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

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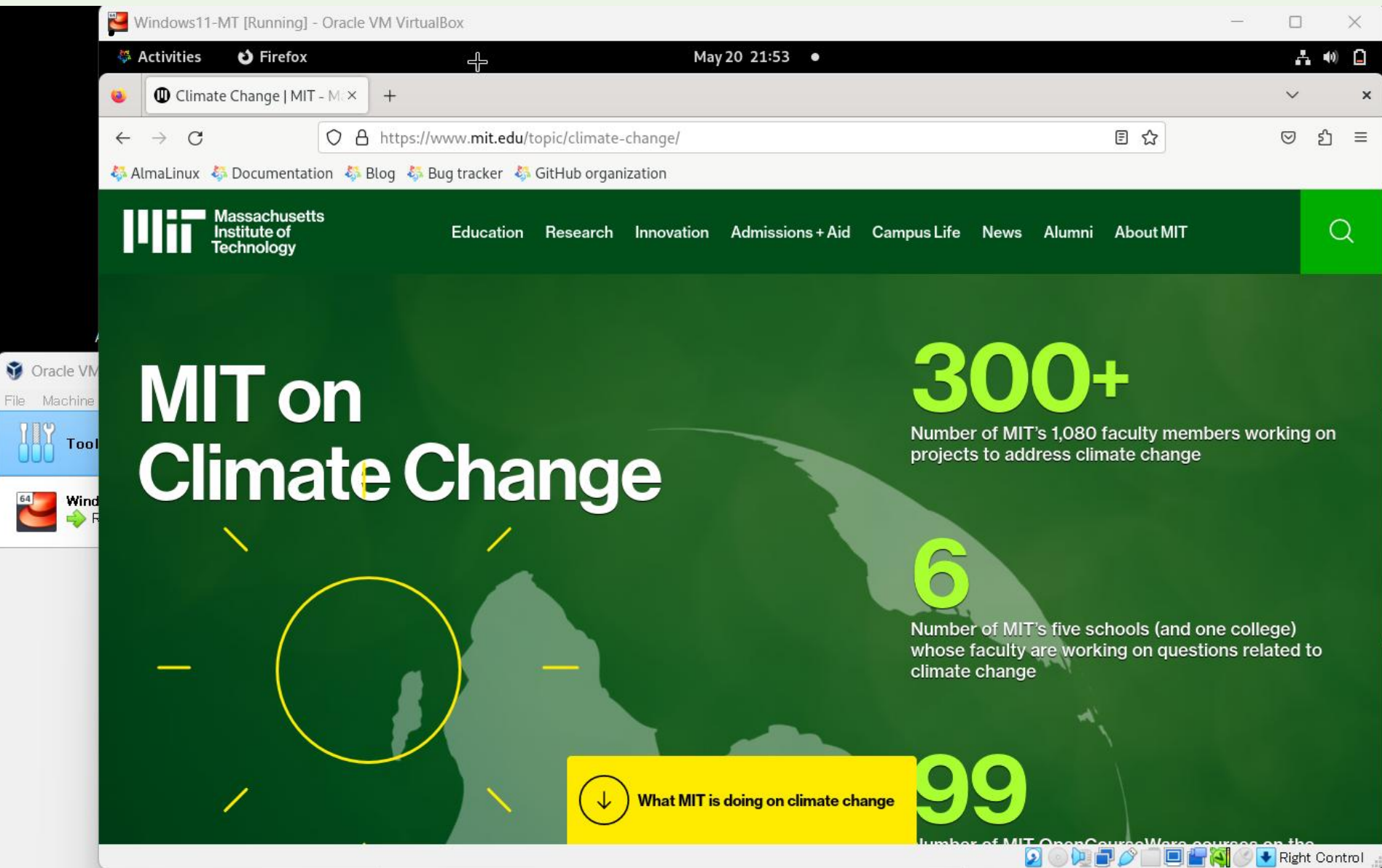
https://github.com/Mtanaka77/

Settings and tests for simulations

Installation of AlmaLinux-9, May 2024, and Debian 12, Nov. 2024
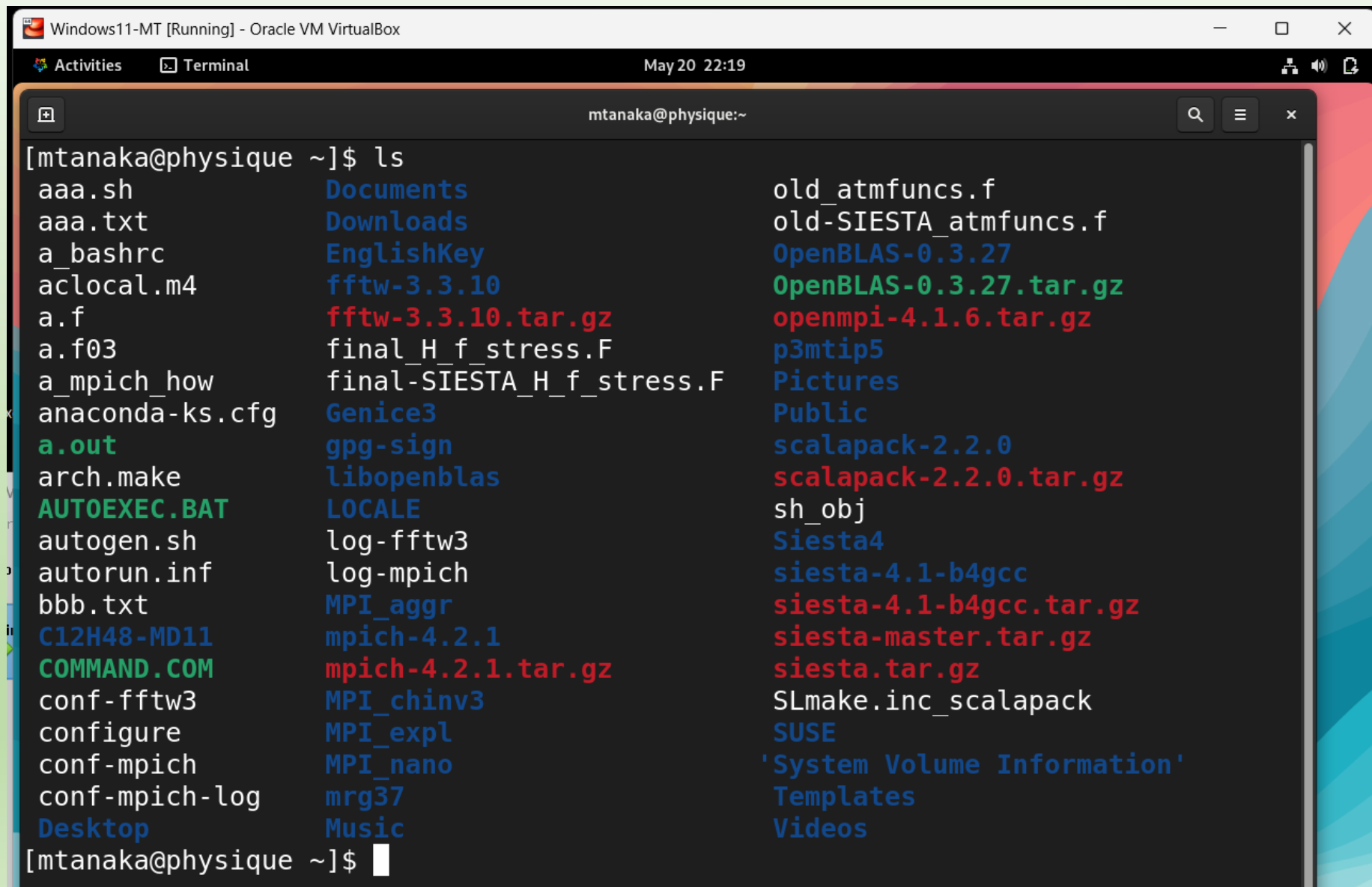
Use Windows 11, VirtualBox 7
Linux gfortran and pip packages

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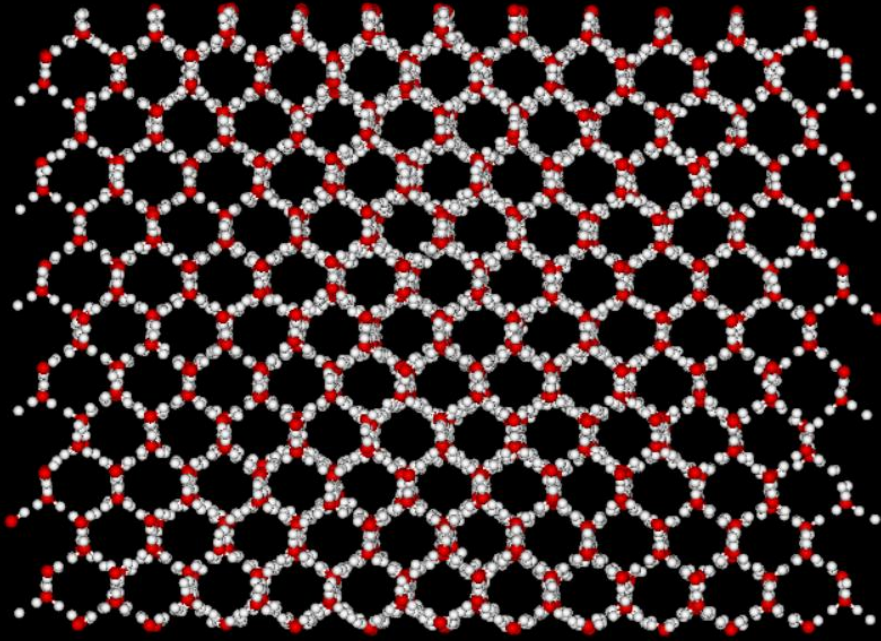
Firefox works with AlmaLinux and MIT sites

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

Test of MD @p3mtip5p07a.f03, 5-points water with 8640 atoms

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 in the genice software in AlmaLinux-9.

Debian 12 OS
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 OK.

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 to avoid non-necessary errors.*

```
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, while it is all right on CentOS 7 OS.

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