

Simulation Tests of AlmaLinux-9 Operating System

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May 27, 2024

Settings and tests of simulations

Install the linux, AlmaLinux-9, Mar. 2024

Use the Windows 11, VirtualBox 7.0.14

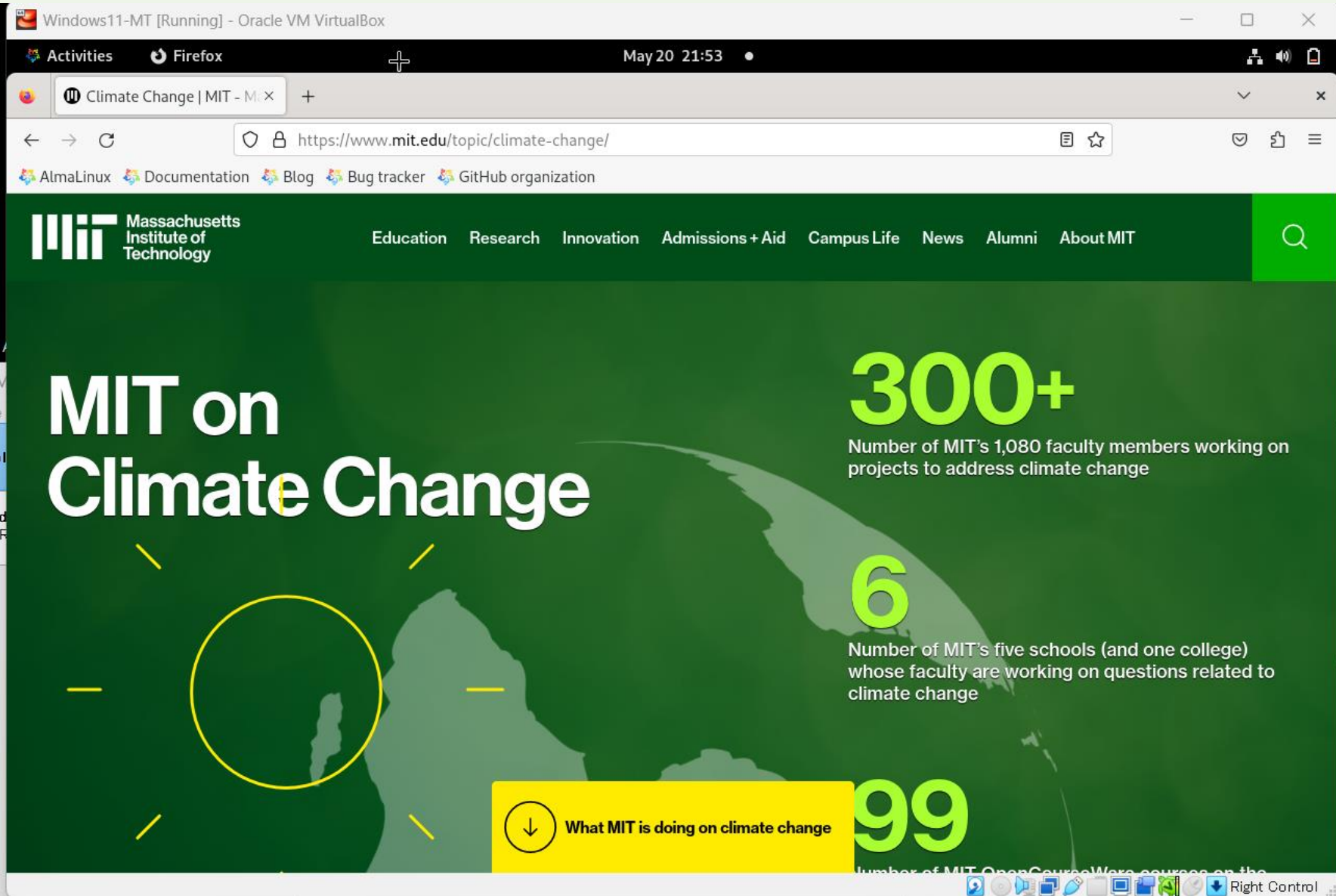
Open gfortran and pip packages

Simulations

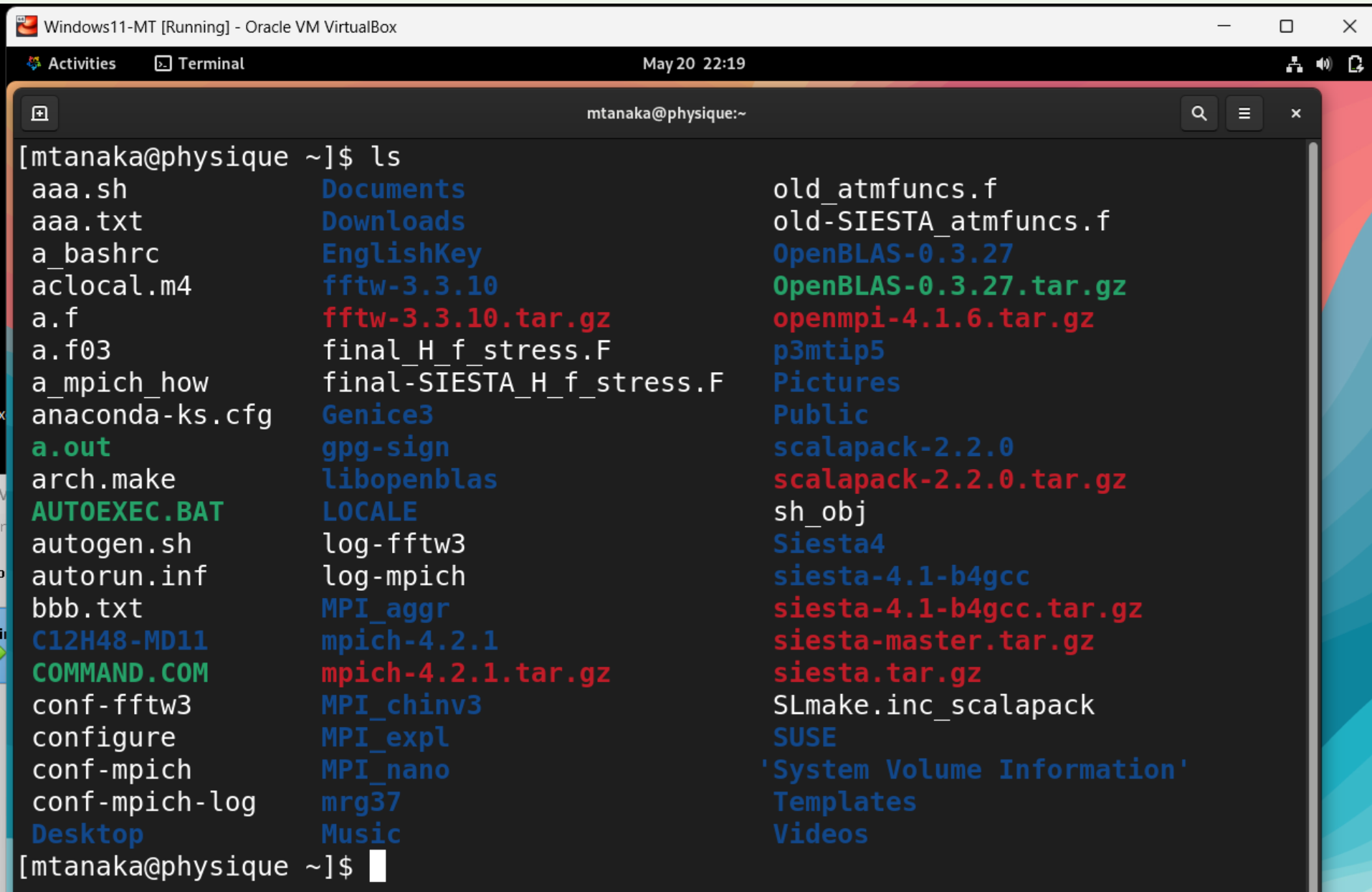
*>> three-dimensional ES p3m code, with tip5,
Ewald sum*

*>> 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



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 three columns. The files include scripts, source code, configuration files, and archives for various software packages like fftw, mpich, and siesta. The terminal window has a dark theme and standard window controls.

```
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
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     siesta-master.tar.gz
conf-fftw3           MPI_chinv3             siesta.tar.gz
configure            MPI_expl               SLmake.inc_scalapack
conf-mpich           MPI_nano               SUSE
conf-mpich-log       mrg37                  'System Volume Information'
Desktop             Music                   Templates
[mtanaka@physique ~]$
```

Test of Siesta-4.1b on AlmaLinux-9

```
Siesta Version   : v4.1-b4
Architecture     : gfortran-MPI
Compiler version: GNU Fortran (GCC) 11.4.1 20231218 (Red Hat 11.4.1-3)
Compiler flags   : mpifort -O2 -fPIC -ftree-vectorize -march=native -fallow-argument-mismatch
PP flags         : -DMPI -DFC_HAVE_ABORT
Libraries        : -lgomp -L/opt/openblas/lib -lopenblas -L/opt/scalapack/lib -lscalapack
PARALLEL version

* Running on 6 nodes in parallel
>> Start of run: 19-MAY-2024 9:47:54

*****
*   WELCOME TO SIESTA   *
*****
```

In the arch.make, the keyword -fallow-argument-mismatch is added of AlmaLinux-9 to avoid non-necessary errors.