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3D Parallel and High-Performance Molecular Dynamics Simulation

Motohiko Tanaka, and Yasunari Zempo[1]
Graduate School of Engineering, Chubu University, Aichi, Japan
[1] Computer and Information Sciences, Hosei University, Tokyo, Japan

During the annual 2021 year, we executed "Parallel Development of Electromagnetic Molecular Dynamics Simulations". There are several themes including "Electromagnetic carbon-gold-atom nanotube accelerator", "Vector-parallel SIESTA-4.1b code", "Development of spectrum analysis code due to maximum entropy method". In this report, we report the vector-parallel SIESTA code in the NIFS Simulator.

In NEC's SX-Aurora TSUBASA of vector-and-parallel simulator, the parallel SIESTA code does not compile at all. On the other hand, Intel's intel-lx compiles SIESTA-4.1b after making some modifications, about which we well report here.

First, one downloads the SIESTA-4.1b code by internet. On our Linux, one does 'tar -xfzv siesta-4.1-b4.tar.gz'. Under the NEC's compiler, one invokes the 'module load intel-lx', and does 'sh ../Src/obj_setup.sh' for SIESTA Obj directory; one siesta-4.1b's MPICH+OMP script should be,

```
CC= mpiicc -O2 -qopenmp
FPP= $(FC) -E -P -x c
FC= mpiifort
MPI_INTERFACE = libmpi_f90.a
MPI_INCLUDE = .
FC_SERIAL= ifort
FFLAGS = -O2 -fPIC -qopenmp
LIBS =    -L${MKLROOT}/lib/intel64 -lmkl_scalapack_lp64 -lmkl_intel_lp64 -lmkl_sequential -lmkl_core ¥
          -lmkl_blacs_intelmpi_lp64 -mkl -qopenmp -lpthread -lm -ldl
```

Then, one proceeds the 'make' step. For NEC's own compiler problems, one must add additional terms. For the six files including "iokp.f", "m_mixing.F90", "m_ts_contour_neq.f90", "m_ts_electype.F90", "m_ts_weight.F90" and " ofc.f90", one changes the correct statement as 'e12.6' by 'e13.6'. Next point is that one must omit the $OMP lines of "inal_H_f_stress.F" as:

```
!!$OMP parallel default(shared)
!!$OMP workshare
        H_tmp = 0.0_dp
!!$OMP end workshare nowait
!!$OMP single
!       Initialize forces and stress .....................
        nullify(fal)
        call re_alloc( fal, 1, 3, 1, na_u, 'fal', 'final_H_f_stress' )
!!$OMP end single
!!$OMP workshare
        fa(1:3,1:na_u) = 0.0_dp
        fal(1:3,1:na_u) = 0.0_dp
        stress(1:3,1:3) = 0.0_dp
        stressl(1:3,1:3) = 0.0_dp
!!$OMP end workshare nowait
!!$OMP end parallel
```

The vector lines must be changed as "novector" in the "old_atmfuncs.f" file:

```
!NEC$ novector
            do 5 izeta=1,nzetasave(l,nsm,is)
              norb=norb+(2*l+1)
              indx=indx+1
              if(norb.ge.io) goto 30
 5          continue
```

They are the lines at 426, 43648 , 492, 502, 523, 570, 580, 605, 666, 712, 724 and 756 of "old_atmfuncs.f" file. The file "normalize_dm.F90" undergoes an error, thus one just skips as '! call die(msg)' at the line 95. One compiles the rest of the code.

Finally for execution of the SIESTA code, one must write:

```
#PBS -v NQSV_MPI_VER= 2020update0
#PBS -v OMP_NUM_THREADS=4
module load intel-lx/$NQSV_MPI_VER
```

Figure 1 and 2 are the run results of the SIESTA-4.1b code for CH4 molecules by Nose thermostat. It goes over 48 MPI slots which takes about 200 minutes.

References:

1. SIESTA-4.1 https://siesta-project.org/SIESTA_MATERIAL/Docs/Manuals/manuals.html
2. M. Tanaka and Y. Zempo, Annual Report of 2022, National Institute of Fusion Science, Japan.

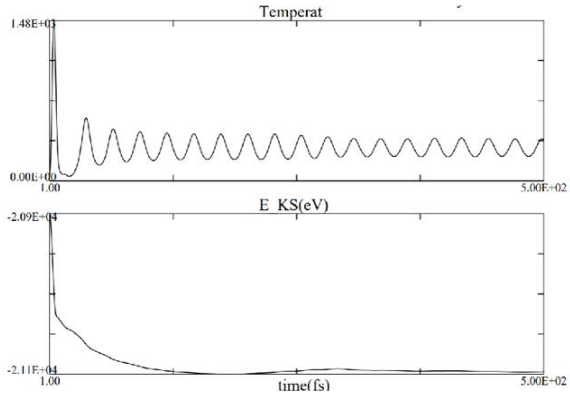

Fig.1 By Nose thermostat, temperature and KS energy up to 500 steps, Dt=1 fs.

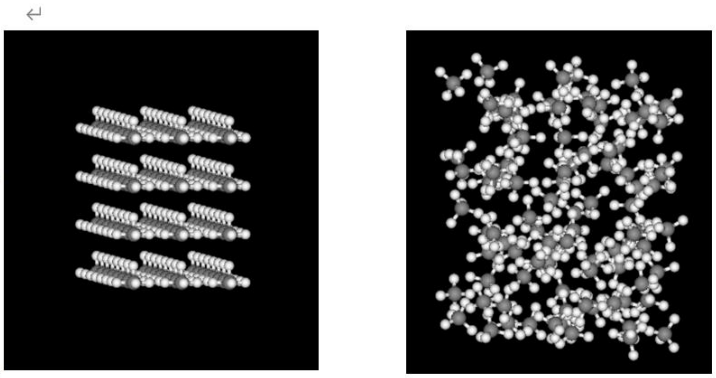

Fig.2 Initial and final states of CH4 molecules, C96H384, about elapsed 200 minutes/48_MPI-1_OMP by Intel-LX.