Simulations of Molecular Dynamics by AlmaLinux v.s. Debian-12 OS

Motohiko Tanaka, Ph.D., Japan

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https://github.com/Mtanaka77/

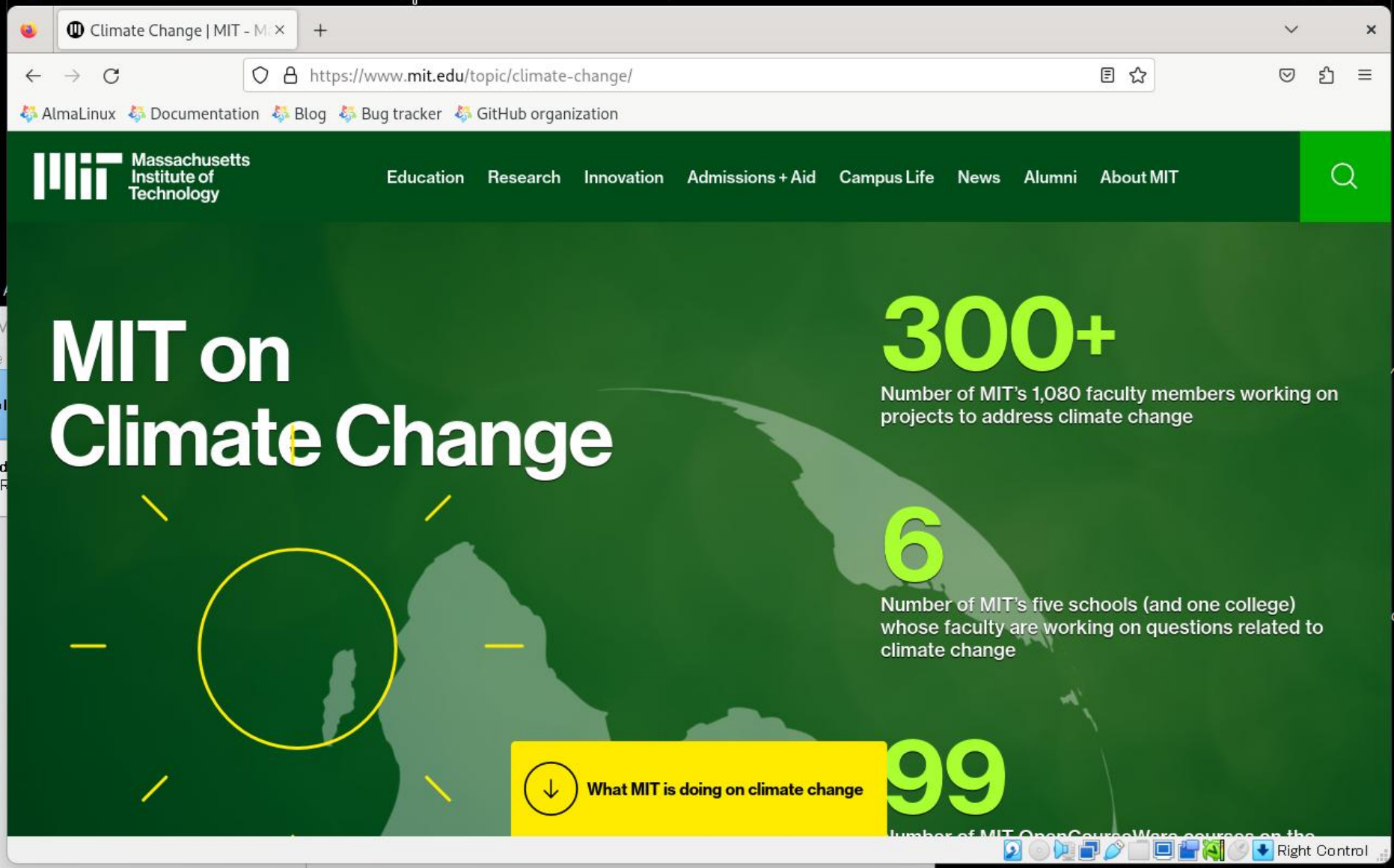
Settings and tests of simulations

Installation of AlmaLinux-9, May 2024, and Debian-12, Nov. 2024

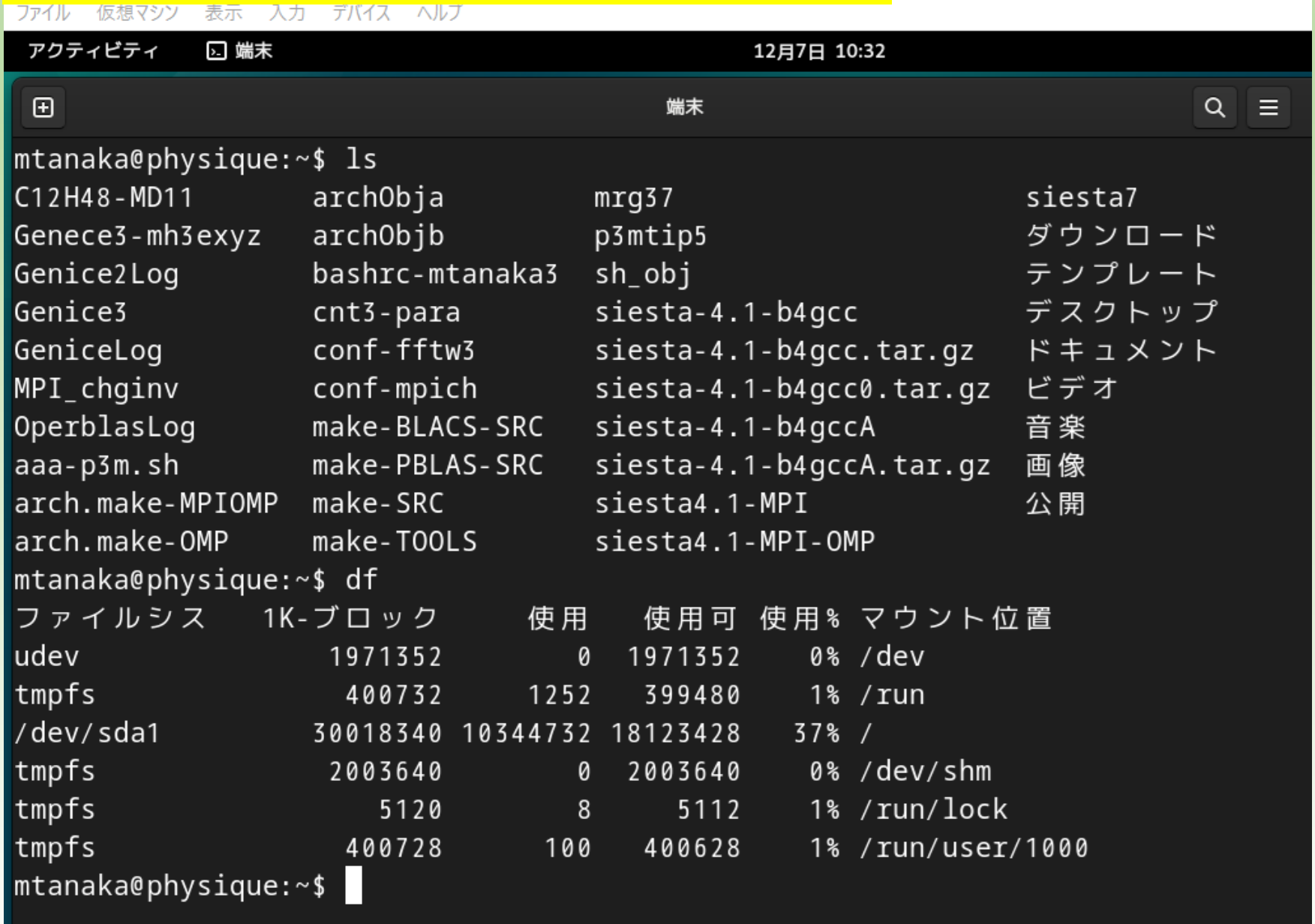
Use Windows 11, VirtualBox 7 to login Linux OS
Linux gfortran and pip3 packages

Simulations, cf. https://github.com/Mtanaka77/
>> Three-dimensional electrostatic p3mtip5 code, with tip5p and Ewald sums
>> Siesta-4.1b, with mpich4 fft3w, OpenBLAS, and Scalapack

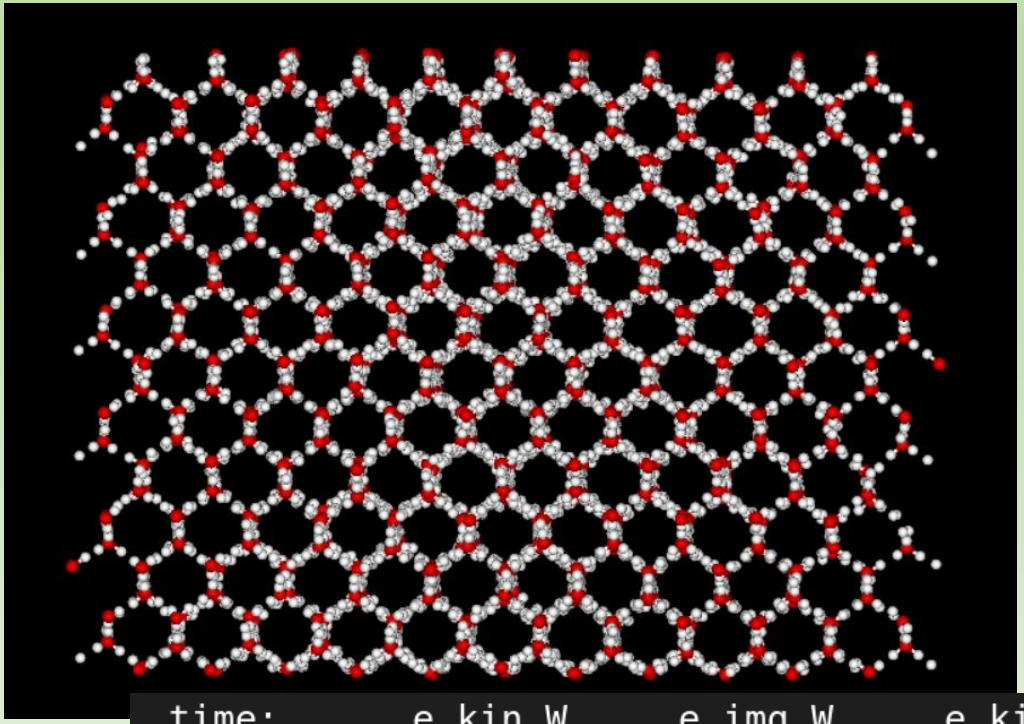
Firefox works for AlmaLinux and Debian OS
Debian can view all of internet, but AlmaLinux is quite limited



Windows to Linux terminal: Installation of mpich4, fftw3 Tests of p3mtip5, and Siesta-4.1b codes



Test of MD: @p3mtip5p07a.f03, by 5-points water model



This simulation run is OK, but timing is highly variable in time because the simulation in VirtualBox competes with many tasks of Windows 11. The cpu2 which should be 0.6 sec at least is different with the time steps.

```
  time:       e_kin.W     e_img.W     e_kin(M)    e_c_r       e_lj        e_p3m
     e_tot          walltm     vm          exc         <ekin>     <eimg>         cpu
0         cpu1         cpu2         cpu3
t=     20.0  1.7095E+00  1.9537E-01  0.0000E+00 -1.6974E+02  3.0997E+01  5.1888E
-04 -1.3684E+02    8.656D+02  1.353D-01  0.000D+00  9.893D-04  1.131D-04     1.1
15D+00   4.028D-04   1.106D+00   8.584D-03
t=     25.0  1.7269E+00  1.9599E-01  0.0000E+00 -1.6972E+02  3.0949E+01  5.3564E
-04 -1.3685E+02    1.076D+03  1.095D-01  0.000D+00  9.993D-04  1.134D-04     1.7
43D+00   3.641D-04   1.734D+00   8.680D-03
t=     30.0  1.7385E+00  2.0207E-01  0.0000E+00 -1.6976E+02  3.0940E+01  5.4725E
-04 -1.3688E+02    1.295D+03  1.117D-01  0.000D+00  1.006D-03  1.169D-04     5.6
95D-01   3.855D-04   5.607D-01   8.385D-03
```

Related pip3 packages

The initial configuration of water and hydrate are constructed (Dr. Matsumoto,https://github.com/vitroid/)
$ pip3 install genice2

Compilation goes OK in genice2 software of CentOS 7. However, it goes errors in the pairlist package and thus not go forward in AlmaLinux-9.

The Debian-12 OS has been installed, and is tested by "mrg37" which is quite OK. The pip3 packages and 'pip3 install genice2' is successfully installed.
The initial water configuration turns to be perfect.

To compile Scalapack Ver. 2

"This is the inside story of Scalapack's make."

One downloads scalapack-2.2.0.tgz and expands it.
In BLACS, PBLAS, SRC, TOOLS, do $ make (no option),
except one difference in SRC.

Give -fallow-argument-mismatch at Makefile's $(FC)
line in SRC, then type $ make –k when one meets errors.

Scalapack is 10.7 MB for libscalapack.a

Test of ab-initio Siesta-4.1b code

A keyword -fallow-argument-mismatch is added in the arch.make file of Siesta-4.1b for AlmaLinux-9 and Debian-12

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```
Siesta Version  : v4.1-b4
Architecture    : mpifort-MPI
Compiler version: GNU Fortran (Debian 12.2.0-14) 12.2.0
Compiler flags  : mpifort  -O2 -ftree-vectorize -fprefetch-loop-arrays -march=na
tive -fallow-arrgument-mismatch -fPIE
PP flags        : -DMPI -DFC_
Libraries       :  -lgomp -L/
calapack.a
PARALLEL version

* Running on 6 nodes in paral
>> Start of run:   4-DEC-2024

reinit: Reading from c12h48.f
```

```
siesta: Cell volume =        720.000000 Ang**3

siesta: Pressure (static):
siesta:                  Solid           Molecule  Units
siesta:          0.00029221          0.00031048  Ry/Bohr**3
siesta:          0.02683002          0.02850685  eV/Ang**3
siesta:         42.98689824         45.67350469  kBar
(Free)E+ p_basis*V_orbitals  =       -2615.811581
(Free)Eharris+ p_basis*V_orbitals  =       -2615.811581

dhscf: Vacuum level (max, mean) =   -0.569552   -0.682007 eV

>> Start of run:   4-DEC-2024  17:38:16
>> End of run:     4-DEC-2024  17:39:58
                                1:42 min./10 cycles/6-MPI

Job completed
```

Overall Results of AlmaLinux and Debian OS

The tests of classic and ab-initio molecular dynamics on AlmaLinux-9 OS were successful. Some alterations must be necessary on this specific operating system.

Many internet sites including FFTW3 failed by busy signal, the pip3 compilation of pairlist was wrong in AlmaLinux-9.

Debian 12 OS was installed, and gcc, make, mpich, fftw3 were set up on top. It was tested with MD and water initial cof pip3 (by Dr. Matsumoto) and Siesta-4.1b, all of which were very favorable on Debian.