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

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https://github.com/Mtanaka77/

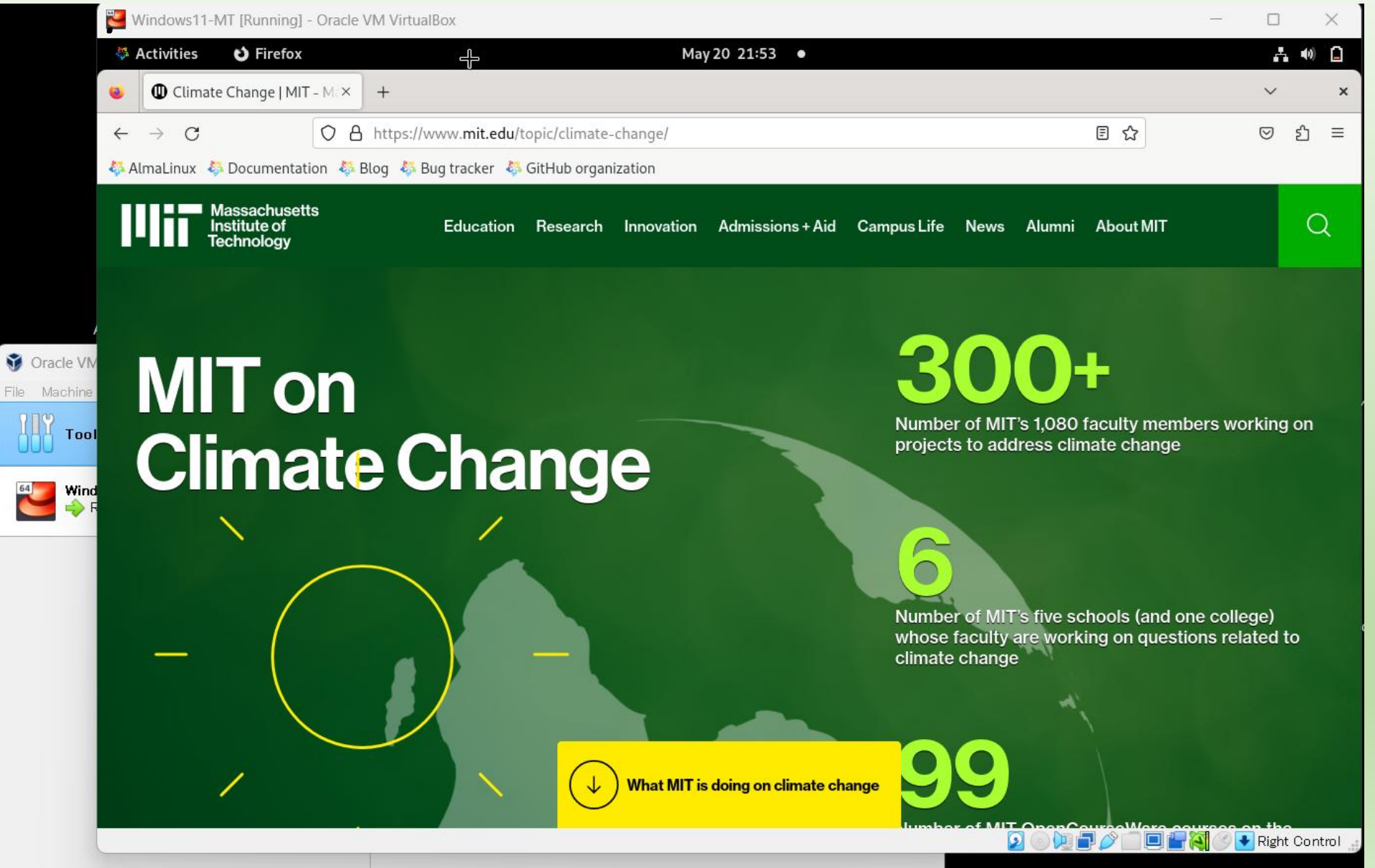
Settings and tests for simulations

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

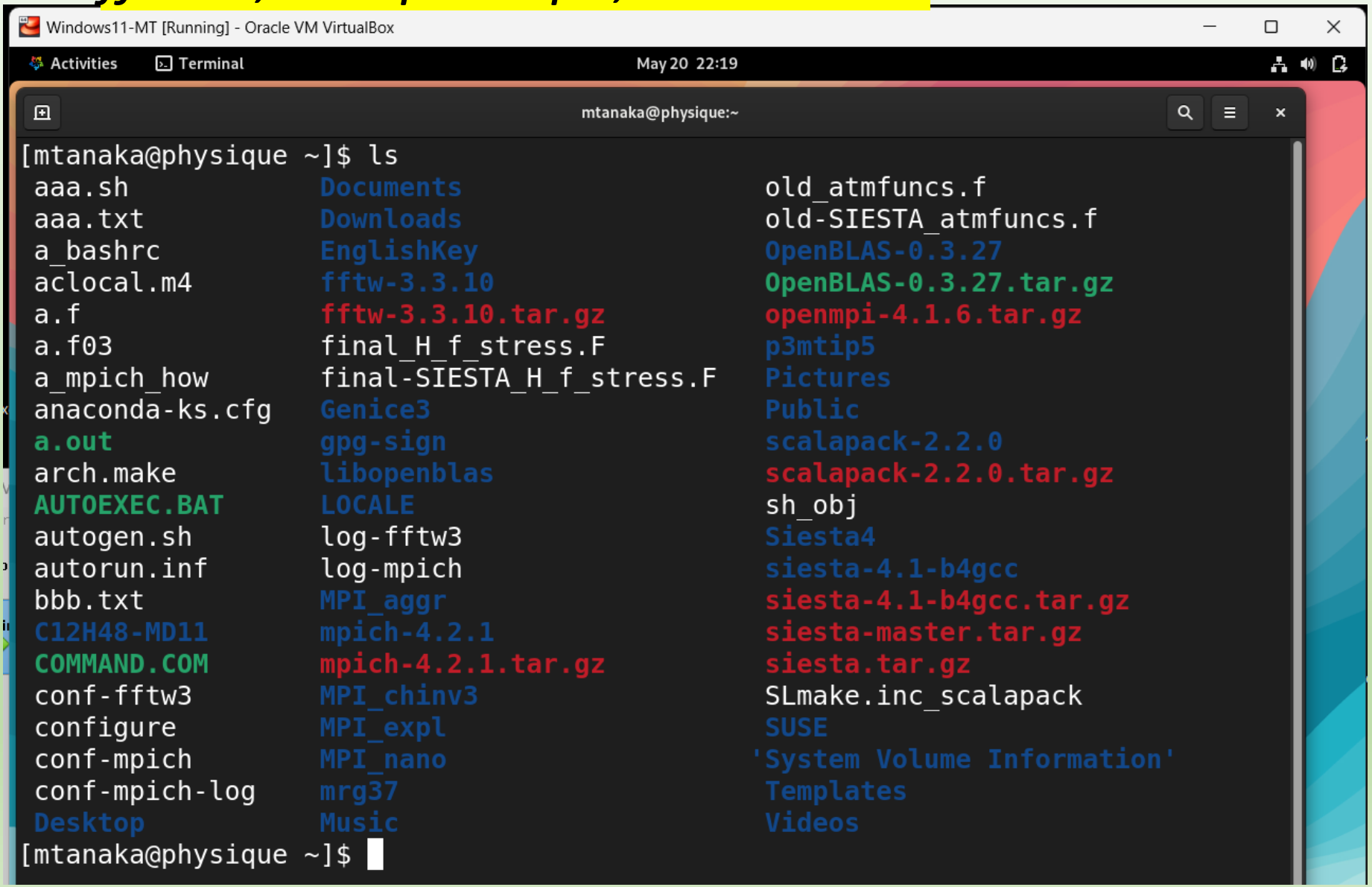
Use Windows 11, VirtualBox 7
Linux gfortran and pip packages

Simulations, https://github.com/Mtanaka77/
>> Three-dimensional electrostatic p3m code,
with tip5p and Ewald sums
>> Siesta-4.1b, with mpich, fft3w, OpenBLAS,
Scalapack

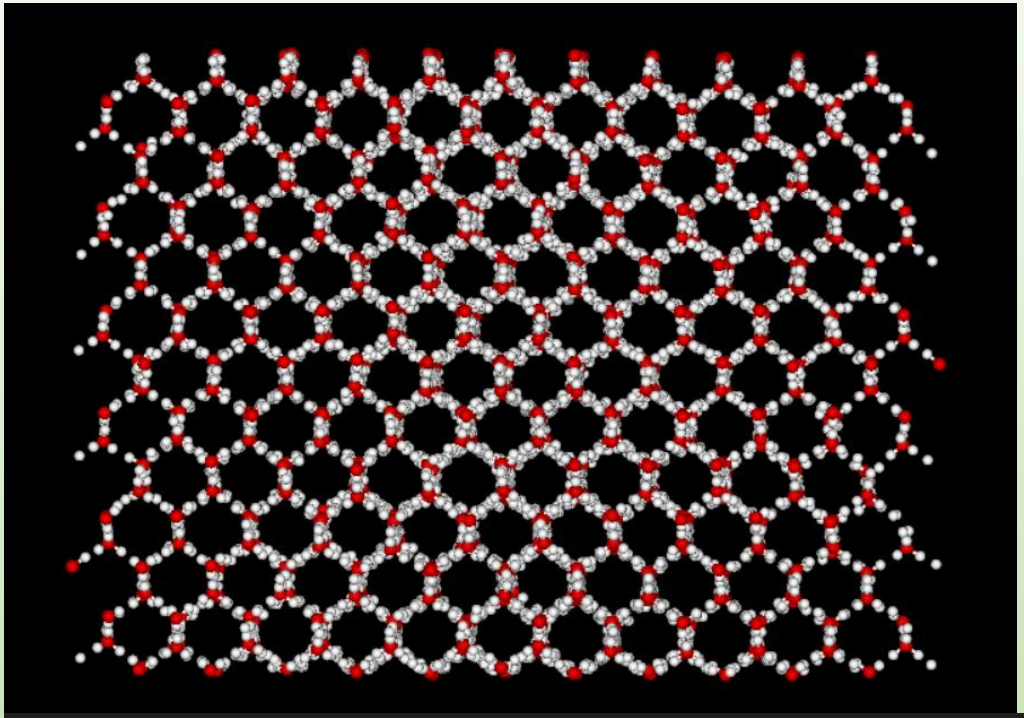
Firefox works for AlmaLinux and Debian



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



Test of MD @p3mtip5p07a.f03, 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 states of water and hydrate are constructed (Dr. Matsumote, https://github.com/vitroid/).
$ pip3 install genice

Compilation goes all right for the genice software of CentOS 7. However, it goes the 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. Pip3 packages and 'pip3 install genice2' is successfully installed. The initial water configuration is perfect.

To compile Scalapack v.2

Download scalapack.2-2-0 and expand it.
In BLACS, PBLAS, SRC, TOOLS, do $ make (no option), except one difference is SRC.

Give –fallow-argument-mismatch at Makefile's $ (FC) line of SRC, and type $ make –k when errors are shown.

Scalapack is 10.7 MB for libscalapack.a

Test of ab-initio Siesta-4.1b code

A keyword -fallow-argument-mismatch in the arch.make file is added 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 results

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, other sites including FFTW3 software fail by busy signal. The scalapack software is on unresolved errors. The pip3 of pairlist goes wrong in AlmaLinux-9.

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