

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

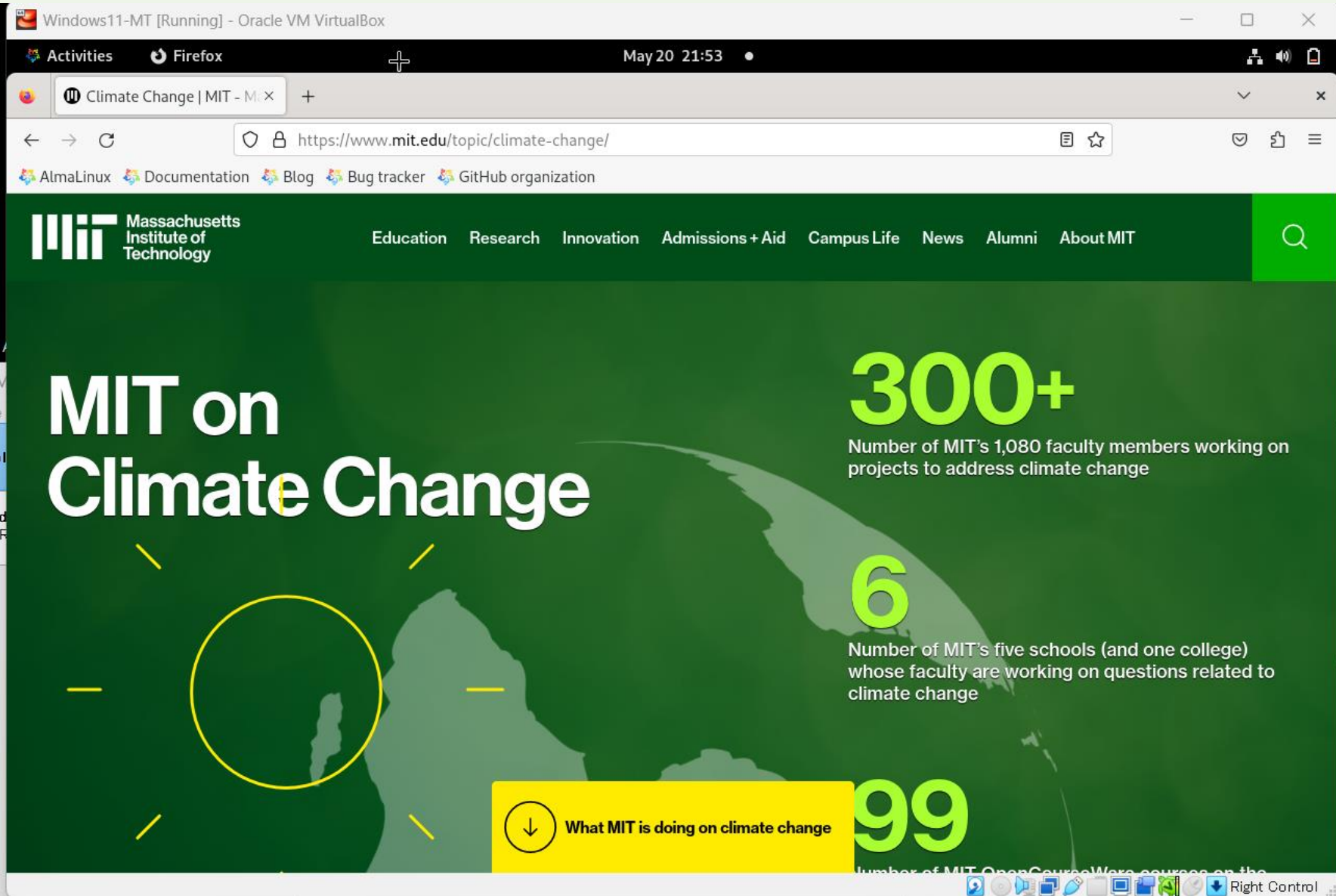
Open gfortran and pip packages

Simulations

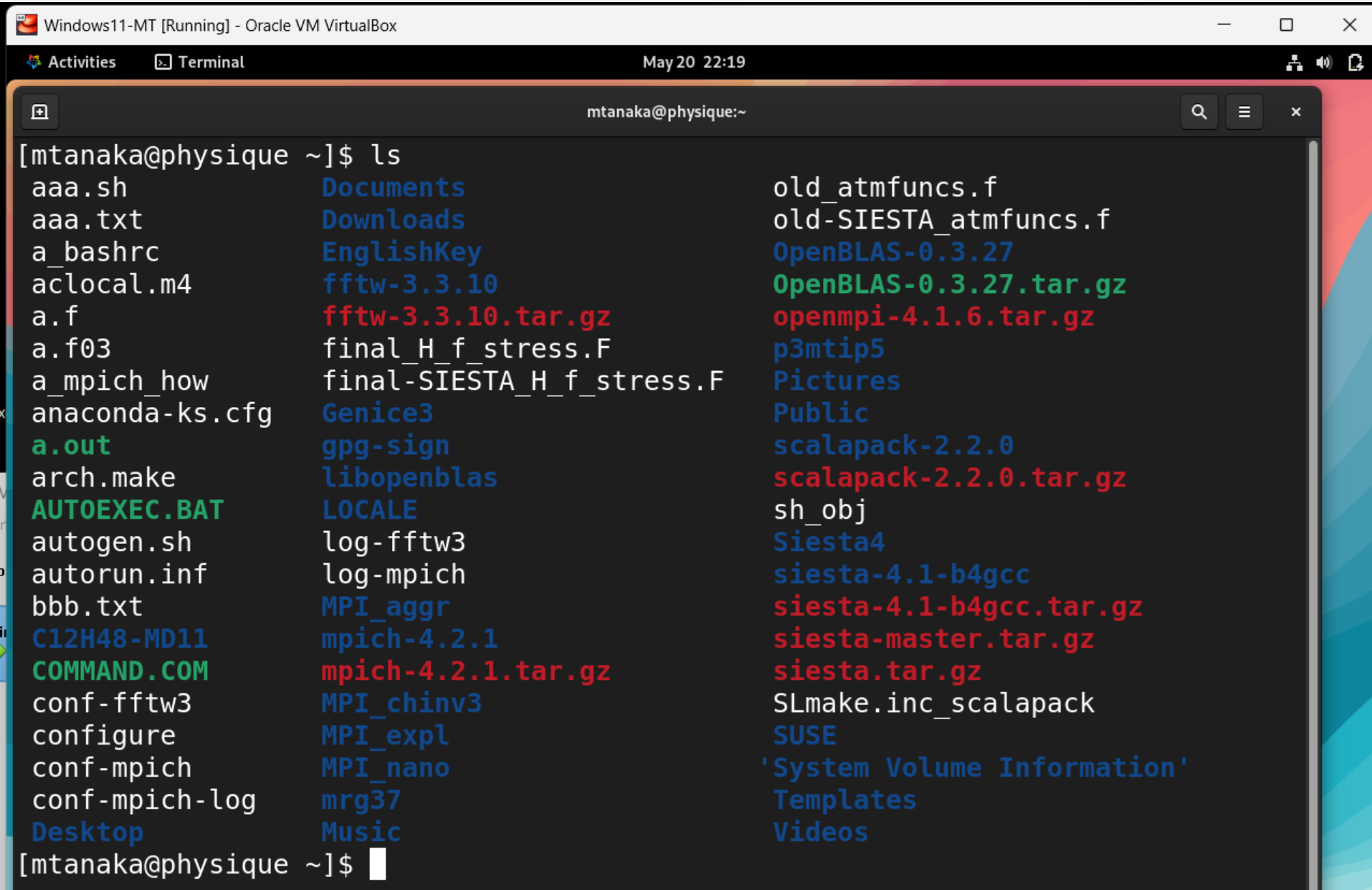
*>> three-dimensional ES p3m code, with tip5,
Ewald sum*

*>> Siesta-4.1b, with mpich, fft3w, OpenBLAS,
Scalapack*

Firefox works for showing AlmaLinux and MIT sites



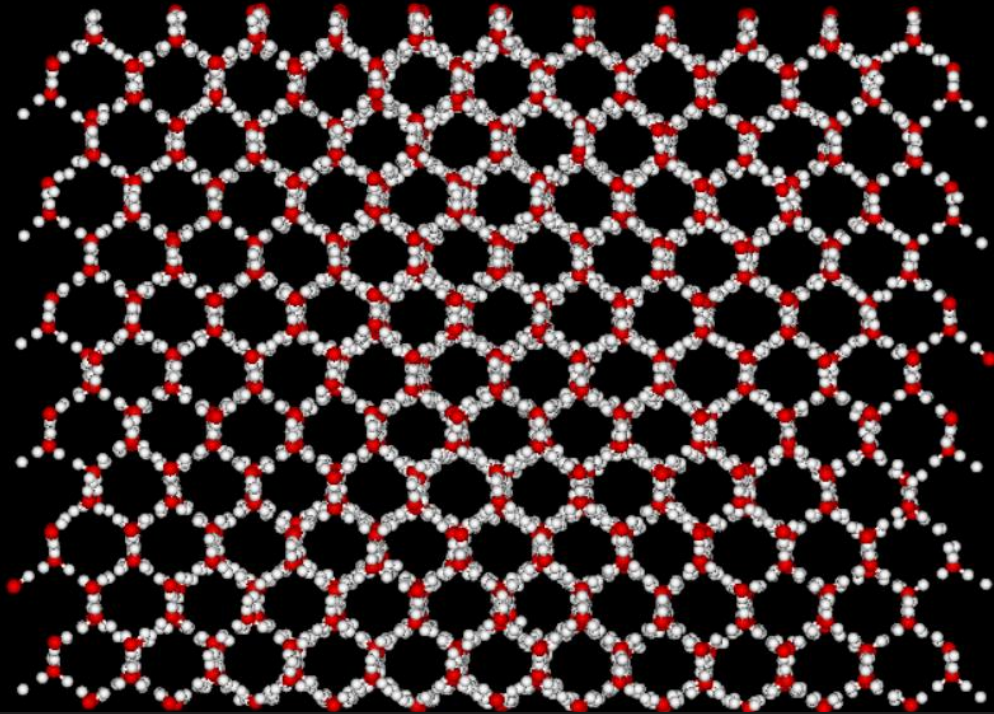
Terminal showing mpich-4, fftw-3 and Siesta-4.1



The image shows a terminal window titled "Windows11-MT [Running] - Oracle VM VirtualBox". The terminal is running a Linux environment with the user "mtanaka@physique". The command "ls" has been executed, displaying a list of files and directories in a three-column format. The files include various scripts, configuration files, and source code for FFTW, MPI, and SIESTA. The directories include standard Linux user directories like Documents, Downloads, and Desktop, as well as project-specific directories like Siesta4 and Videos.

```
Windows11-MT [Running] - Oracle VM VirtualBox
May 20 22:19
mtanaka@physique:~
[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     openmpi-4.1.6.tar.gz
a.f03                 final_H_f_stress.F     p3mtip5
a_mpich_how           final-SIESTA_H_f_stress.F Pictures
anaconda-ks.cfg       Genice3                Public
a.out                 gpg-sign               scalapack-2.2.0
arch.make             libopenblas            scalapack-2.2.0.tar.gz
AUTOEXEC.BAT          LOCALE                 sh_obj
autogen.sh            log-fftw3              Siesta4
autorun.inf           log-mpich              siesta-4.1-b4gcc
bbb.txt               MPI_aggr               siesta-4.1-b4gcc.tar.gz
C12H48-MD11           mpich-4.2.1            siesta-master.tar.gz
COMMAND.COM           mpich-4.2.1.tar.gz     siesta.tar.gz
conf-fftw3            MPI_chinv3             SLmake.inc_scalapack
configure             MPI_expl               SUSE
conf-mpich            MPI_nano               'System Volume Information'
conf-mpich-log        mrg37                  Templates
Desktop              Music                   Videos
[mtanaka@physique ~]$
```

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 30.000000000000000
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 *
*****

reinit: Reading from c12h48.fdf

its
//Bohr**3
//Ang**3
κBar
42.98098303 43.0130218
(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
```