

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

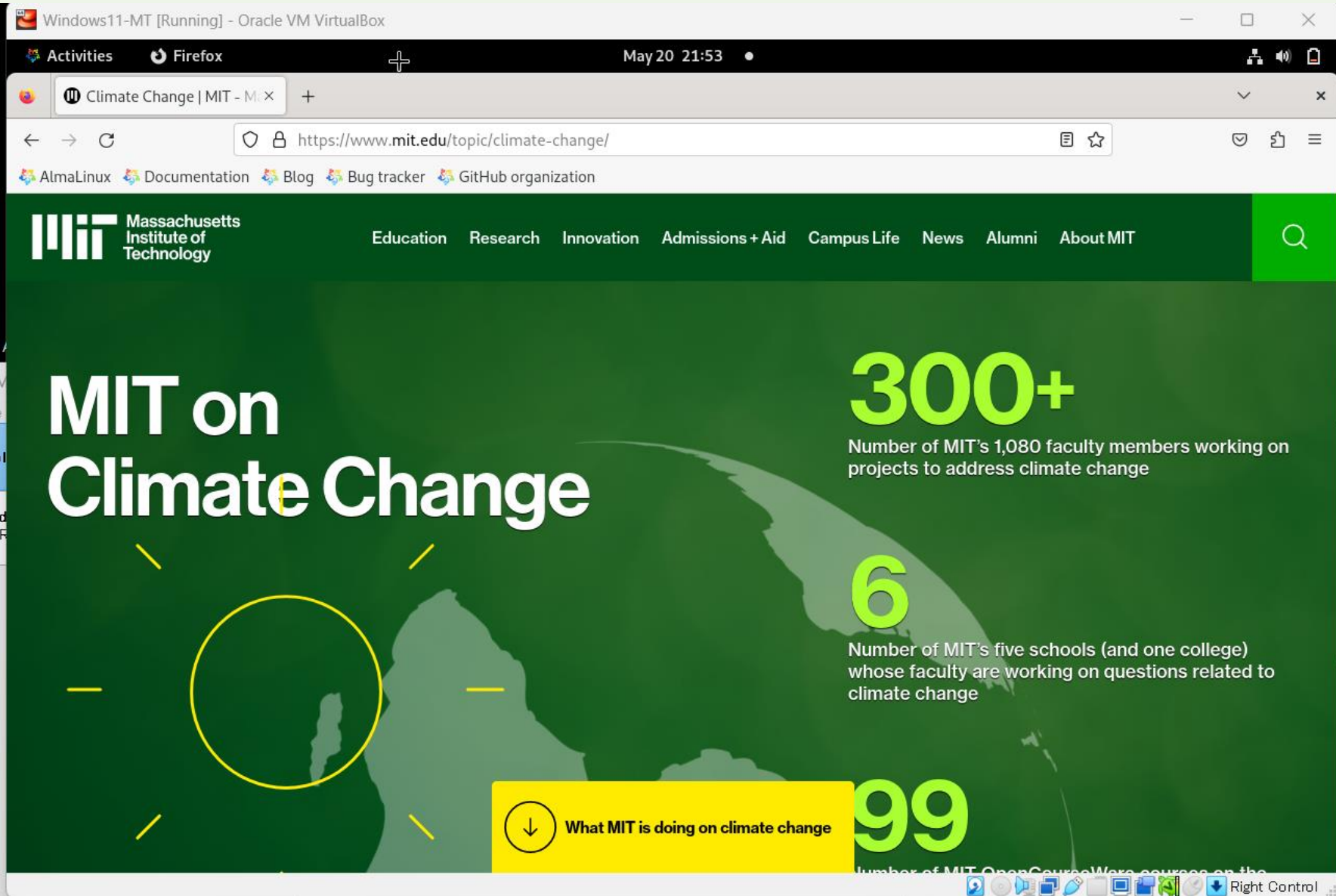
Open gfortran and pip packages

Simulations

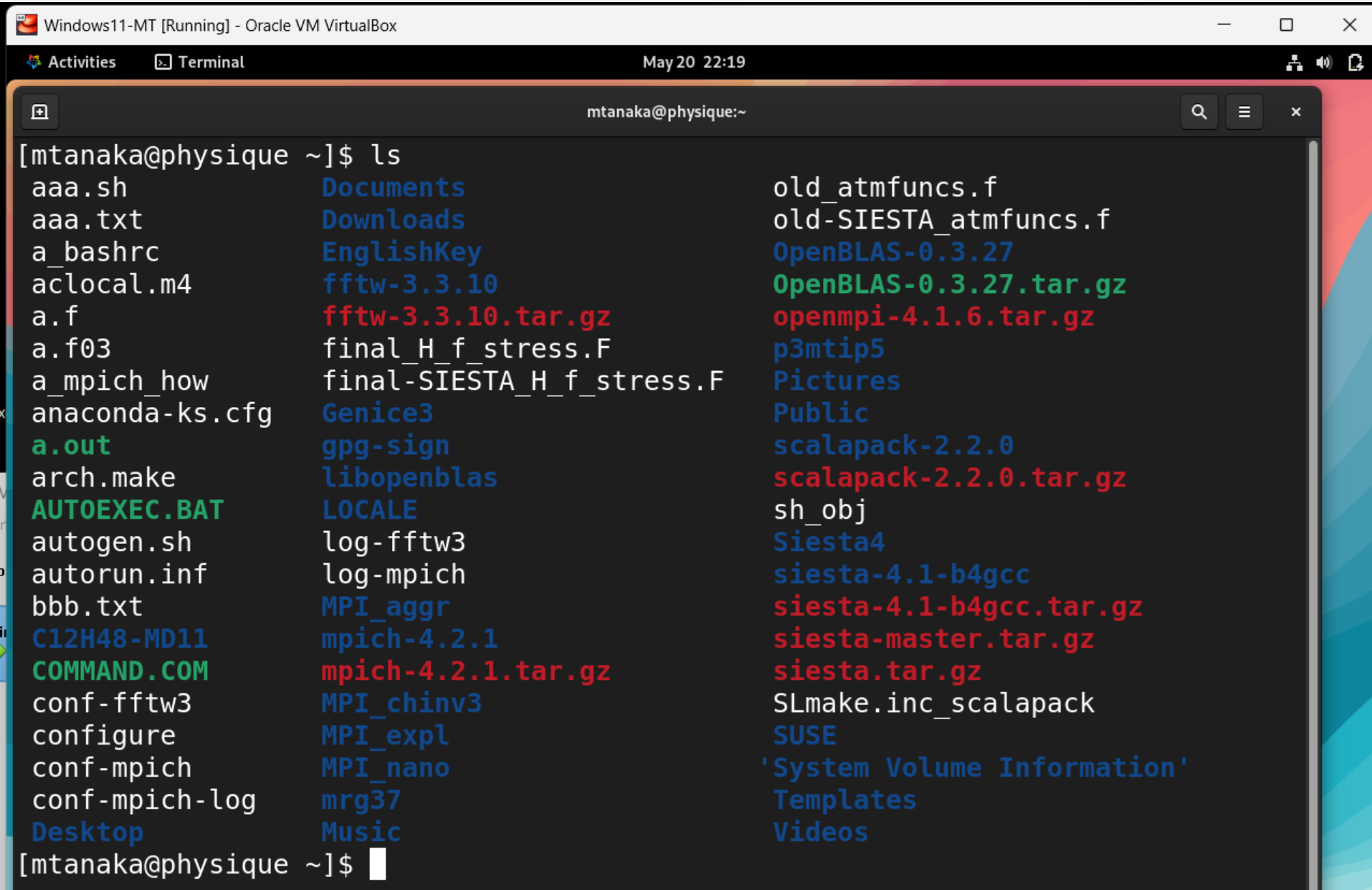
*>> three-dimensional ES p3m code, with tip5,
Ewald sum*

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

Firefox works for showing AlmaLinux and MIT sites



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



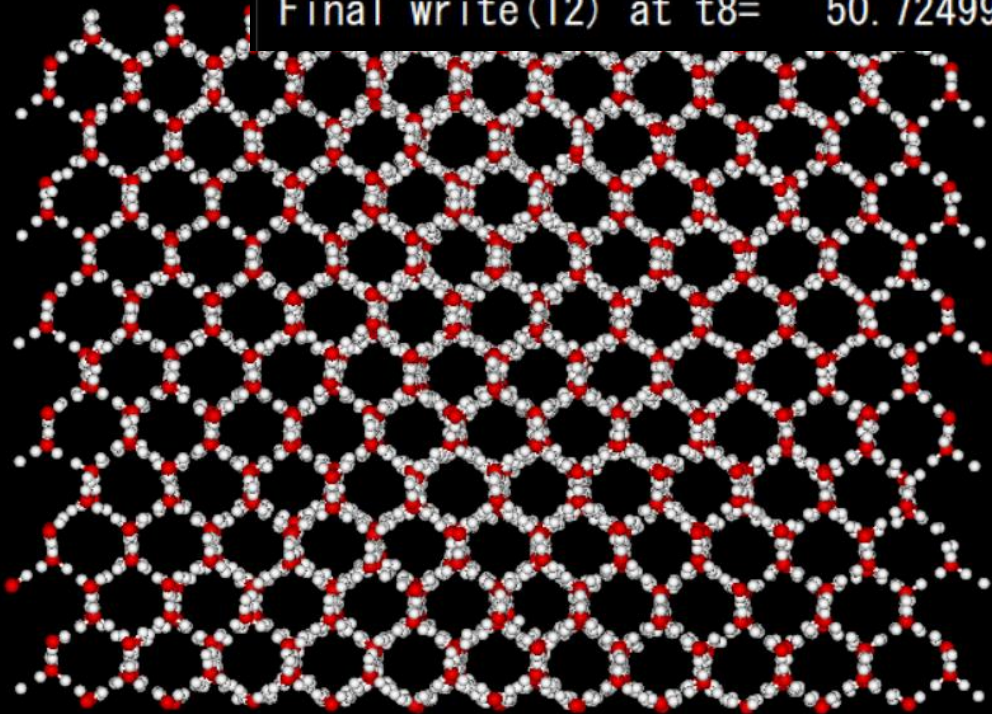
The image shows a terminal window titled "Windows11-MT [Running] - Oracle VM VirtualBox". The terminal is running a Linux environment with the user "mtanaka@physique". The command "ls" has been executed, displaying a list of files and directories in a three-column format. The files include shell scripts, text files, configuration files, and various software packages and their source archives. 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     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
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, 6 cpu/3 GHz

```
t= 30.0 1.5047E+00 1.8313E-01 0.0000E+00 -1.7020E+02 3.0737E+01
5.1659E-04 -1.3778E+02 4.282D+02 1.024D-01 0.000D+00 8.708D-04
1.060D-04 3.571D-01 2.404D-04 3.511D-01 5.815D-03
t= 40.0 1.4686E+00 1.9438E-01 0.0000E+00 -1.7059E+02 3.1085E+01
5.1197E-04 -1.3784E+02 5.707D+02 9.719D-02 0.000D+00 8.499D-04
1.125D-04 3.556D-01 2.392D-04 3.495D-01 5.795D-03
t= 50.0 1.5077E+00 2.0854E-01 0.0000E+00 -1.7075E+02 3.1106E+01
4.9661E-04 -1.3793E+02 7.130D+02 9.940D-02 0.000D+00 8.725D-04
1.207D-04 3.551D-01 2.391D-04 3.493D-01 5.572D-03
Final: t8, it, tmax= 50.72499999998190 2030 50.5000
000000000000
Final write(12) at t8= 50.72499999998190
```



Test of Siesta-4.1b on AlmaLinux-9

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
```