Performance Evaluation of Hartree-Fock Program developed by Ruby Scripting Language

Hiroaki Honda[a,d,1)], **Yuichi Inadomi** [b,d,2)], **Jun Maki** [c,3)]

[a] Research Institute of Information Technology, Kyushu University
6-10-1 Hakozaki, Higashi-ku, Fukuoka 812-8581, Japan,
[b] Graduate School of Information Science and Electrical Engineering, Kyushu University,
744 Motooka Nishi-ku, Fukuoka 819-0395 Japan
[c] Institute of Systems, Information Technologies and Nanotechnologies
2-1-22, Momochihama, Sawara-ku, Fukuoka, 814-0001, Japan,
[d] CREST-JST

[1)] honda.hiroaki.971@m.kyushu-u.ac.jp
[2)] inadomi@soc.ait.kyushu-u.ac.jp
[3)] maki@isit.or.jp

ABSTRACT

Currently, molecular orbital (MO) calculation is known as accurate quantum theoretical method for chemistry and widely used for purely theoretical chemistry research, designing functional material, and drug discovery, and so on. But if we want implement new theoretical ideas in a conventional MO program, we soon realize it is not so easy, because current practical MO programs are quite large and detailed source code documents are not often disclosed. Therefore, it takes a lot of time to modify even fundamental data like molecular integral values, Fock and Density matrices.

In this research, we are developing new MO calculation prototyping environment based on Ruby scripting language. This prototyping environment has two objects: first, as educational programming materials with famous quantum chemistry text book for students, second, as rapid prototyping method of new ideas for researchers. If researchers understand their new method is effective with our environment, they can implement again to conventional promising program system. This environment is for prototyping but has to be sufficiently high performance, because quantum chemistry calculation is often too time consuming.

We implemented parallel restricted Hartree-Fock programming environment by Ruby language. For high-performance calculations, we used C-language native code libraries for Array class and other utilities for quantum chemistry calculations using Ruby foreign language extensions. We already prepared binding utilities NArray class library[2], ruby-mpi MPI library[3], BLAS/Lapack libraries, and molecular integrals calculation libraries based on Obara's algorithm[4].

We evaluated and compared program sizes and parallel efficiencies of our new Ruby and native C-language implantations with static load balancing algorithm. For code size, number of Ruby program steps except comments is almost 450, while C program is 2298. For parallelization efficiencies, Ruby implementation archived 48.4 % efficiency. This result is sufficient enough, compared with 52.5 % parallel efficiency by C implementation.

Currently, we are developing Configuration State Function based Configuration Interaction (CI) method. After this CI program is completed, our prototyping environment will be opened.

REFERENCES

[1] Gordon Group/GAMESS Homepage, [On line]. Available: < http://www.msg.ameslab.gov/gamess/>.
[2] Ruby/NArray, [On line]. Available: <https://github.com/masa16/narray>.
[3] A ruby binding of MPI, [On line]. Available: <https://github.com/seiya/ruby-mpi>.
[4] S.Obara *et al.*, *J.Chem.Phys.*, Vol.84, pp.3963-3974, 1986.