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3D Parallel and High-Performance Molecular Dynamics Simulation

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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-and-parallel SIESTA code in the NIFS Simulator.

In NEC's SX-Aurora TSUBASA of vector-and-parallel simulator, the generic parallel SIESTA code did not work at all. On the other hand, the Intel compiler works for SIESTA-4.1b after making some modifications, about which we will report here.

First, we download the SIESTA-4.1b by internet and decompress the code by 'tar -xfzv siesta-4.1-b4.tar.gz'. Under the NEC's compiler, we invoke by 'module load intel-lx', and do 'sh ../Src/obj_setup.sh' on the SIESTA Obj directory; the 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, we proceed on the 'make' step. For NEC's own compiler problems, we must do additional works. 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", we change the correct statement as 'e13.6' from 'e12.6'. Next point is that we must comment out 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 operation must be changed by "novector" of !NEC$ line in the "old_atmfuncs.f" file as,

```
!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
```

These are the lines of 426, 43648 , 492, 502, 523, 570, 580, 605, 666, 712, 724 and 756 of "old_atmfuncs.f". Finally, the file "normalize_dm.F90" undergoes an error, thus we just comment out as '! call die(msg)' at the line 95. We compile the rest of the code.

For execution of the SIESTA code, we use the script in the NIFS-Intel Simulator:

```
#PBS -T intmpi
#PBS -v NQSV_MPI_VER= 2020update0
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 cores which takes about elapsed 200 minutes on the Intel LX machine.

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.

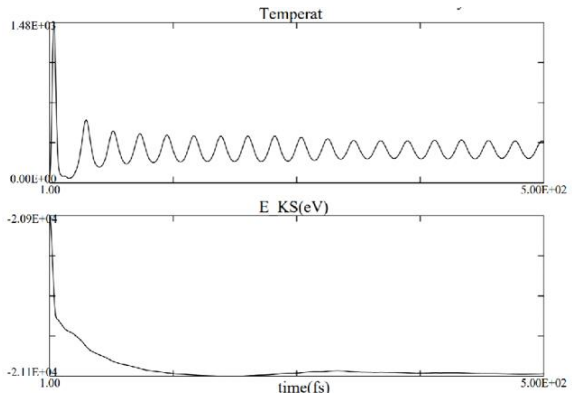

Fig.1 By Nose thermostat, temperature and KS energy up to 500 steps, Dt=1 fs.

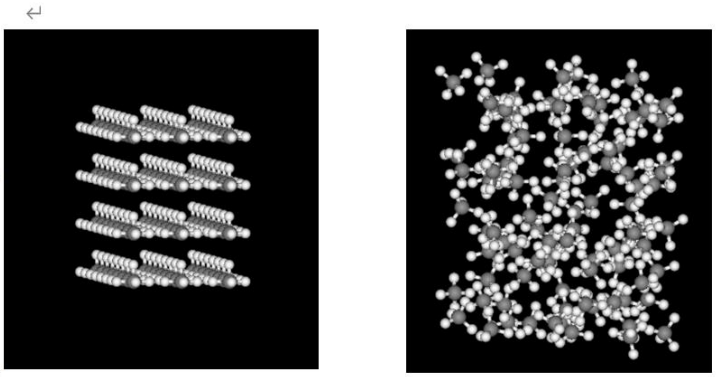

Fig.2 Initial and final states of CH4 molecules, C96H384, about elapsed 200 minutes/48_MPI-1_OMP by Intel-LX.