Partition-of-unity finite elements for large, accurate quantum mechanical materials calculations

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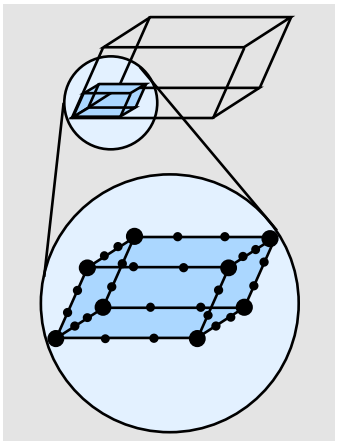
$$-\tfrac{1}{2}\nabla^2\psi_i(\mathbf{x}) + \hat{V}_{\mathit{eff}}\psi_i(\mathbf{x}) = \varepsilon_i\psi_i(\mathbf{x}),$$
$$\hat{V}_{\mathit{eff}} = V_I^{\ell} + \hat{V}_I^{n\ell} + V_H + V_{xc},$$
$$V_I^{\ell} = \sum_a V_{I,a}(\mathbf{x}),$$
$$\hat{V}_I^{n\ell}\psi_i = \sum_a \int d\mathbf{x}' V_{I,a}^{n\ell}(\mathbf{x},\mathbf{x}')\psi_i(\mathbf{x}'),$$
$$V_H = -\int d\mathbf{x}' \frac{\rho_e(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|},$$
$$V_{xc} = V_{xc}(\mathbf{x};\rho_e),$$
$$\rho_e = -\sum_i f_i\psi_i^*(\mathbf{x})\psi_i(\mathbf{x}),$$

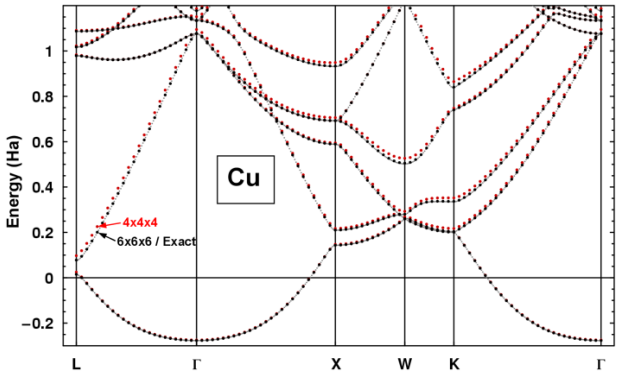
DFT

+



FEM

⇒



materials properties

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Introduction

- Goal: **Completely general electronic-structure method (metals and insulators, high-symmetry and low) for large problems involving "hard atoms".**
- Approach: **Solve the Kohn-Sham equations in a partition-of-unity (PU) finite-element (FE) basis**
- Why **PUFE?**

	PW	FD	FE	PUFE	.. DG!
General, systematically improvable	✓	✓	✓	✓	...
Variational (upper bounds, convergence)	✓	✗	✓	✓	...
Local (refinement, parallelization, O(N))	✗	✓	✓	✓	...
Efficient repr. (↓ storage, CPU time)	✓	✗	✗	✓✓	...

What's new

Initial results show order of magnitude improvement over current state of the art

Outline

- Problem: Kohn-Sham equations
- FE basis
- Formulation of solution in FE basis
  - Nonlocal operators
  - Boundary conditions
  - Long-range interactions
- Band structures, total energies: metals and insulators
- Problem: too many degrees of freedom
- Solution: partition-of-unity basis
- Comparison to FE, FE-AMR, and planewaves for “hard” atoms
- Parallelization
- Quadrature
- Solver
- All-electron calculations

Problem: Kohn-Sham equations in an infinite crystal — for large, complex cells of arbitrary symmetry

Kohn-Sham equations

$$-\tfrac{1}{2}\nabla^2\psi_i(\mathbf{x}) + \hat{V}_{eff}\psi_i(\mathbf{x}) = \varepsilon_i\psi_i(\mathbf{x}),$$

(Schrödinger)

$$\hat{V}_{eff} = V_I^{\ell} + \hat{V}_I^{n\ell} + V_H + V_{xc},$$

$$V_I^{\ell} = \sum_a V_{I,a}(\mathbf{x}),$$ (long-range, divergent)

$$\hat{V}_I^{n\ell}\psi_i = \sum_a \int d\mathbf{x}' V_{I,a}^{n\ell}(\mathbf{x},\mathbf{x}')\psi_i(\mathbf{x}'),$$ (all-space)

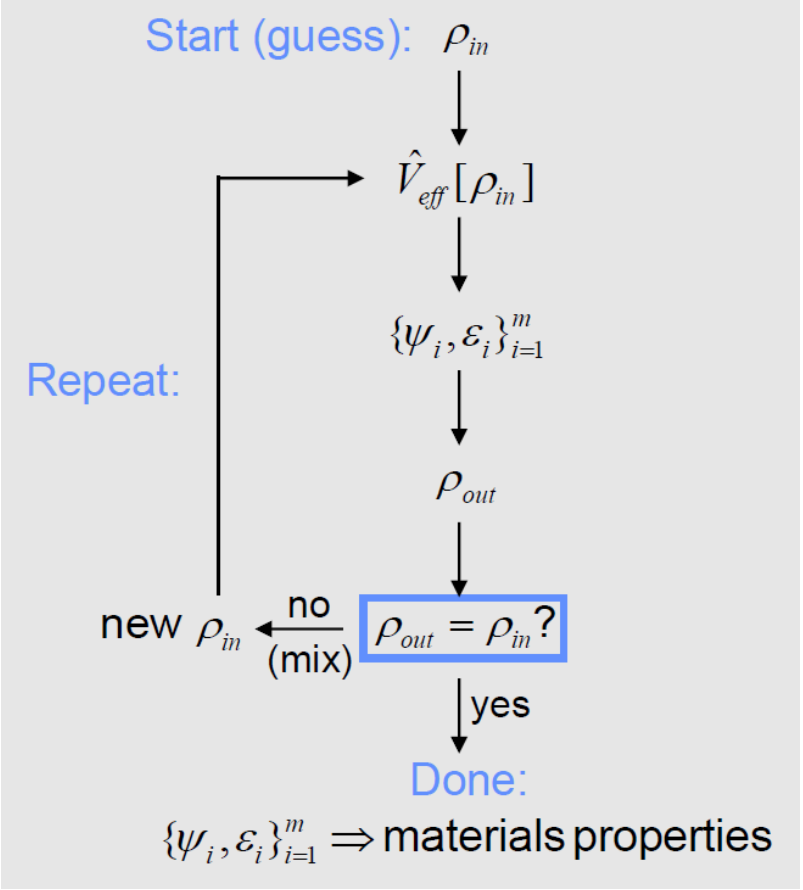
$$V_H = -\int d\mathbf{x}' \frac{\rho_e(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|},$$ (long-range, div.) (Poisson)

$$V_{xc} = V_{xc}(\mathbf{x};\rho_e),$$

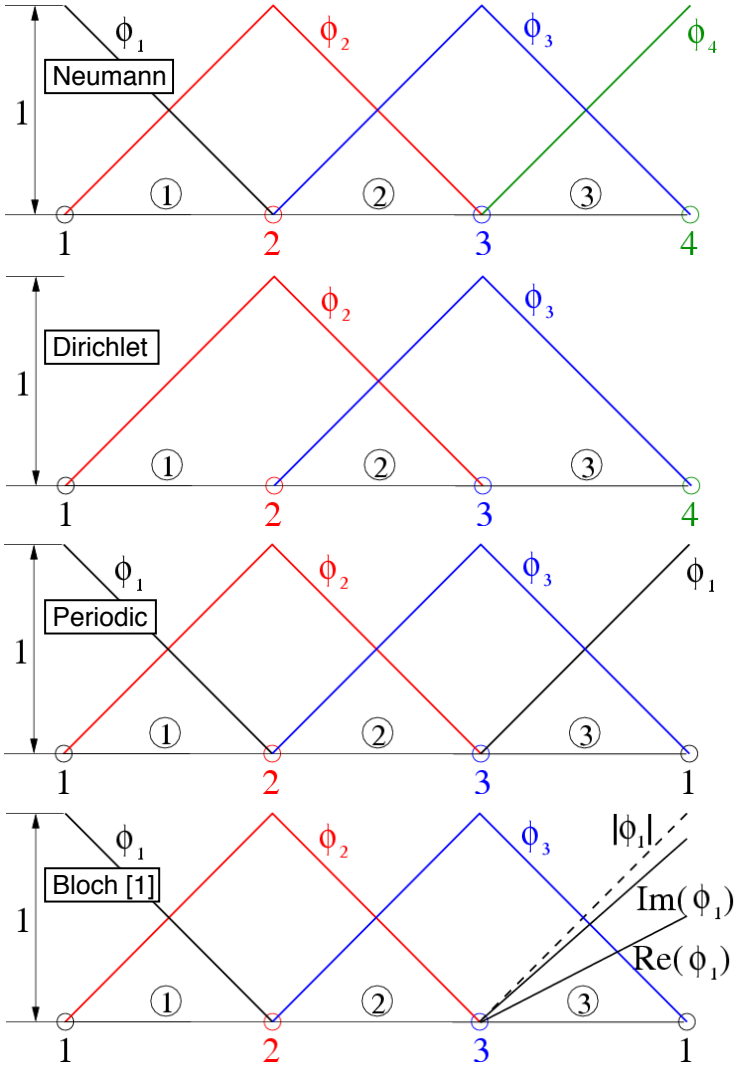
$$\rho_e = -\sum_i f_i\psi_i^*(\mathbf{x})\psi_i(\mathbf{x}),$$ (degenerate states, fractional occ.)

~ 10^3 atoms/eigenfunctions

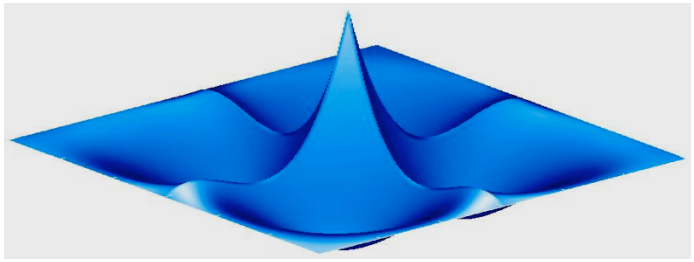
Self-consistent field (SCF) solution process



FE basis: strictly local, piecewise polynomials



1D linear finite element bases



3D cubic basis function

$$\phi_i(b) = \phi_i(a) = 0$$

$$\phi_i(b) = \phi_i(a)$$

$$\phi_i(b) = e^{ik(b-a)}\phi_i(a)$$

- **Polynomial →**
  - **General, systematically improvable**
  - **Flexible boundary conditions**
- **Strictly local →**
  - **Variable resolution in real space**
  - **Sparse matrices**
  - **Well suited to parallel implementation**
- **However, unlike planewaves:**
  - **Finite**
  - **C^0 (continuous but not smooth)**
  - **Periodic in value only**
  - **Nonorthogonal**

[1] Sukumar, Pask, Int. J. Numer. Meth. Eng. **77**, 1121 (2009)

Hard part: Schrödinger

Formulation: Schrödinger problem in the infinite crystal is reduced to a boundary value problem in the finite unit cell

- **The FE basis is defined in a finite domain.**
- **To find ψ satisfying**

$$-\tfrac{1}{2}\nabla^2\psi + V^{\ell}\psi + \hat{V}^{n\ell}\psi = \varepsilon\psi$$

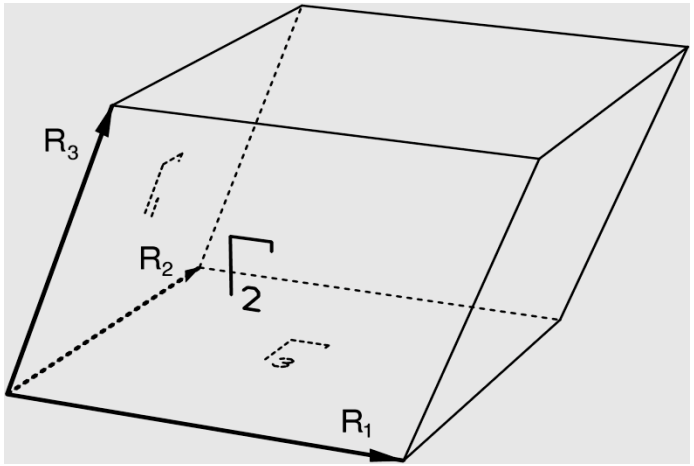
$$\psi(\mathrm{x}+\mathrm{R}) = e^{i\mathbf{k}\cdot\mathbf{R}}\psi(\mathrm{x}) \quad \textbf{(Bloch's Thm)}$$

in the infinite crystal, we solve an equivalent problem in the finite unit cell [1,2]:

$$-\tfrac{1}{2}\nabla^2\psi + V^{\ell}\psi + \hat{V}^{n\ell}\psi = \varepsilon\psi \quad \text{in } \Omega$$

$$\psi(\mathrm{x}+\mathrm{R}_{\ell}) = e^{i\mathbf{k}\cdot\mathbf{R}_{\ell}}\psi(\mathrm{x}), \quad \mathrm{x}\in\Gamma_{\ell}$$

$$\nabla\psi(\mathrm{x}+\mathrm{R}_{\ell})\cdot\hat{\mathrm{n}} = e^{i\mathbf{k}\cdot\mathbf{R}_{\ell}}\nabla\psi(\mathrm{x})\cdot\hat{\mathrm{n}}, \quad \mathrm{x}\in\Gamma_{\ell}$$



Unit cell

- **Laplacian? [1]**
- **Derivative BC? [1]**
- **Crystal potential? [2]**
- **Nonlocal operator? [2]**

[1] Sukumar, Pask, Int. J. Numer. Meth. Eng. **77**, 1121 (2009)
[2] Pask, Sterne, Modelling Simul. Mater. Sci. Eng. **13**, R71 (2005) **(Review)**

Nonlocal operators are transformed to the finite unit cell

- **The domain of the nonlocal potential operator is all space.**
- **The domain of the problem is the finite unit cell; the basis is defined only in the finite unit cell.**
- **For a separable potential of the usual form**

$$\hat{V}^{n\ell}(\mathrm{x},\mathrm{x}') = \sum_{n,a,L} v_L^a(\mathrm{x}-\tau_a-\mathrm{R}_n)h_L^a v_L^a(\mathrm{x}'-\tau_a-\mathrm{R}_n)$$

the nonlocal term is

$$\hat{V}^{n\ell}\psi = \sum_{n,a,L} v_L^a(\mathrm{x}-\tau_a-\mathrm{R}_n)h_L^a \int d\mathrm{x}'\, v_L^a(\mathrm{x}'-\tau_a-\mathrm{R}_n)\psi(\mathrm{x}')$$

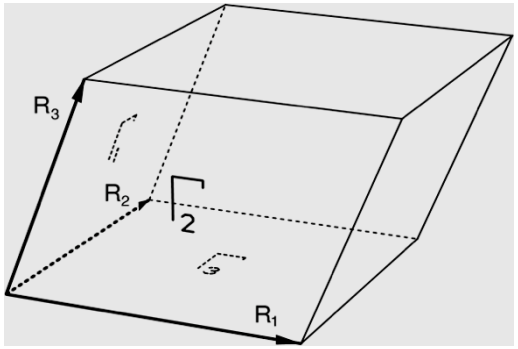
- **Transforming to the unit cell gives [1]**

$$\hat{V}^{n\ell}\psi = \sum_{a,L}\sum_{n} e^{i\mathbf{k}\cdot\mathbf{R}_n} v_L^a(\mathrm{x}-\tau_a-\mathrm{R}_n)h_L^a \int_\Omega d\mathrm{x}' \sum_{n'} e^{-i\mathbf{k}\cdot\mathbf{R}_{n'}} v_L^a(\mathrm{x}'-\tau_a-\mathrm{R}_{n'})\psi(\mathrm{x}')$$

[1] Pask, Sterne, Modelling Simul. Mater. Sci. Eng. **13**, R71 (2005)

Laplacian and boundary condition issues are resolved by reformulating in weak form

- **Laplacian of C^0 functions is singular at cusps.**
- **Basis does not satisfy derivative BC.**
- **Resolution — weak formulation with derivative BC built in [1,2]:**



Unit cell

Find the scalars $\varepsilon \in \mathbb{R}$ and functions $\psi \in \mathcal{W}$ such that

$$\int_\Omega \left(\tfrac{1}{2} \nabla v^* \cdot \nabla \psi + v^* V^\ell \psi + v^* \hat{V}^{n\ell} \psi \right) d\mathbf{x} = \varepsilon \int_\Omega v^* \psi \, d\mathbf{x} \quad \forall v \in \mathcal{W}$$

where $\mathcal{W} = \{ w \in H^1(\Omega) : w(\mathbf{x} + \mathbf{R}_\ell) = e^{i\mathbf{k}\cdot\mathbf{R}_\ell} w(\mathbf{x}),\ \mathbf{x} \in \Gamma_\ell \}$

- **Highest derivative of order 1 → finite discontinuities at interelement boundaries.**
- **Basis need only satisfy value-periodic condition: solution will satisfy value condition exactly and derivative condition asymptotically (weakly).**

[1] Pask, Klein, Fong, Sterne, Phys. Rev. B **59**, 12352 (1999)
[2] Sukumar, Pask, Int. J. Numer. Meth. Eng. **77**, 1121 (2009)

Discretization in the FE basis produces a sparse generalized eigenproblem

- **Discretization in the FE basis yields a sparse Hermitian generalized eigenproblem for the eigenvalues and eigenfunction coefficients:**

$$\sum_j H_{ij} c_j = \varepsilon \sum_j S_{ij} c_j$$

$$H_{ij} = \int_\Omega \left(\tfrac{1}{2} \nabla \phi_i^* \cdot \nabla \phi_j + \phi_i^* V^\ell \phi_j + \phi_i^* \hat{V}^{n\ell} \phi_j \right) d\mathbf{x}$$

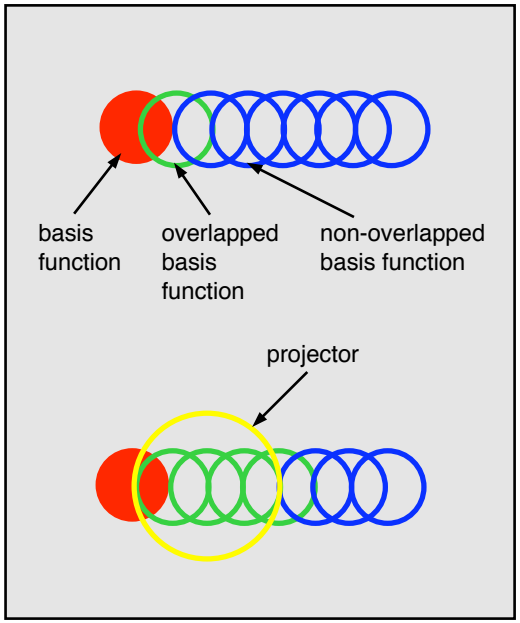
$$S_{ij} = \int_\Omega \phi_i^* \phi_j \, d\mathbf{x}$$

- **For a separable potential, the nonlocal term becomes [1]**

$$\int_\Omega d\mathbf{x} \, \phi_i^* \hat{V}^{n\ell} \phi_j = \sum_{a,L} f_L^{ai} h_L^a (f_L^{aj})^*$$

where

$$f_L^{ai} = \int_\Omega d\mathbf{x} \, \phi_i^*(\mathbf{x}) \sum_n e^{i\mathbf{k}\cdot\mathbf{R}_n} v_L^a(\mathbf{x} - \boldsymbol{\tau}_a - \mathbf{R}_n)$$



[1] Pask, Sterne, Modelling Simul. Mater. Sci. Eng. **13**, R71 (2005)

Kohn-Sham: crystal potential, total energy

Crystal potential can be constructed efficiently in real space by replacing long-range *V* by equivalent localized *ρ*

- $V \sim -Z/r,\ r > r_c \Rightarrow$ *V* equivalent to total charge *Z* localized within $r = r_C$.

- **Upon replacing long-range ionic potentials by equivalent localized densities, total Coulomb potential can be computed at once by Poisson solution with net neutral electronic + localized-ionic charge as source term [1]:**

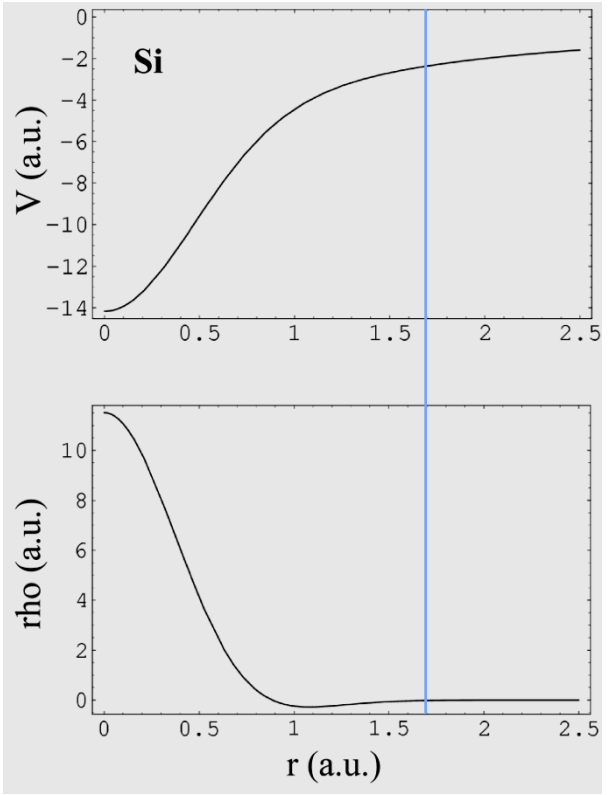
$$\rho_I = \sum_a \rho_{I,a}(\mathrm{x})$$

$$\rho = \rho_I + \rho_e$$

$$\nabla^2 V_C(\mathrm{x}) = 4\pi\rho(\mathrm{x}) \qquad \textbf{(periodic BCs)}$$

$$\hat{V}_{eff} = V_I^{\ell} + \hat{V}_I^{n\ell} + V_H + V_{xc} = V_C + \hat{V}_I^{n\ell} + V_{xc}$$

- **Long-range potential sum replaced by short-range charge sum and Poisson solution in cell.**



Local part of HGH [2] pseudopotential and associated charge density.

[1] Pask, Sterne, Phys. Rev. B **71**, 113101 (2005)
[2] Hartwigsen, Goedecker, Hutter, Phys. Rev. B **58**, 3641 (1998)

Total energy can be constructed efficiently in real space by replacing long-range *V* by equivalent localized *ρ*

- **Total energy in density-functional theory:**

$$E_{tot} = T_s + E_{eI}^{\ell} + E_{eI}^{n\ell} + E_{ee} + E_{II} + E_{xc}$$

- **In an infinite crystal:**

E_{eI}^{ℓ} is divergent and negative while E_{ee} and E_{II} are divergent and positive

$E_C = E_{eI}^{\ell} + E_{ee} + E_{II}$ is finite.

- **Using total charge ρ and Coulomb potential V_C, E_C can be determined at once:**

$$E_C = -\tfrac{1}{2}\int_{\Omega} d\mathrm{x}\, \rho(\mathrm{x}) V_C(\mathrm{x}) - E_s \qquad E_s = -\tfrac{1}{2}\sum_a \int d\mathrm{x}\, \rho_{I,a}(\mathrm{x}) V_{I,a}(\mathrm{x})$$

- **No Fourier transforms, structure factors, Ewald sums: O(N) ops in real space.**

- **Total energy then reduces to** $E_{tot} = T_s + E_C + E_{eI}^{n\ell} + E_{xc}$

- **Kohn-Sham orbital dependence in kinetic and nonlocal terms can be eliminated using KS equations to determine the relation**

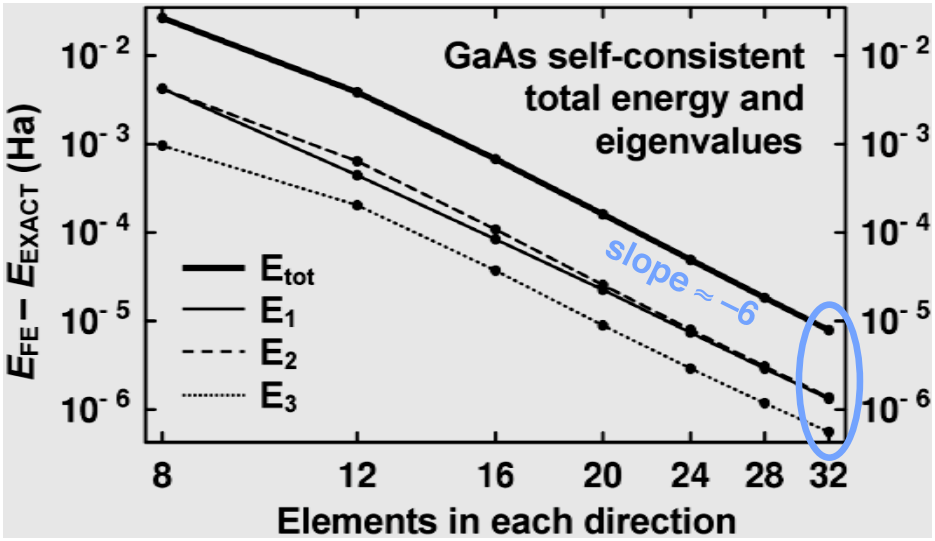
$$T_s - \int_{\Omega} d\mathrm{x}\, \rho_e(\mathrm{x}) V_{eff}^{\ell}(\mathrm{x}) + E_{eI}^{n\ell} = \sum_i f_i \varepsilon_i$$

Method converges systematically and variationally to the self-consistent solution

$$E_{tot} = \underbrace{\sum_i f_i \varepsilon_i + \int_\Omega d\mathrm{x}\ \left[\rho_e(\mathrm{x}) V^{\ell}_{eff}(\mathrm{x})\right]}_{T_s + E^{nl}_{eI}} - \tfrac{1}{2}\rho(\mathrm{x}) V_C(\mathrm{x}) - \rho_e(\mathrm{x})\varepsilon_{xc}(\mathrm{x};\rho_e)\Big] + \tfrac{1}{2}\sum_a \int d\mathrm{x}\,\rho_{I,a}(\mathrm{x}) V_{I,a}(\mathrm{x})$$

E_{xc}

E_C

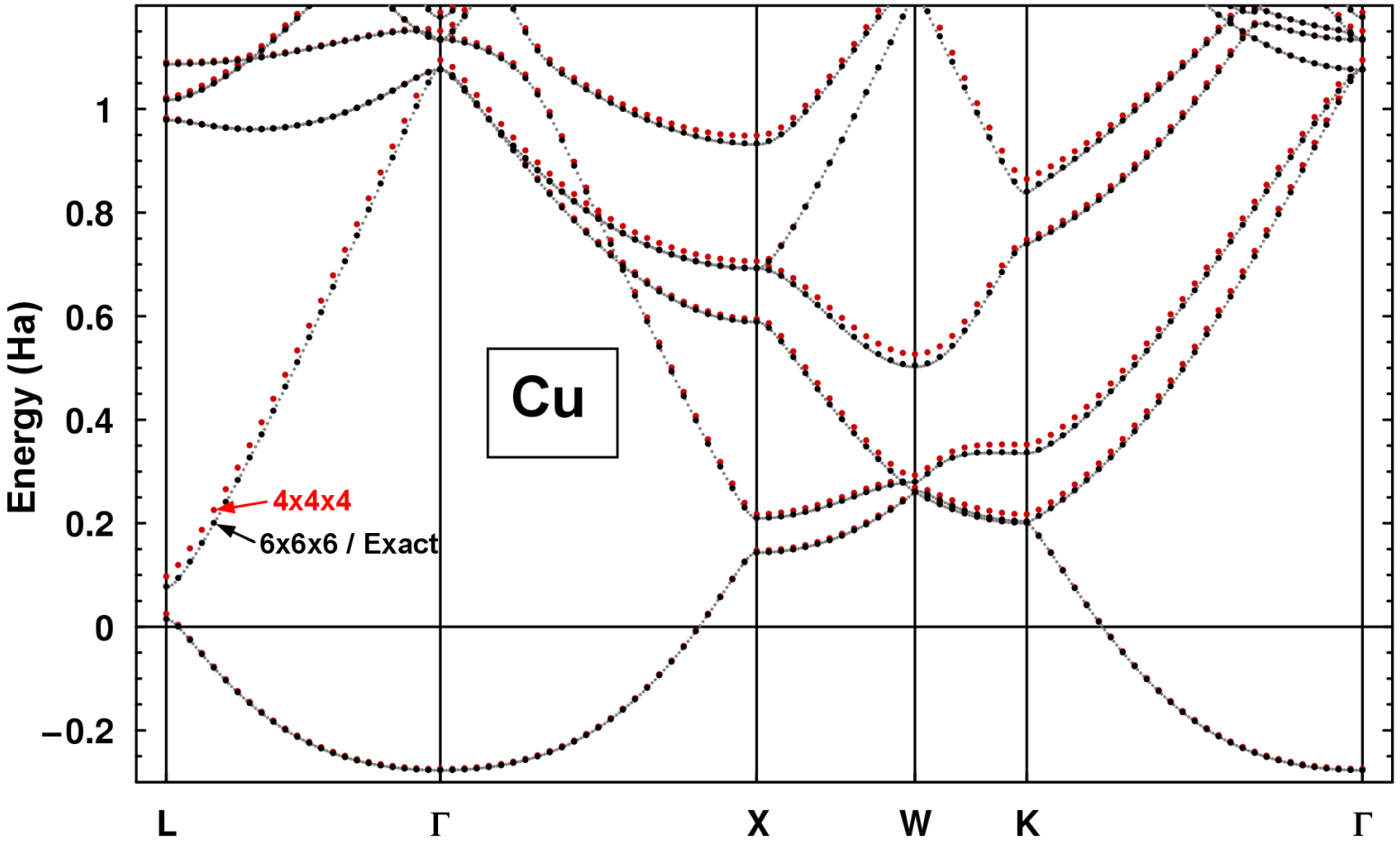


Convergence of self-consistent FE total energy and eigenvalues to exact values with increasing number of elements.

- **Self-consistent total energy converges uniformly and variationally to the exact solution as the number of elements is increased.**
- **Optimal theoretical rate consistent with cubic completeness of basis: error $O(h^6)$, where h is the mesh spacing.**

[1] Pask, Sterne, Phys. Rev. B **71**, 113101 (2005)

Method applies equally well to metals



Convergence of FE to exact self-consistent band structure for Cu.

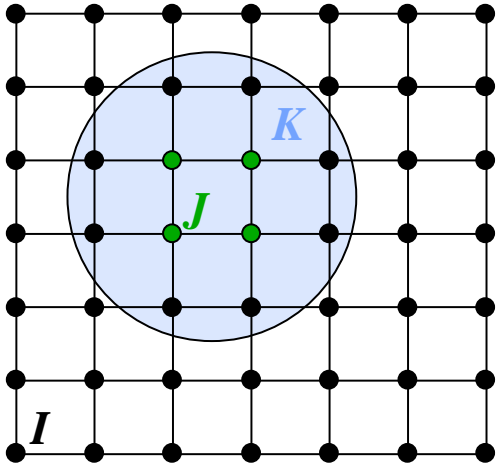
Problem: Too many degrees of freedom

Partition of Unity Finite Element Method [1]

- **Trial function:**

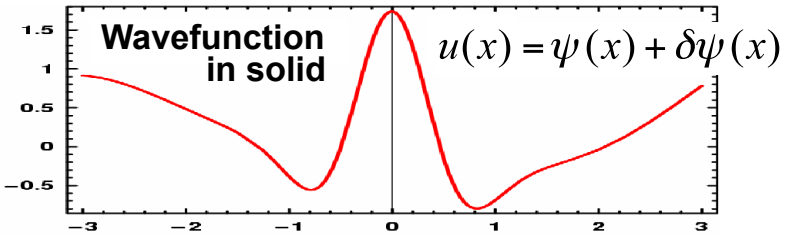
$$u^h(\mathbf{x}) = \underbrace{\sum_{i \in I} c_i \phi_i(\mathbf{x})}_{\text{FE contribution}} + \underbrace{\sum_{j \in J,\, k \in K} d_{jk} \phi_j^{PU}(\mathbf{x}) \psi_k(\mathbf{x})}_{\text{Enriched contribution}}$$

  - I = **nodes in mesh**
  - $J \subseteq I$ = **nodes to be enriched**
  - K = **enrichment function indices**
  - $\{\phi_i(\mathbf{x})\}$ = **FE basis functions**
  - $\{\phi_j^{PU}(\mathbf{x})\}$ = **PU basis functions,** $\sum_j \phi_j^{PU}(\mathbf{x}) = 1$
  - $\psi_k(\mathbf{x})$ = **enrichment functions**

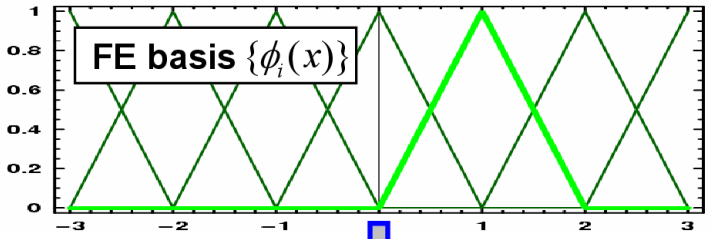


[1] Melenk, Babuska, Comp. Meth. Appl. Mech. Eng. **139**, 289 (1996)

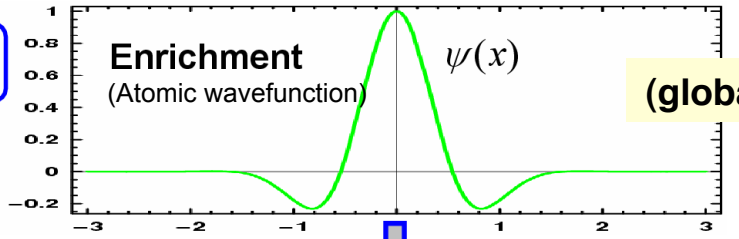
Partition of unity finite elements in quantum mechanical calculations



PU = Partition of unity
FE = Finite element



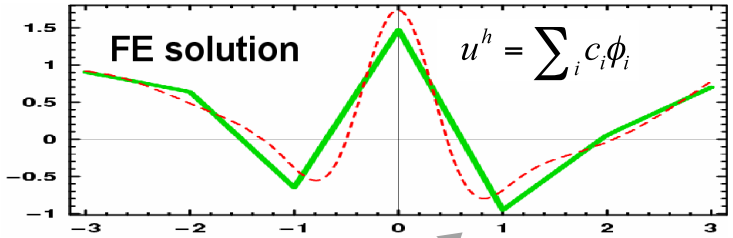
Add physics

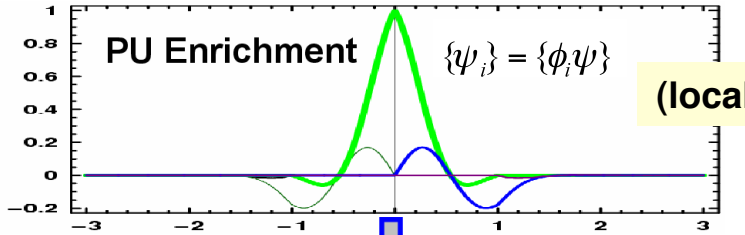


(global)

(Solve)

(Partition)

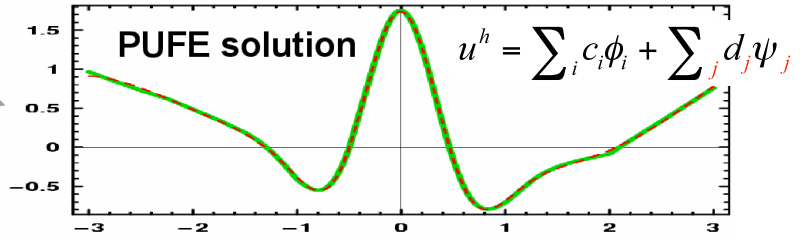




(local)

(Solve)

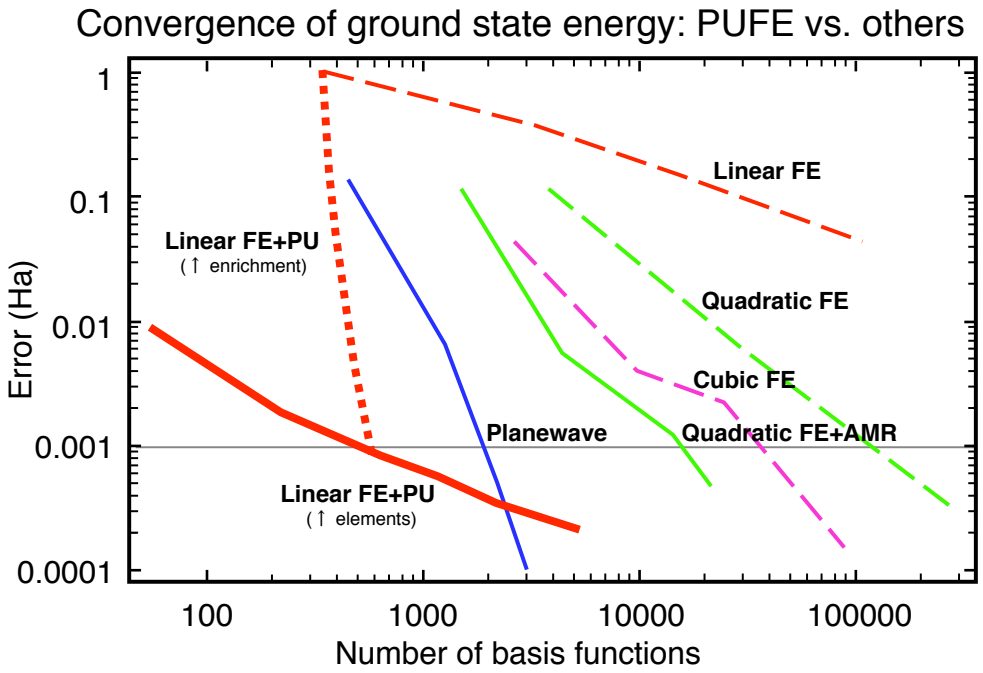
(6-element solutions)

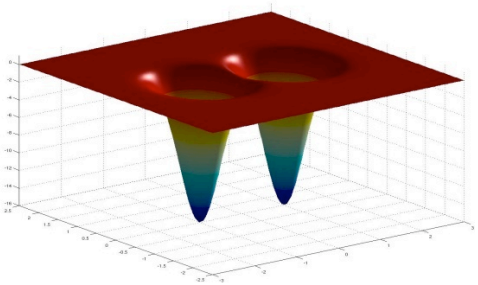


- Known physics incorporated
- Accuracy increased
- Strict locality retained

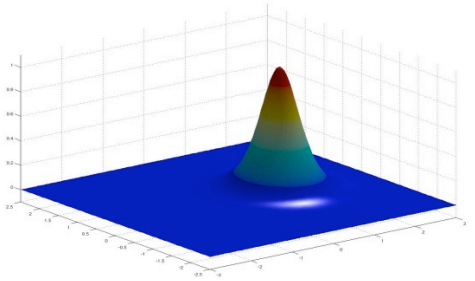
PUFE vs. current state-of-the-art: model problem

- **Conventional Planewave, FE, and new PUFE methods applied to standard test problem [1,2]: deep, localized potential, as for *d*- or *f*- electron metal**





Potential – 2 a.u. separation

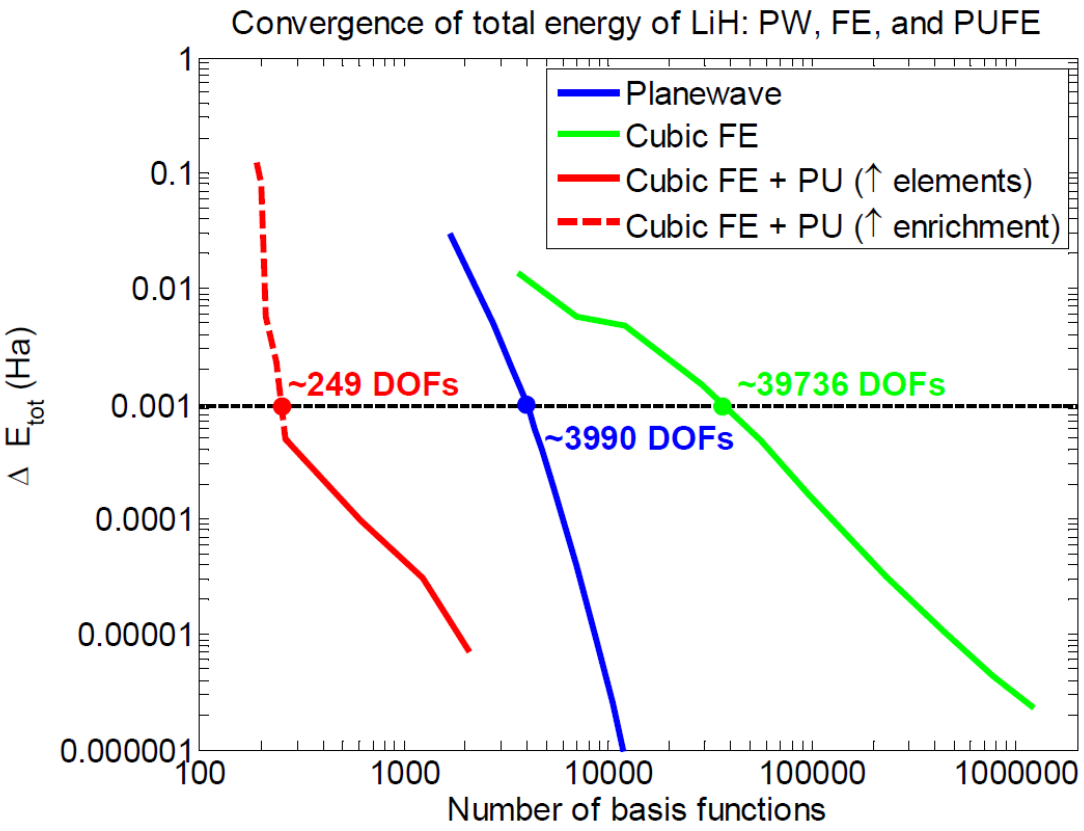


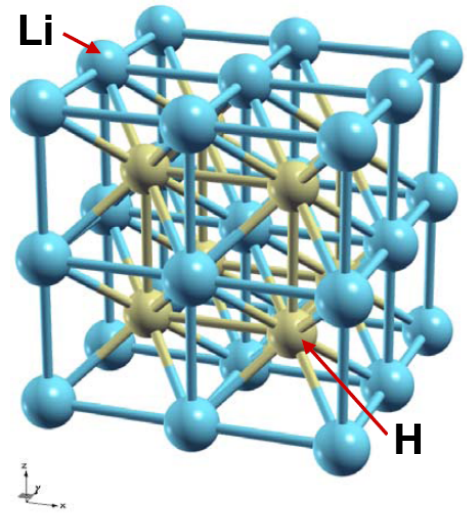
Enrichment function

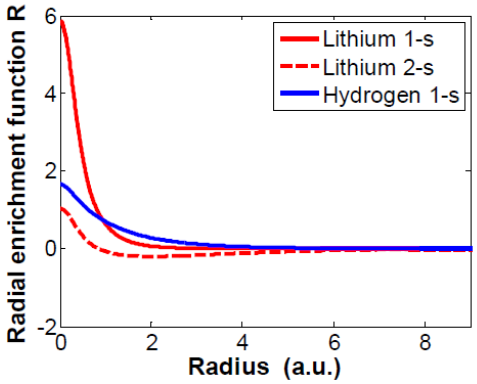
- **Factor of 30 reduction in basis functions relative to best conventional FE**
- **Factor of 4 reduction relative to PW**
- **⇒ Order of magnitude reduction in total solution time relative to PW**

[1] Gygi, Europhys. Lett. **19**, 617 (1992) [2] Tsuchida, Tsukada, Phys. Rev. B **54**, 7602 (1996)

PUFE vs. current state-of-the-art: real materials



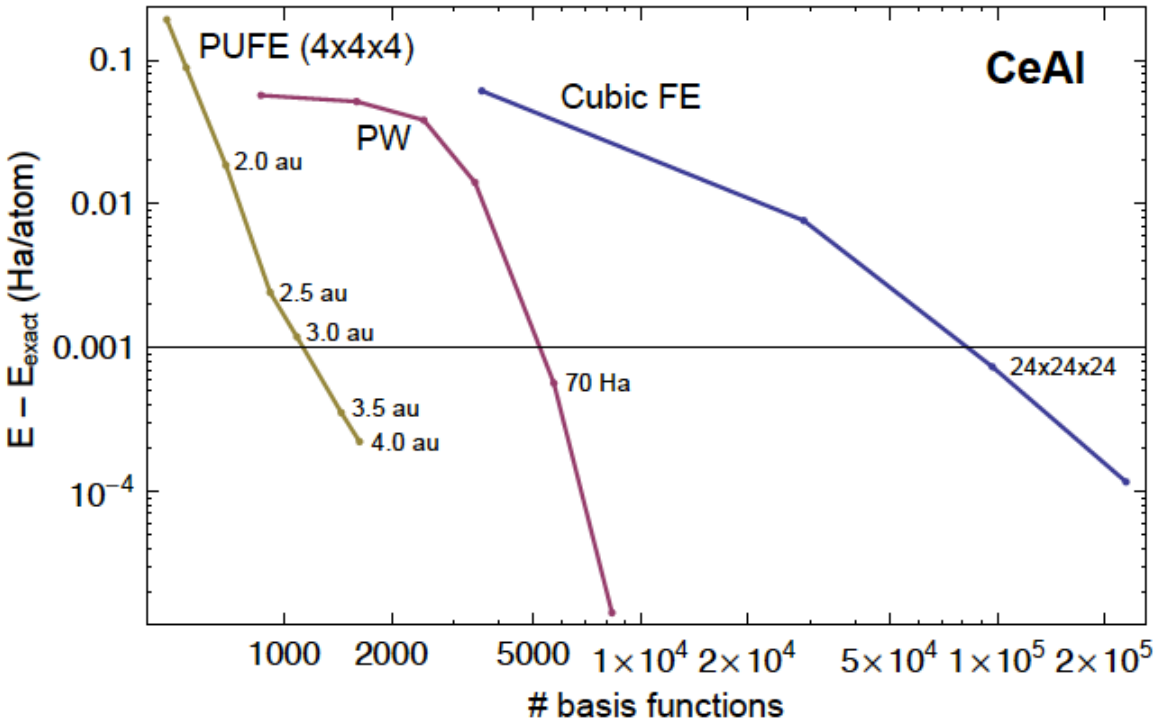


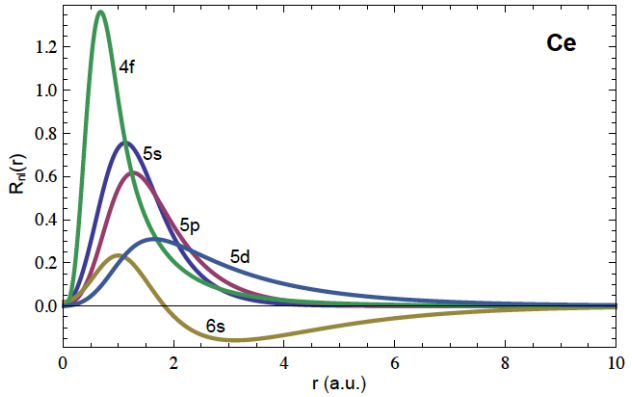


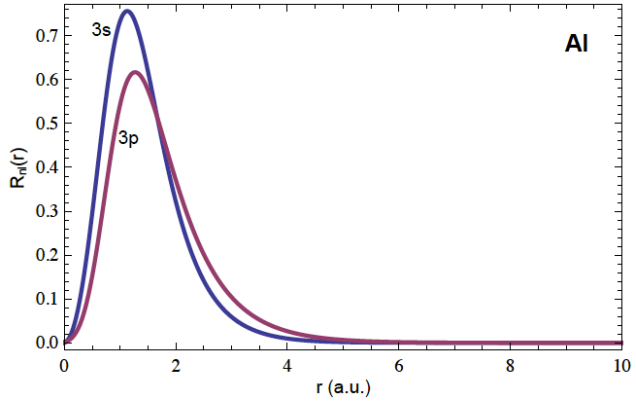
Order of magnitude advance

PUFE vs. current state-of-the-art: worst case

- Triclinic CeAl, atoms displaced
- 17 enrichment functions for Ce: s, p, d, and f orbitals



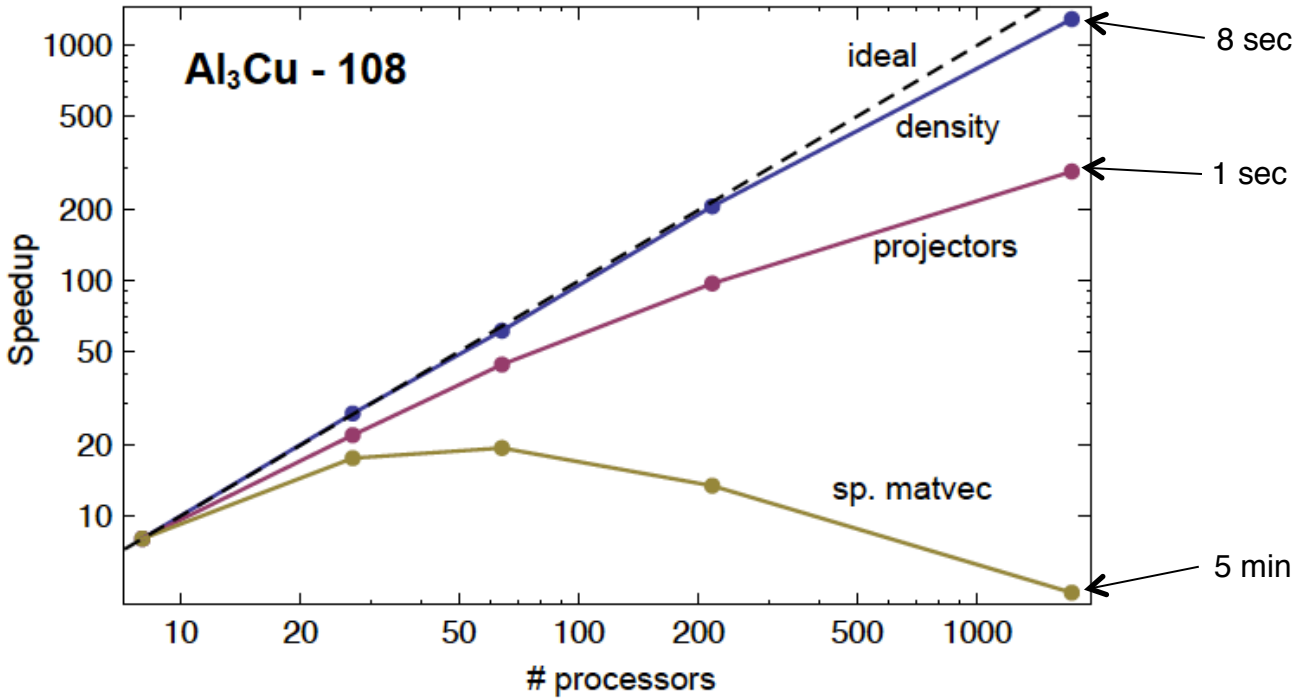




Still, factor of 5

Parallel Implementation

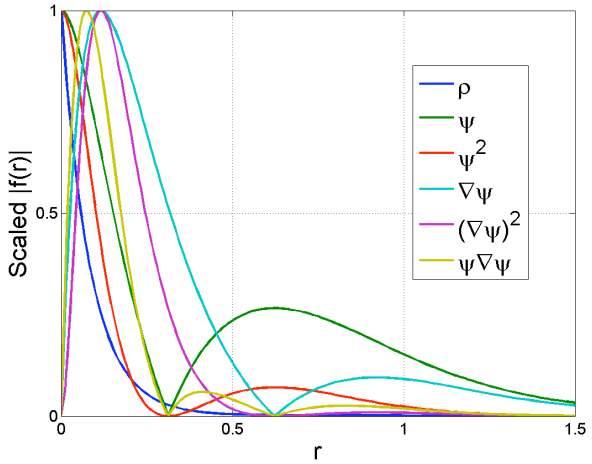
- Fortran 90 + MPI
- Parallelized density construction, matrix element integrals, sparse matvecs
- Test: CuAl cell, 108 atoms
- 8 – 1728 procs., LLNL sierra cluster, 12 cores per node



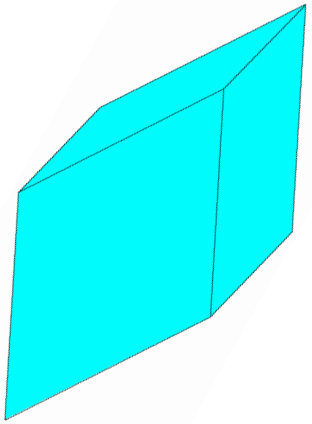
Sparse matvecs: reduce gather-scatters

•Integrands and integration domain

•Linear scale



•Unit cell



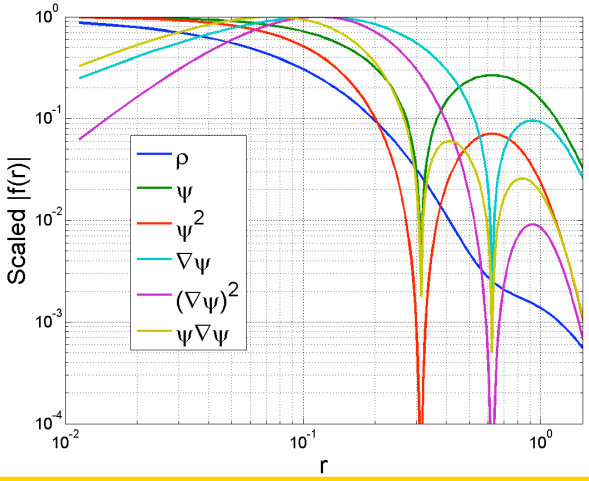
$$a_1 = a/2(0,1,1),$$

$$a_2 = a/2(1,0,1),$$

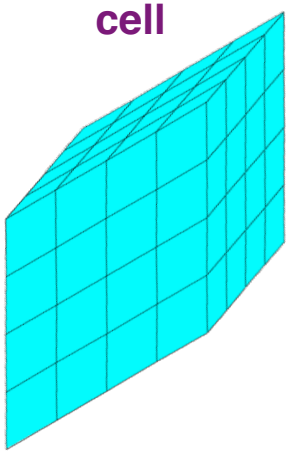
$$a_3 = a/2(1,1,0),$$

$$a = 6.75\ bohr$$

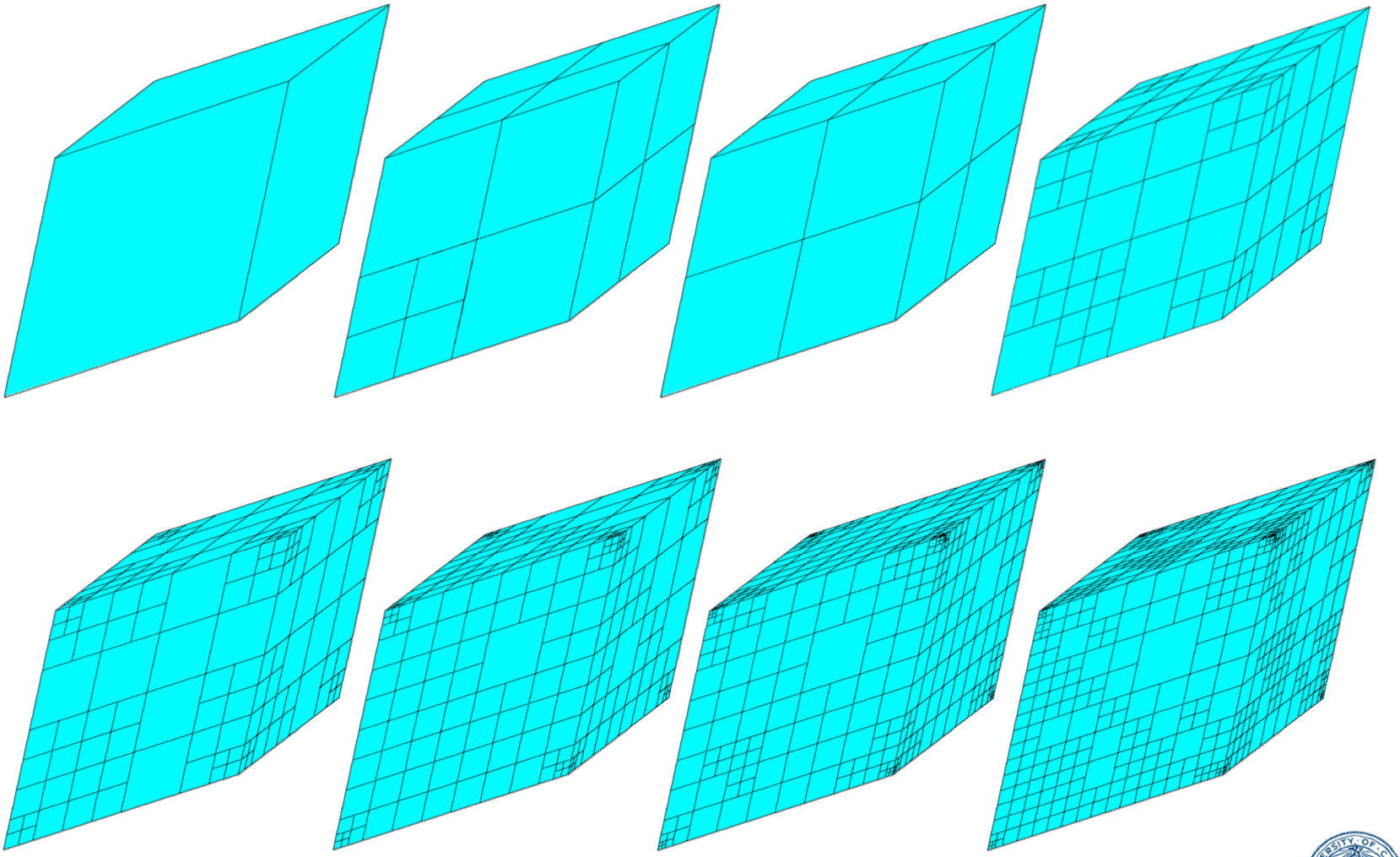
•Logarithmic scale



•Finite element discretization of the unit cell



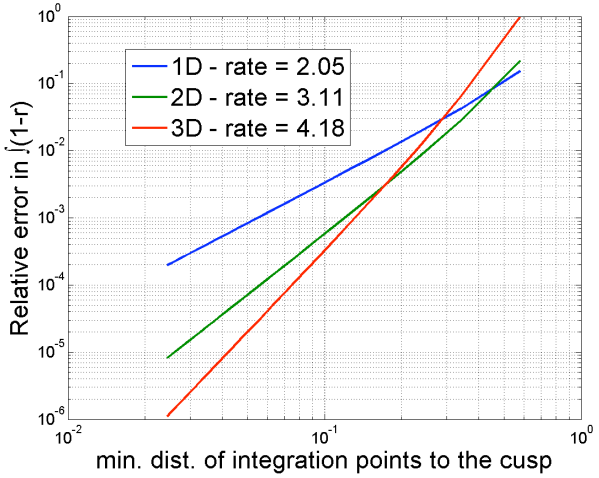
- **Adaptive integration**

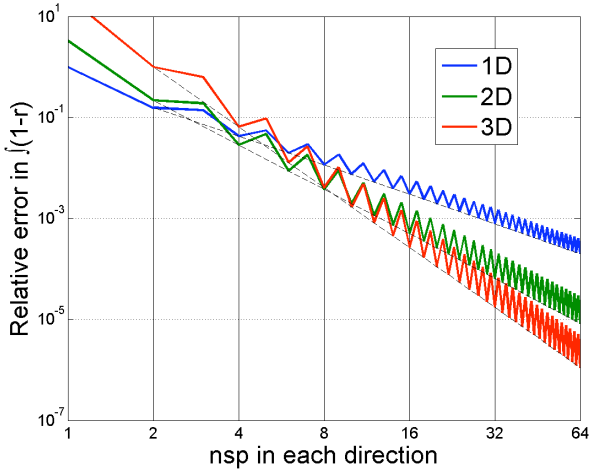


•Adaptive integration

- For each element:
  1. Integrate over the element using a tensor product rule
  2. Divide the element into 8 similar partitions and integrate over each of them
  3. If the difference is below the tolerance, return the quadrature over the element.
  4. If the difference is above the tolerance, repeat the process for each of the 8 partitions separately.

•Performance of adaptive integration for functions with a cusp:





Blessing of dimensionality!

•Adaptive integration – Poisson solve

Mesh	Error tolerance	Number of integration points		
		Tensor-product•*	Adaptive quadrature	Pure FE
2	7×10^{-3}	512000	128750	1000
4	2×10^{-3}	169000	72750	8000
7	3×10^{-4}	—	141750	42875
8	2×10^{-4}	624000	137500	64000
12	2×10^{-5}	1840000	297375	216000
16	6×10^{-6}	14020000	540000	512000
20	4×10^{-6}	27196000	1171500	1000000
24	7×10^{-7}	46852000	1896000	1728000
32	2×10^{-7}	—	4369000	4096000

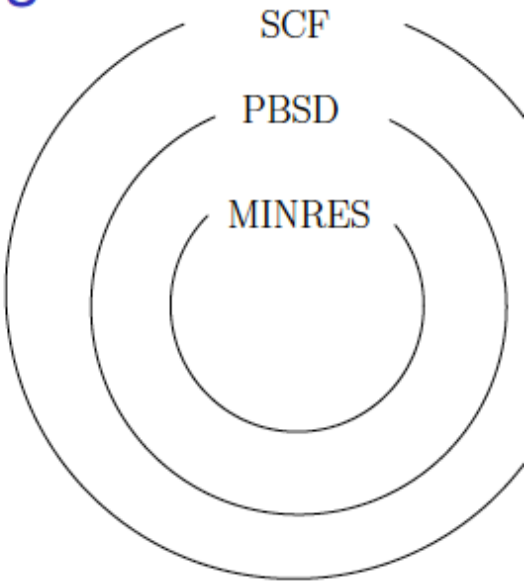
•* Pask et al., IJMCE, in press

Order of magnitude speedup

Detecting MINRES stagnation and setting tolerance

Eigensolver's innermost loop solves $(A - \widehat{\lambda} B)p = r$

- solve inexactly by MINRES
- dominant cost ($\sim 70\%$ of total runtime)



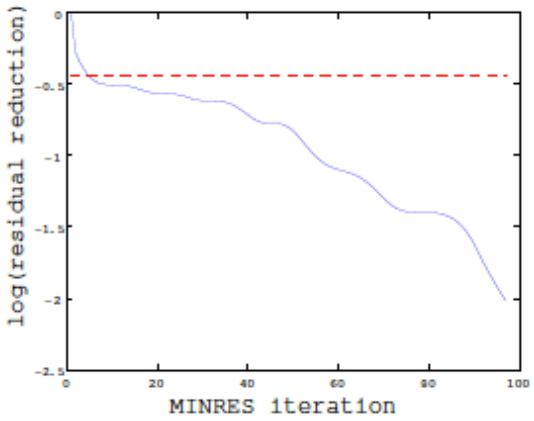
New bound for sth MINRES residual:

$$\frac{\|r_s\|_2}{\|r_0\|_2} \leq 2\Delta^{[s/2]}\sqrt{1-\tau^2} + \tau$$

$\rightarrow$ 0 rapidly $\quad$ $\rightarrow$constant

Idea: **estimate τ and set MINRES tolerance**

MINRES convergence (blue) and stopping tolerance (red)



FEM-KS solver CuAl simulations

mesh: $7 \times 9 \times 10 \times 11 = 6930$

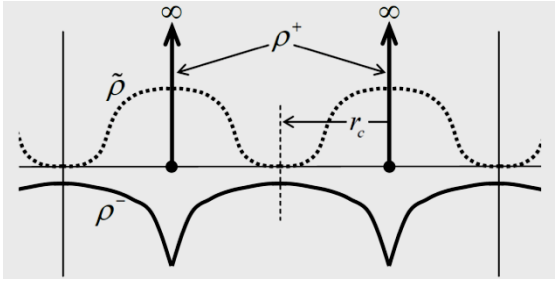
	Total time(s)	# MINRES
standard	76.5	9230
new	40.4	3643

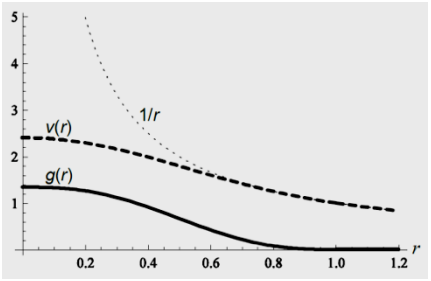
mesh: $7 \times 18 \times 20 \times 22 = 55440$

	Total time(s)	# MINRES
standard	8409	96459
new	2986	27964

All-electron problem

All-electron calculations: O(*N*) Coulomb potential and energy [1]





- **Introduce smooth, analytic, strictly local neutralizing function → solve singular part analytically, non-singular remainder numerically, both O(N)**

- **No "distributed nucleus" approx., sphere-interstitial matching, FFTs, Ewald, etc.**

$$\rho(\mathbf{x}) = \rho^+(\mathbf{x}) + \rho^-(\mathbf{x}) = \underbrace{\rho^+(\mathbf{x}) - \tilde{\rho}(\mathbf{x})} + \underbrace{\rho^-(\mathbf{x}) + \tilde{\rho}(\mathbf{x})} = \tilde{\rho}^+(\mathbf{x}) + \tilde{\rho}^-(\mathbf{x})$$

$$V(\mathbf{x}) = V^+(\mathbf{x}) + V^-(\mathbf{x}) = \tilde{V}^+(\mathbf{x}) + \tilde{V}^-(\mathbf{x}) \quad \text{(in } H^1\text{)}$$

$$\tilde{V}^+(\mathbf{x}) = \sum_I \frac{q_i}{|\mathbf{x} - \tau_I|} - \tilde{V}_I(\mathbf{x}) \quad \text{(analytic)} \qquad \nabla^2 \tilde{V}^-(\mathbf{x}) = -4\pi\tilde{\rho}^-(\mathbf{x}) \quad \text{(numerical)}$$

$$E = \tfrac{1}{2}\int_\Omega d^3x\, \rho(\mathbf{x})V(\mathbf{x}) = \tfrac{1}{2}\int_\Omega d^3x\, (\tilde{\rho}^+(\mathbf{x}) + \tilde{\rho}^-(\mathbf{x}))(\tilde{V}^+(\mathbf{x}) + \tilde{V}^-(\mathbf{x})) = E^{++} + E^{+-} + E^{--}$$

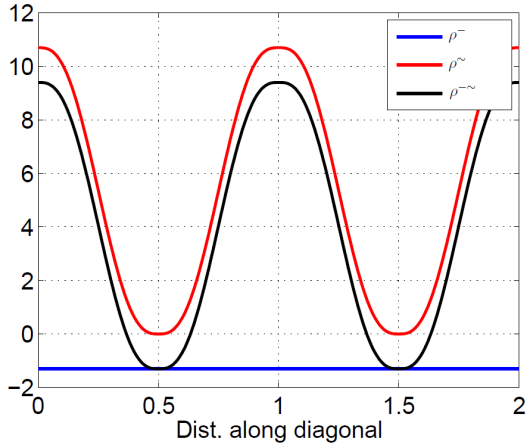
$$E - E_{self} = \sum_i [q_i \tilde{V}^-(\tau_i) - \tfrac{1}{2}q_i^2(v(0) + I_g)] + \int_\Omega d^3x\, (\tfrac{1}{2}\tilde{\rho}^-(\mathbf{x}) - \tilde{\rho}(\mathbf{x}))\tilde{V}^-(\mathbf{x}) \quad \text{(pointwise)}$$

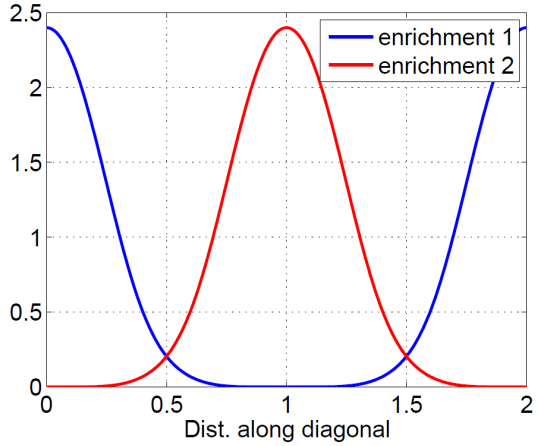
$$= \sum_i \tfrac{1}{2}q_i^2(I_g - v(0)) + \sum_i q_i \int_{\Omega_i} d^3x\, \rho^-(\mathbf{x})(1/r_i - v(r_i)) + \tfrac{1}{2}\int_\Omega d^3x\, \tilde{\rho}^-(\mathbf{x})\tilde{V}^-(\mathbf{x}) \quad \text{(integral)}$$

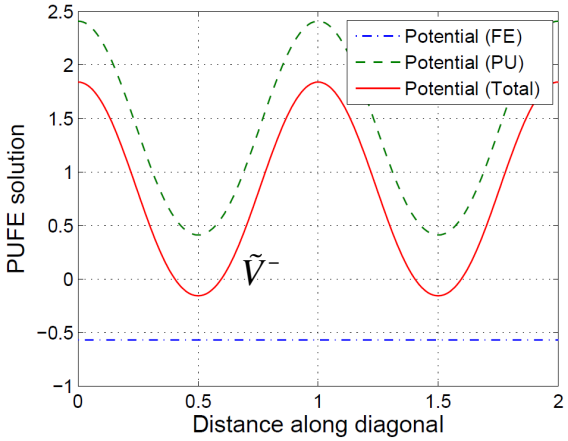
[1] Pask, Sukumar, Mousavi (2010): arXiv:1004.1765

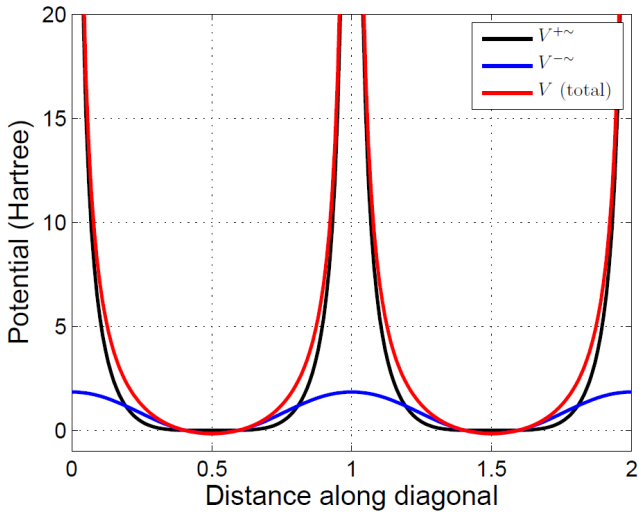
All-electron calculations: Ewald problem

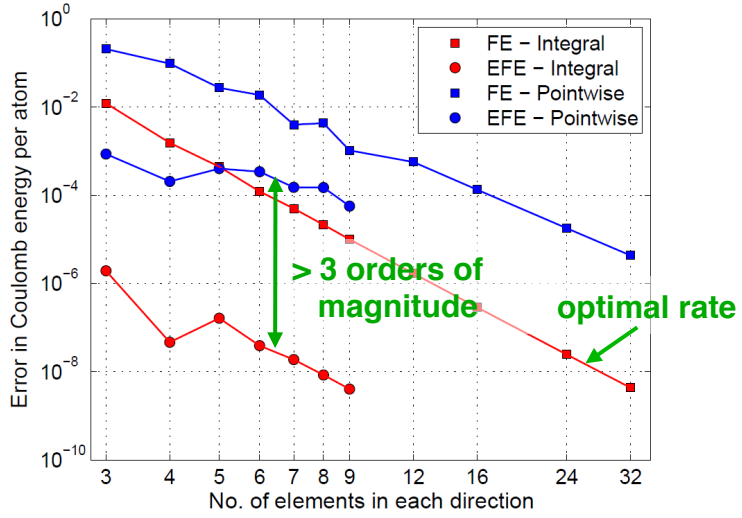
- **bcc crystal: unit spacing, unit nuclear charges, uniform electronic density**





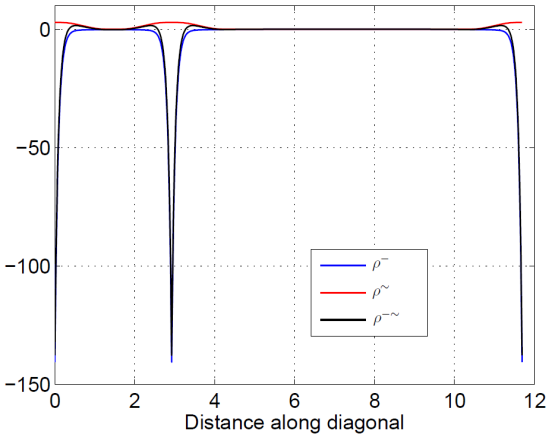


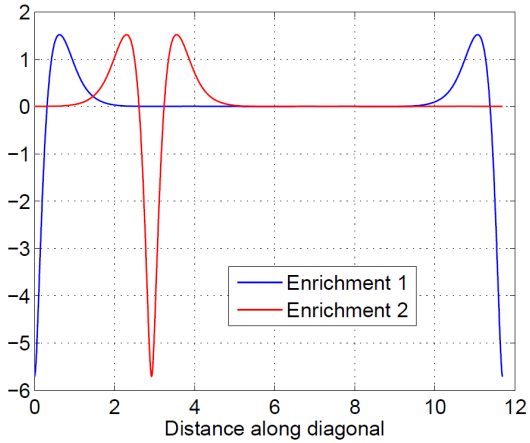


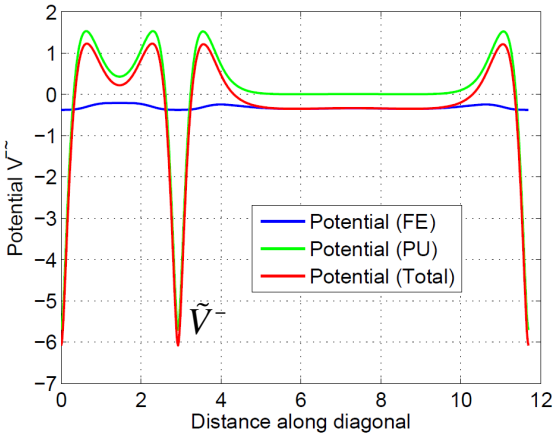


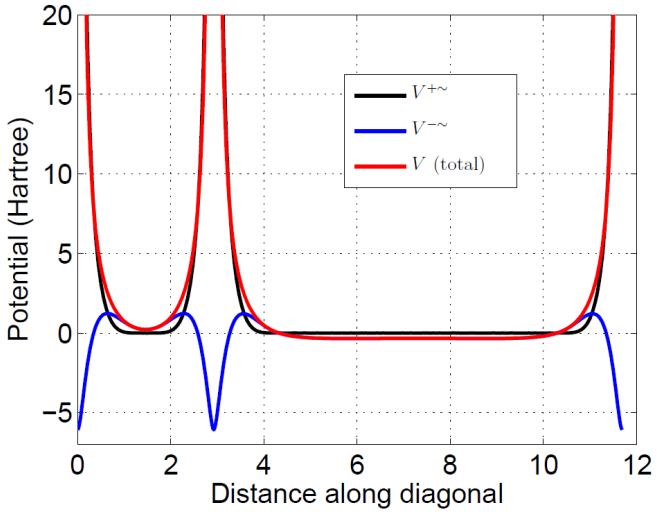
All-electron calculations: Diamond

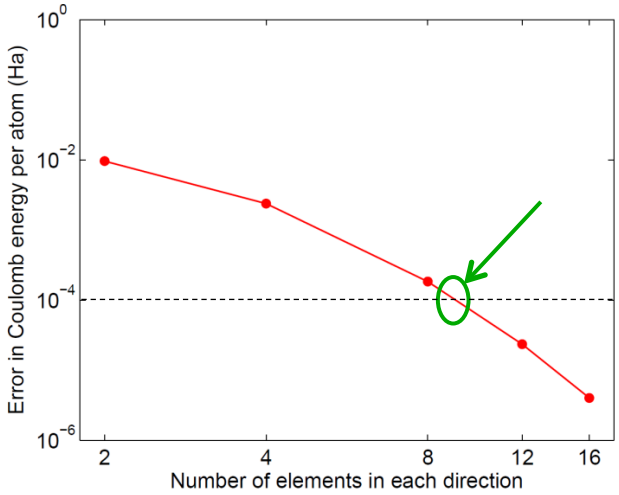
- **Enrichment functions from isolated atom densities**











Summary

- General, systematically improvable ab initio electronic-structure calculations in a partition-of-unity FE basis: arbitrary unit cells, Brillouin zone sampling, metals and insulators.
- Strictly local, piecewise polynomial basis → well suited to large, accurate calculations on massively parallel architectures.
- Initial results show order-of-magnitude advantage relative to present state-of-the-art.
- New state-or-the-art? Parallelization/optimization will tell.

Issues / in progress / future:

- Metallic QMD at extreme conditions
- Forces: Pulay-like corrections?
- Problem formulation: all-electron? PAW?
- Basis: order? modal? hierarchical? spectral?
- Memory and solver optimizations: preconditioning, SD?, CG?, Anderson (RMM)? …
- Parallel implementation: data distribution
- O(N)

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