New computational methodologies for accelerating *ab initio* molecular dynamics simulation

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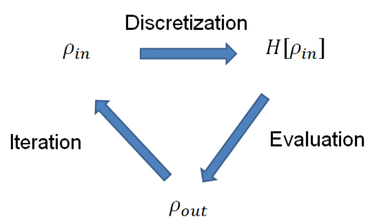
Objective

Develop fast *ab initio* molecular dynamics (AIMD) strategies for large scale disordered systems.

Kohn-Sham density functional theory (KSDFT):

$$\left(-\frac{1}{2}\Delta + V_{ext}[\{R_j\}_{j=1}^{M}] + \int dx' \frac{\rho(x')}{|x-x'|} + V_{xc}[\rho]\right)\psi_i(x) = \varepsilon_i \psi_i(x)$$

$$\rho(x) = 2\sum_{i=1}^{N/2} |\psi_i(x)|^2, \qquad \int dx\, \psi_i^*(x)\psi_j(x) = \delta_{ij}$$

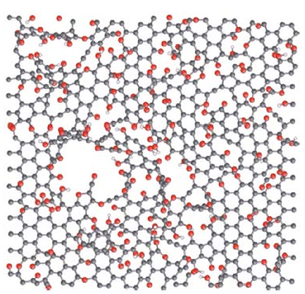


Energy and force

$$E_{tot}\left[\{R_j\}_{j=1}^{M}\right] = \sum_{i=1}^{\frac{N}{2}} \varepsilon_i - \frac{1}{2}\iint dxdy \frac{\rho(x)\rho(y)}{|x-y|} + E_{xc}[\rho(x)] - \int dx\, V_{xc}[\rho](x)\rho(x)$$

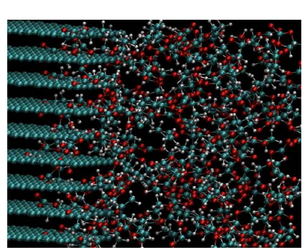
$$F_i = -\frac{\partial E_{tot}}{\partial R_i}$$

SciDAC Applications



Advanced Modeling of Ions in Solutions, on Surfaces, and in Biological Environments

Team: R. Car, W. E, M. Klein, X. Wu, E. Ng, C. Yang, L. Lin



Discontinuous methods for accurate, massively parallel quantum molecular dynamics: Lithium ion interface dynamics from first principles

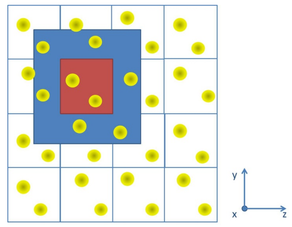
Team: J. Pask, V. Lordi, L. Lin, C. Yang, E.W. Draeger

Methodology: ALB-DG

ALB-DG: Adaptive Local Basis functions in a Discontinuous Galerkin Framework

Objective: Systematic reduction of the number of basis functions, starting from a complete basis set such as planewaves.

Obtain the basis functions adaptively in local domains



Solve the global problem using the discontinuous Galerkin method

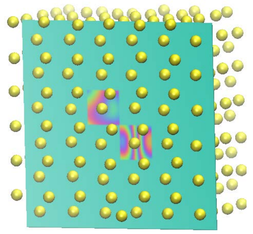
$$E_{DG}(\{\psi_i\}) = \frac{1}{2}\sum_{i=1}^{N}\langle \nabla\psi_i, \nabla\psi_i\rangle_{\mathcal{T}} + \langle V_{\text{eff}}, \rho\rangle_{\mathcal{T}} + \sum_{\ell}\gamma_\ell \sum_{i=1}^{N} |\langle b_\ell, \psi_i\rangle_{\mathcal{T}}|^2 \quad \text{Kohn-Sham}$$

$$-\sum_{i=1}^{N}\langle \{\{\nabla\psi_i\}\}, [\![\psi_i]\!]\rangle_{\mathcal{S}} + \frac{\alpha}{h}\sum_{i=1}^{N}\langle [\![\psi_i]\!], [\![\psi_i]\!]\rangle_{\mathcal{S}}. \quad \text{New terms}$$

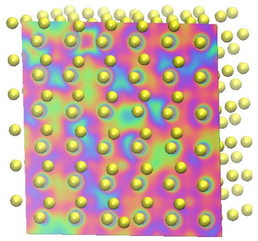
average and jump operators across surfaces $\mathcal{S}$:

$$\{\{q\}\} = \tfrac{1}{2}(q_1 + q_2) \quad \text{on } \mathcal{S}.$$

$$[\![u]\!] = u_1 n_1 + u_2 n_2 \quad \text{on } \mathcal{S}.$$

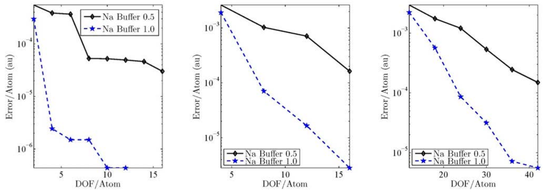


Na: Local basis functions



Na: Global electron density

Accuracy and efficiency



Quasi 1D Quasi 2D 3D

Methodology: PEXSI

PEXSI: Pole EXpansion and Selected Inversion

Objective: Accurate evaluation of the electron density, energy and atomic force with at most $O(N^2)$ scaling.

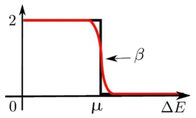
KSDFT in the form of the Fermi operator

$$\rho(x) = 2\sum_{i=1}^{N/2}|\psi_i(x)|^2$$

$$= (\psi_1(x) \;\; \dots \;\; \psi_{N_t}(x)) \begin{pmatrix} \chi(\varepsilon_1 - \mu) & & \\ & \ddots & \\ & & \chi(\varepsilon_{N_t} - \mu) \end{pmatrix} \begin{pmatrix} \psi_1(x) \\ \vdots \\ \psi_{N_t}(x) \end{pmatrix}$$

$$= \{\chi(H[\rho] - \mu I)\}_{x,x}$$

- μ : Chemical potential such that $\#\{\sigma(H) \le \mu\} = N/2$
- χ : Heaviside function satisfying $\chi(x) = \begin{cases} 2, & x \le 0, \\ 0, & x > 0 \end{cases}$

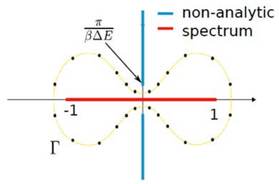


$$\rho = \text{diag}\frac{2}{1 + e^{\beta(H[\rho]-\mu I)}}$$

- Finite temperature, Fermi-Dirac
- Zero temperature, Heaviside

Pole expansion based on complex analysis

$$\rho \approx \text{diag}\sum_{i=1}^{Q}\frac{\omega_i}{H - z_i I}$$



Optimal expansion cost

$$Q \sim \log \beta\Delta E$$

Selected inversion: compute selected elements of a Green's function without the full inversion

- LDL^T factorization

$$A = \begin{pmatrix} A_{11} & A_{21}^T \\ A_{21} & \hat{A}_{22} \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ L_{21} & I \end{pmatrix}\begin{pmatrix} A_{11} & 0 \\ 0 & S_{22} \end{pmatrix}\begin{pmatrix} 1 & L_{21}^T \\ 0 & I \end{pmatrix}$$

$$L_{21} = A_{21}A_{11}^{-1}, \qquad S_{22} = \hat{A}_{22} - A_{21}L_{21}^T$$

- Inversion

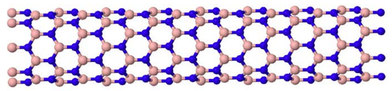
$$A^{-1} = \begin{pmatrix} A_{11}^{-1} + L_{21}^T S_{22}^{-1} L_{21} & -L_{21}^T S_{22}^{-1} \\ -S_{22}^{-1}L_{21} & S_{22}^{-1} \end{pmatrix}$$

A^{-1} restricted to the non-zero pattern of L is "self-contained"

Cost of selected inversion: at most $O(N^2)$ scaling

Quasi-1D	$O(N)$
Quasi-2D	$O(N^{1.5})$
3D bulk	$O(N^2)$

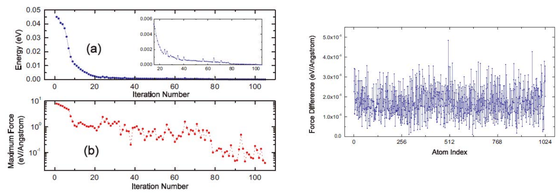
Accuracy



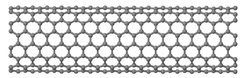
Boron nitride nanotube (BNNT)

# Poles	$E_{\text{PEXSI}} - E_{\text{ref}}$ (eV)	MAE Force (eV/Angstrom)
20	5.868351108	0.400431
40	0.007370583	0.001142
60	0.000110382	0.000026
80	0.000000360	0.000002

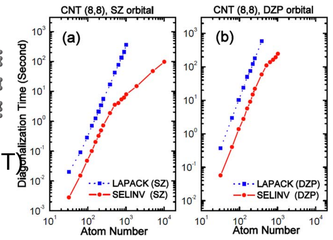
Geometry optimization for BNNT with 1024 atoms (DZP basis, PEXSI solved on a single core)



Efficiency (single SCF, PEXSI solved on a single core)



Carbon nanotube (CNT)



References

L. Lin, L. Ying, Element orbitals for Kohn-Sham density functional theory, Phys. Rev. B 85, 235144, 2012

L. Lin, J. Lu, L. Ying and W. E, Optimized local basis function for Kohn-Sham density functional theory, J. Comput. Phys 231, 4515, 2012

L. Lin, J. Lu, L. Ying and W. E, Adaptive local basis set for Kohn-Sham density functional theory in a discontinuous Galerkin framework I: Total energy calculation, J. Comput. Phys. 231, 2140, 2012

L. Lin, C. Yang, J. Lu, L. Ying and W. E, A Fast Parallel algorithm for selected inversion of structured sparse matrices with application to 2D electronic structure calculations, SIAM J. Sci. Comput. 33, 1329, 2011

L. Lin, C. Yang, J. Meza, J. Lu, L. Ying and W. E, SelInv -- An algorithm for selected inversion of a sparse symmetric matrix, ACM Trans. Math. Software 37, 40, 2011

L. Lin, J. Lu, L. Ying and W. E, Pole-based approximation of the Fermi-Dirac function, Chin. Ann. Math. 30B, 729, 2009

L. Lin, J. Lu, L. Ying, R. Car and W. E, Fast algorithm for extracting the diagonal of the inverse matrix with application to the electronic structure analysis of metallic systems, Commun. Math. Sci. 7, 755, 2009

L. Lin, M. Chen, C. Yang and L. He, Accelerating atomic orbital-based electronic structure calculation via pole Expansion plus selected inversion, submitted, 2012

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