Simulations of Molecular Dynamics by Debian-13 v.s. AlmaLinux-9

Motohiko Tanaka, Ph.D., Japan
https://github.com/Mtanaka77/

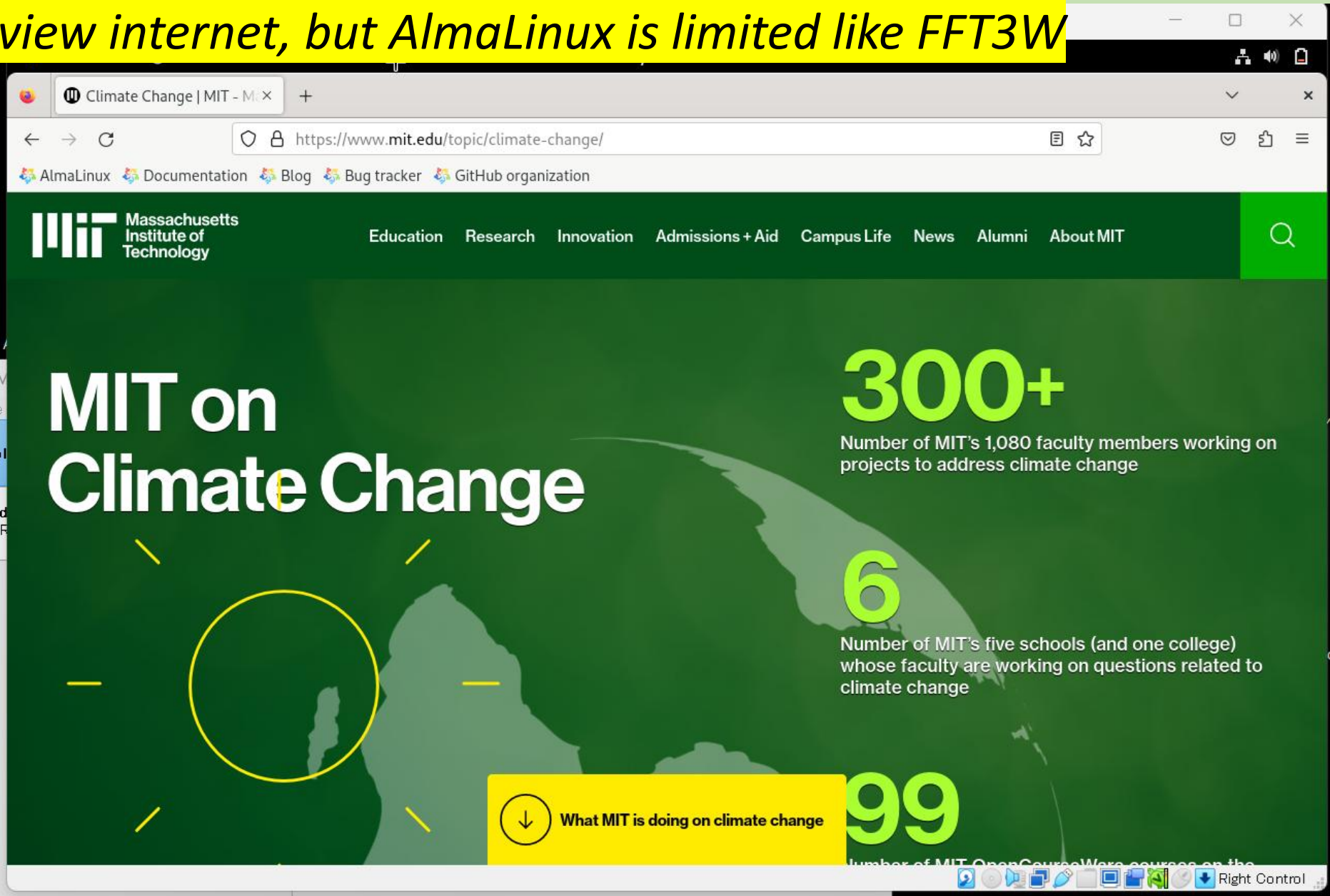
Setting tests for simulations

Installation of AlmaLinux-9 and Debian-13

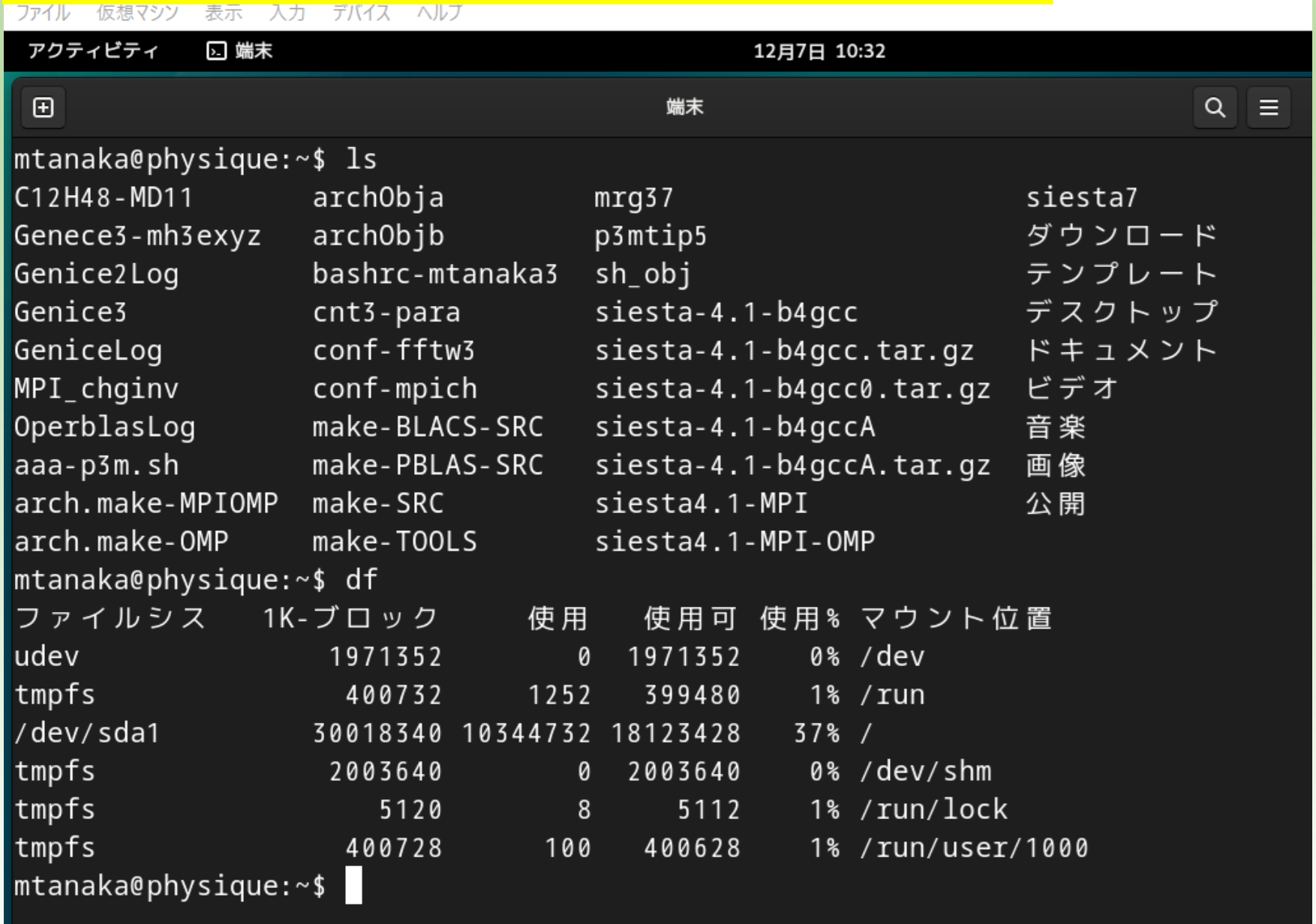
Use Windows 11, and VirtualBox 7.5 to login Linux
Linux gfortran and pip3 packages

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

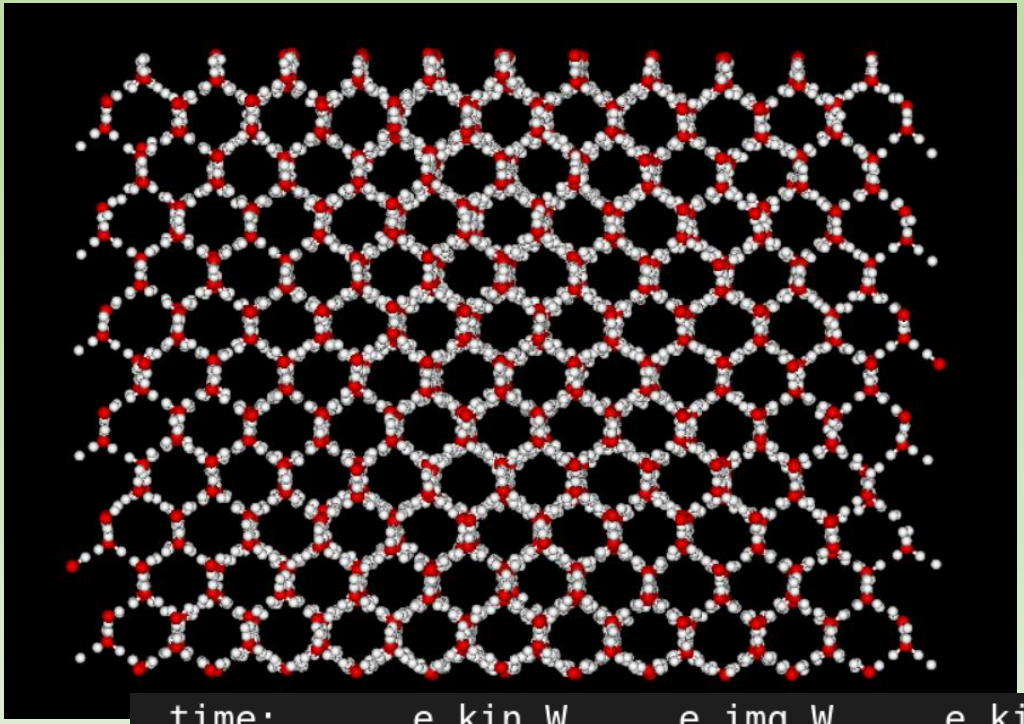
Firefox works for AlmaLinux and Debian OS. Debian can view internet, but AlmaLinux is limited like FFT3W



(1) Linux terminal from Windows: 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
```

(2) Related pip3 packages, Genice2

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

Compilation goes well in genice2 software for Debian. However, it goes with strange errors in "genice CS1…" for AlmaLinux-9.6.

The Debian-13 has been installed, and is tested by "mrg37" which is quite OK. The pip3 packages and 'pip3 install genice2' is successfully installed. "genice CS1…" generates water molecules which is perfect.

(3.a) To compile Scalapack Ver. 2

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

One downloads scalapack-2.2.2.tgz and expands it.
Give -fallow-argument-mismatch and
-Wno-implicit-function-declaration at Slmake.make,
of Debian-13. And $ make in TOOLS, SRC, PBLAS,
BLACS, and BLACS/Install directories.
It comes with 11 MB of libscalapack.a.

(3.b) 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 Debian-13 (Nov. 2025).

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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's

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 errors at "genice CS1 …" in AlmaLinux-9.6.

Debian 13 OS was installed, and gcc, gfortran, mpich, fftw3 were set up on top. It was tested with MD, water code "Genice2" (by Dr. Matsumoto), and Siesta-4.1b, and all of which were very favorable on Debian.