

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

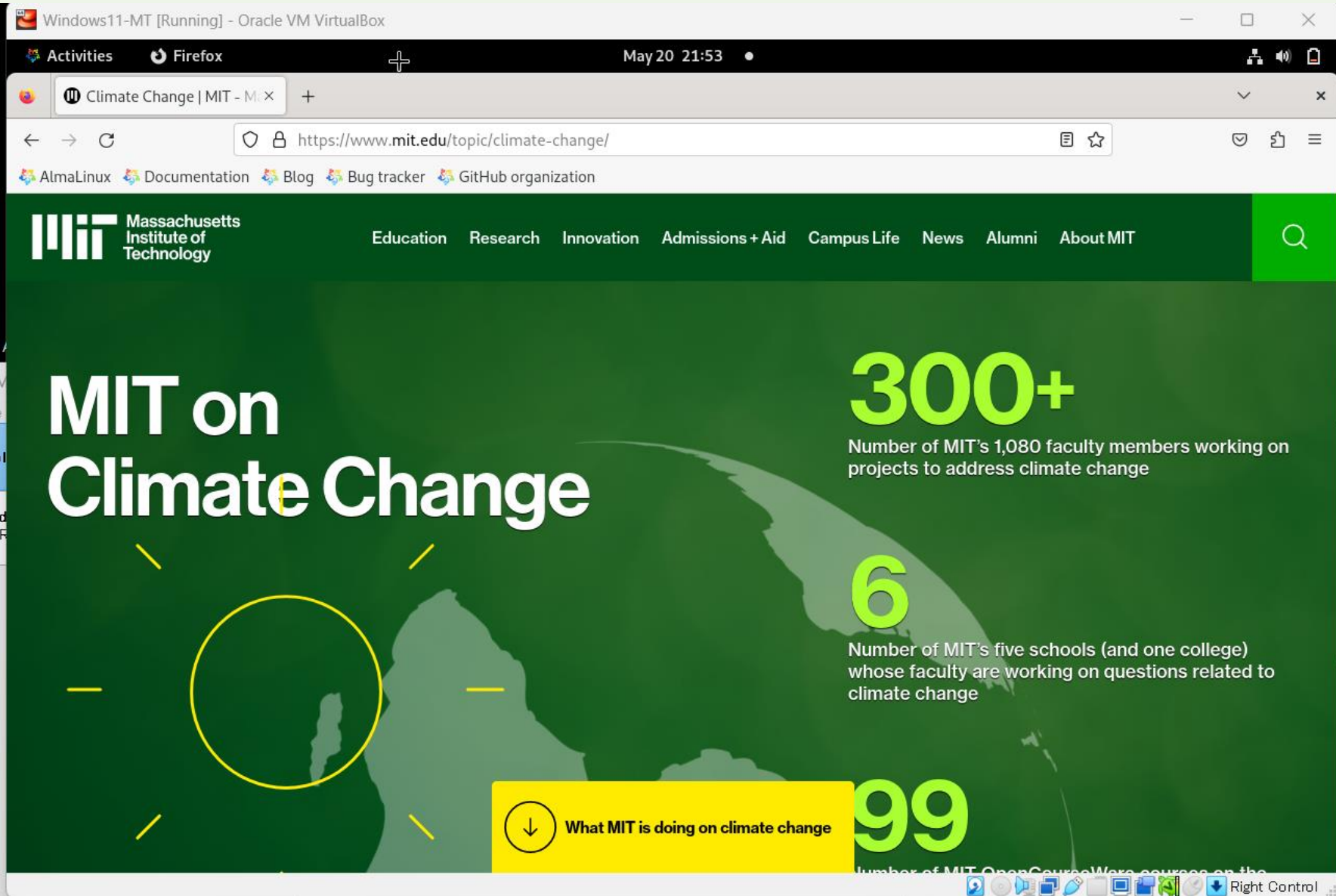
Open gfortran and pip packages

Simulations

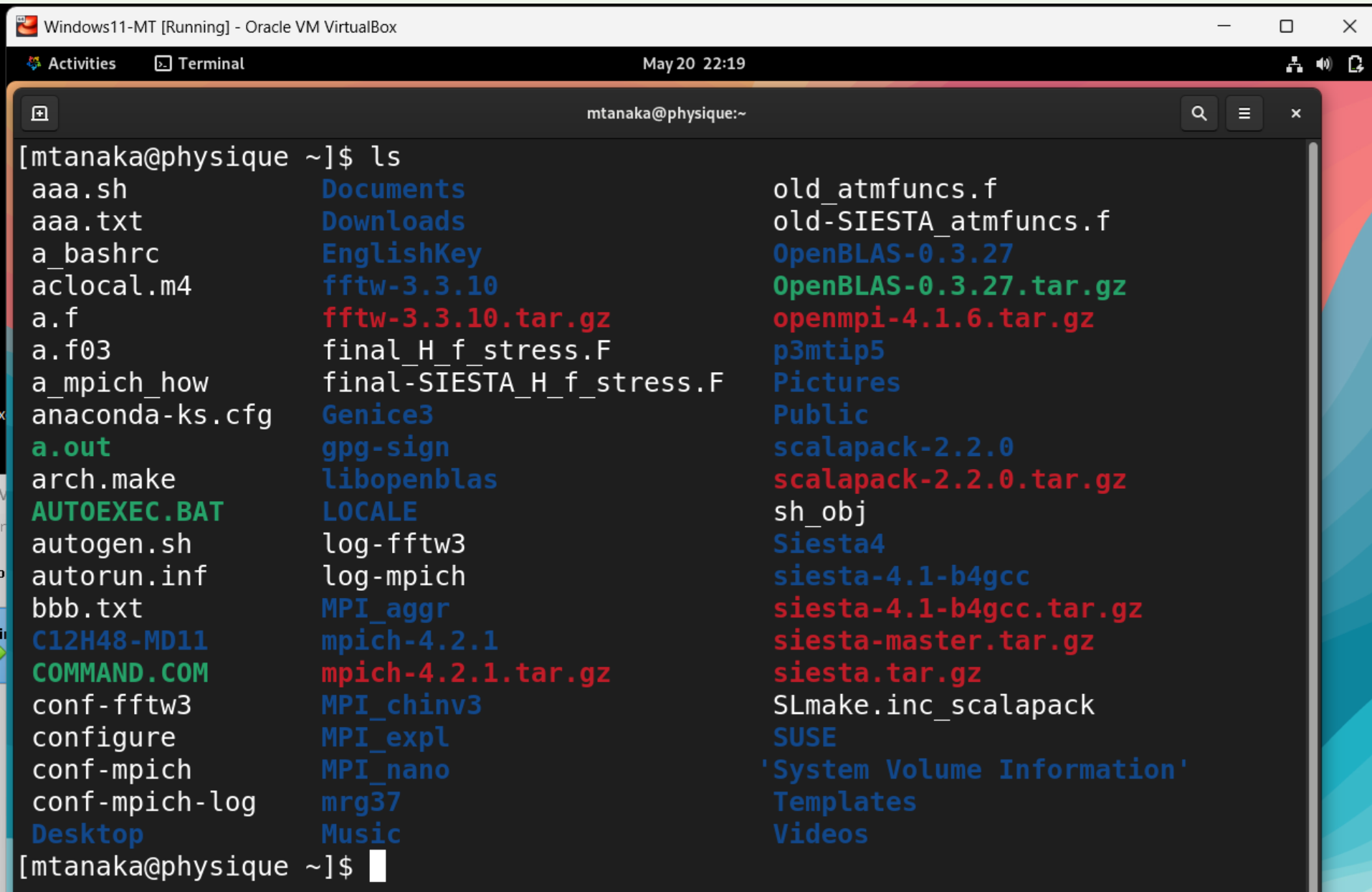
*>> three-dimensional ES p3m code, with tip5,
Ewald sum*

*>> 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

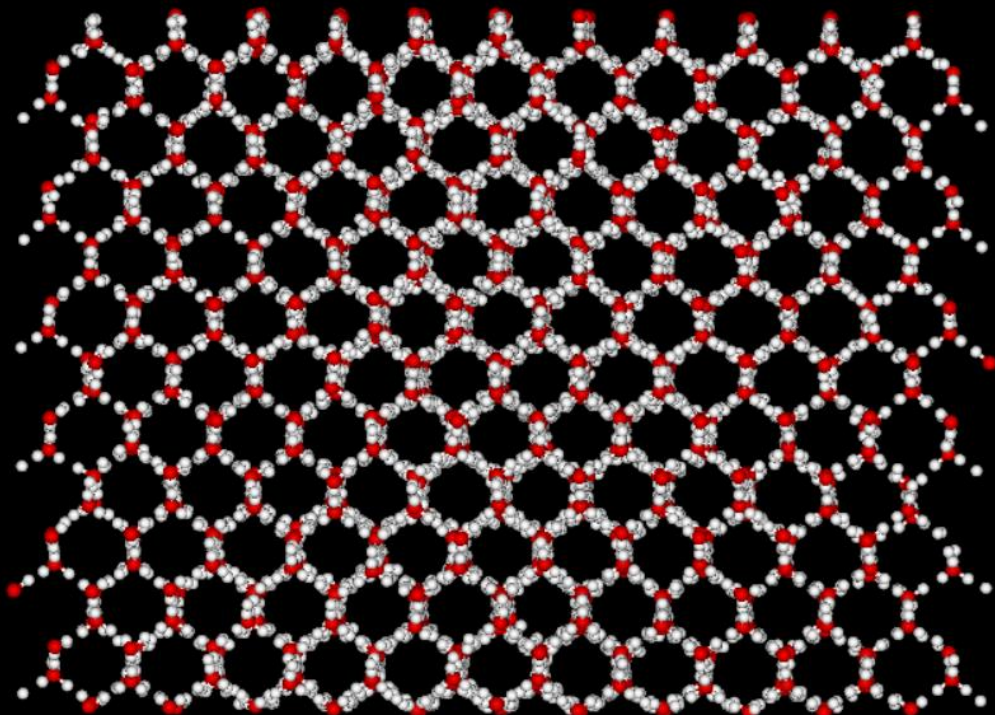


The image shows a terminal window titled "Windows11-MT [Running] - Oracle VM VirtualBox". The terminal is running a Linux environment with the prompt "mtanaka@physique:~". The user has entered the command "ls", and the output is displayed in three columns. The files and directories are listed in alphabetical order. 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
```

The terminal window also shows the prompt "[mtanaka@physique ~]" and a cursor at the end of the line.

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 30.00000000000000
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 -lscalapack
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
ar
```

```
reinit: Reading from c12h48.fdf
```

```
(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
```