Simulation Tests of AlmaLinux-9 Operating System

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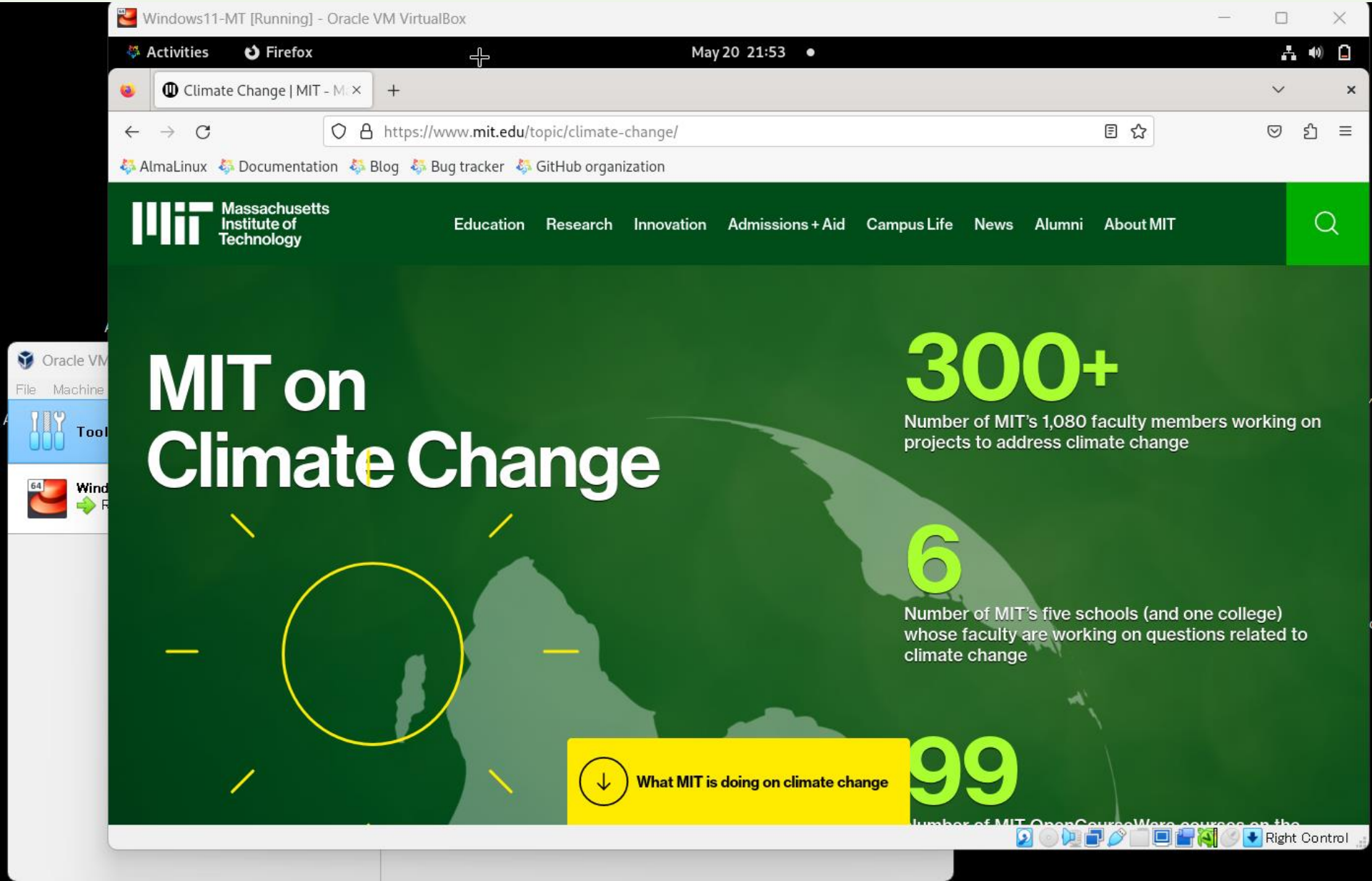
Settings and tests of simulations

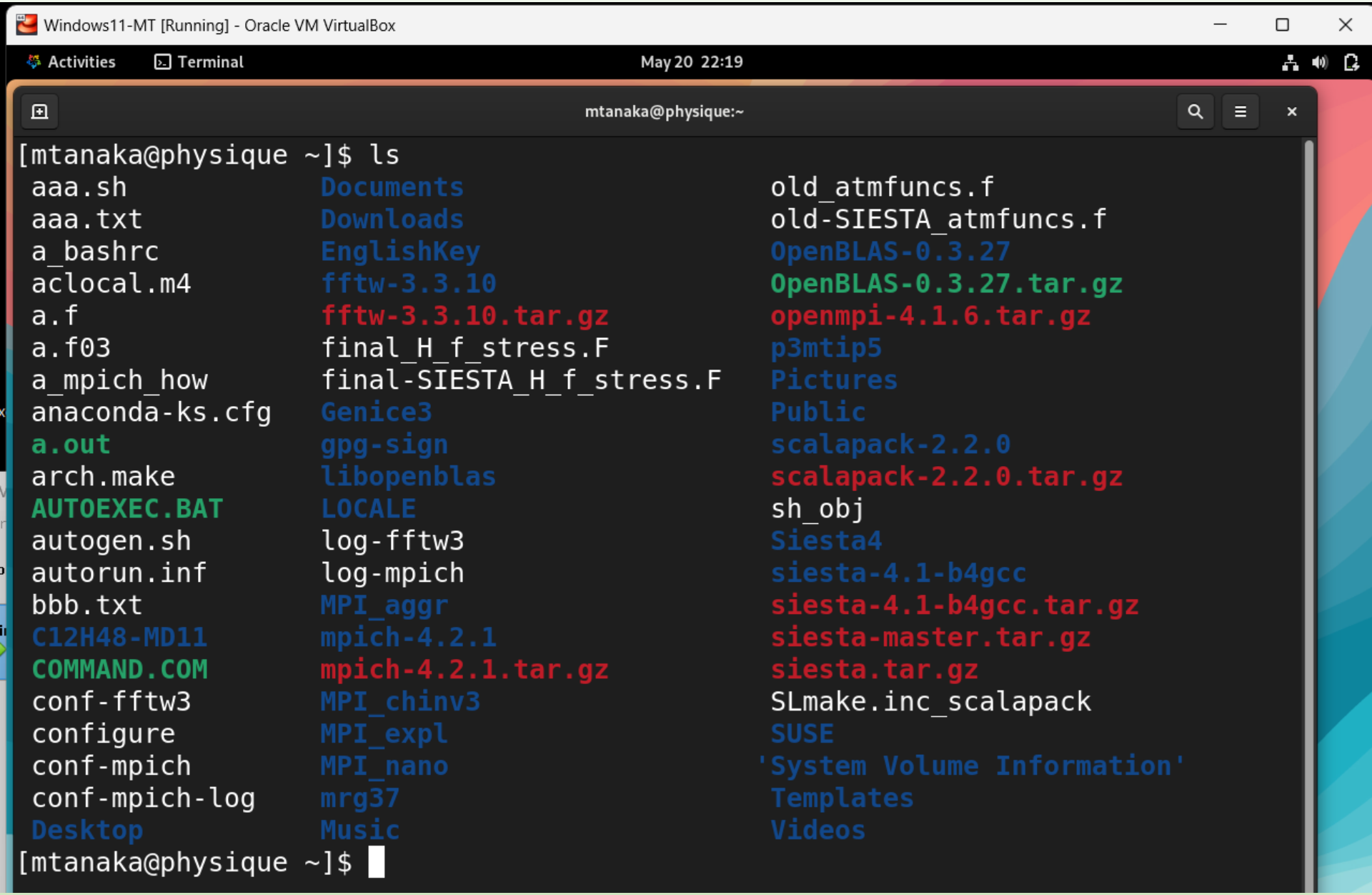
Install the linux, AlmaLinux-9, Mar. 2024
Use the Windows 11, VirtualBox 7.0.14
Open gfortran and pip packages

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

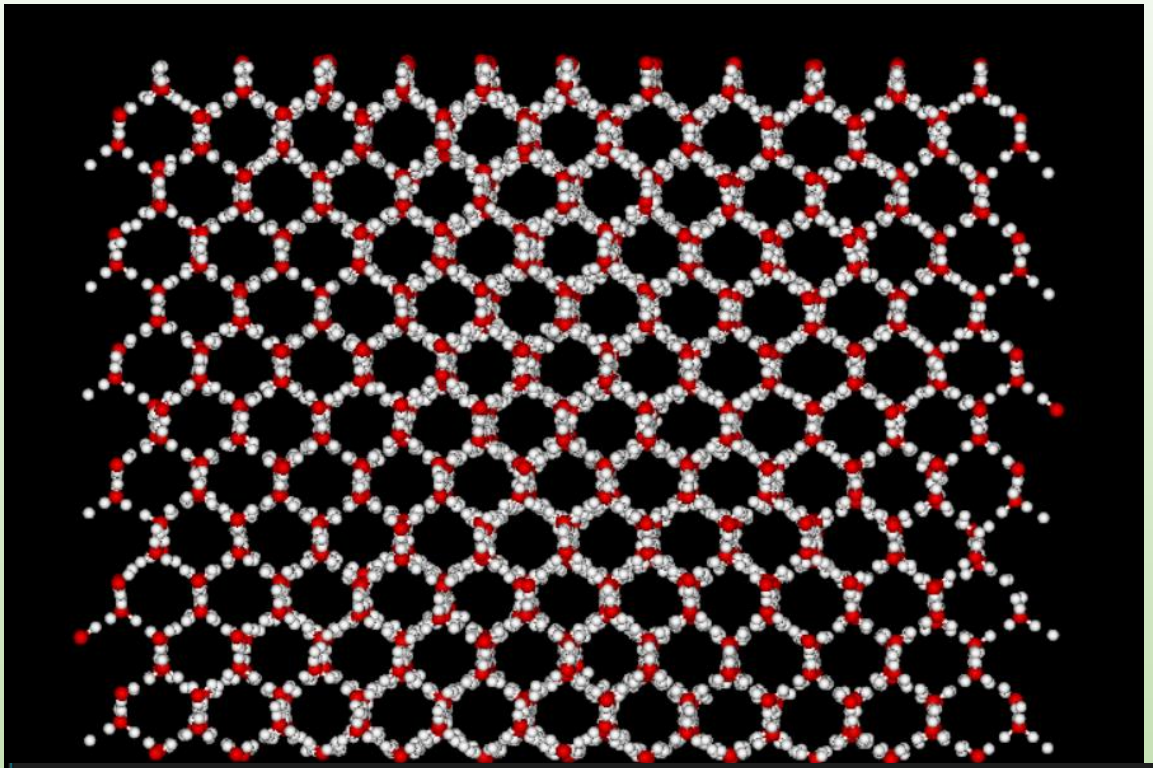
Firefox works for showing AlmaLinux and MIT sites



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



Test of @p3mtip5p07a.f03 H2O 8640 atoms



```
t=     30.0  1.7385E+00  2.0207E-01  0.0000E+00 -1.6976E+02  3.0940E+01  5.4725E
-04 -1.3688E+02    9.692D+02  1.117D-01  0.000D+00  1.006D-03  1.169D-04     8.1
82D-01   3.394D-04   8.099D-01   7.924D-03
   Final: t8, it, tmax=   30.224999999999351            1210   30.000000000000
00
 Final write(12) at t8=   30.224999999999351

 *ipar, wall_time(sec)=           1   976.62514873099997

 % 4 cpu on HP
```

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
```