Recent developments of Discontinuous Galerkin Density functional theory

Lin Lin

Department of Mathematics, UC Berkeley;
Computational Research Division, LBNL

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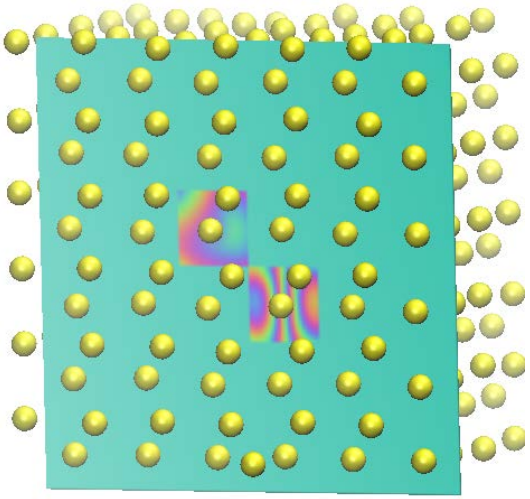
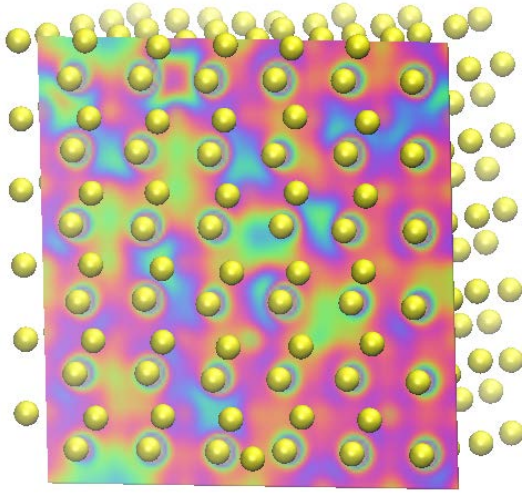
Brief description of DGDFT

- Kohn-Sham DFT (LDA/GGA)
- Discontinuous basis functions
  - Continuous density?
  - Finite kinetic energy?
- Relatively simple control of accuracy
- Relatively small number of basis per atom



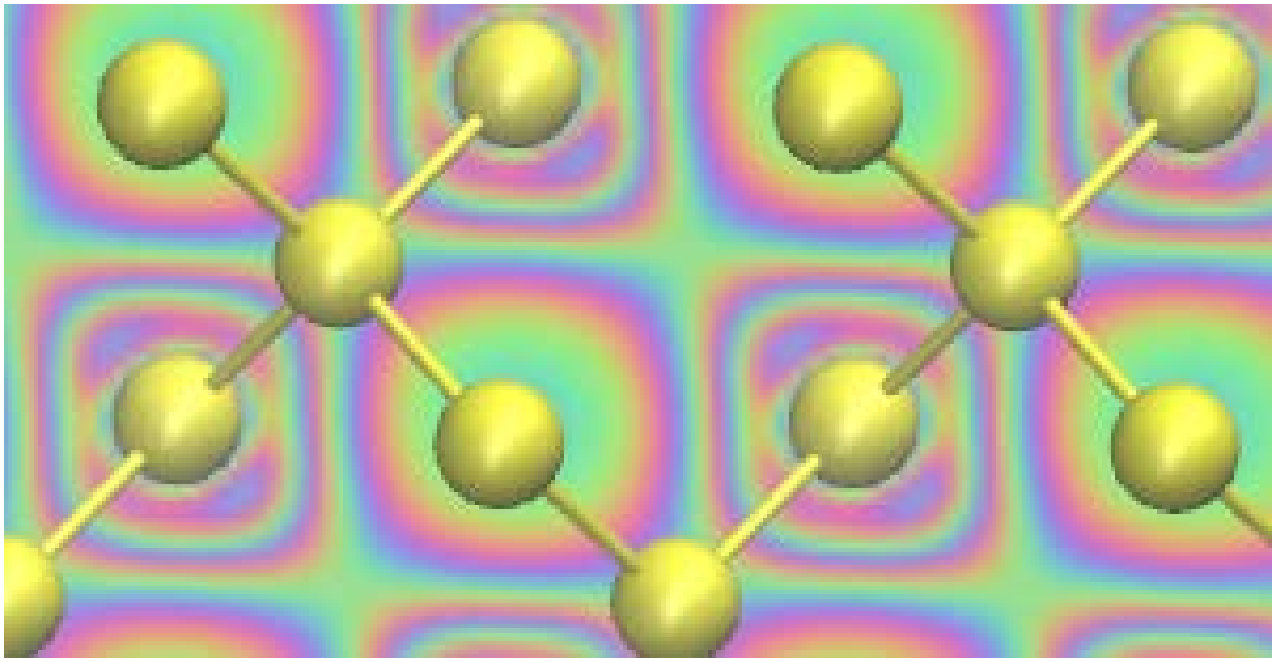


Feature of DGDFT

- Real space formulation (Discontinuous Galerkin)
- Exchange-correlation used by libxc
- HGH norm conserving pseudopotential.
- Geometry optimization
- Molecular dynamics (NVE/NVT)
- Massively parallel (>50000 procs)
- Compatible with the Pole Expansion and Selected Inversion method (PEXSI) for overcoming O(N^3) wall

[LL-Lu-Ying-E, J. Comput. Phys. 231, 2140 (2012)]

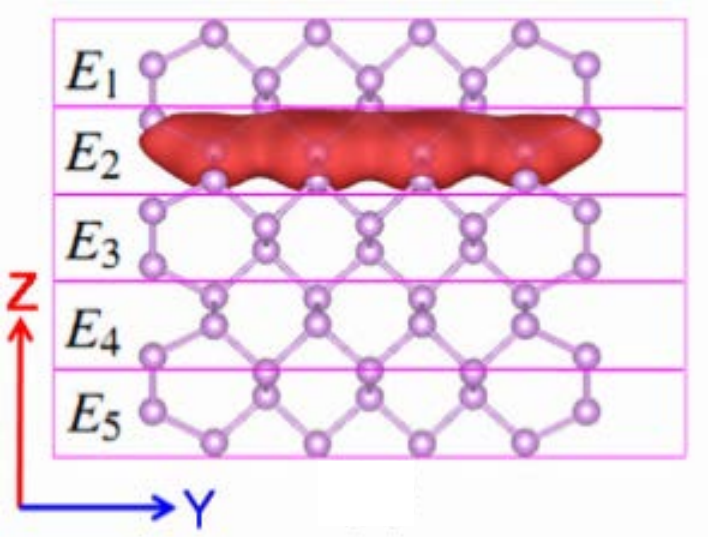
Why another basis set



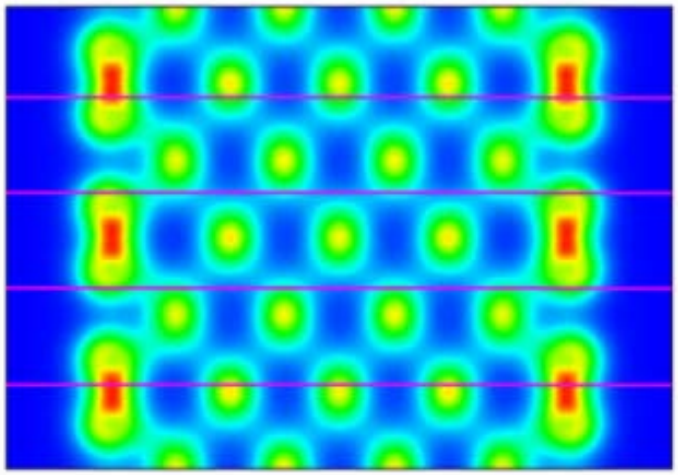
Example: electron density of Si
(HGH pseudopotential)

Our goal: Automatic dimension reduction

- Construct the local basis functions adaptively by solving a small part of the system, and obtain discontinuous basis functions.
- Discontinuous Galerkin (DG) framework to patch basis functions together.



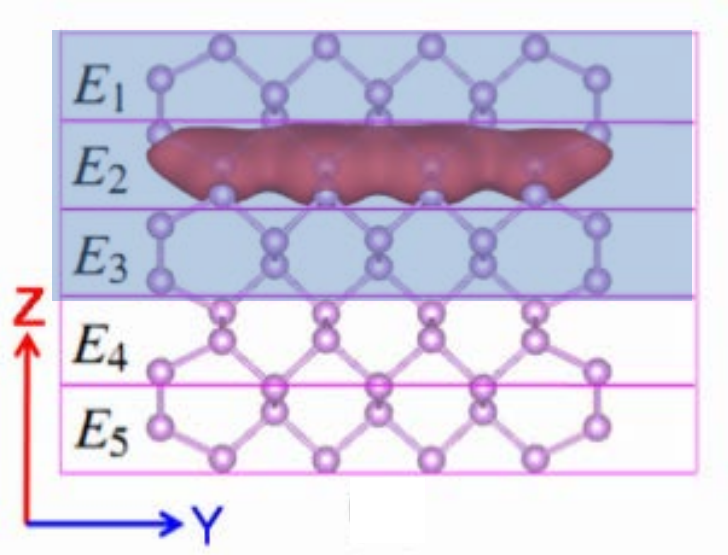
Basis (discontinuous)



Density (nearly continuous)

Adaptive local basis functions

- Element: E_k, Extended element: Q_k.
- Solving the linear eigenvalue problem (NO pseudo-hydrogen saturation etc.) inside the extended element region with periodic boundary conditions.

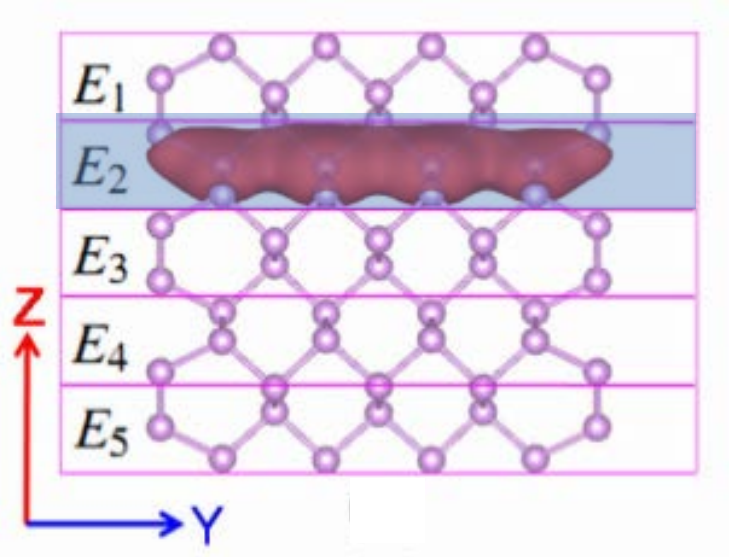


$$H_{\mathrm{eff},Q_k}\widetilde{\varphi}_{k,j} = \varepsilon_{k,j}\widetilde{\varphi}_{k,j}.$$

Here $Q_2 = E_1 \cup E_2 \cup E_3$

Adaptive local basis functions

- Restrict $\tilde{\varphi}_{k,j}$ from extended element to element $\varphi_{k,j}$
- Orthogonalize $\varphi_{k,j}$ (via singular value decomposition): adaptive local basis functions.

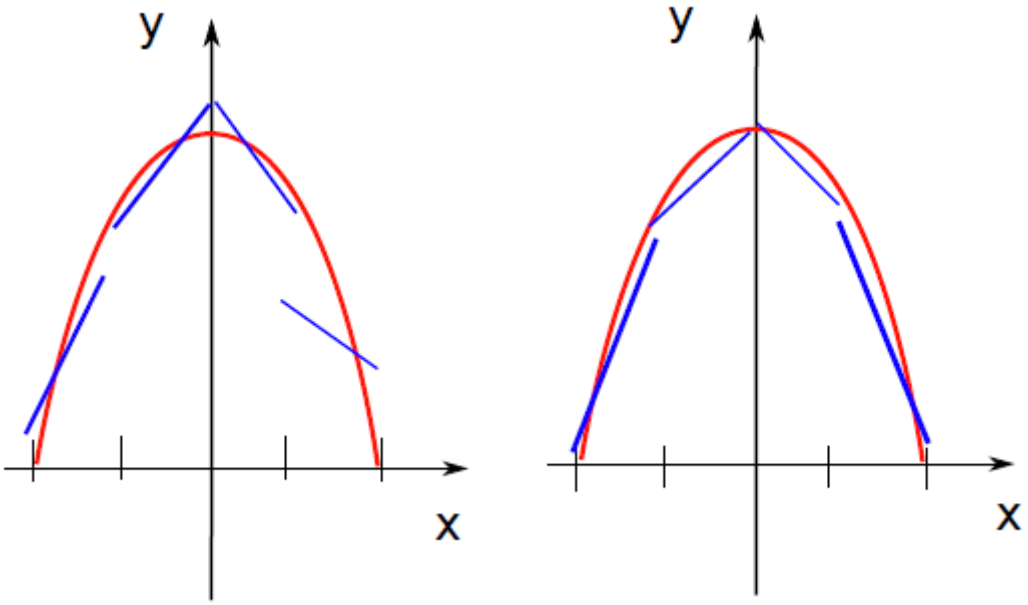


$$H_{\mathrm{eff},Q_k}\tilde{\varphi}_{k,j} = \varepsilon_{k,j}\tilde{\varphi}_{k,j}.$$

$$\varphi_{k,j} = \tilde{\varphi}_{k,j}\big|_{E_k}.$$

Discontinuous Galerkin method

- Finite element method with discontinuous basis functions.
- Inter-element continuity (consistency): e.g. Penalty on the inter-element jump [Arnold, 1982]



Kohn-Sham energy functional

Fix the electron density ρ, and consider the linear problem (i.e. one step SCF iteration)

$$H_{\text{eff}} = -\frac{1}{2}\Delta + V_{\text{eff}} + \sum_{\ell} \gamma_\ell |b_\ell\rangle\langle b_\ell|$$

with orthonormality constraints $\langle \psi_i, \psi_j \rangle = \delta_{ij}$.
The effective one-body potential

$$V_{\text{eff}}[\rho](x) = V_{\text{ext}}(x) + \int \frac{\rho(y)}{|x-y|}\,\mathrm{d}y + \epsilon'_{\text{xc}}[\rho(x)].$$

Kohn-Sham energy functional

The linear problem minimizes the following quadratic functional

$$E_{\text{eff}}(\{\psi_i\}) = \frac{1}{2}\sum_{i=1}^{N}\int |\nabla\psi_i(x)|^2\,\mathrm{d}x + \int V_{\text{eff}}(x)\rho(x)\,\mathrm{d}x$$

$$+\sum_{\ell}\gamma_\ell\sum_{i=1}^{N}|\langle b_\ell,\psi_i\rangle|^2,$$

Discontinuous Galerkin method

Kohn-Sham

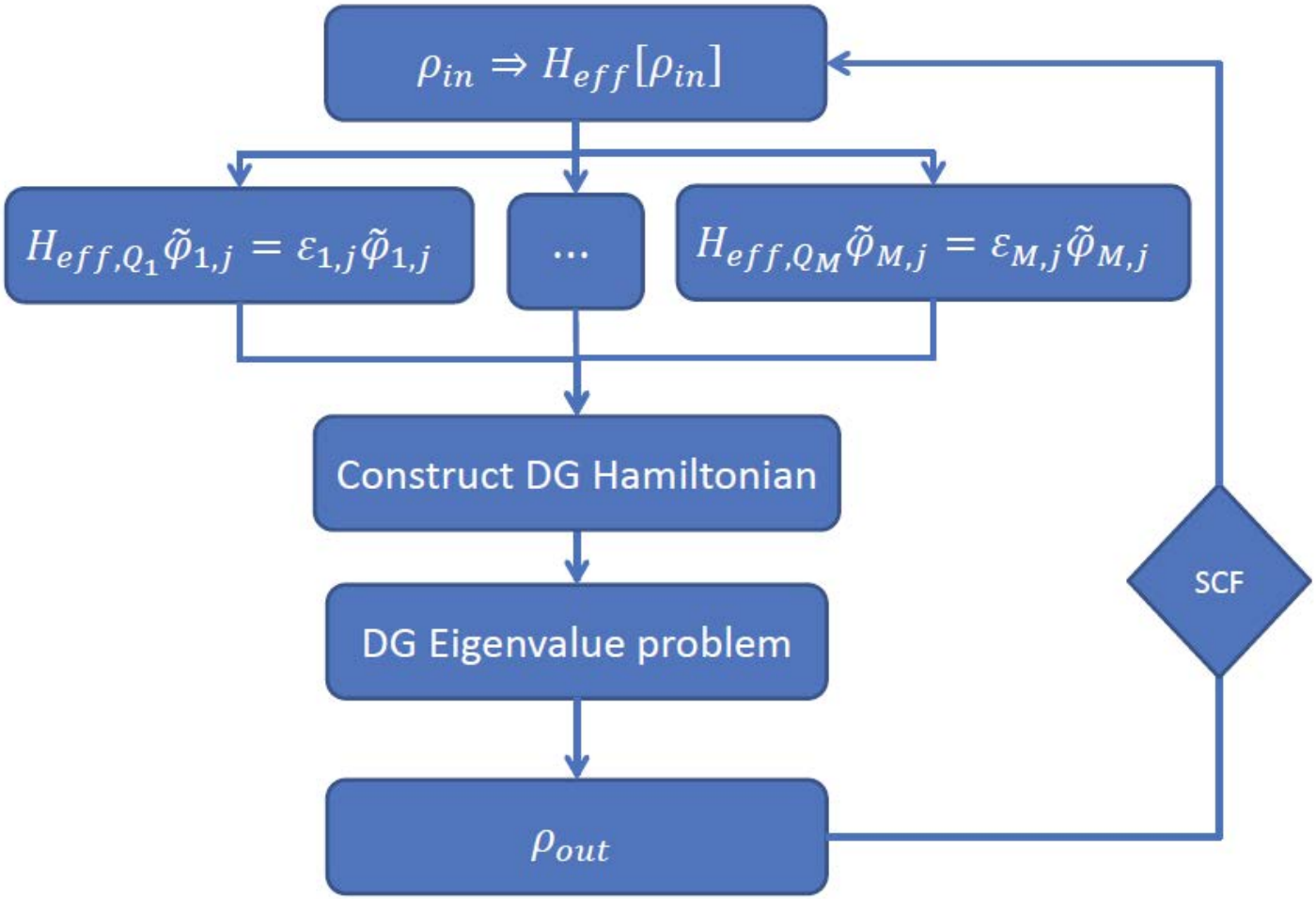
$$E_{\mathrm{DG}}(\{\psi_i\}) = \frac{1}{2}\sum_{i=1}^{N}\langle\nabla\psi_i,\nabla\psi_i\rangle_{\mathcal{T}}+\langle V_{\mathrm{eff}},\rho\rangle_{\mathcal{T}}+\sum_{\ell}\gamma_\ell\sum_{i=1}^{N}|\langle b_\ell,\psi_i\rangle_{\mathcal{T}}|^2$$

$$-\sum_{i=1}^{N}\langle\{\{\nabla\psi_i\}\},[[\psi_i]]\rangle_{\mathcal{S}}+\alpha\sum_{i=1}^{N}\langle[[\psi_i]],[[\psi_i]]\rangle_{\mathcal{S}}.$$

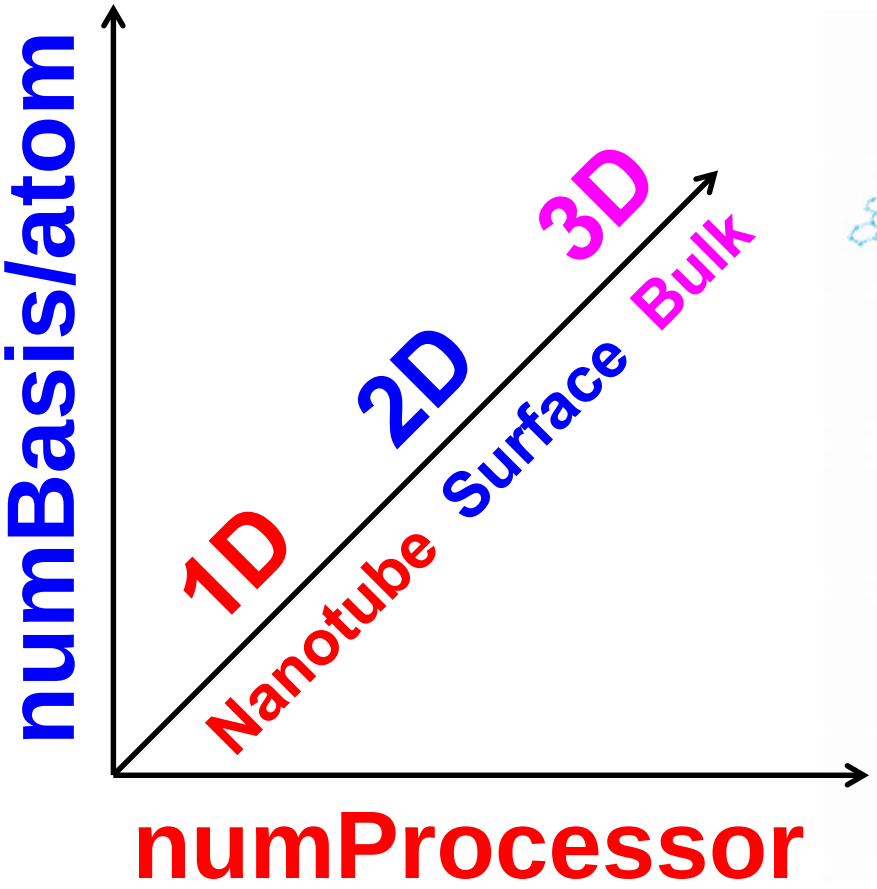
New terms

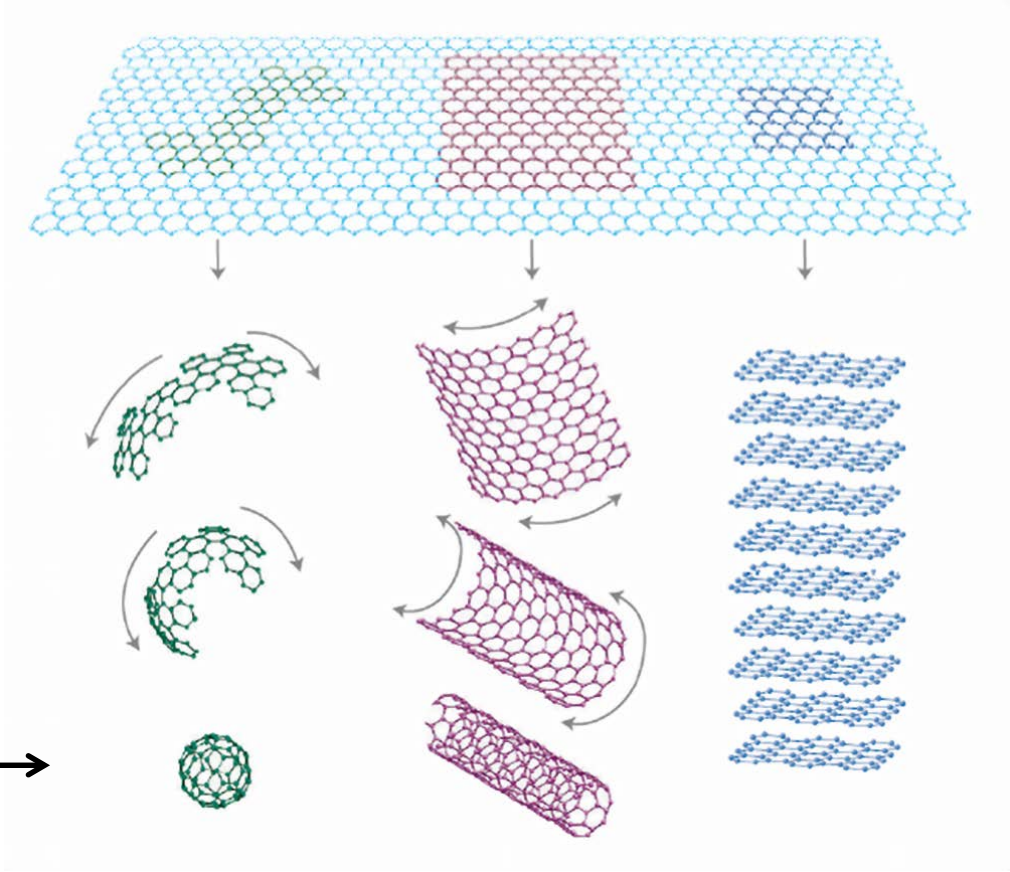
- [LL-Lu-Ying-E, J. Comput. Phys. 231, 2140 (2012)]
- Interior penalty method [Arnold, 1982]

Flowchart of adaptive local basis functions



Different dimensional systems



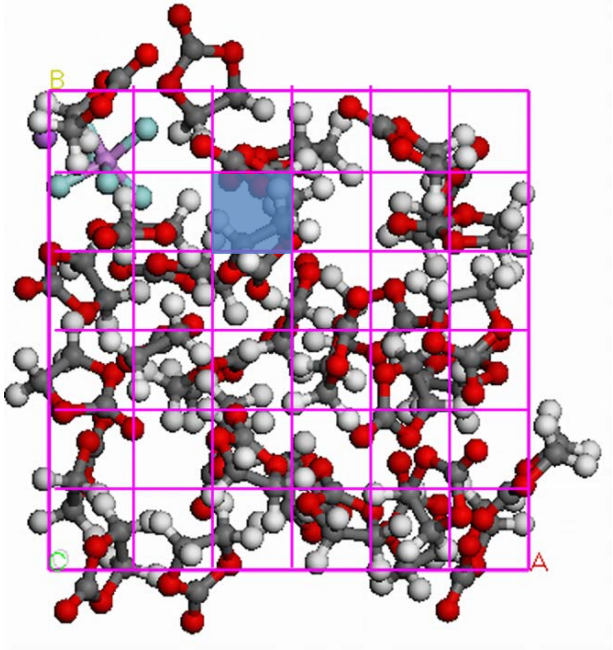


Two level parallelization in DGDFT

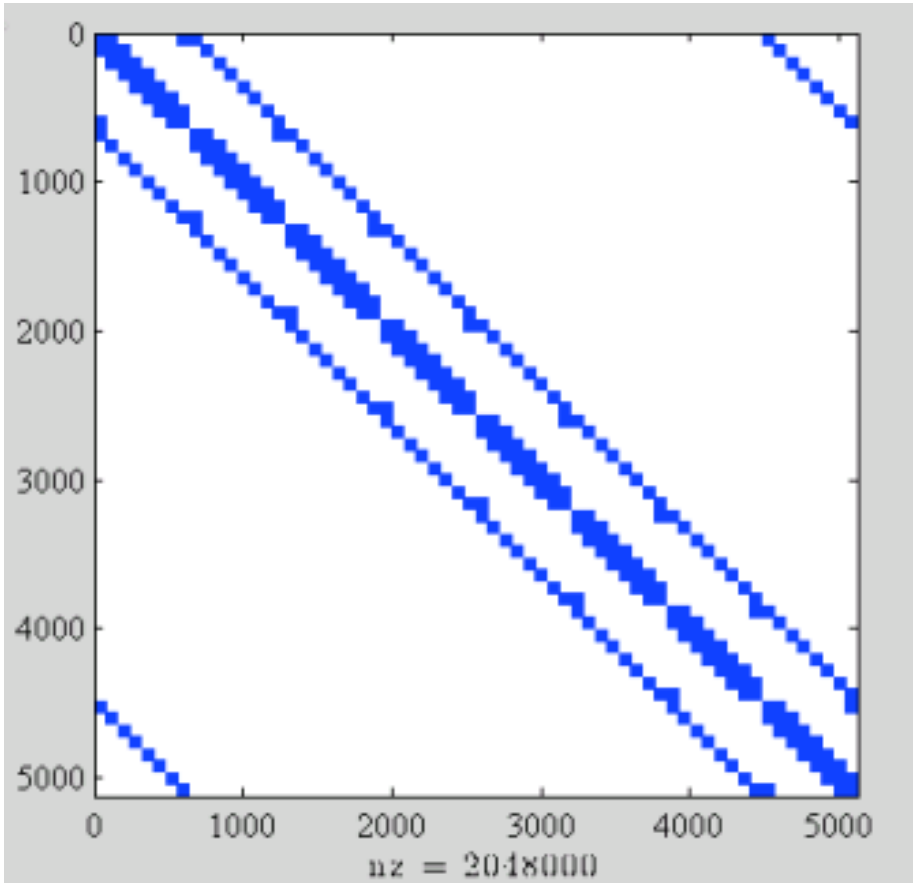
1. Intra-element parallelization
numBasis: 10 ~ 100 procs

2. Inter-element parallelization
numElement: 4 ~ 1,000 procs

Scale to **100,000** procs or more



DG matrix as a block finite difference stencil



Sparsity pattern of a DG matrix for a graphene system with 128 atoms (40 basis per atom)

Pole EXpansion and Selected Inversion

Pole expansion, $Q \sim O(\log(\beta \Delta E))$; $Q = 40 \sim 80$ in practice

$$\rho(x) \approx \sum_{i=1}^{Q} \frac{\omega_i}{H - z_i I}(x, x)$$

Selected Inversion

- Scale at most as $O(N^2)$ even for metals (zero gap).
- Rely on sparsity of H rather than near-sightedness

[LL-Lu-Ying-E, Chin. Ann. Math. 30B 729, 2009]
[LL-Lu-Ying-Car-E, Commun. Math. Sci. 7, 755, 2009]
[LL-Yang-Meza-Lu-Ying-E, ACM Trans. Math. Software 37, 40, 2011]
[LL-Chen-Yang-He, J. Phys. Condens. Matter 25, 295501, 2013]
[LL-Garcia-Huhs-Yang, J. Phys. Condens. Matter 26, 305503, *2014*]

http://www.pexsi.org/

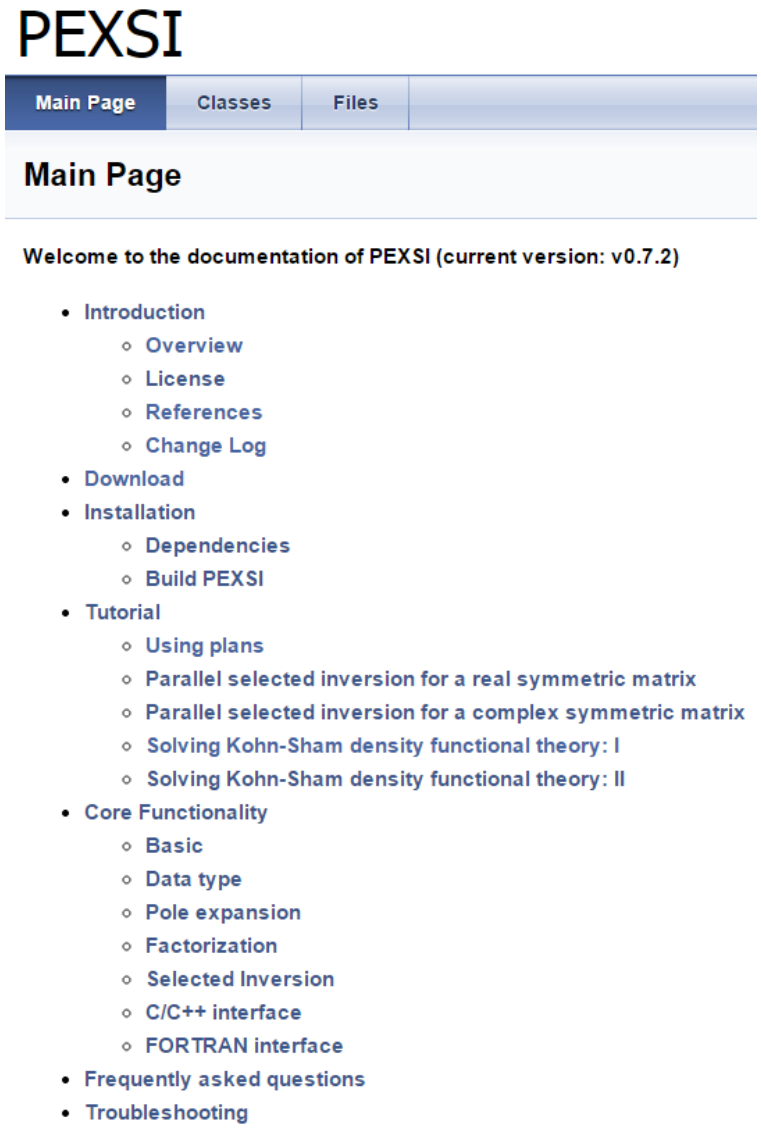
- Work with sparse H, S matrices

- Integrated with SIESTA as SIESTA-PEXSI

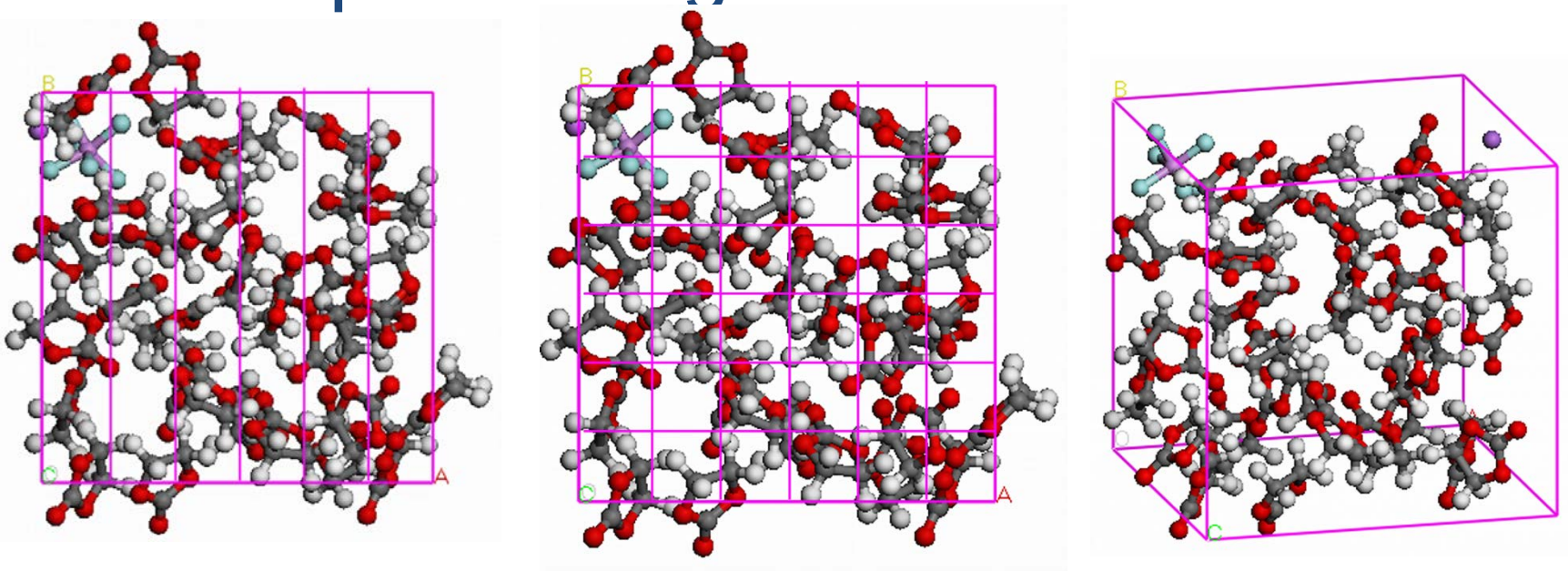
[LL-Garcia-Huhs-Yang, J. Phys. Condens. Matter 26, 305503, *2014*]

Scale to >10,000 processors

for over 20000 atoms solved in DZP basis set.



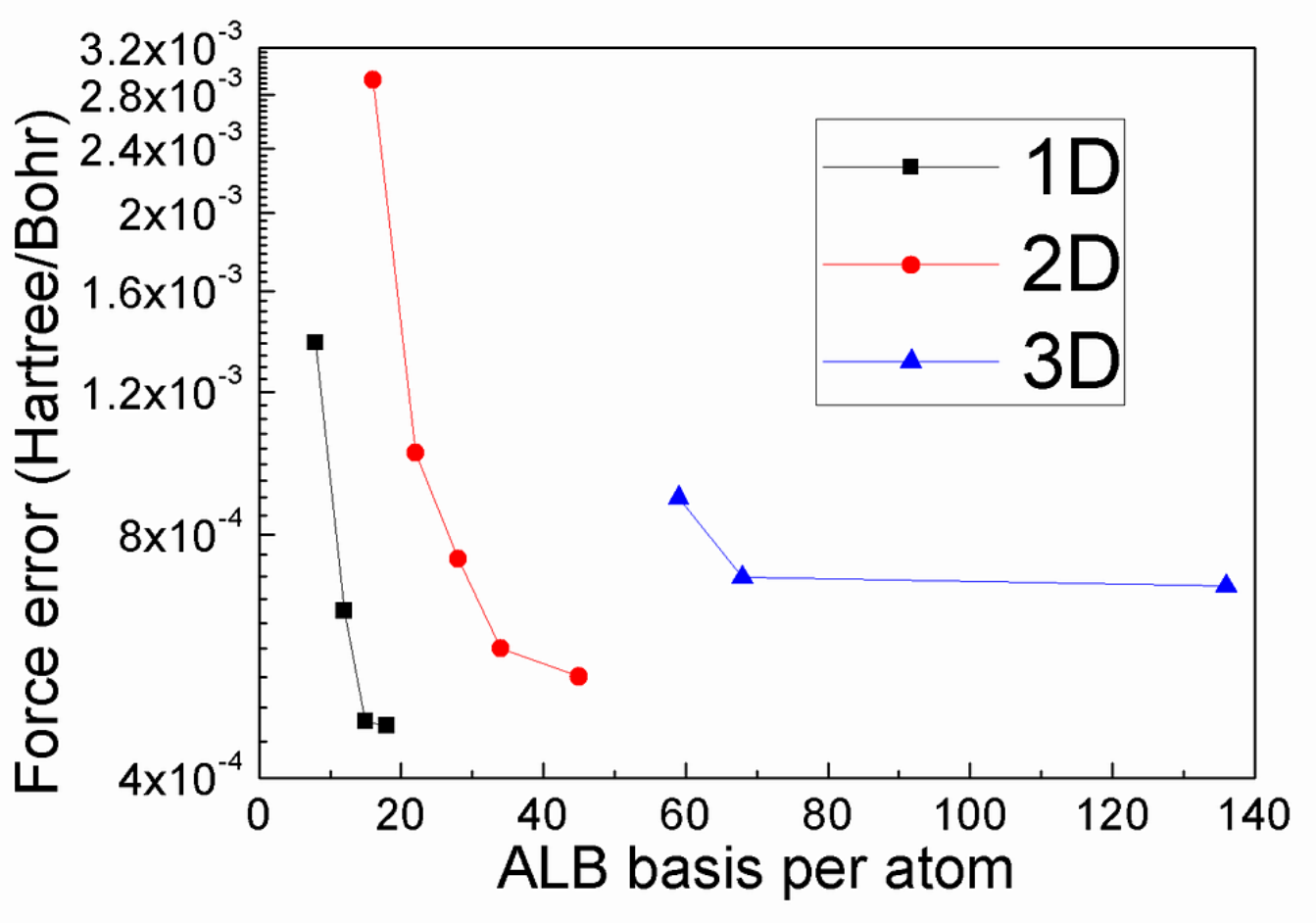
DGDFT for the same system but with different partitioning



Three kinds of partition: **1D**, **2D** and **3D**

Partition	numBasis/element	numProcessors
1D 6*1*1	600 (**12** basis/atom)	6*600 = 3600
2D 6*6*1	300 (**34** basis/atom)	36*300 = 10800
3D 6*6*6	100 (**68** basis/atom)	216*100 = 21600

1D, 2D and 3D Partition

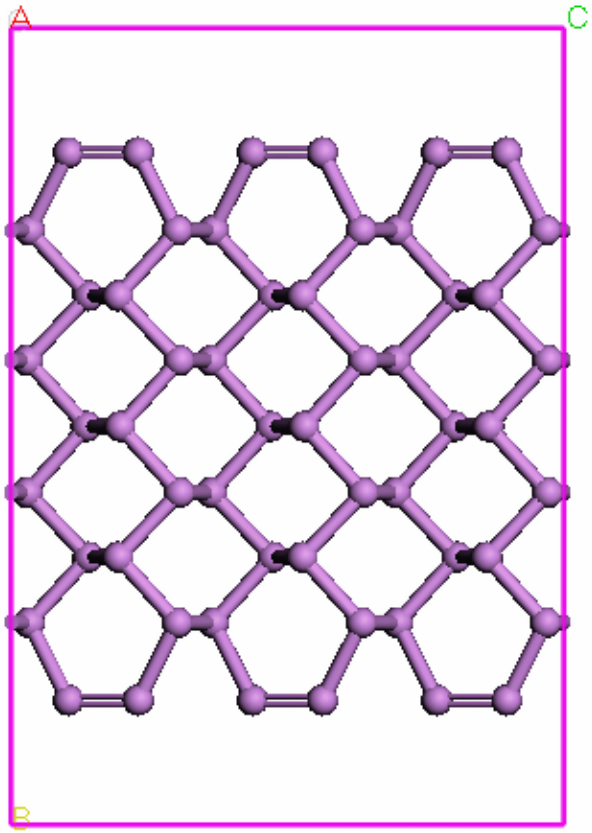


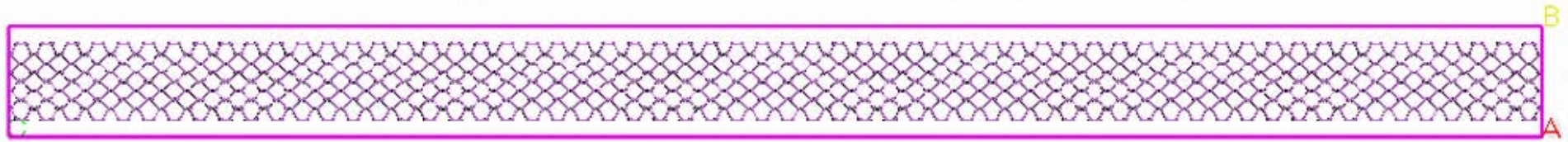
Energy can be as accurate as 1×10^{-5} au/atom.

Compared to converged planewave calculation using ABINIT

PhosphoreneNanoribbons

ACPNR4_3: 54 atoms
ACPNR4_60: 1080 atoms
ACPNR4_120: 2160 atoms
ACPNR4_240: 4320 atoms



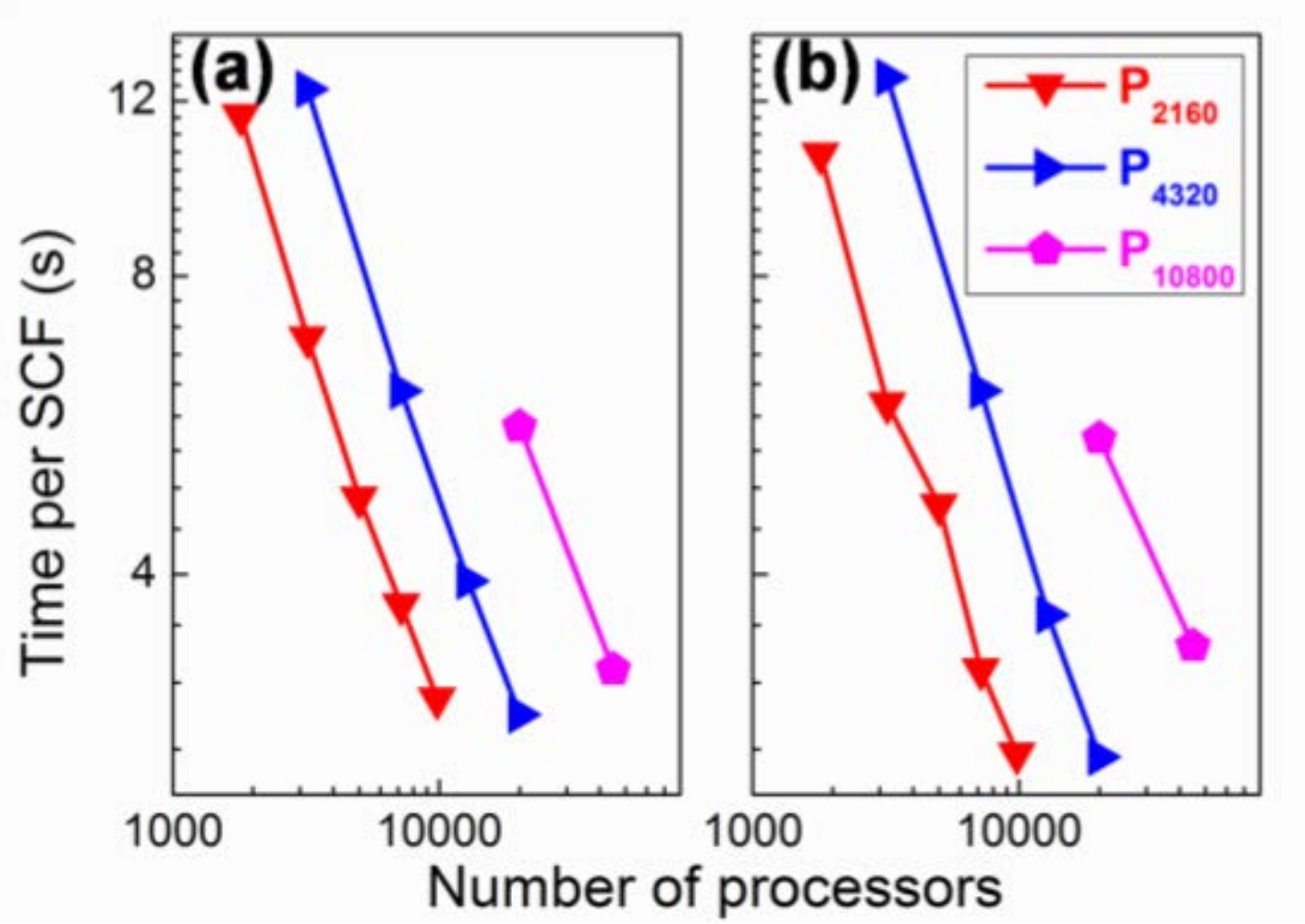


Accuracy

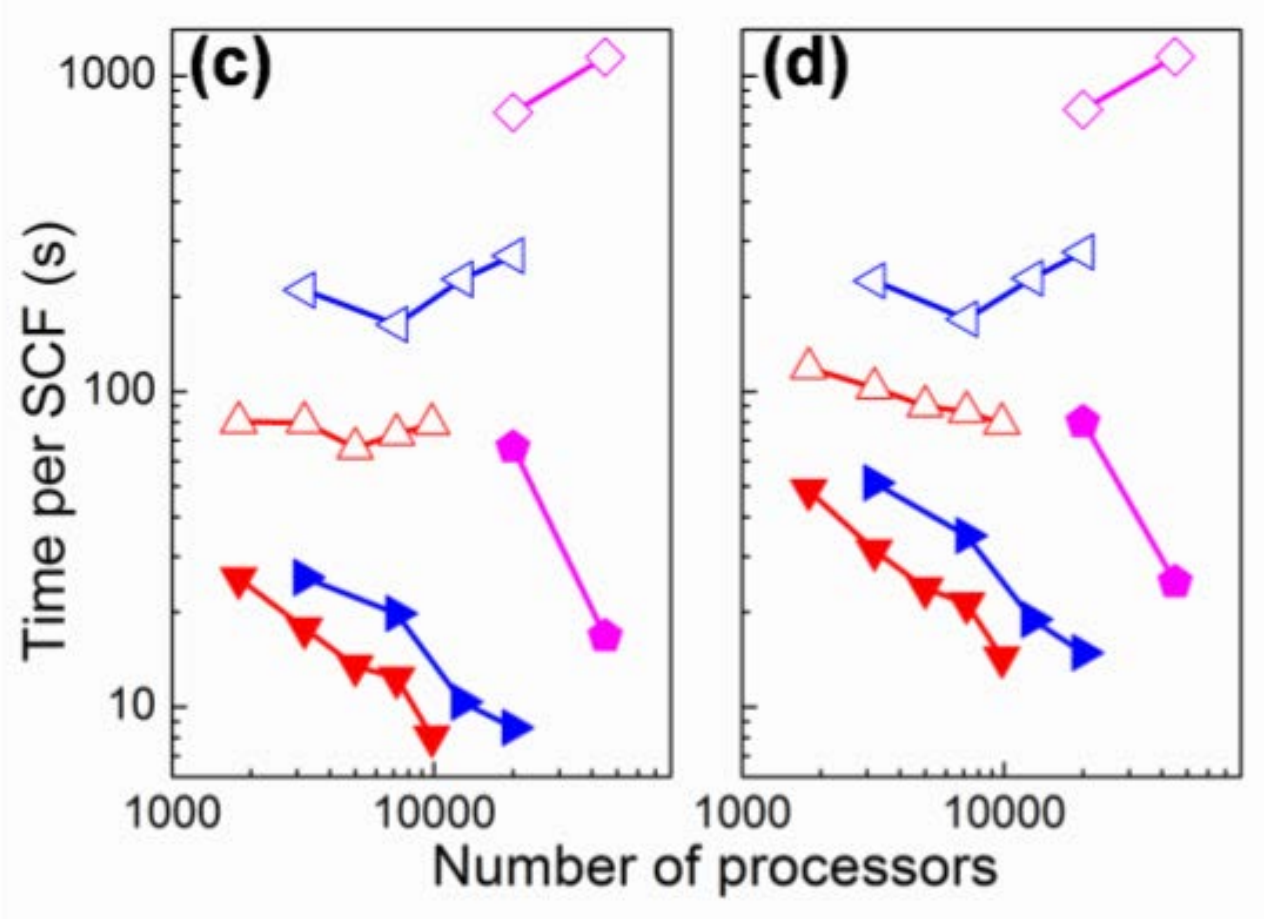
DGDFT P_{54}		DIAG		PEXSI	
Ecut	ALB	ΔE	ΔF	ΔE	ΔF
10	28	1.94E-02	4.81E-02	1.94E-02	4.81E-02
20	28	6.49E-04	5.12E-03	5.39E-04	1.67E-02
40	10	1.28E-03	1.52E-02	1.21E-03	4.19E-03
40	12	5.54E-04	2.17E-03	6.45E-04	2.17E-03
40	15	1.87E-04	9.54E-04	1.16E-04	9.57E-04
40	19	7.00E-05	4.00E-04	7.12E-05	4.13E-04
40	28	9.64E-06	2.90E-04	4.21E-05	2.84E-04
100	28	8.25E-06	1.24E-04	2.90E-05	1.31E-04
200	28	6.62E-06	9.43E-05	3.66E-05	9.09E-05

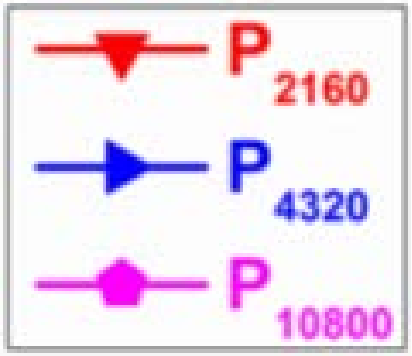
All units are atomic unit. Accuracy compared to converged ABINIT results.

Efficiency: Construction of basis (a) and Hamiltonian (b)



Efficiency: Diagonalization (c) and Total wall clock time (d)





Empty: DIAG
Filled: PEXSI

Molecular dynamics

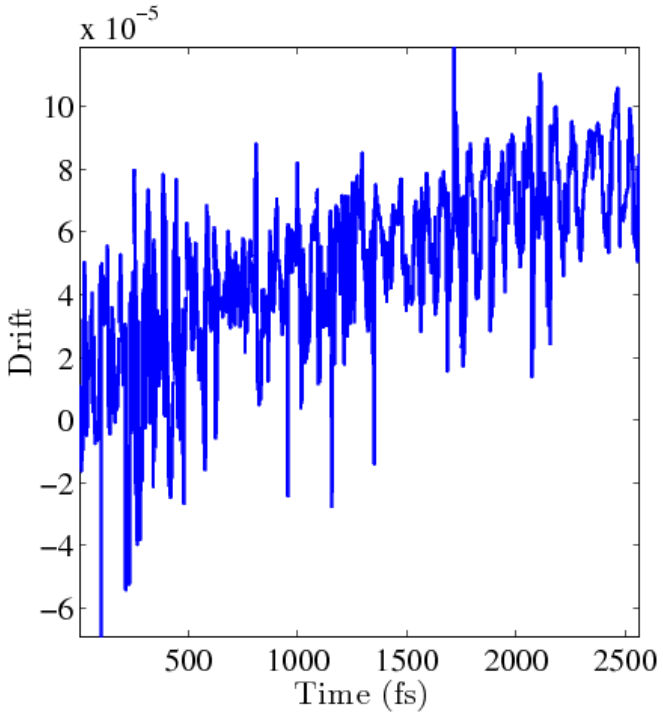
- Single level Nose-Hoover thermostat. Temperature: 300 K
- Time step: 2 fs

- Conserved quantity

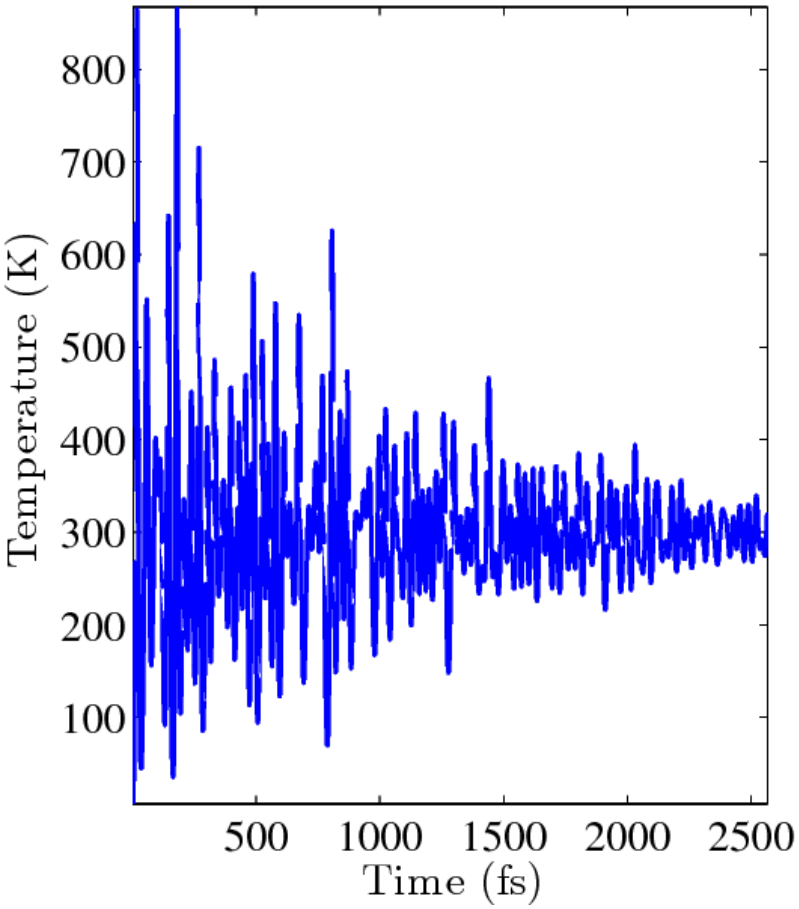
$$H = \sum_{I=1}^{M} \frac{p_I^2}{2M_I} + V + \frac{p_\eta^2}{2Q} + 3Nk_BT\eta$$

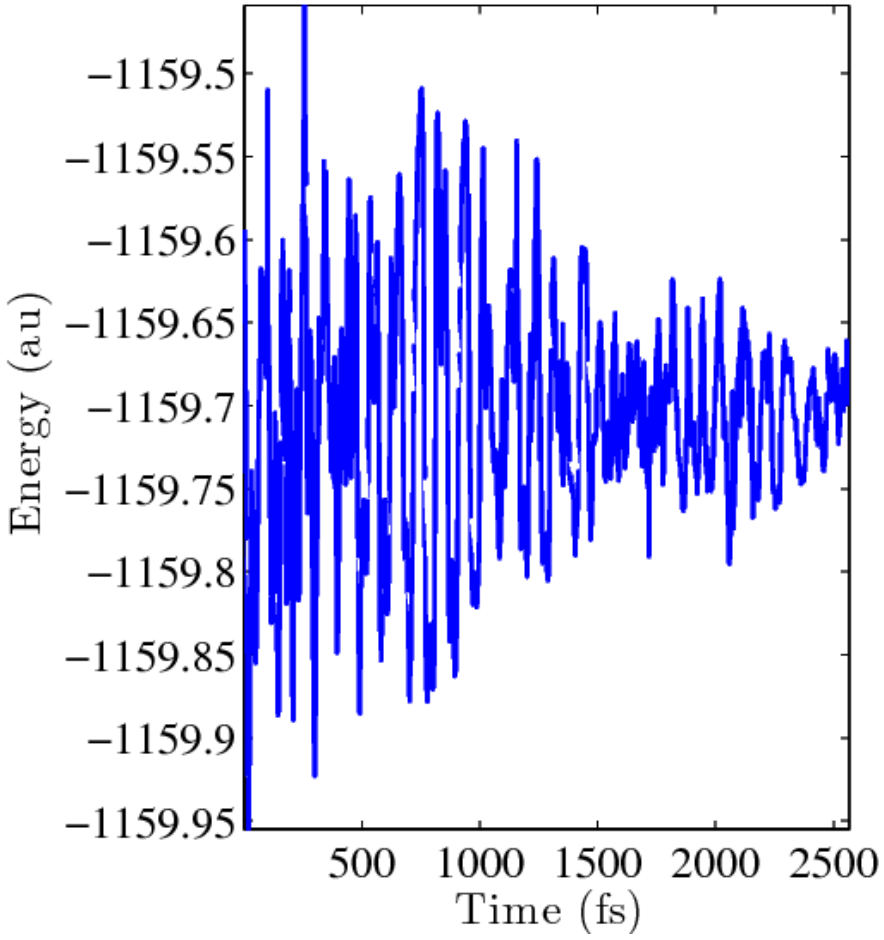
- $Drift = \frac{|H(t)-H(0)|}{|H(0)|}$

or 2.6×10^{-4} au/ps per atom

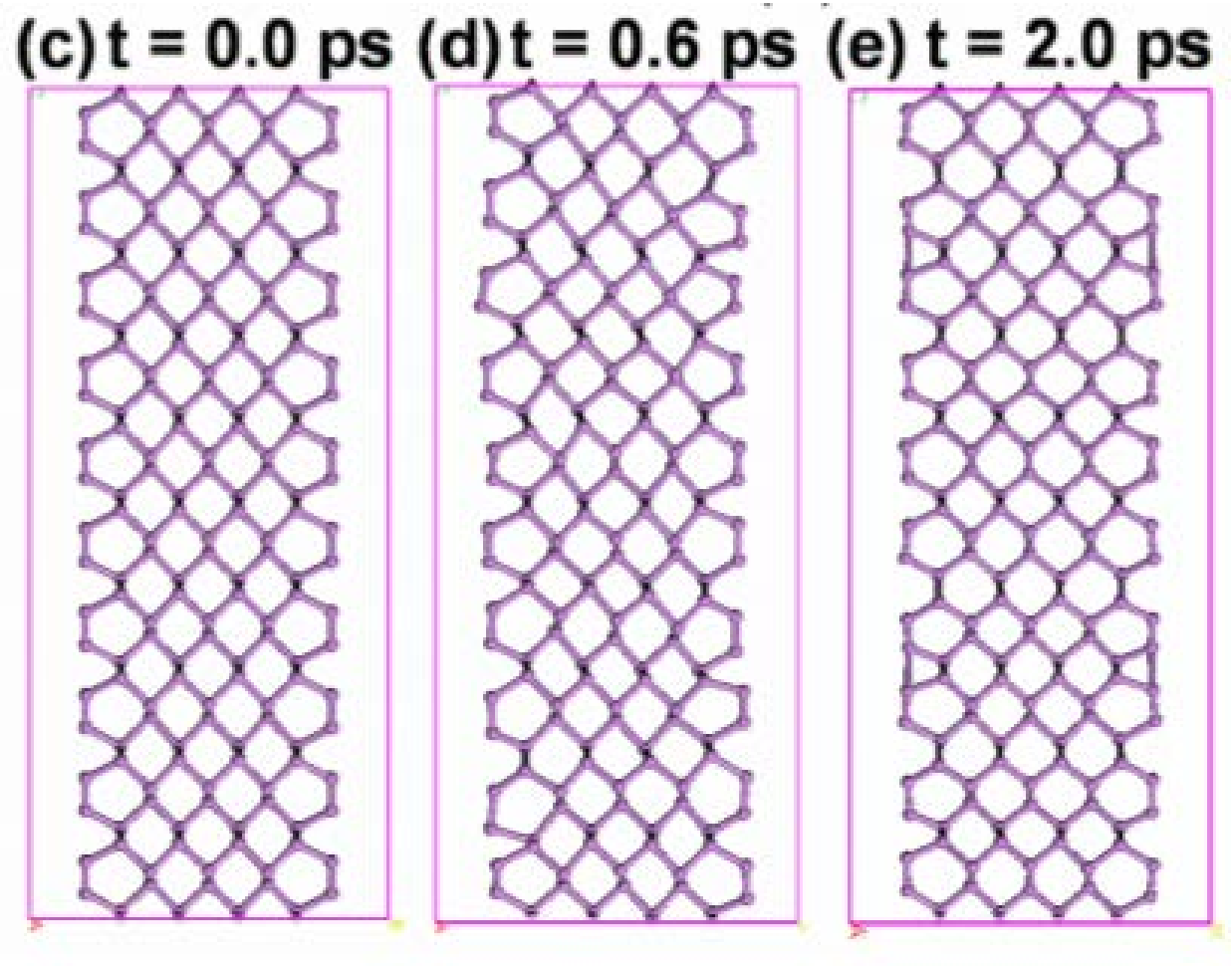


Molecular dynamics





Edge reconstruction of ACPNR



Conclusion

- Adaptive local basis functions (ALB). Automatic dimension reduction
- Atomic and environmental effect
- Accurate and small number of basis per atom.
- Local Hamiltonian matrix. Parallel computing.
- Combined with the pole expansion and selected inversion algorithm for low order scaling computation (at most $O(N^2)$ scaling) of KSDFT.

Acknowledgment

Joint work with

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