Usage Report for Fiscal Year 2015

Project Title:

Development of new long-range corrected density functional theory

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1. Background and purpose of the project, relationship of the project with other projects

In quantum chemical computations, the evaluation of two-electron integrals is the most time-consuming bane for the applications to pragmatically large systems. While tremendous effort to accelerate Coulomb integration has borne useful fruits, such as the fast multipole moment method, the acceleration scheme for HF exchange integrals has been still tediously slow. Therefore, the high demand of computational cost for long-tailed HF exchange integral is now a critical bottle-neck of the broad and active applications of hybrid and long-range corrected (LC) DFT functionals to real-sized systems, such as nano-materials, solid state materials, surface chemical systems, biomolecules, and so on.

In this project, we presented a new method to speed up the evaluation of long-range HF exchange integrals, which is of critical importance in the applications of LC-DFT to real-sized systems. Specifically, we proposed a new attenuating operator that employs Gaussian functions for which a new screening method that we very recently developed will be actively used. We then showed that this new method reproduces the energies and properties of LC-DFT with shorter computational time for systems under the periodic boundary condition (PBC), as well as for large molecular systems.

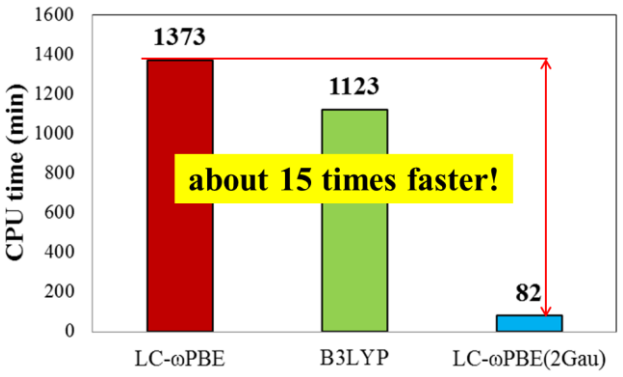
2. Specific usage status of the system and calculation method

In this project, we used RICC (mpc) machines for estimating the CPU time for the two-electron HF exchange integration accelerated by newly proposed methods.

3. Result

We implemented our newly-proposed algorithm which uses a new attenuating operator consisting of two Gaussian functions in our development version of Gaussian09 and found that new algori

Figure shows that the CPU time spent for achieving the energy convergence of the 1st self-consistent field cycle of periodic diamond system according to LC-ωPBE, B3LYP, and new algorithm for LC-ωPBE [LC-ωPBE(2Gau)] obtained using Gaussian09. As shown in the figure, new algorithm succeeds in accelerating the evaluation time for long-range HF exchange integrations.



4. Conclusion

We found that new algorithm results in achieving 15 times faster convergence of the 1st SCF cycle than the conventional LC-ωPBE calculations.

5. Schedule and prospect for the future

We expect to propose an improved algorithm for evaluating two electron HF exchange integrals of Gaussian function operator in the near future, which will accelerate much more LC-DFT calculations.

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Fiscal Year 2015 List of Publications Resulting from the Use of the supercomputer

[Publication]

1. "Long-Range Corrected Density Functional Theory with Accelerated Hartree-Fock Exchange Using a Two-Gaussian Operator [LC-ωPBE(2Gau)]" J.-W. Song and K. Hirao, *J. Chem. Phys.* **143**, 144112 (2015).
2. "Efficient method of evaluation for Gaussian Hartree-Fock exchange operator for Gau-PBE functional" J.-W. Song and K. Hirao, *J. Chem. Phys.* **143**, 024102 (2015) [DOI:10.1063/1.4923264].
3. "Molecules relevant for Organic Photovoltaics: A Range Separated Density Functional Study" R. Kar, M. P. Borpuzari, J.-W. Song, and K. Hirao, *Mol. Phys.* (Special Issue in Honour of Sourav Pal) **113**, 2930 (2015) [DOI:10.1080/00268976.2015.1059512].
4. "Towards the Complete Range Separation of Non-Hybrid Exchange–Correlation Functional" Bun Chan, J.-W. Song, Y. Kawashima, and K. Hirao, *J. Comput. Chem.* **36**, 871 (2015).

[Proceedings, etc.]

1. "Long-range Corrected Density Functional Theory with Linearly-Scaled HF exchange" J.-W. Song and K. Hirao, ICCMSE2015, *AIP Conf. Proc.*, **1702**, 090062 (2015).

[Oral presentation at an international symposium]

1. "Adsorption energy calculations using long-range corrected density functional theory between CO and metal system" J.-W. Song Kawai, K. Yamashita, and K. Hirao, The 9th Annual Meeting of Japan Society for Molecular Science (2015), Tokyo, JAPAN.

[Others (Press release, Science lecture for the public)]

N/A