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3D Parallel and High-Performance Molecular Dynamics Simulation

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During the annual year 2021, 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 problem, one must add additional terms. At first 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, 436, 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, 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 Figure 2 are the run result of SIESTA-4.1b code for CH4 mollecules by Nose thermostat. It goes by 48 MPI 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.

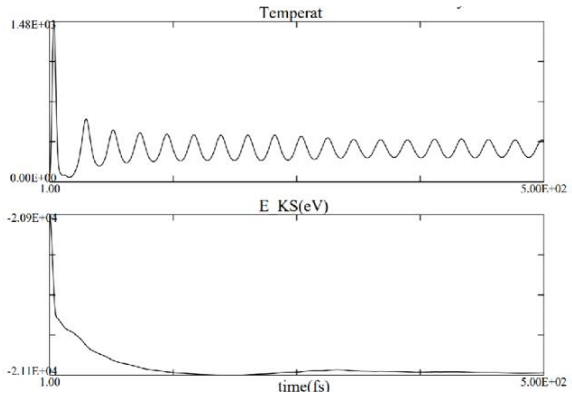

Fig.1 By Nose thermostat, temperature and KS energy up to 500 steps, Dt=1 fs.

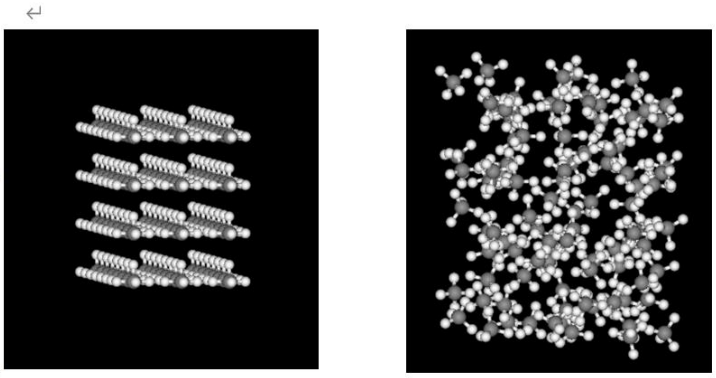

Fig.2 Initial and final states of CH4 molecules, C96H384, about elapsed 200 minutes/48_MPI-1_OMP by Intel-LX.