Simulation Tests of AlmaLinux-9 Operating System

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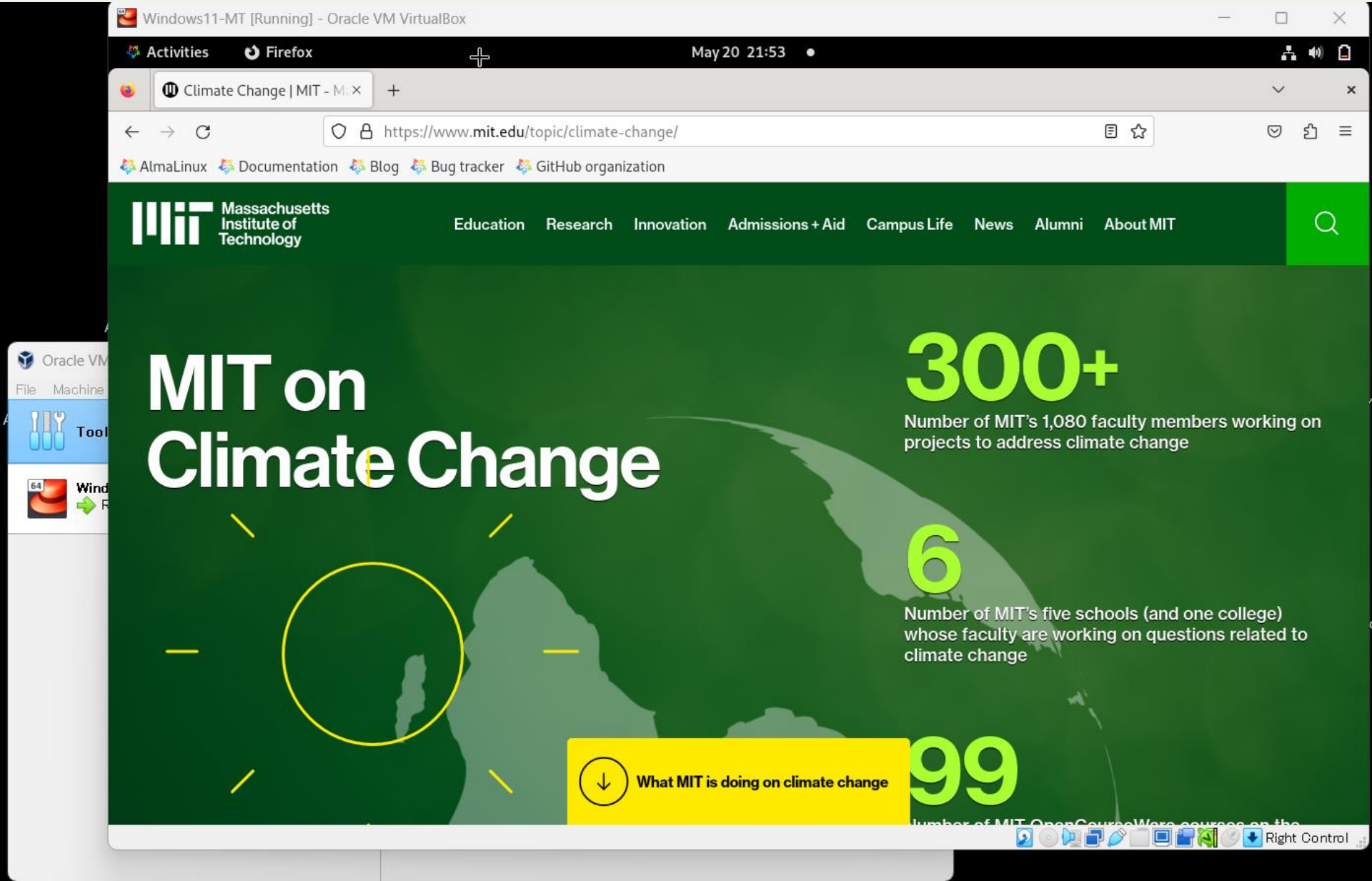
Settings and tests of simulations

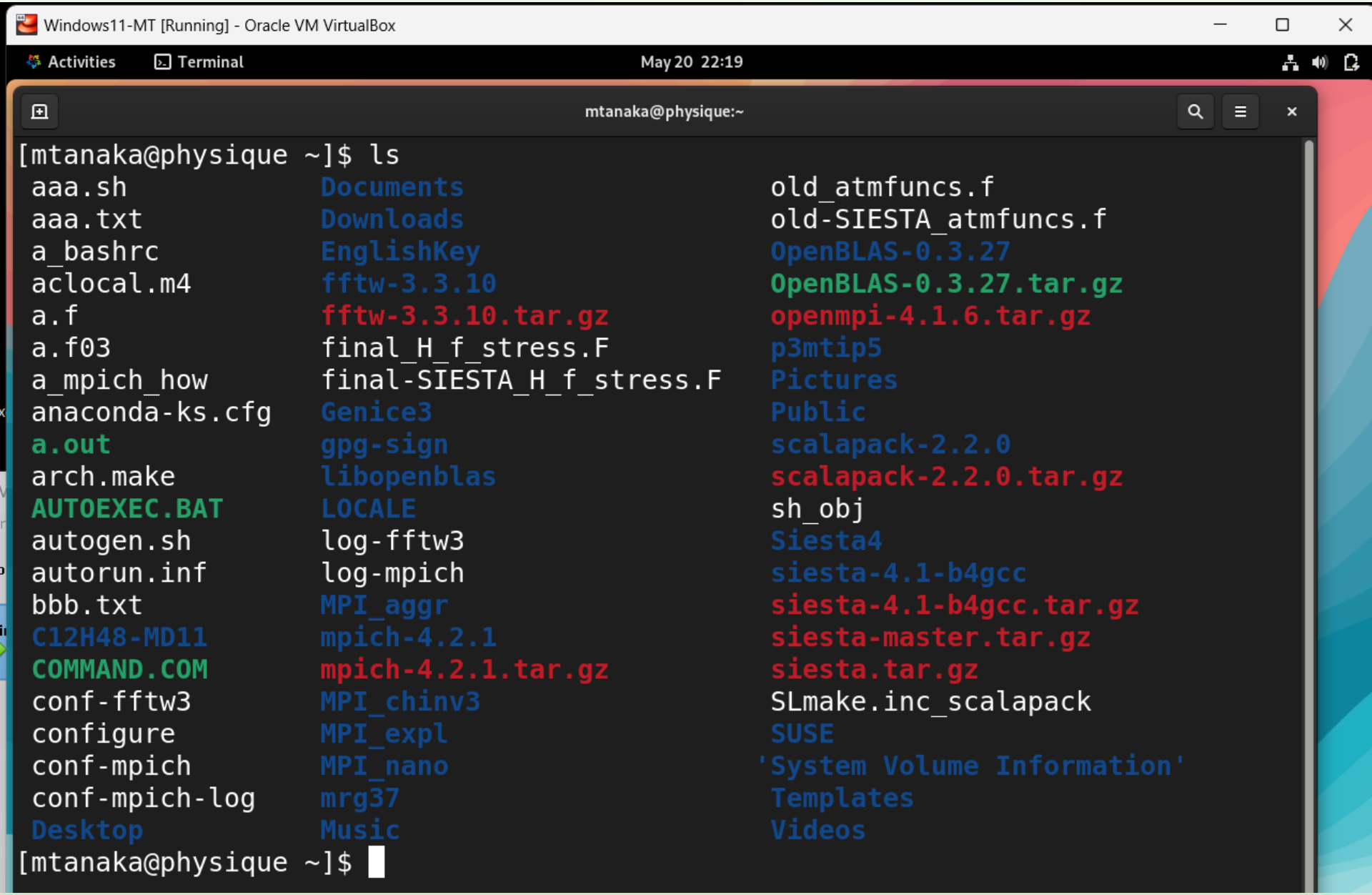
Install the linux, AlmaLinux-9, Mar. 2024
Use the Windows 11, VirtualBox 7.0.14
Open gfortran and pip packages

Simulations
>> three-dimensional ES p3m code, with tip5, Ewald sum
>> Siesta-4.1b, with mpich, fft3w, OpenBLAS, Scalapack

Firefox works for showing AlmaLinux and MIT sites

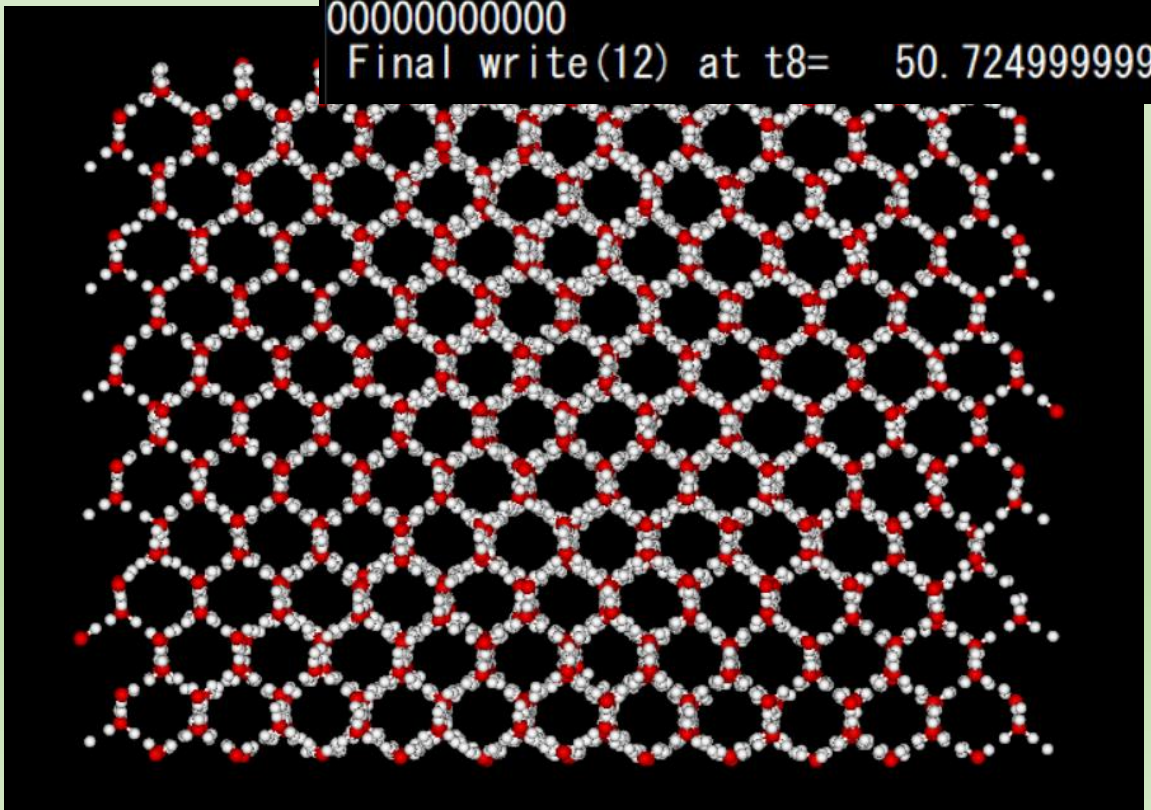


Terminal using mpich-4, fftw-3 and Siesta-4.1



Test of @p3mtip5p07a.f03 H2O 8640 atoms, 6 cpu/3 GHz

```
t=      30.0  1.5047E+00  1.8313E-01  0.0000E+00 -1.7020E+02  3.0737E+01
  5.1659E-04 -1.3778E+02    4.282D+02  1.024D-01  0.000D+00  8.708D-04
 1.060D-04     3.571D-01   2.404D-04   3.511D-01   5.815D-03
t=      40.0  1.4686E+00  1.9438E-01  0.0000E+00 -1.7059E+02  3.1085E+01
  5.1197E-04 -1.3784E+02    5.707D+02  9.719D-02  0.000D+00  8.499D-04
 1.125D-04     3.556D-01   2.392D-04   3.495D-01   5.795D-03
t=      50.0  1.5077E+00  2.0854E-01  0.0000E+00 -1.7075E+02  3.1106E+01
  4.9661E-04 -1.3793E+02    7.130D+02  9.940D-02  0.000D+00  8.725D-04
 1.207D-04     3.551D-01   2.391D-04   3.493D-01   5.572D-03
   Final: t8, it, tmax=   50.724999999998190          2030    50.5000
00000000000
 Final write(12) at t8=   50.724999999998190
```



Test of Siesta-4.1b on AlmaLinux-9

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  *                        its
                         ************************                        /Bohr**3
                                                                         /Ang**3
reinit: Reading from c12h48.fdf                                          ar
(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
```