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

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.
- 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.

Three dimensions

One dimension

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

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

Evaluation

Fig. 7: Linear scaling with 2,048 cores and the diamond structure on XT5.

Fig. 8: Weak scaling with the diamond structure on XT5.

Fig. 9: Strong scaling on the K computer: 131,072 diamond atoms (left) and 26,000 atoms in the DNA structure (right) with OpenMX and O(ω) 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.

Future work
- Evaluate our method with non-linear scaling methods.

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References

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