

Simulation Tests for AlmaLinux Operating System

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Settings and tests for simulations

Installation of AlmaLinux-9, May 2024

Use the Windows 11, VirtualBox 7.0.14

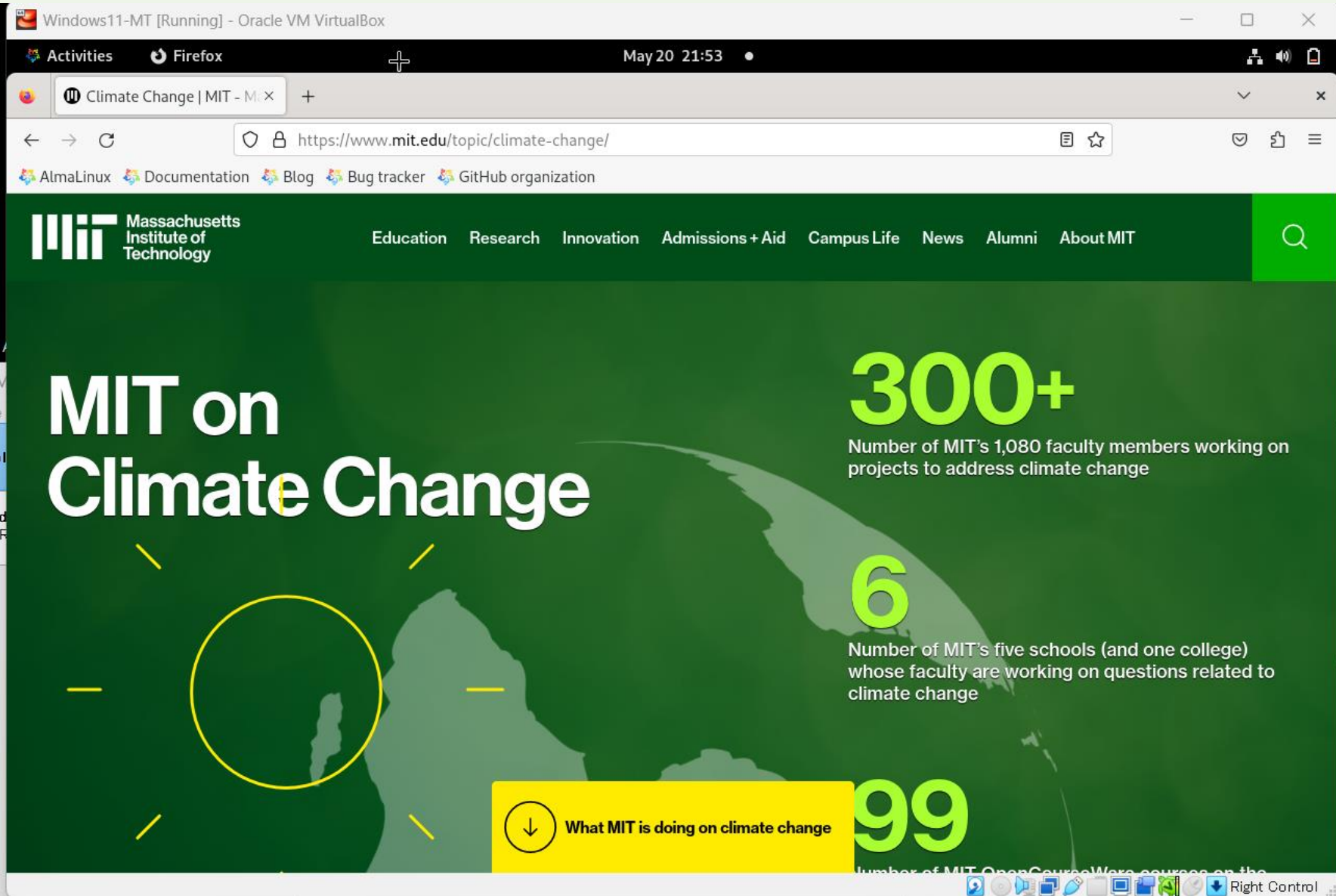
Open gfortran and pip packages

Simulations

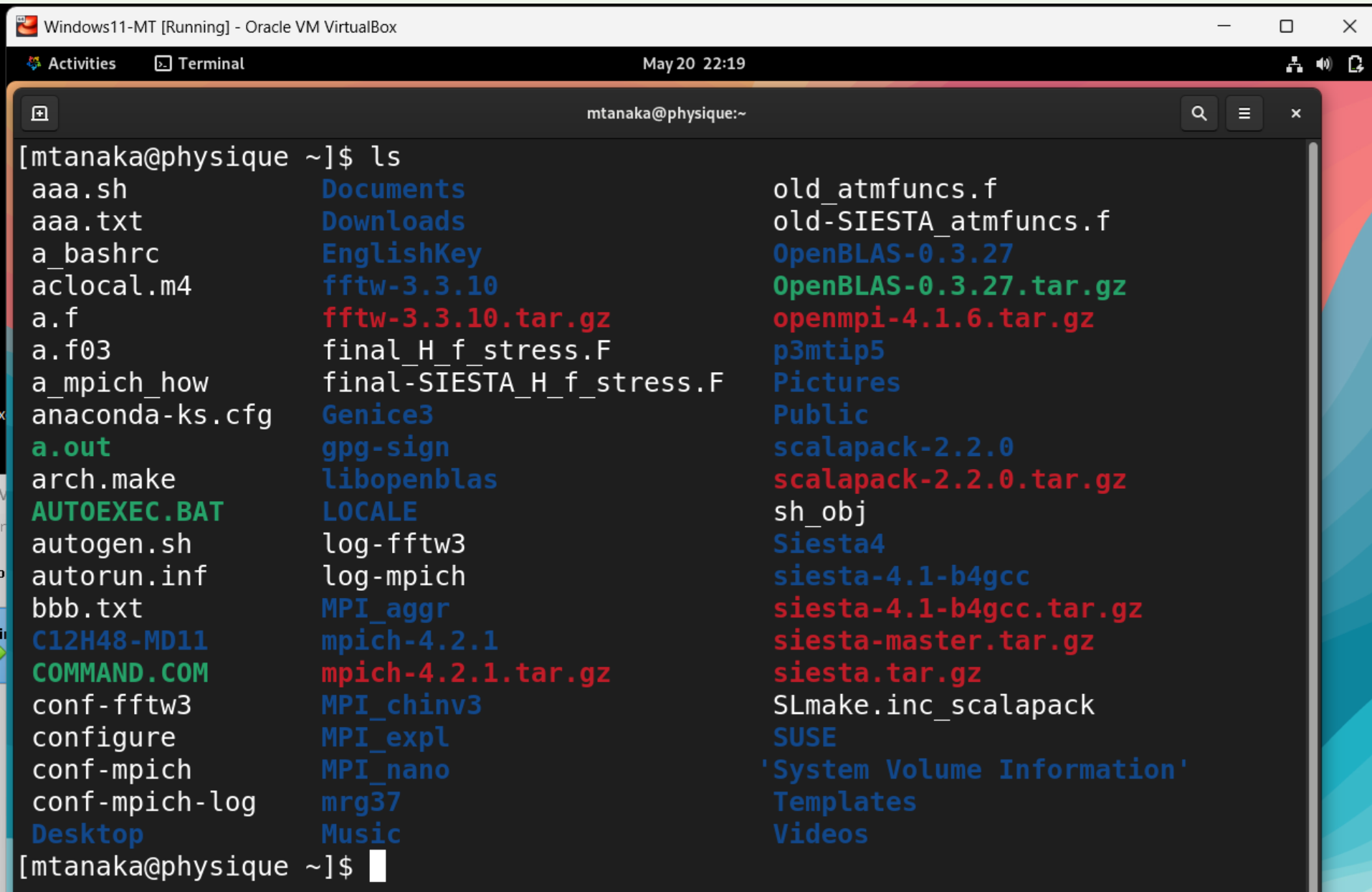
*>> Three-dimensional electrostatic p3m code,
with tip5p and Ewald sums*

*>> 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

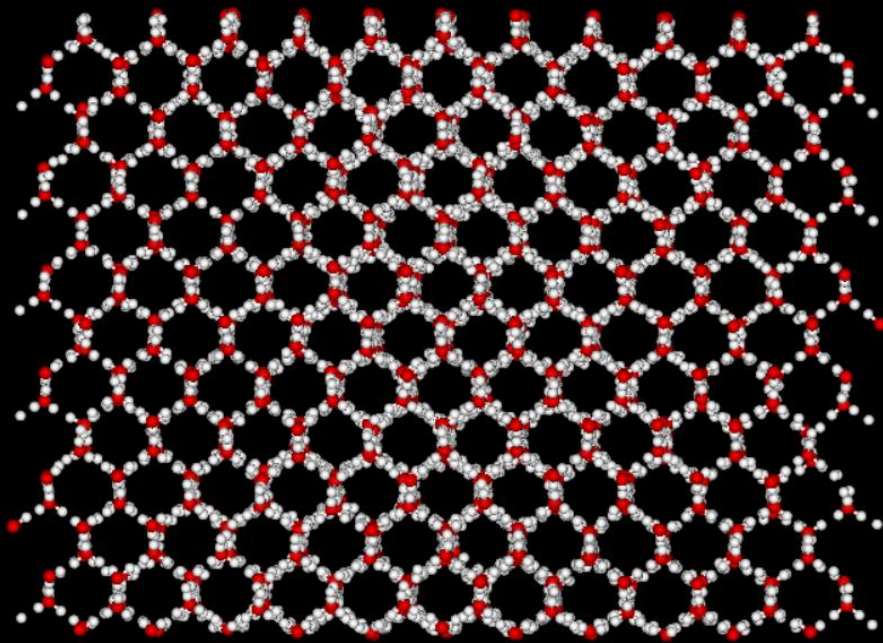


The image shows a terminal window titled "Windows11-MT [Running] - Oracle VM VirtualBox". The terminal is running a Linux environment with the user "mtanaka" at the host "physique". The command "ls" has been executed, displaying a list of files and directories in a three-column format. The files are color-coded: blue for directories, green for executables, red for archives, and cyan for scripts. The output is as follows:

```
[mtanaka@physique ~]$ ls
aaa.sh          Documents      old_atmfuncs.f
aaa.txt         Downloads     old-SIESTA_atmfuncs.f
a_bashrc        EnglishKey    OpenBLAS-0.3.27
aclocal.m4      fftw-3.3.10   OpenBLAS-0.3.27.tar.gz
a.f             fftw-3.3.10.tar.gz
a.f03           final_H_f_stress.F
a_mpich_how     final-SIESTA_H_f_stress.F
anaconda-ks.cfg Genice3       Pictures
a.out           gpg-sign      Public
arch.make       libopenblas   scalapack-2.2.0
AUTOEXEC.BAT    LOCALE        scalapack-2.2.0.tar.gz
autogen.sh      log-fftw3     sh_obj
autorun.inf     log-mpich     Siesta4
bbb.txt         MPI_aggr      siesta-4.1-b4gcc
C12H48-MD11     mpich-4.2.1   siesta-4.1-b4gcc.tar.gz
COMMAND.COM     mpich-4.2.1.tar.gz
conf-fftw3      MPI_chinv3    siesta-master.tar.gz
configure       MPI_expl      siesta.tar.gz
conf-mpich      MPI_nano      SLmake.inc_scalapack
conf-mpich-log  mrg37         SUSE
Desktop         Music          'System Volume Information'
               Templates
               Videos
```

[mtanaka@physique ~]\$

Test of @p3mtip5p07a.f03, H2O: 5-points 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

\$ pip3 install genice

Compilation goes all right for the genice software of CentOS 7. However, it goes with errors in the pairlist package and thus not in the genice software in AlmaLinux-9.

Test of Siesta-4.1b

A keyword -fallow-argument-mismatch in the arch.make file 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 -lscalapack
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
```

| | | | Jnits |
|--|--|--|------------|
| | | | ry/Bohr**3 |
| | | | eV/Ang**3 |

```
siesta:          42.98698303          45.67350218 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
```