Simulation Tests for AlmaLinux Operating System

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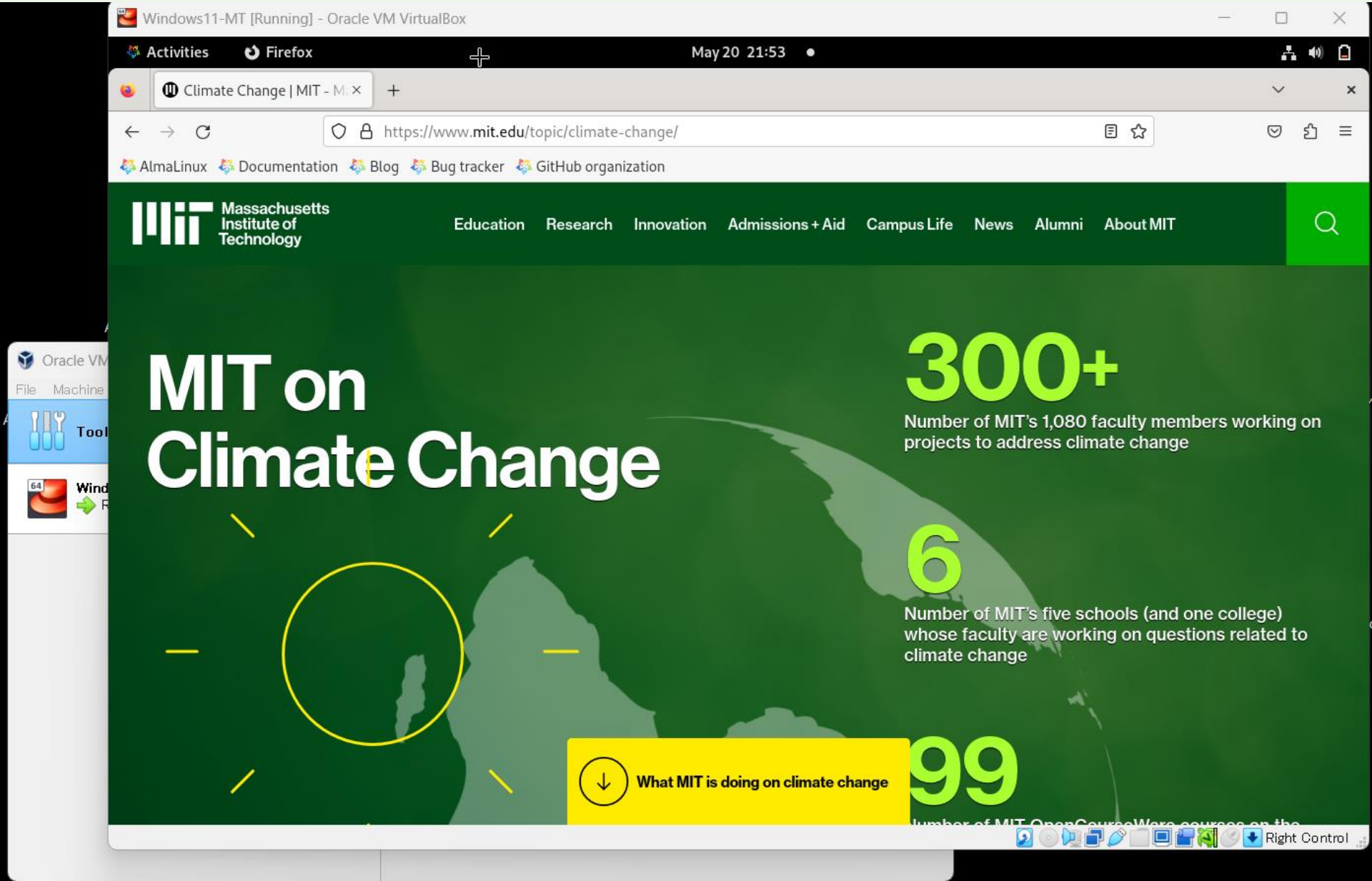
Settings and tests for simulations

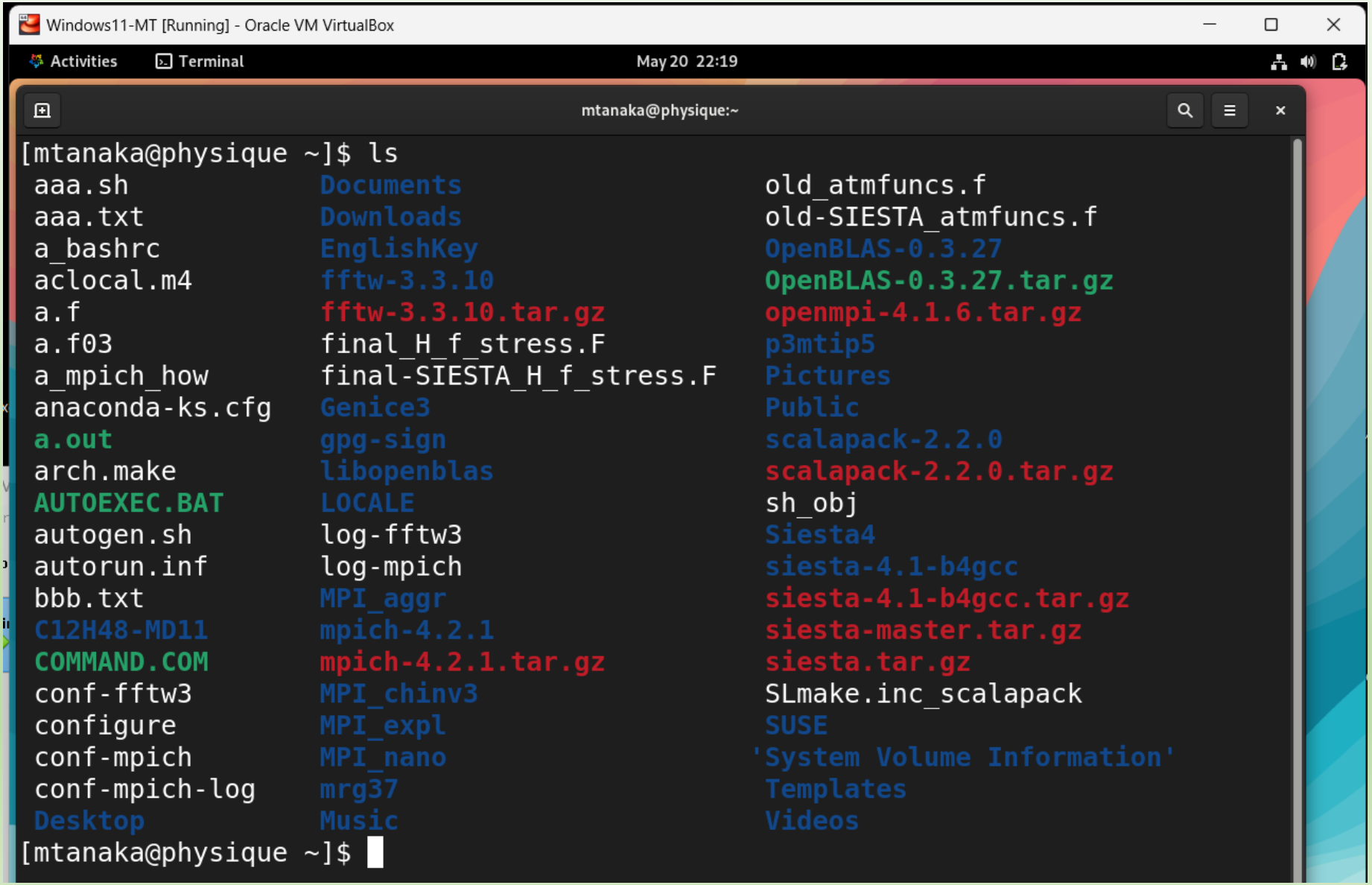
Installation of AlmaLinux-9, May 2024
Use Windows 11, VirtualBox 7.0.14
Linux gfortran and pip packages

Simulations
>> Three-dimensional electrostatic p3m code, with tip5p and Ewald sums
>> Siesta-4.1b, with mpich, fft3w, OpenBLAS, Scalapack

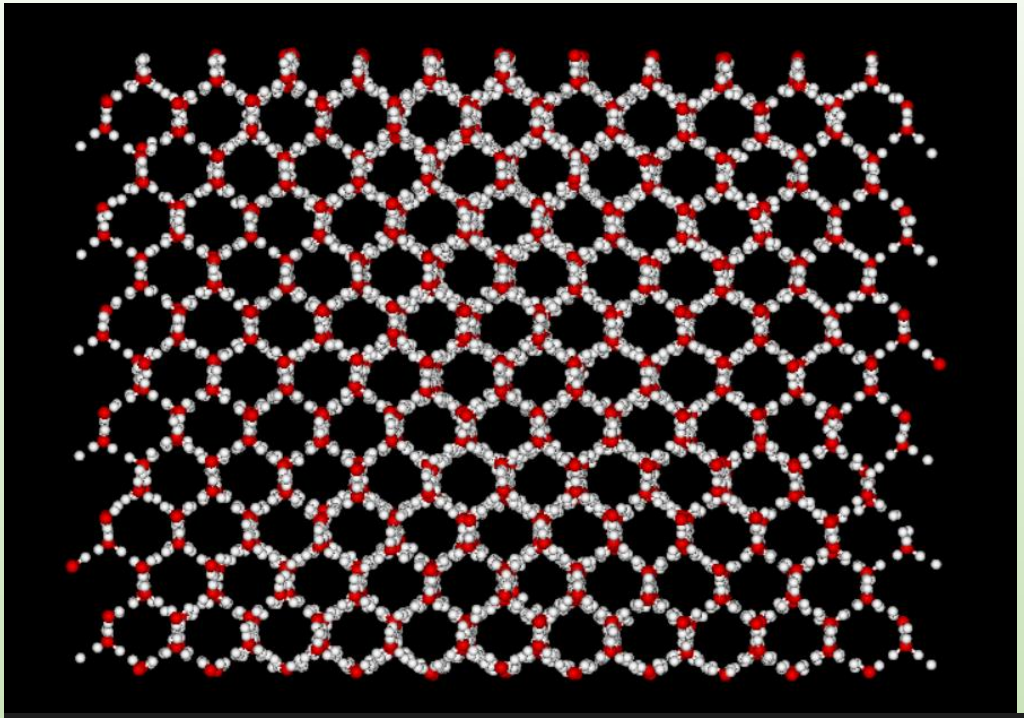
Firefox works with AlmaLinux and MIT sites



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



Test of @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 state of water and hydrate is 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.

Test of ab-initio Siesta-4.1b

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:         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
```