Simulation Tests of AlmaLinux-9 Operating System

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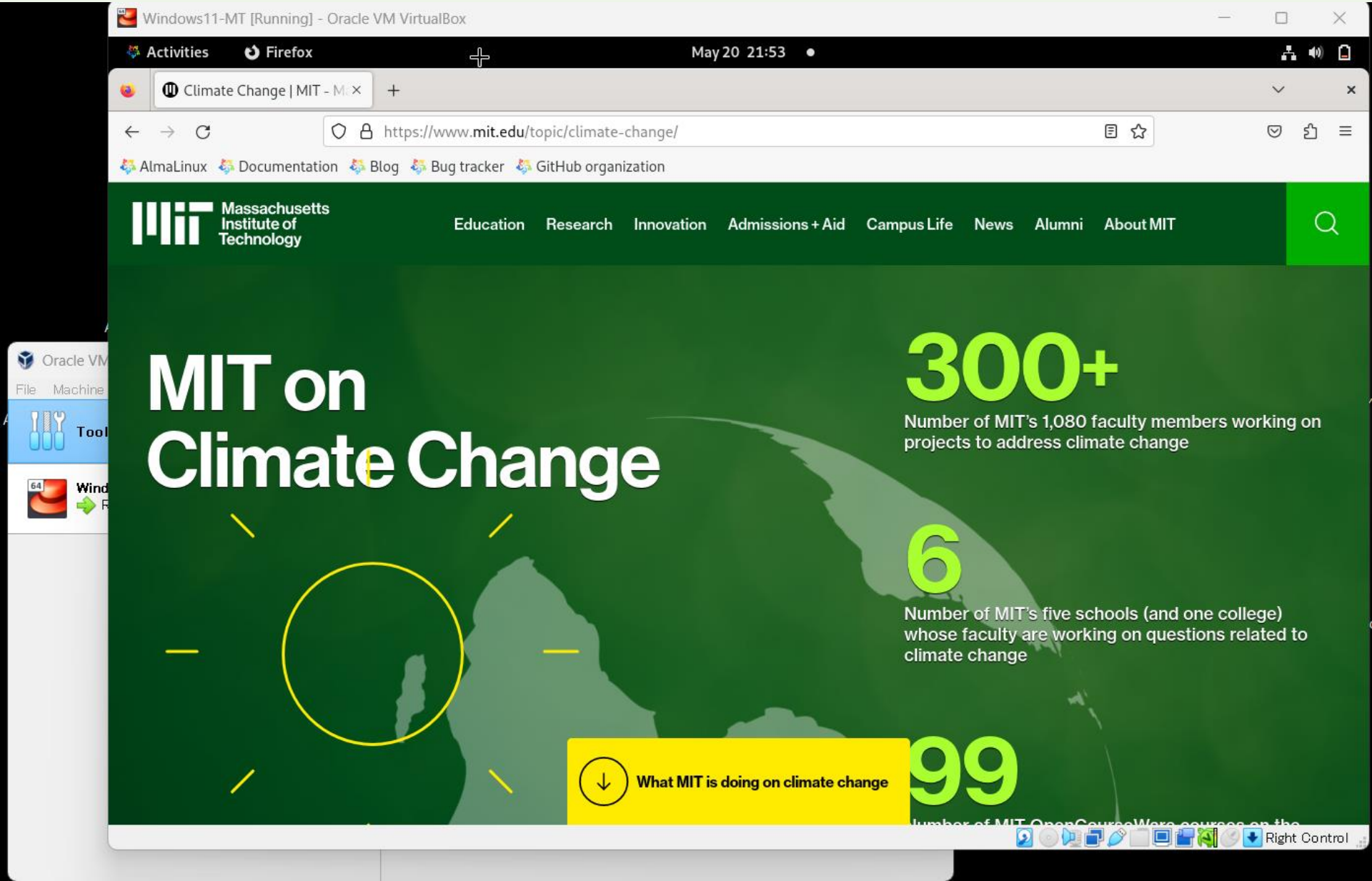
Settings and tests of simulations

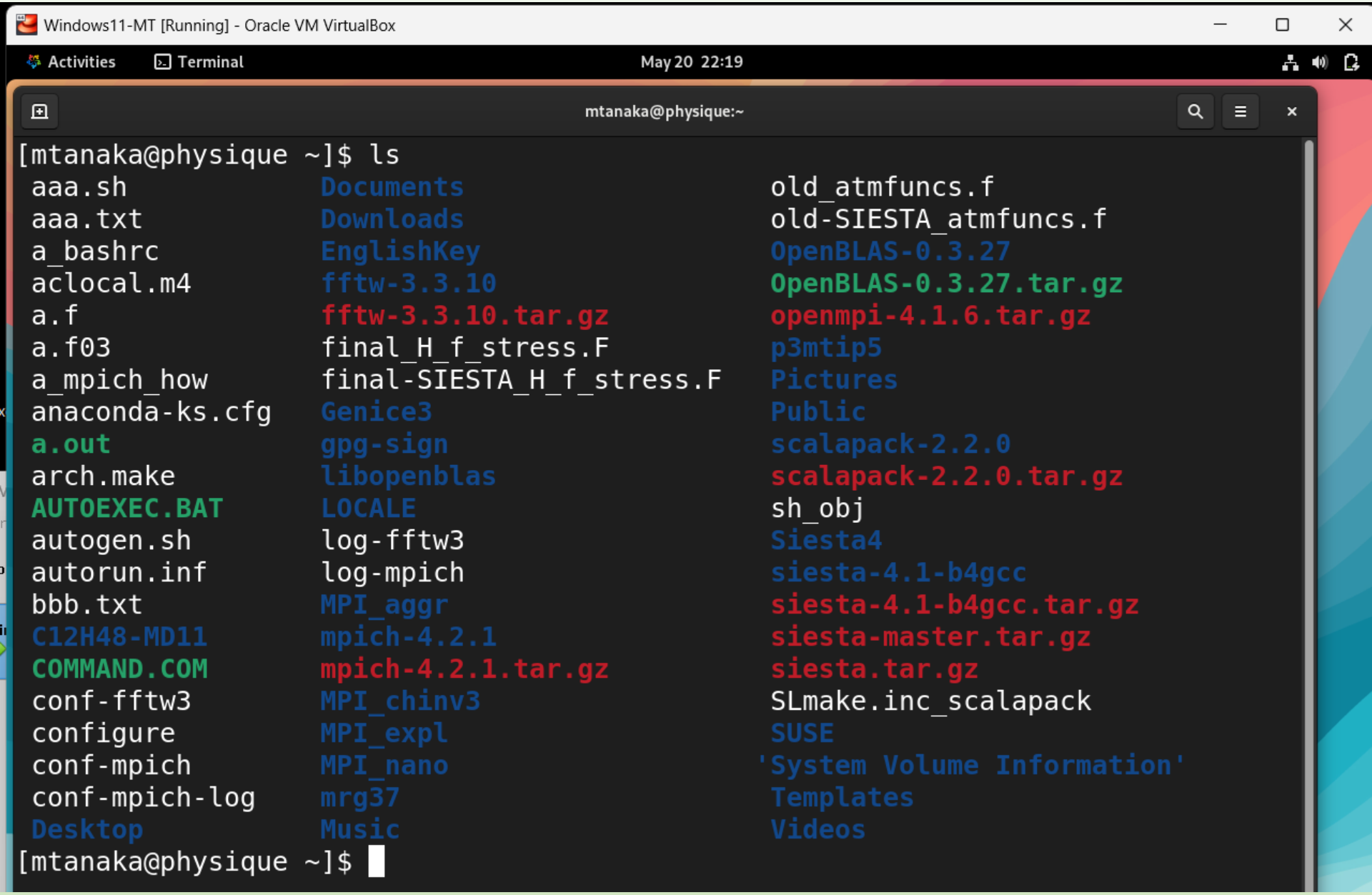
Installation of AlmaLinux-9, March 2024
Use the Windows 11, VirtualBox 7.0.14
Open gfortran and pip packages

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

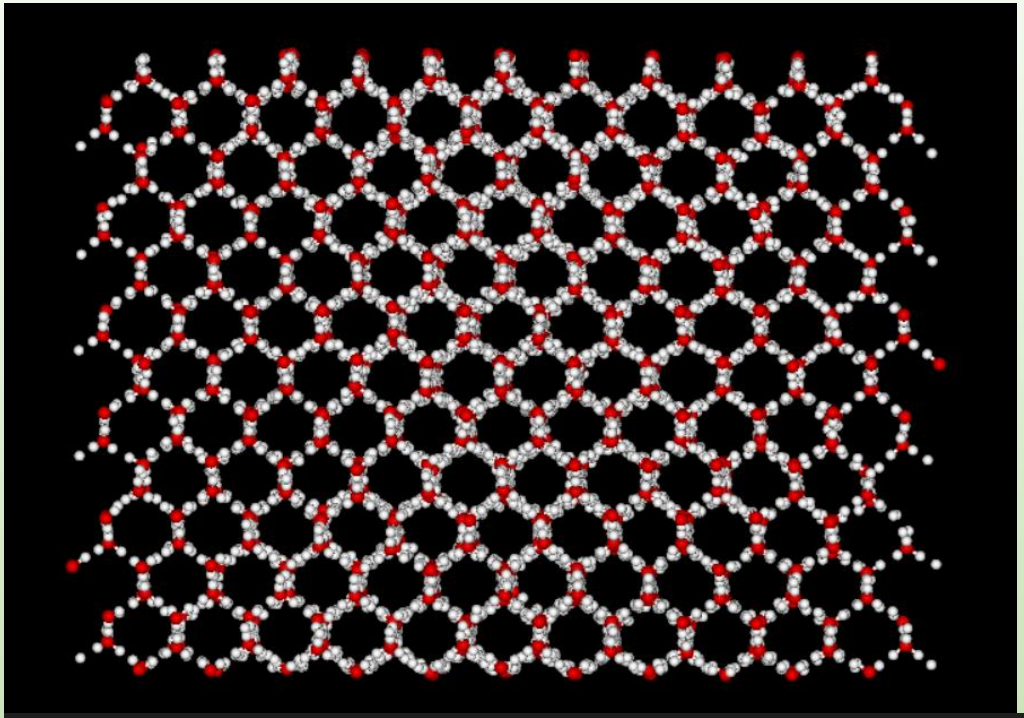
Firefox works with AlmaLinux and MIT sites



Terminal showing mpich-4, fftw-3 and Siesta-4.1



Test of @p3mtip5p07a.f03 H2O: 5-points, 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 is very different in 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
```

Test of Siesta-4.1b

In the arch.make, the keyword -fallow-argument-mismatch is added of AlmaLinux-9 to avoid non-necessary errors.

```
Siesta Version  : v4.1-b4
Architecture    : gfortran-MPI
Compiler version: GNU Fortran (GCC) 4.8.5 20150623 (Red Hat 4.8.5-44)
Compiler flags  : mpifort  -O2 -fPIC -ftree-vectorize -march=native
PP flags        : -DMPI -DFC_HAVE_ABORT
Libraries       :  -lgomp -L/opt/openblas/lib -lopenblas_omp  -L/opt/sc
alapack-2.2.0/lib -lscallapack
PARALLEL version

* Running on 6 nodes in parallel
>> Start of run:  10-MAY-2024  17:39:33

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

reinit: Reading from c12h48.fdf
                                                              nits
                                                              /Bohr**3
                                                              /Ang**3
siesta:          42.98698303          45.07350218  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
>> End of run:  10-MAY-2024  17:40:33
Job completed
```