

Massive Parallelization of a Linear Scaling DFT Code OpenMX

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Motivation

Density functional theory (DFT)

Quantum mechanical modeling method used to investigate the electronic structure of many-body systems in physics and chemistry.

Petaflops era and beyond

- The K computer with approximately 700,000 cores.
- Exaflops machines with millions of cores expected to arrive by 2020.

OpenMX (Open source package for Material eXplorer)

- Linear scaling DFT code.
- Large-scale calculations demanded.



Purpose

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Develop a domain decomposition method for enabling large-scale DFT calculations with hundreds of thousands of atoms and cores.

Objectives

- Approximately the same computational amount for each process.
- Locality held: nearby atoms assigned to the same process.
- Inter-process communications minimized.
- Applicable to any numbers of atoms and processes.
- Applicable to any distribution patterns of atoms in space.
- Computationally inexpensive.

Method

1. Atom Decomposition Method

Two key ideas: (i) the modified recursive bisection method for recursively decomposing the domain by constructing a binary tree, and (ii) the moment of inertia tensor for finding a principal axis of each sub-domain to reorder the atoms based on their projection on the axis and divide them into two sub-domains to fit the binary tree structure.

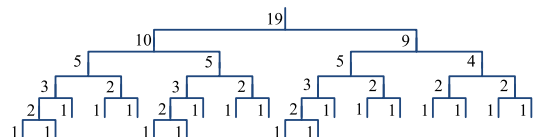


Fig. 1: The modified recursive bisection method with the binary tree for 19 processes.

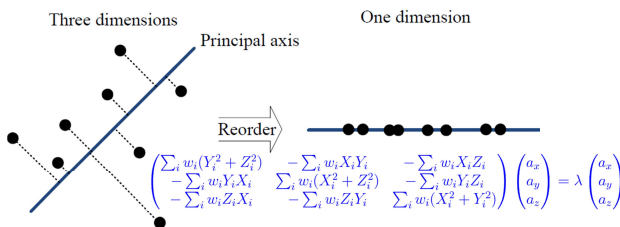


Fig. 2: The moment of inertia tensor for 3D-to-1D atom reordering.

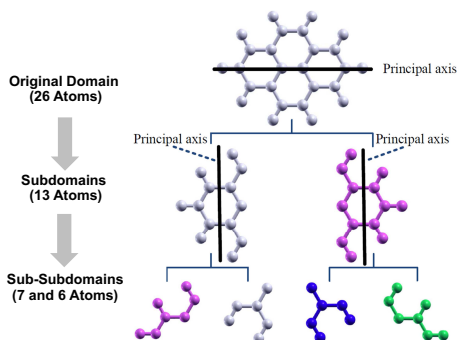


Fig. 3: Example of the atom decomposition method with 26 atoms.

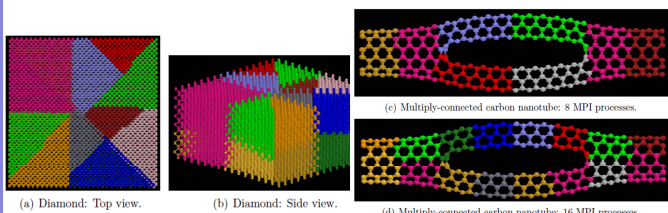


Fig. 4: Atom decomposition with 16,384 diamond atoms and 19 processes, and CNTs.

2. Grid Decomposition Method

Define four data structures to make data locality consistent with that of the clustered atoms for minimizing inter-process communications.

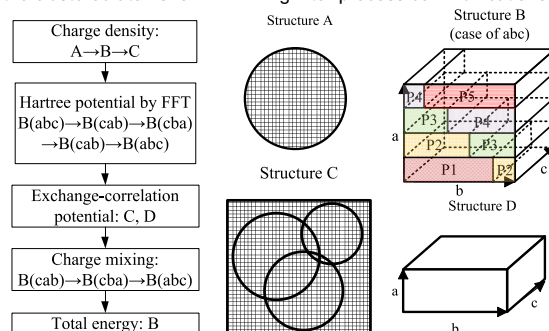
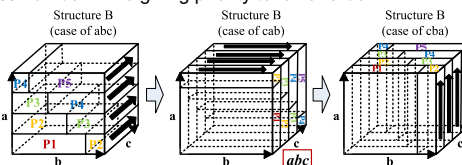


Fig. 5: Data structures and the calculation flow.

3. 3D Adaptive Order-Aware Decomposition Method for 3D FFT

Automatically decompose in 1D, 2D, or 3D depending on the process number while giving priority to lower order.



N_p : Number of processes	cab	acb	abc	cab	cba	bca	cba	acb	bca
$N_p \leq N$	$N^2 \cdot N^2 / N_p$	$2(N^2 \cdot N^2 / N_p)$	$2(N^2 \cdot N^2 / N_p)$	$N^2 \cdot N^2 / N_p$	$2(N^2 \cdot N^2 / N_p)$	$2(N^2 \cdot N^2 / N_p)$	$N^2 \cdot N^2 / N_p$	$N^2 \cdot N^2 / N_p$	$N^2 \cdot N^2 / N_p$
$N < N_p < N^2$	$2(N \cdot N_p) / N^2$	$2(N \cdot N_p) / N^2$	$2(N \cdot N_p) / N^2$	$2(N \cdot N_p) / N^2$	$2(N \cdot N_p) / N^2$	$2(N \cdot N_p) / N^2$	$2(N \cdot N_p) / N^2$	$2(N \cdot N_p) / N^2$	$2(N \cdot N_p) / N^2$
$N_p = N^2$	$2(N \cdot N_p) / N^2$	$2(N \cdot N_p) / N^2$	$2(N \cdot N_p) / N^2$	$2(N \cdot N_p) / N^2$	$2(N \cdot N_p) / N^2$	$2(N \cdot N_p) / N^2$	$2(N \cdot N_p) / N^2$	$2(N \cdot N_p) / N^2$	$2(N \cdot N_p) / N^2$
$N^2 < N_p < N^3$	$N^2 + 2(N_p \cdot N) / N^2$	$N^2 + 2(N_p \cdot N) / N^2$	$N^2 + 2(N_p \cdot N) / N^2$	$N^2 + 2(N_p \cdot N) / N^2$	$N^2 + 2(N_p \cdot N) / N^2$	$N^2 + 2(N_p \cdot N) / N^2$	$N^2 + 2(N_p \cdot N) / N^2$	$N^2 + 2(N_p \cdot N) / N^2$	$N^2 + 2(N_p \cdot N) / N^2$
$N_p = N^3$	$3(N \cdot N_p) / N^2$	$3(N \cdot N_p) / N^2$	$3(N \cdot N_p) / N^2$	$3(N \cdot N_p) / N^2$	$3(N \cdot N_p) / N^2$	$3(N \cdot N_p) / N^2$	$3(N \cdot N_p) / N^2$	$3(N \cdot N_p) / N^2$	$3(N \cdot N_p) / N^2$

Fig. 6: The decomposition method in 2D row-wise and the communication amount.

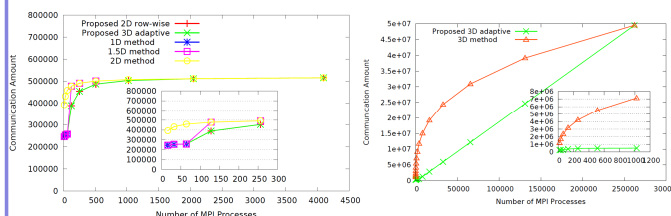


Fig. 7: Comparison with other methods.

Evaluation

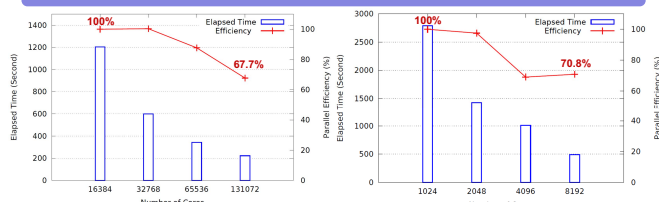


Fig. 8: Strong scaling on the K computer: 131,072 diamond atoms (left) and 13,000 and 26,000 atoms in the DNA structure (right) with OpenMX and $O(N)$ Krylov subspace method.

Summary

Our method

- Atom decomposition method + Grid decomposition method.
- 3D adaptive order-aware decomposition method for 3D FFT.
- The parallel efficiency at 131,072 cores is 67.7% compared to the baseline of 16,384 cores with 131,072 diamond atoms.

Ongoing and future work

- Tune subroutines to enhance single-node performance.
- Generalize the decomposition method for N -D FFT.

Acknowledgements

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References

[1] T.V.T. Duy and T. Ozaki, arXiv:1209.4506 (2012).