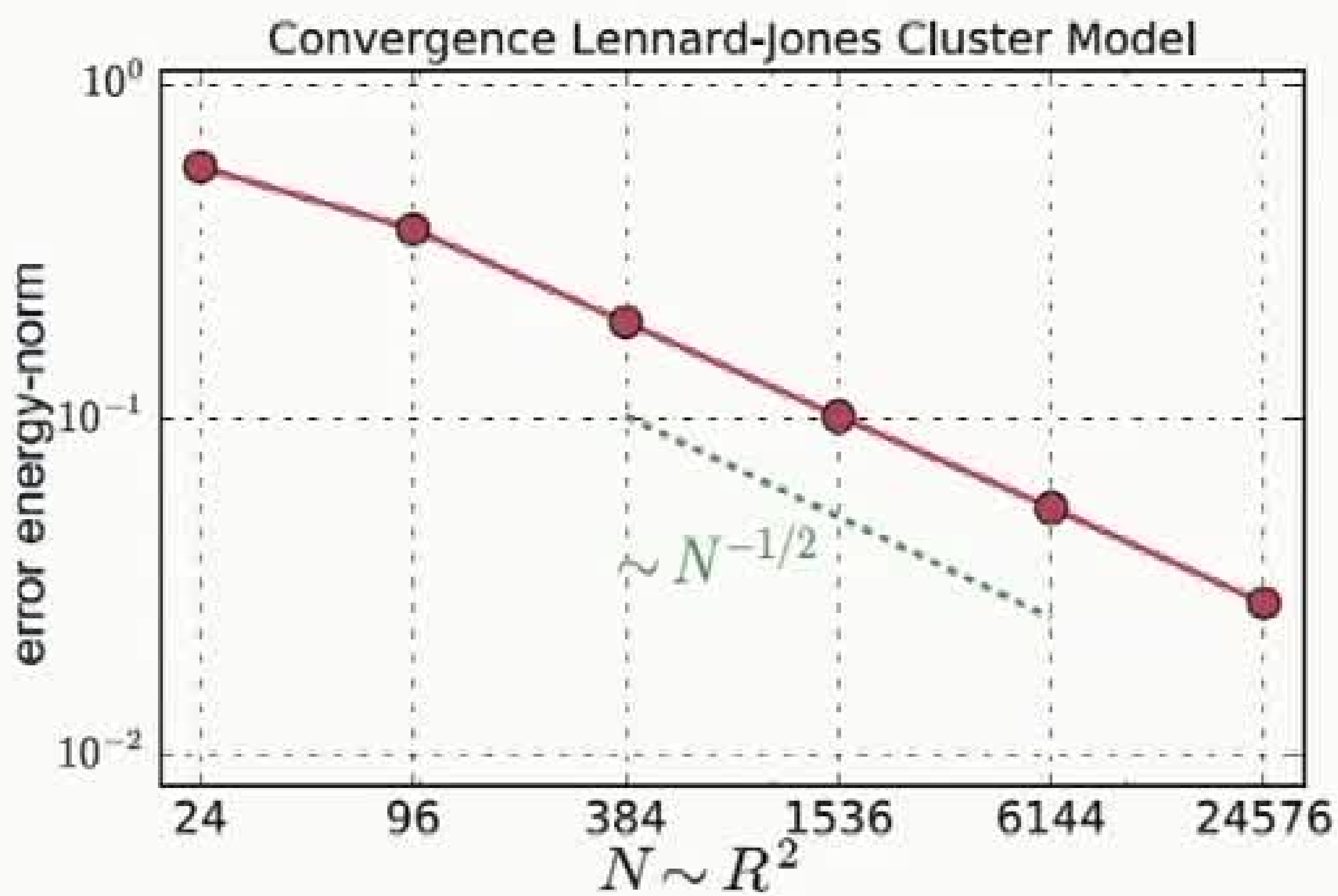
2. **Cell Problem as Galerkin Approx:**

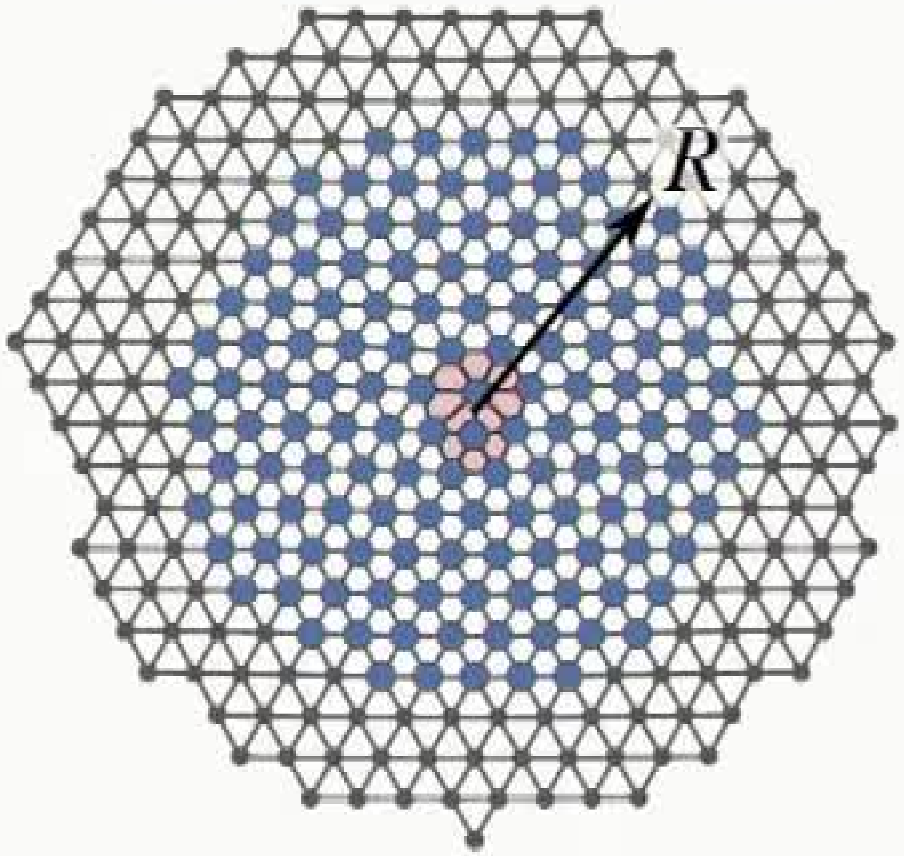
$$\bar{u}_R \in \arg\min \{ \mathcal{E}(u) \,|\, u \in \mathcal{H}_R \}$$

3. **Convergence Rate:**

$$\|\bar{u} - \bar{u}_R\|_E \lesssim R^{-1} \approx N^{-1/2}$$





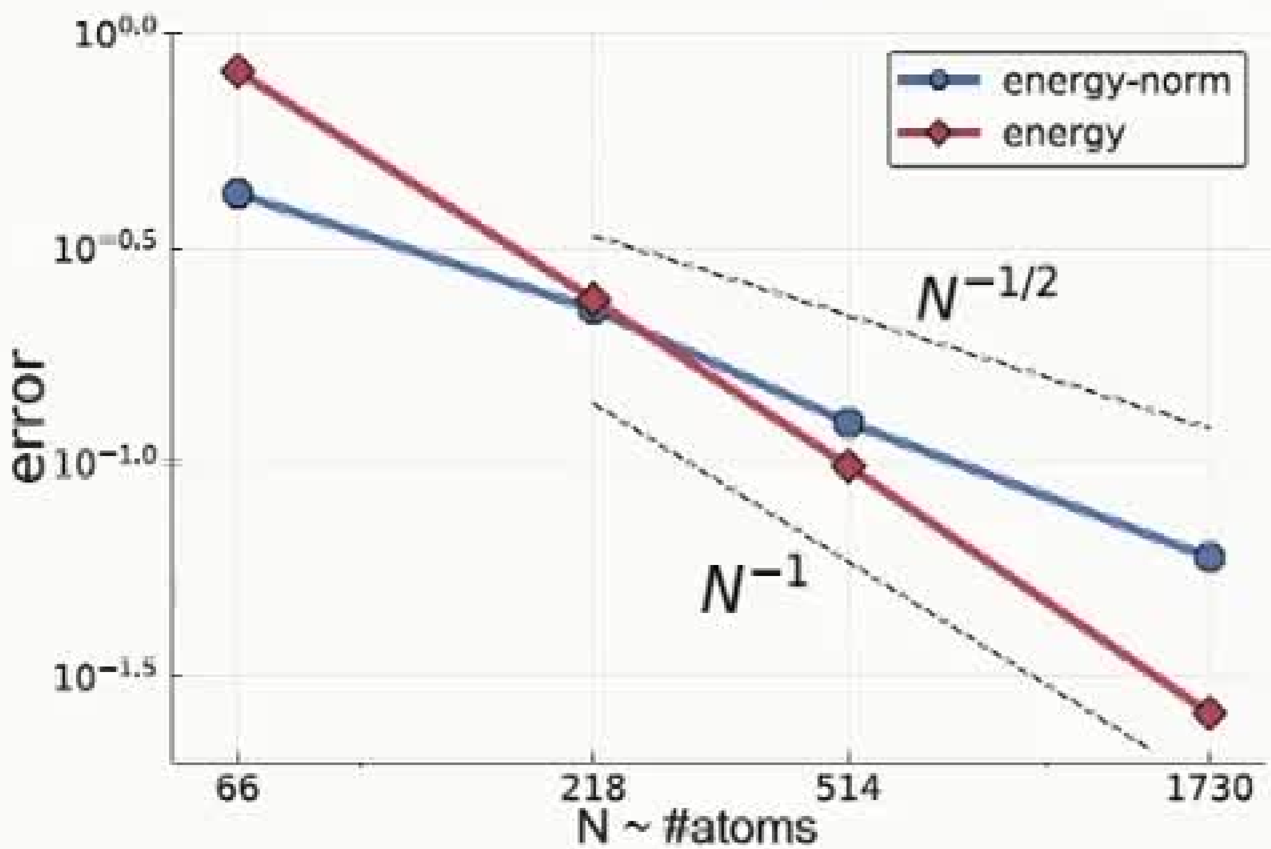


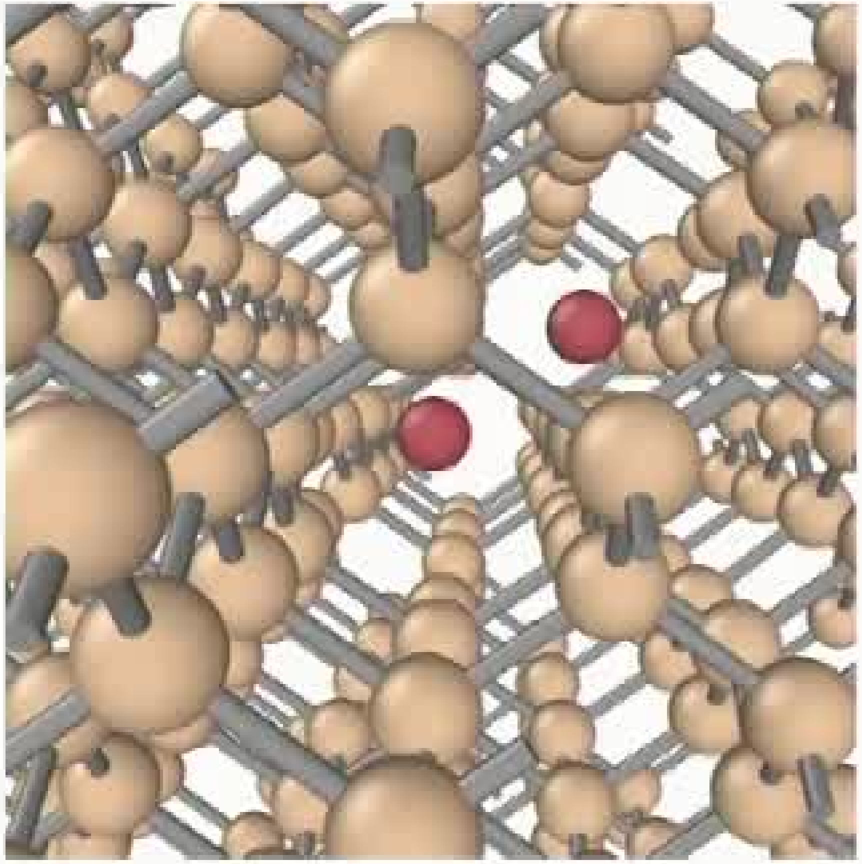
The rate $N^{-1/2}$ is UN-surprisingly generic

$$\|\bar{u} - \bar{u}_R\|_E \lesssim N^{-1/2} \log^r N$$

- all point defects (2D and 3D) in Bravais and multi-lattices [Olson, CO, 2017]

Di-Insterstitial, bulk Si, Stillinger-Weber Potential





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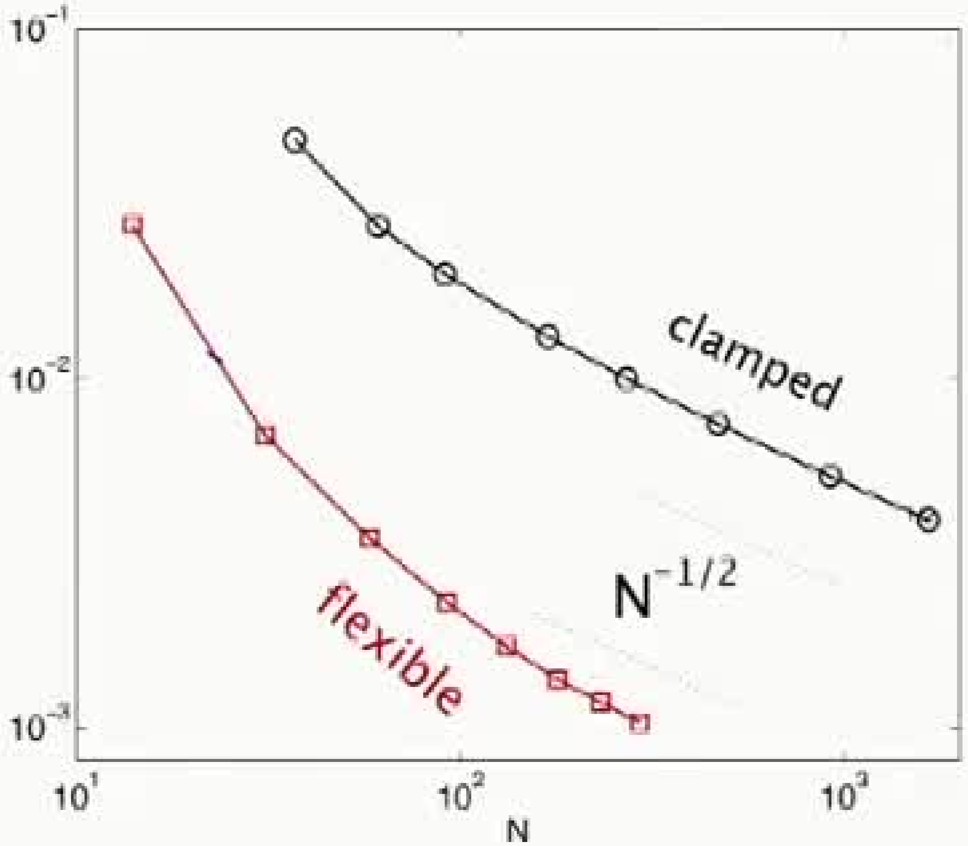
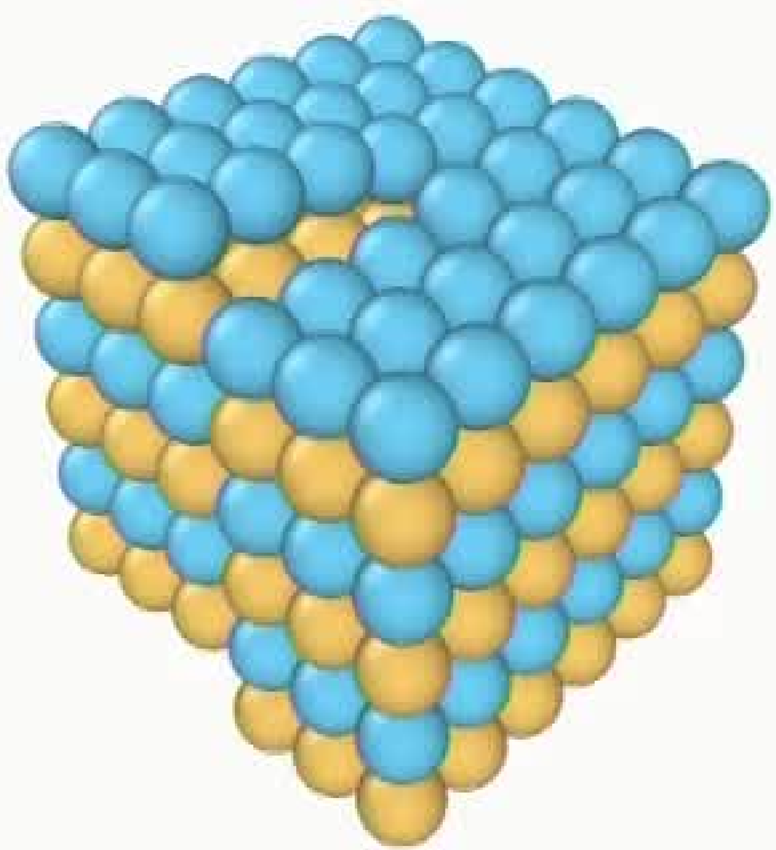
- all straight dislocations (Bravais and high-symmetry multi-lattice)
- clamped, periodic and flexible boundary conditions

Screw Dislocation (EAM Toy Model)





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- all point defects (2D and 3D) in Bravais and multi-lattices [Olson, CO, 2017]
- all straight dislocations (Bravais and high-symmetry multi-lattice)
- clamped, periodic and flexible boundary conditions

General Question: Improve the bdry condition to improve the rate?

Thu 04:30, Room # D129 Julian Braun: A Hierarchy of Boundary Conditions for Crystal Defect Calculations

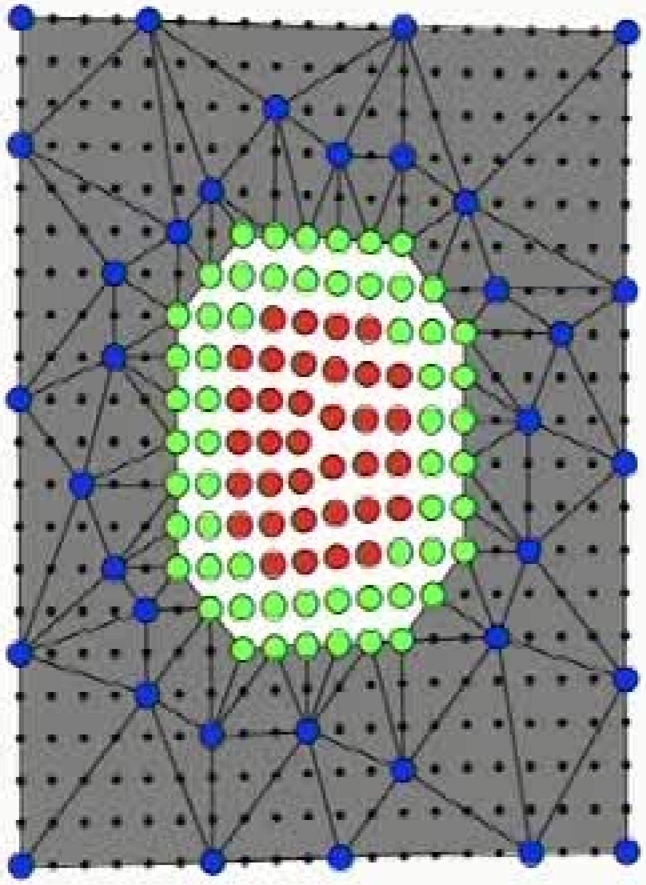
Rest of the Talk: Beat $N^{-1/2}$ using multi-scale approaches.

II. A/C Coupling
Quasicontinuum

joint work with
Mitch Luskin (UMN), A Shapeev (Skoltech), Derek Olson (RPI), Xingjie Li (UNC), Brian Van Koten (Amherst), Matthew Dobson (Amherst), Hao Wang (Sichuan), Lei Zhang (Jiaotong), Endre Süli (Oxford), Charalambos Makridakis (Sussex).

- C. Ortner and L. Zhang, Atomistic/Continuum Blending with Ghost Force Correction, SIAM J. Sci. Comput., 2016
- X. H. Li and C. Ortner and A. Shapeev and B. Van Koten, Analysis of blended atomistic/continuum hybrid methods, Numer. Math., 2016
- C. Ortner and A. Shapeev and L. Zhang, (In-)Stability and Stabilisation of QNL-Type Atomistic-to-Continuum Coupling Methods, SIAM Multiscale Model. Simul., 2014
- D. Olson and X. Li and C. Ortner and B. Van Koten, Force-Based Atomistic/Continuum Blending for Multilattices, to appear in Numer. Math.

Sharp-Interface Coupling



$y^{\mathrm{AC}} \in \arg\min \{ E^{\mathrm{AC}} \,|\, \text{b.c.} \}$

$$E^{\mathrm{AC}}(y) = \sum_{\ell \in \Omega^{\mathrm{A}}} E_\ell^{\mathrm{A}}(y) + \sum_{\ell \in \Omega^{\mathrm{I}}} E_\ell^{\mathrm{I}}(y) + \int_{\Omega^{\mathrm{C}}} W(\nabla y)$$

E_ℓ^{I} is chosen to minimise spurious interface forces, in particular "ghost forces": $\nabla E^{\mathrm{AC}}(Fx) = \mathrm{GF}(F)$

- $\boxed{E_\ell^{\mathrm{I}} = E_\ell^{\mathrm{A}}}$: Original Quasicontinuum Method

  [Tadmor, Ortiz, Phillips, 1996]

  Cauchy–Born Model: $W(F) \propto E_\ell^{\mathrm{A}}(Fx)$

- $\boxed{E_\ell^{\mathrm{I}}(y) = E_\ell^{\mathrm{A}}(R_\ell y)}$: Geometric Reconstruction Method

  [Shimokawa et al (2004); E, Lu, Yang, 2006]

  [Shapeev (2011); Li/Luskin (2012); CO/Zhang (2012,14)]

(Fun Fact: General construction of R_ℓ still open)

Sharp Interface Coupling: Error Estimate

M-Theorem: (Lax/Richtmyer, 1956)

ERROR ≈ STABILITY × CONSISTENCY

$$y^{\mathrm{A}} - y^{\mathrm{AC}} \approx \big[\nabla^2 E^{\mathrm{AC}}\big]^{-1}\big[\nabla E^{\mathrm{A}} - \nabla E^{\mathrm{AC}}\big]$$

Theorem: [Dobson/Luskin/2009; CO/2012; Dobson/2014; ...]

If y^{A} is a stable defect, the A/C method is stable, and GF is suff. small, then $\exists y^{\mathrm{AC}} \in \arg\min E^{\mathrm{AC}}$ s.t.

$$\|y^{\mathrm{A}} - y^{\mathrm{AC}}\|_E \lesssim C_{\mathrm{stab}}\big(\|\mathrm{GF}\|_{L^2(\Omega^{\mathrm{I}})} + \|\nabla^3 y^{\mathrm{A}}\|_{L^2(\Omega^{\mathrm{C}})} + \text{FEM-ERR.} + R_{\mathrm{C}}^{-d/2}\big)$$

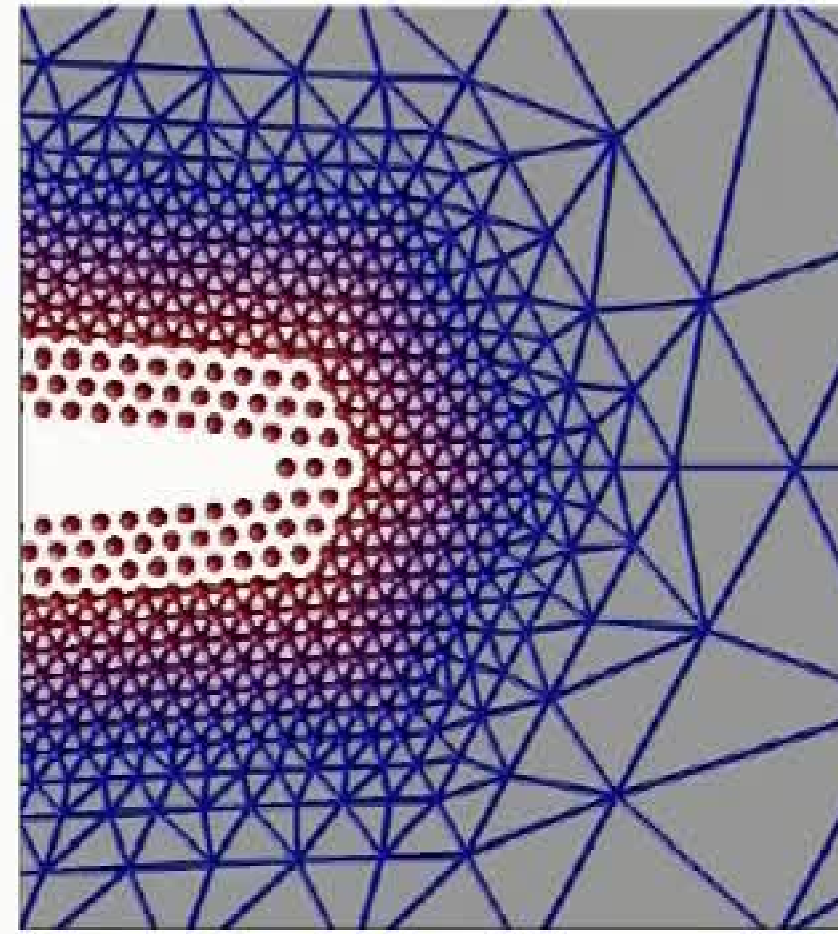
But unfortunately ...

Theorem: [CO, Shapeev, Zhang; 2014]

For every sharp-interface A/C method, there exist interatomic potentials such that $\nabla^2 E^{\mathrm{A}}(x) > 0$ but $\nabla^2 E^{\mathrm{AC}}$ is indefinite or even singular. 

Blending: The first "complete" result

$$E^{\mathrm{BQC}}(y) = \sum_{\ell \in \Omega^{\mathrm{A}}} (1 - \beta(\ell)) E_\ell^{\mathrm{A}}(y) + \int_{\Omega^{\mathrm{C}}} \beta W(\nabla y)$$



β : smooth blending function

Belytschko/Xiao (2004); Badia et al (2008); Baumann et al (2008); Lusking/VanKoten(2011); Luskin/CO/VanKoten (2012)

Theorem: Luskin/VanKoten (2011); Li/CO/Shapeev/VanKoten (2016)

If y^{A} is a stable defect, Ω^{A} is suff. large and β "suff. well adapted", then

1. Universal Stability: $\nabla^2 E^{\mathrm{BQC}}(y) > 0$ for $y \approx y^{\mathrm{A}}$ 
2. There exists $y^{\mathrm{BQC}} \in \arg\min E^{\mathrm{BQC}}$ s.t.

$$\|y^{\mathrm{BQC}} - y^{\mathrm{A}}\|_E \lesssim \|\nabla^2 \beta\|_{L^2(\Omega^{\mathrm{I}})} + \|\nabla^3 y^{\mathrm{A}}\|_{L^2(\Omega^{\mathrm{C}})} + \text{FEM ERR.} + R_{\mathrm{C}}^{-d/2}$$

Universal Stability

Task: $\langle \nabla^2 E^{\mathrm{BQC}}(y)v, v \rangle \geq c\|v\|_E^2$

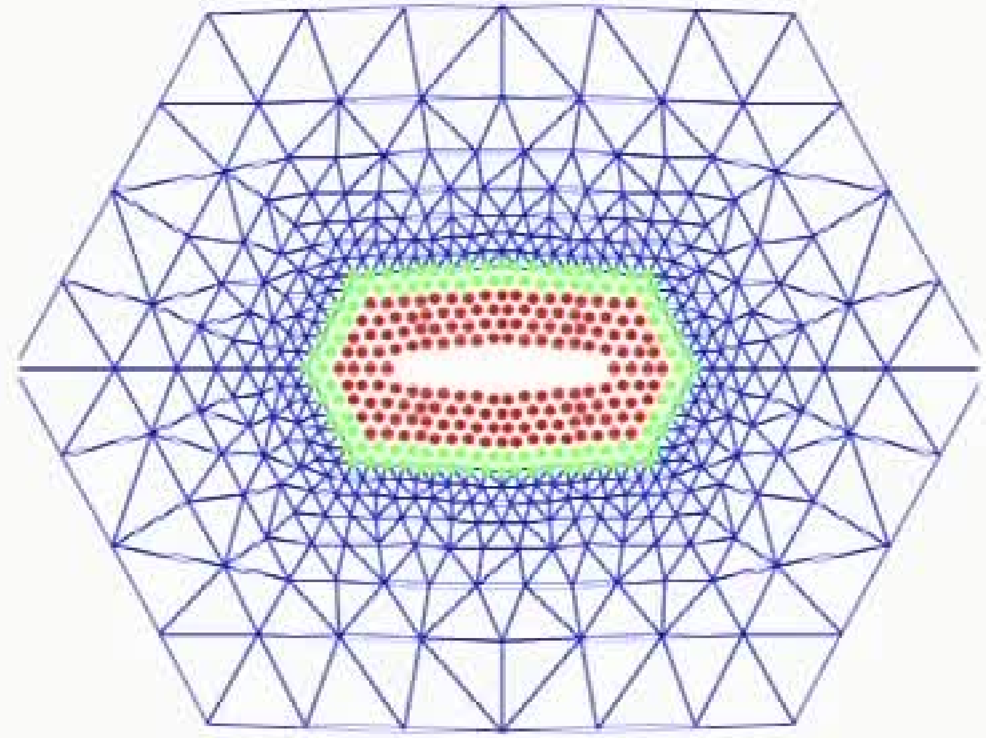
Decompose into three scales: $v = v^{\mathrm{A}} + v^{\mathrm{B}} + v^{\mathrm{C}}$

$$
\begin{aligned}
\langle \nabla^2 E^{\mathrm{BQC}}(y)v, v \rangle = &\ \langle \nabla^2 E^{\mathrm{A}}(y)v^{\mathrm{A}}, v^{\mathrm{A}} \rangle && \text{defect core is stable} \\
&+ \langle \nabla^2 E^{\mathrm{BQC}}(x)v^{\mathrm{B}}, v^{\mathrm{B}} \rangle && ??????? \\
&+ \langle \nabla^2 E^{\mathrm{C}}(x)v^{\mathrm{C}}, v^{\mathrm{C}} \rangle && \text{bulk continuum is stable} \\
&+ \text{ cross terms }.
\end{aligned}
$$

Key Issue:

- v^{B} converges weakly but converges strongly after rescaling.
- $\langle \nabla^2 E^{\mathrm{BQC}} v^{\mathrm{B}}, v^{\mathrm{B}} \rangle \approx \langle \nabla^2 E^{\mathrm{C}} v^{\mathrm{B}}, v^{\mathrm{B}} \rangle$

Numerical Test



Setup: Micro-crack surrounded by atomistic region

Remember: $|\nabla^j (y^{\mathrm{A}} - x)| \lesssim |x|^{1-d-j}$

$$\|y_R^{\mathrm{A}} - r^{\mathrm{A}}\|_E \lesssim R_{\mathrm{A}}^{-1}$$

$$\|y^{\mathrm{QC}} - y^{\mathrm{A}}\|_E \lesssim \|\nabla^3 y^{\mathrm{A}}\|_{L^2(\Omega^{\mathrm{C}})} + R_{\mathrm{C}}^{-1} + \mathrm{FEM} + \mathrm{GF}$$

$$\sim R_{\mathrm{A}}^{-3} \qquad \sim R_{\mathrm{A}}^{-2} \qquad \gtrsim 1$$

$$\|y^{\mathrm{GR}} - y^{\mathrm{A}}\|_E \lesssim \|\nabla^3 y^{\mathrm{A}}\|_{L^2(\Omega^{\mathrm{C}})} + R_{\mathrm{C}}^{-1} + \mathrm{FEM} + \|\nabla^2 y^{\mathrm{A}}\|_{L^2(\Omega^{\mathrm{I}})}$$

$$\sim R_{\mathrm{A}}^{-3} \qquad \sim R_{\mathrm{A}}^{-2} \qquad \sim R_{\mathrm{A}}^{-5/2}$$

$$\|y^{\mathrm{BQC}} - y^{\mathrm{A}}\|_E \lesssim \|\nabla^3 y^{\mathrm{A}}\|_{L^2(\Omega^{\mathrm{C}})} + R_{\mathrm{C}}^{-1} + \mathrm{FEM} + \|\nabla^2 \beta\|_{L^2}$$

$$\sim R_{\mathrm{A}}^{-3} \qquad \sim R_{\mathrm{A}}^{-2} \qquad \gtrsim R_{\mathrm{A}}^{-1}$$

Optimality: Blending + GFC

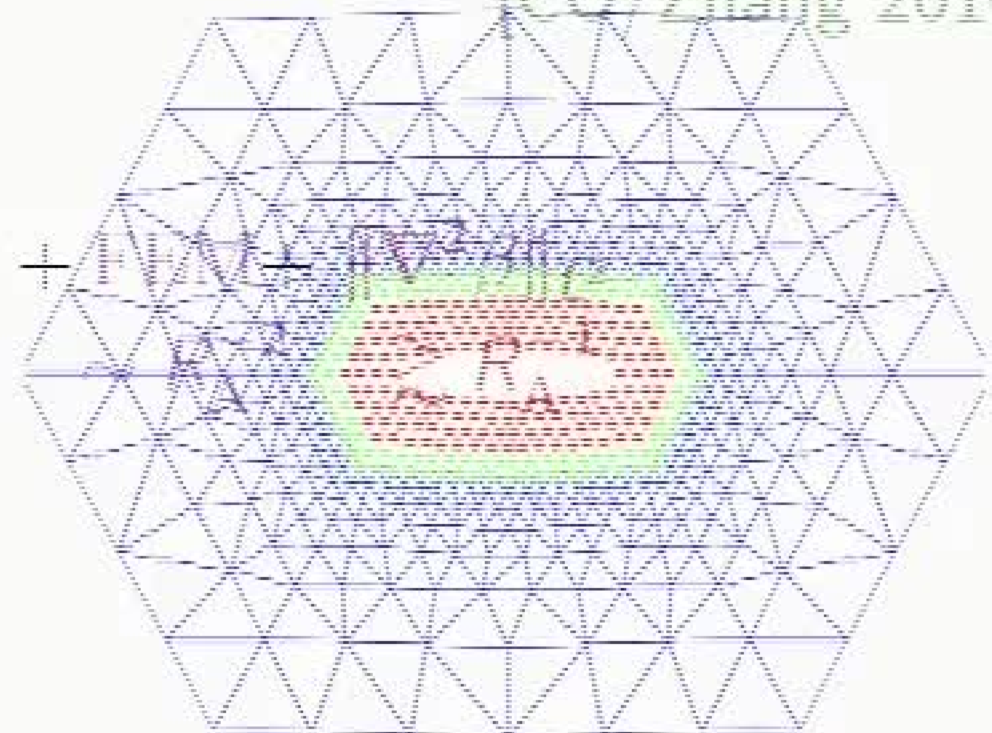
[CO/Zhang 2016]

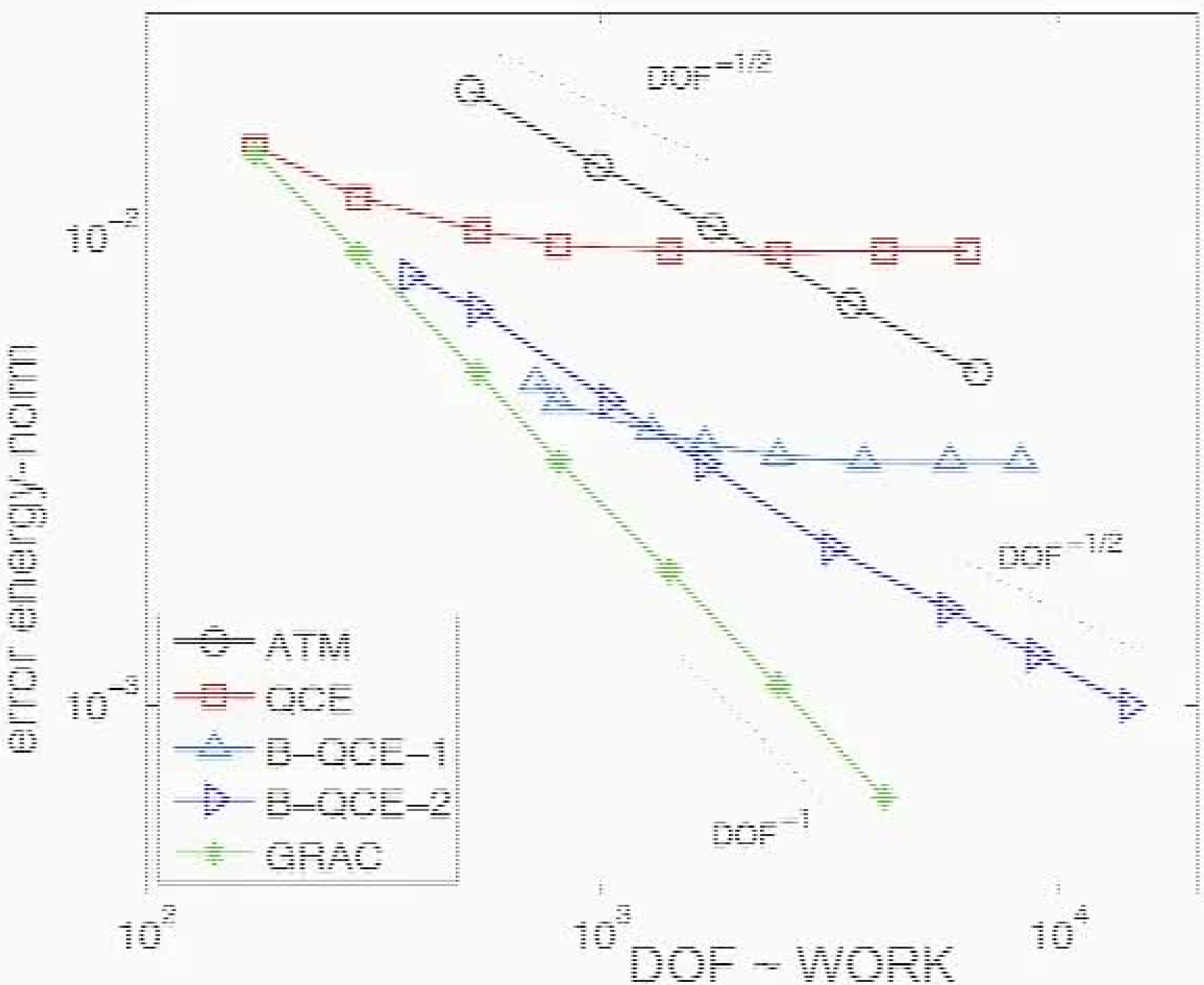
BQC Error:

$$\|y^{BQC} - y^\Lambda\|_E \lesssim \|\nabla^3 y^\Lambda\|_{L^2(\Omega^c)} + R_C^{-1} + \dots \sim R_A^{-3}$$

Setup: Micro-crack surrounded by atomistic region

Remember: $|\nabla^j (y^\Lambda - x)| \lesssim |x|^{1-d-j}$





Optimality: Blending + GFC

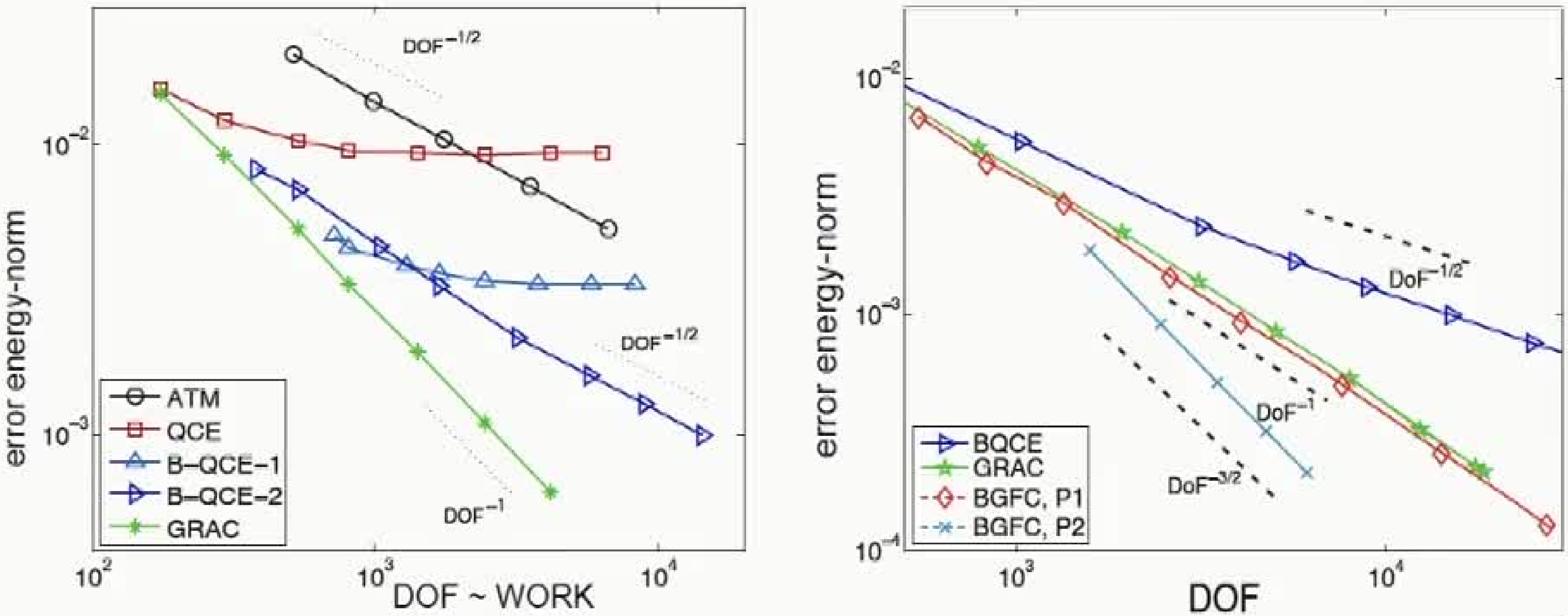
[CO/Zhang 2016]

BQC Error:

$$\|y^{\mathrm{BQC}} - y^{\mathrm{A}}\|_E \lesssim \underbrace{\|\nabla^3 y^{\mathrm{A}}\|_{L^2(\Omega^{\mathrm{C}})}}_{\sim R_{\mathrm{A}}^{-3}} + R_{\mathrm{C}}^{-1} + \underbrace{\mathrm{FEM}}_{\sim R_{\mathrm{A}}^{-2}} + \underbrace{\|\boxed{\partial W(\nabla y^{\mathrm{A}})} \cdot \nabla^2 \beta\|_{L^2}}_{\gtrsim R_{\mathrm{A}}^{-1}}$$

GFC: $E_\ell(y) \rightsquigarrow E_\ell(y) - \nabla E_\ell(x) \cdot (y - x)$ [Shenoy, Tadmor, Ortiz et al 1999]

$$\|y^{\mathrm{BQC}} - y^{\mathrm{A}}\|_E \lesssim \underbrace{\|\nabla^3 y^{\mathrm{A}}\|_{L^2(\Omega^{\mathrm{C}})}}_{\sim R_{\mathrm{A}}^{-3}} + R_{\mathrm{C}}^{-1} + \underbrace{\boxed{\text{P2-FEM}}}_{\sim R_{\mathrm{A}}^{-3}} + \underbrace{\|\boxed{\nabla u^{\mathrm{A}}} \cdot \nabla^2 \beta\|_{L^2}}_{\sim R_{\mathrm{A}}^{-3}}$$



Many Further Works, Variations and Extensions

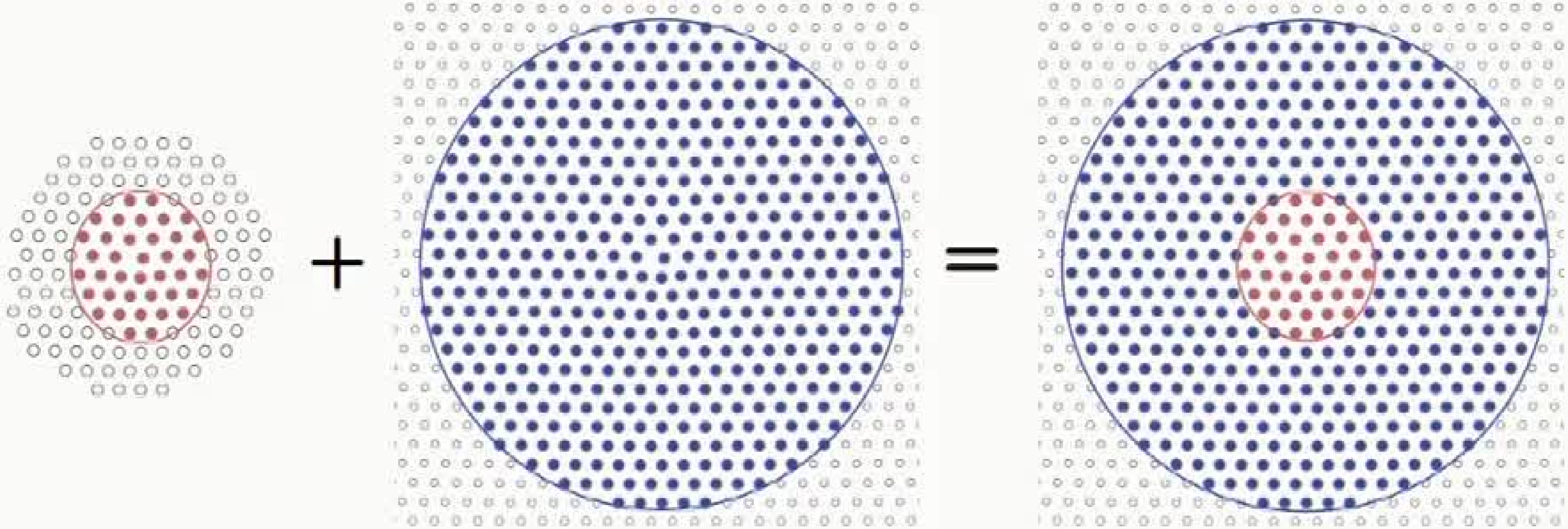
1. Force-based A/C schemes: Dobson/CO/Luskin (2010); Makridakis/CO/Süli (2011); Lu/Ming (2013); Li/Luskin/CO (2013); Li/CO/Shapeev/Vankoten (2016)
2. Domain-decomposition A/C schemes: Olson/Shapeev/Bochev/Luskin (2016); Olson/Bochev/Luskin/Shapeev (2014);
3. Other classes of defects; e.g. cracks Buze/Hudson/CO (in prep), surfaces Binder/CO/Luskin (2017)
4. Multi-lattices: Abdulle/Lin/Shapeev (2013); Abdulle/Lin/Shapeev (2012); Olson/CO (2017); Olson/Li/CO/VanKoten (2018)
5. A posteriori error control Wang/CO (2013), Wang/Zhang/Lin/Liao (2017), Wang/Yang (2018)
6. towards temperature Kim/Perez/Tadmor/Voter (2014), Luskin/Shapeev (2014), Braun/Duong/CO (in prep)
7. towards saddles and TST: Binder/Luskin/Perez/Voter (2015)
8. True dynamics? Little rigorous but see e.g. X Li talk Wed AM.

III. QM/MM Coupling

joint work with
Huajie Chen (Peking Normal), Jianfeng Lu (Duke), Faizan Nazar (Paris Dauphine), Jack Thomas (Warwick)

Acknowledgements: Gabor Csanyi, James Kermode

- F. Q. Nazar and C. Ortner. Locality of the Thomas-Fermi-von Weizsäcker equations. Arch. Ration. Mech. Anal., 224(3), 2017
- H. Chen and C. Ortner. QM/MM methods for crystalline defects. Part 2: Consistent energy and force-mixing. SIAM Multiscale Model. Simul., 15(1), 2017
- H. Chen and C. Ortner. QM/MM methods for crystalline defects. Part 1: Locality of the tight binding model. SIAM Multiscale Model. Simul., 14(1), 2016
- H. Chen and J. Lu and C. Ortner, Thermodynamic Limit of Crystal Defects with Finite Temperature Tight Binding, to appear in Arch. Ration. Mech. Anal.



Energy-Mixing Schemes: (e.g., ChemShell, MAAD, QUASI, ONION, ...)

$$E^{\mathrm{H}}(y) = E^{\mathrm{MM}}(y|_{\mathrm{MM}}) + E^{\mathrm{QM}}(y|_{\mathrm{QM}}) + E^{\mathrm{INT}}(y|_{\mathrm{MM}}, y|_{\mathrm{QM}})$$

- same difficulty as A/C: **how to couple**?
- $\Rightarrow$ Force-mixing methods, e.g., [Csanyi, Kermode, Bernstein, DeVita, ...]
- $\Rightarrow$ Energy-mixing remains an **open problem**

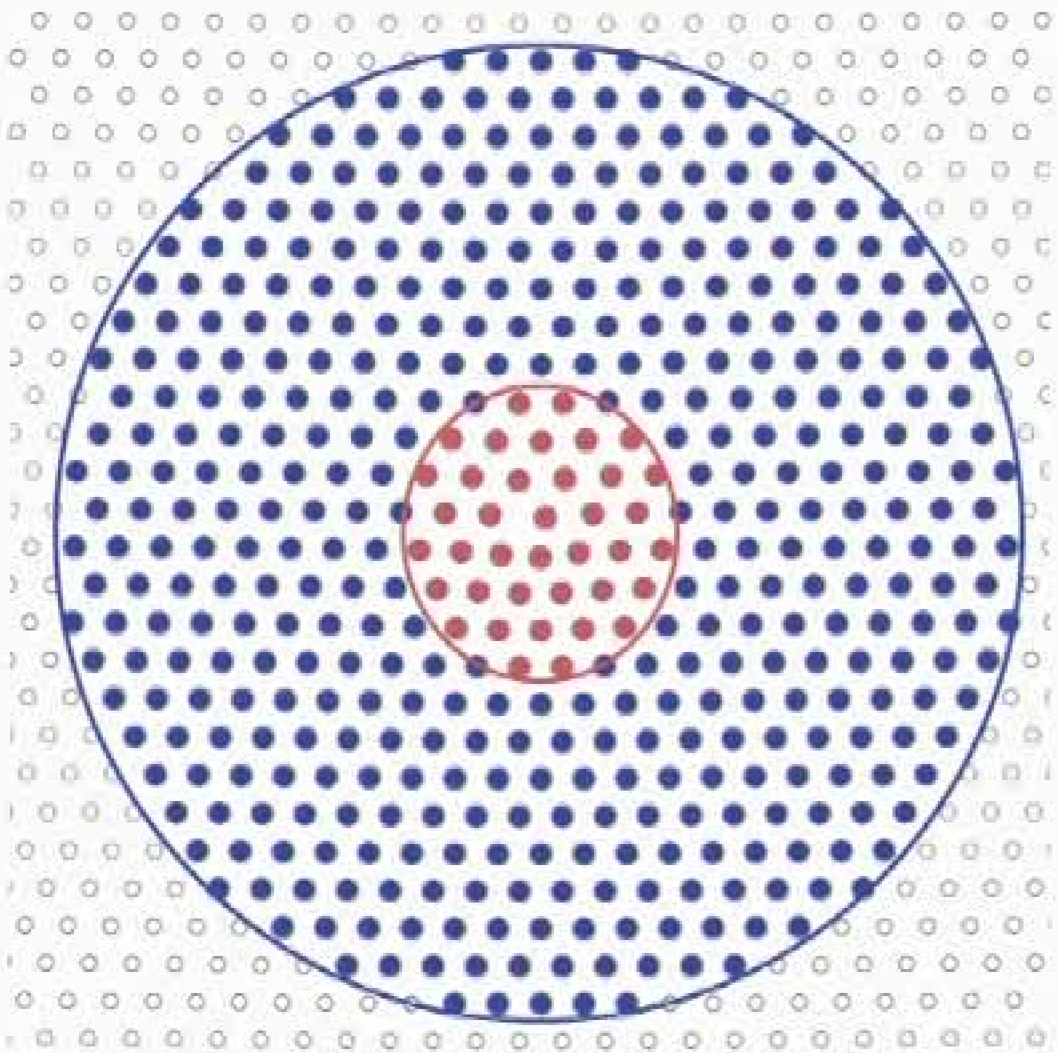
Strong Force Locality

[Csanyi/DeVita/...2005]

A necessary condition for **any** QM/MM:

$$\frac{\partial^2 E^{\mathrm{QM}}(y)}{\partial y_i \partial y_j} \lesssim \omega(r_{ij})$$

where $\omega(r) \to 0$ sufficiently fast.



(In principle, electrostatics is a "special" interaction and can be treated separately, but for now assume it is screened.)

Decomposition of Energy

Coulson, Proc.R.Soc.London A, 1939
Chen, CO, MMS, 2016

$$\mathbf{H}(y)\psi_s = \varepsilon_s\psi_s \rightsquigarrow \qquad E^{\rm QM}(y) = \sum_{s=1}^N f(\varepsilon_s) = \sum_{\ell=1}^N [f(\mathbf{H})]_{\ell\ell} =: \sum_{\ell=1}^N E_\ell(y)$$

(= Bond-Order Potential!)

Theorem: E_ℓ is invariant under permutations and isometries and

local: $$\left|\frac{\partial E_\ell(y)}{\partial y_m}\right| \lesssim e^{-\gamma r_{\ell m}}, \qquad \left|\frac{\partial^2 E_\ell(y)}{\partial y_m \partial y_n}\right| \lesssim e^{-\gamma(r_{\ell m}+r_{\ell n})}, \dots$$

Estimates are robust as $N \to \infty$.

"Analytically, Tight-Binding is just an interatomic potential."

Remarks:

- Justifies strong force locality, but is **much** stronger
- All results from Part I and II generalise to the TB model [Chen/Lu/CO/2018], [Thomas/in prep]
- It is also the basis of understanding interatomic potentials
- For the Mermin model (canonical electrons) the result appears to be false

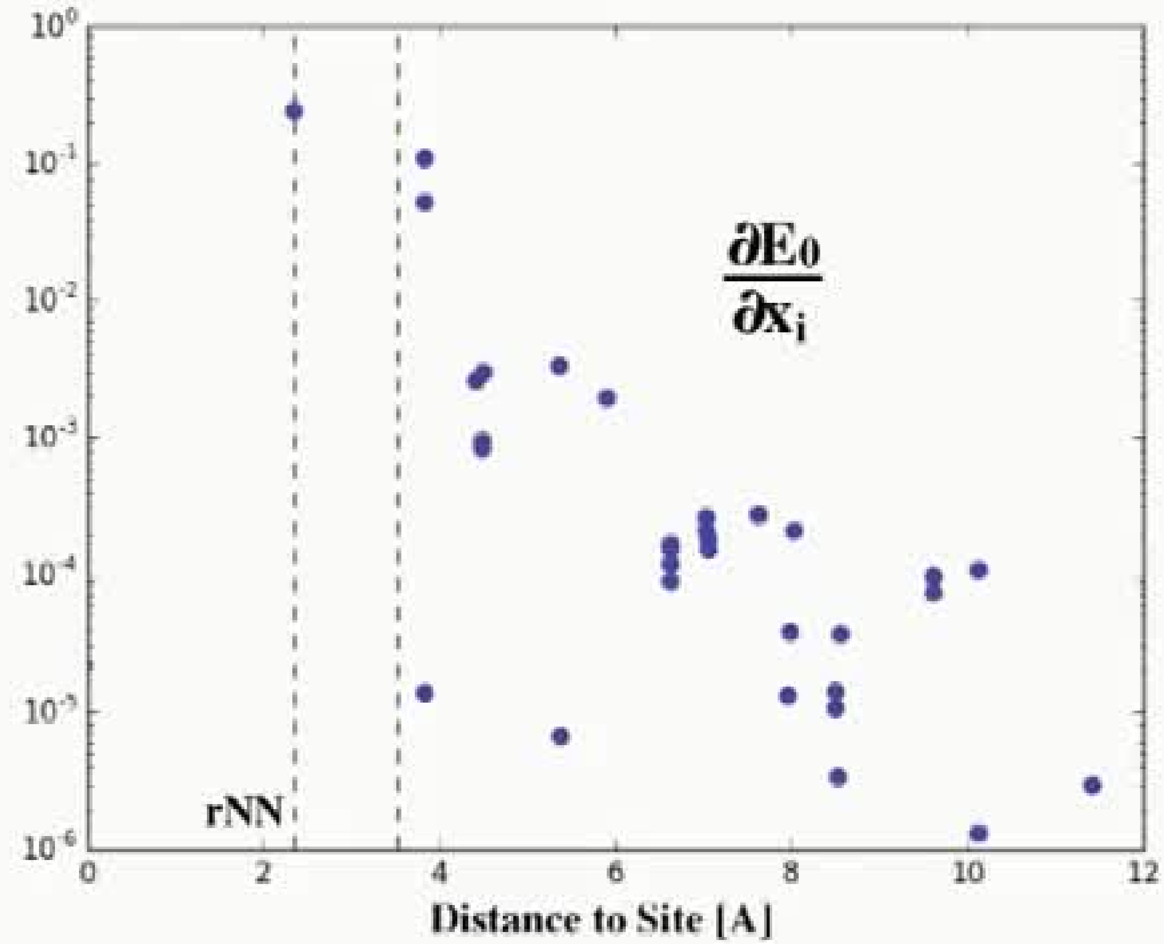
Extensions and Open Problems

All ideas from Part I generalise to TB using **separability of E^{QM}**:

$$E^{\mathrm{QM}}(y) = \sum_s f(\varepsilon_s) = \sum_\ell E_\ell(y)$$

Other Models:

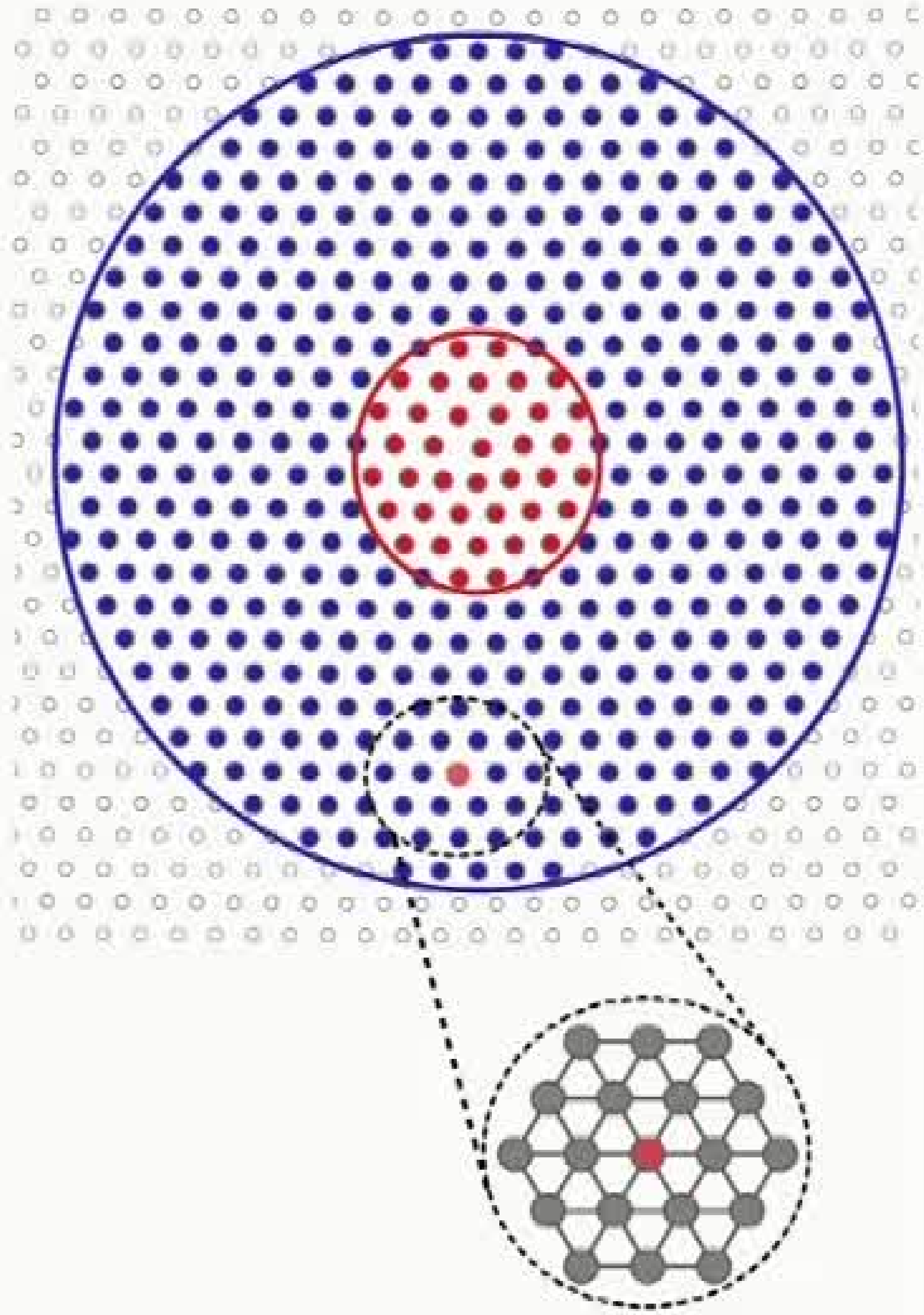
- **[NEW]** TB for insulators (0T): J. Thomas, MSc Thesis
- Hartree-Fock with Yukawa interaction: Chen, Nazar, CO; in prep
- Tomas-Fermi-Weizsäcker: Nazar, CO, ARMA 2017
- **numerical evidence for KS-DFT (LDA, bulk Si):** (with J. Kermode)



Open Problem: metals!

QM/MM Energy Mixing

Chen, CO, MMS, 2017



New Ingredient: $E^{\mathrm{QM}}(y) = \sum_{\ell\in\Lambda} E_\ell(y)$

Hybrid Energy:

$$E^{\mathrm{H}}(y) := \sum_{\ell\in\Lambda^{\mathrm{QM}}} E_\ell(y) + \sum_{\ell\in\Lambda\setminus\Lambda^{\mathrm{QM}}} E_\ell^{\mathrm{MM}}(y)$$

- Key new idea: $E_\ell^{\mathrm{MM}} \approx E_\ell$

$$y^{\mathrm{H}} \in \arg\min \{ E^{\mathrm{H}}(y) \,|\, \text{bdry. cond.} \}$$

What we learned from A/C Coupling:

- match inner and outer models
- match the interaction at the interface

$\Rightarrow$ require $\nabla^j E_\ell^{\mathrm{MM}}(x) = \nabla^j E_\ell(x) \quad \text{for } j = 0, \dots, p$

QM/MM Energy Mixing

Chen, CO, MMS, 2017

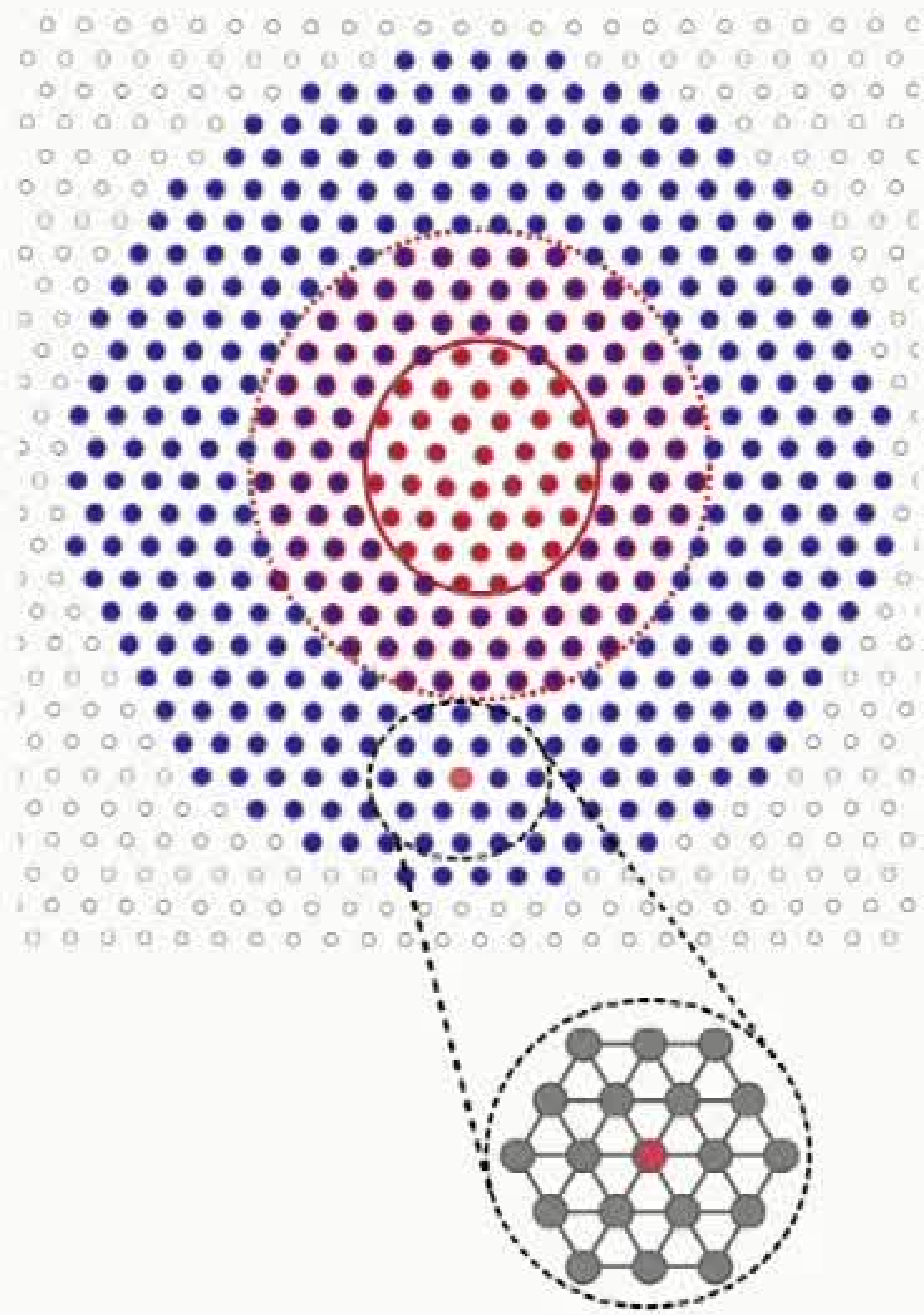
New Ingredient: $E^{\mathrm{QM}}(y) = \sum_{\ell \in \Lambda} E_\ell(y)$

Hybrid Energy:

$$E^{\mathrm{H}}(y) := \sum_{\ell \in \Lambda^{\mathrm{QM}}} E_\ell^{\mathrm{BUF}}(y) + \sum_{\ell \in \Lambda \setminus \Lambda^{\mathrm{QM}}} E_\ell^{\mathrm{MM}}(y)$$

- Key new idea: $\boxed{E_\ell^{\mathrm{MM}} \approx E_\ell}$
- $\mathcal{E}_\ell^{\mathrm{BUF}}$ = site energy with $\Lambda^{\mathrm{QM}} \cup \Lambda^{\mathrm{BUF}}$

$$\boxed{y^{\mathrm{H}} \in \arg\min \left\{ E^{\mathrm{H}}(y) \,\middle|\, \text{bdry. cond.} \right\}}$$



What we learned from A/C Coupling:

- match inner and outer models
- match the interaction at the interface

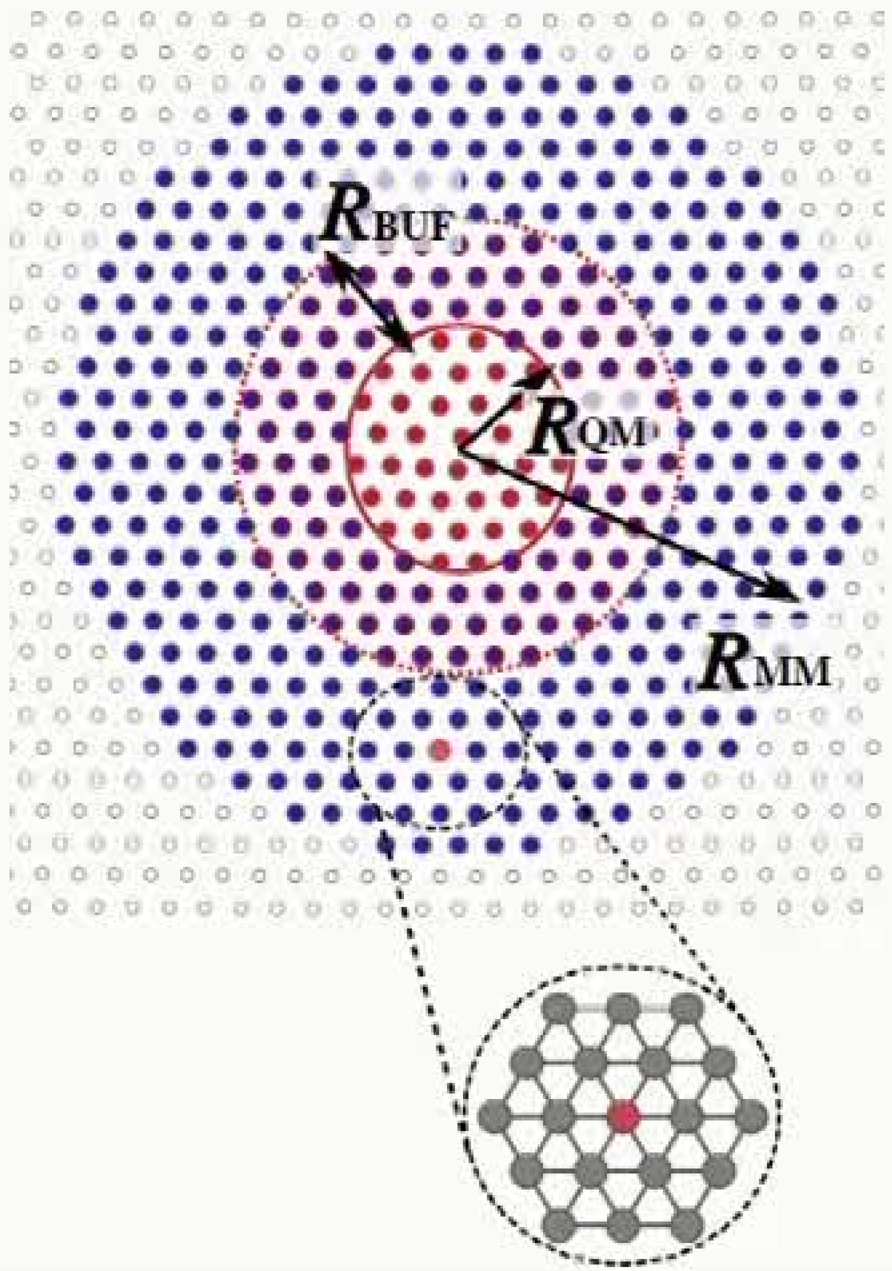
$$\Rightarrow \quad \text{require} \quad \boxed{\nabla^j E_\ell^{\mathrm{MM}}(x) = \nabla^j E_\ell^{\mathrm{BUF}}(x) \quad \text{for } j = 0, \dots, p}$$

Convergence Rate: Edge Dislocation

Theorem: If $E_\ell^{\mathrm{MM}} \sim E_\ell^{\mathrm{BUF}}$ to order $p \geq 2$ and $R_{\mathrm{QM}}, R_{\mathrm{MM}}, R^{\mathrm{BUF}}$ suff. large, then there exists $\bar{y}^{\mathrm{H}}$ s.t.

$$\|\bar{y}^{\mathrm{QM}} - \bar{y}^{\mathrm{H}}\|_E \lesssim \boxed{R_{\mathrm{QM}}^{1-p}} + e^{-cR_{\mathrm{BUF}}} + R_{\mathrm{MM}}^{-1}.$$

- $\boxed{R_{\mathrm{QM}}^{1-p}}$: order of accuracy of MM potential (Taylor expansion)
- $e^{-cR_{\mathrm{BUF}}}$: buffer for QM region and truncation of MM potential
- R_{MM}^{-1} : truncation of elastic far-field



Convergence Rate: Edge Dislocation

Theorem: If $E_\ell^{\mathrm{MM}} \sim E_\ell^{\mathrm{BUF}}$ to order $p \geq 2$ and $R_{\mathrm{QM}}, R_{\mathrm{MM}}, R^{\mathrm{BUF}}$ suff. large, then there exists $\bar{y}^{\mathrm{H}}$ s.t.

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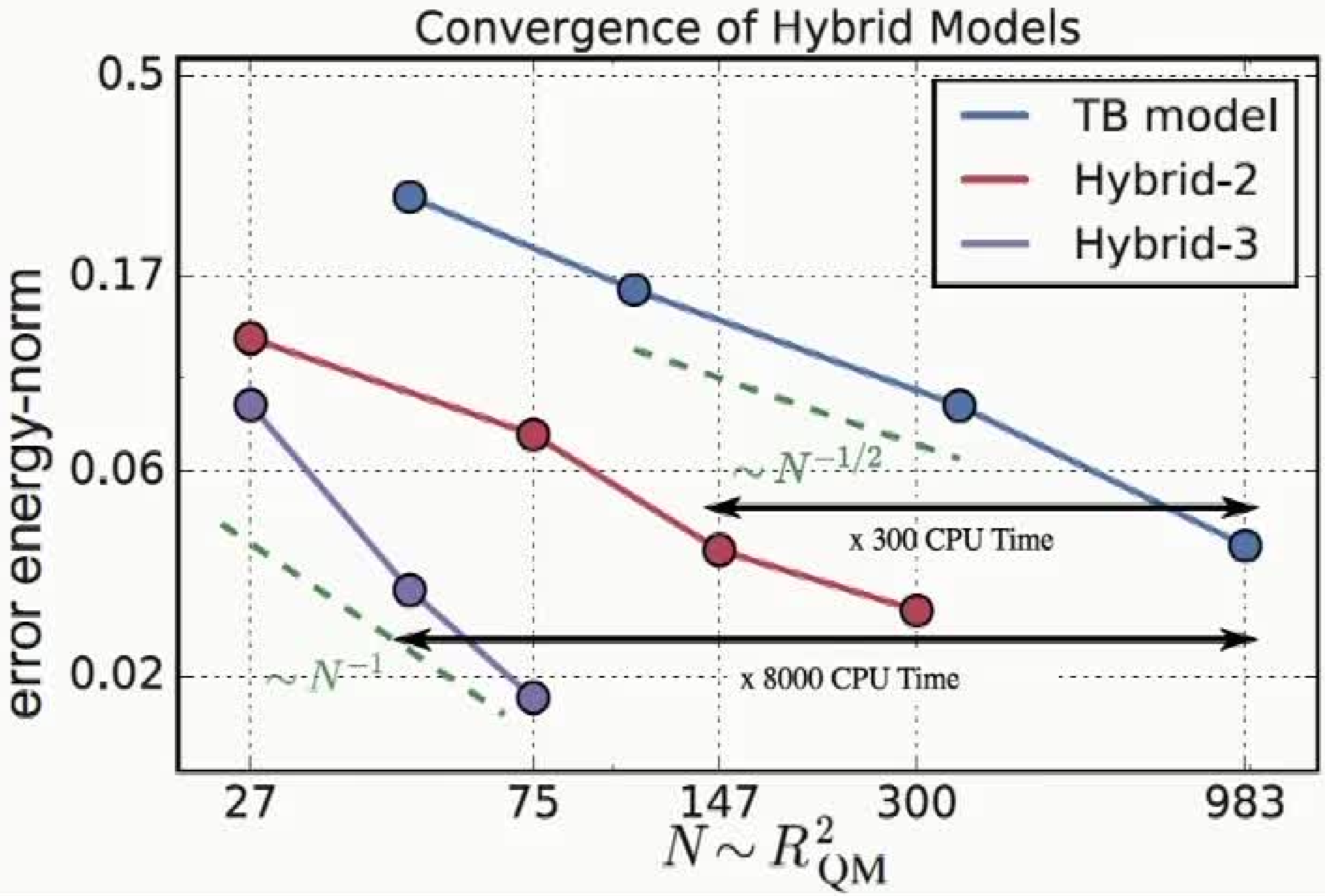

Convergence Rate: Di-Interstitial in Bulk Si

Theorem: For a POINT DEFECT: If $E_\ell^{\mathrm{MM}} \sim E_\ell^{\mathrm{BUF}}$ to order p and $R_{\mathrm{QM}}, R_{\mathrm{MM}}, R^{\mathrm{BUF}}$ suff. large, then there exists $\bar{u}^{\mathrm{H}}$ s.t.

$$\|\bar{u} - \bar{u}^{\mathrm{H}}\|_E \lesssim \boxed{R_{\mathrm{QM}}^{d/2-dp}} + e^{-cR_{\mathrm{BUF}}} + R_{\mathrm{MM}}^{-d/2}.$$