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

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https://github.com/Mtanaka77/

Settings and tests of simulations

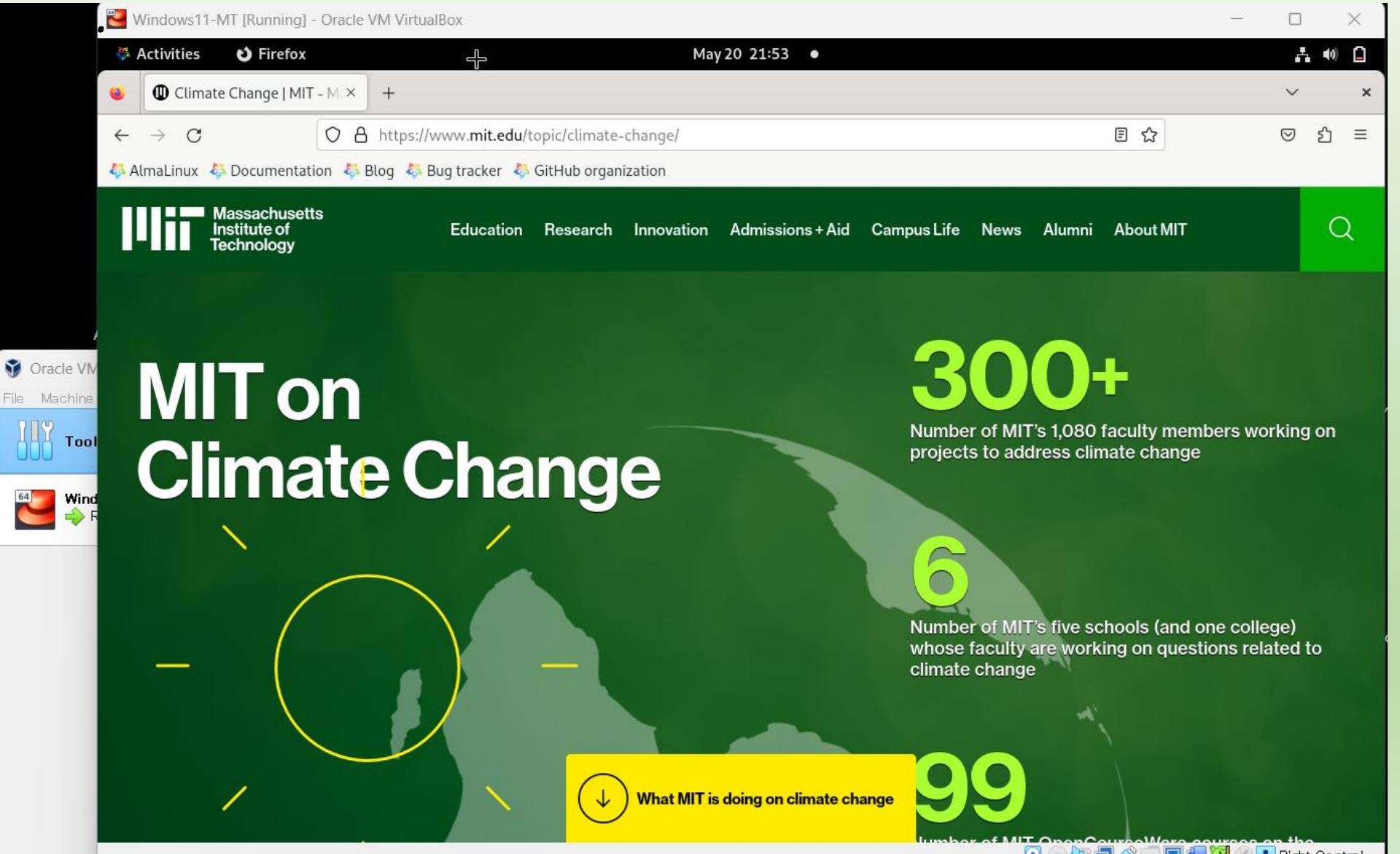
Installation of AlmaLinux-9, May 2024, and
Debian 12, Nov. 2024

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

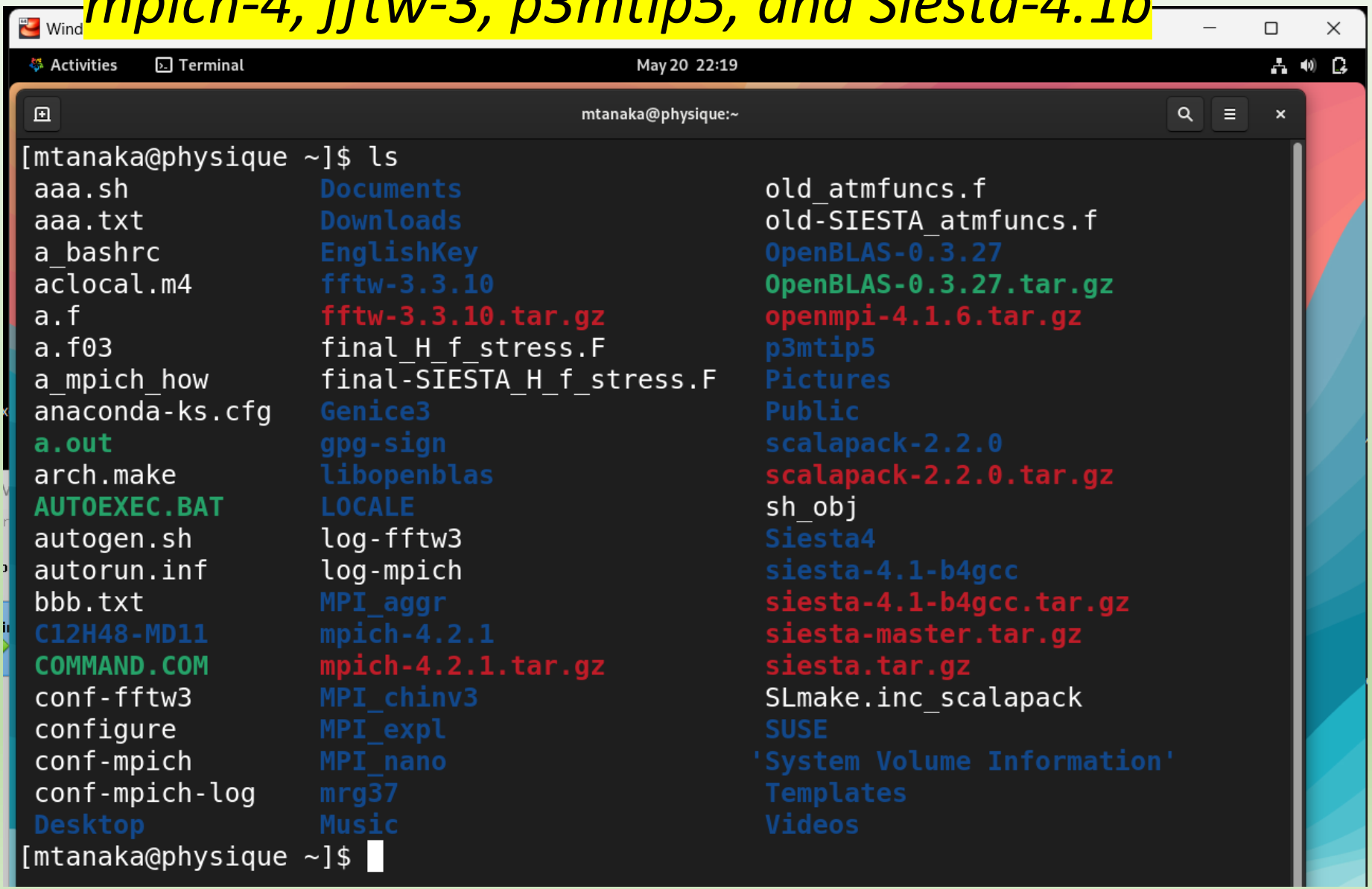
Simulations, cf. https://github.com/Mtanaka77/
>> Three-dimensional electrostatic p3mtip5 code,
with tip5p and Ewald sums
>> Siesta-4.1b, with mpich4 fft3w, OpenBLAS,
and Scalapack

Firefox works for AlmaLinux and Debian

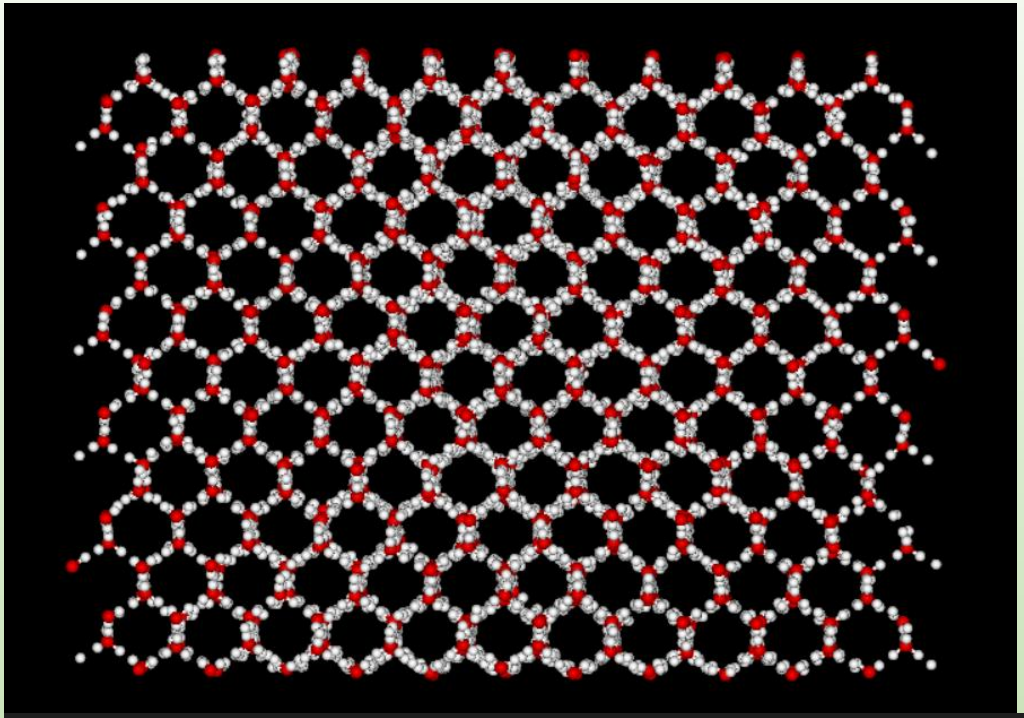
Debian can view all of internet, but AlmaLinux is quite limited



Windows to Linux terminal shows installation of mpich-4, fftw-3, p3mtip5, and Siesta-4.1b



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.

Debian 12
The Debian 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 Version 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

```
Architecture    : gfortran-MPI
Compiler version: GNU Fortran (GCC) 11.4.1 20231218 (Red Hat 11.4.1-3)
Compiler flags  : mpifort  -O2 -fPIC -ftree-vectorize -march=native -fallow-argu
ment-mismatch
PP flags        : -DMPI -DFC_HAVE_ABORT
Libraries       :  -lgomp -L/opt/openblas/lib -lopenblas -L/opt/scalapack/lib -l
scalapack
PARALLEL version

* Running on 6 nodes in parallel
>> Start of run:   2-JUN-2024  10:09:19

                         ************************
                         *  WELCOME TO SIESTA   *
                         ************************

reinit: Reading from c12h48.fdf
siesta:          0.02683007           0.02850685  eV/Ang**3
siesta:         42.98698226          45.67350102  kBar
(Free)E+ p_basis*V_orbitals  =       -2615.811579
(Free)Eharris+ p_basis*V_orbitals  =       -2615.811579

dhscf: Vacuum level (max, mean) =   -0.569553   -0.682007 eV
>> Start of run:   2-JUN-2024  10:09:19
>> End of run:     2-JUN-2024  10:11:55
Job completed
```

Overall Points of AlmaLinux and Debian OS

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

However, internet sites including FFTW3 fail by busy signal. The pip3 compilation of pairlist is wrong in AlmaLinux-9.

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