

# *Simulation Tests of AlmaLinux-9 Operating System*

*Motohiko Tanaka, PhD, Japan*

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# *Settings and tests of simulations*

*Install the linux, AlmaLinux-9, Mar. 2024*

*Use the Windows 11, VirtualBox 7.0.14*

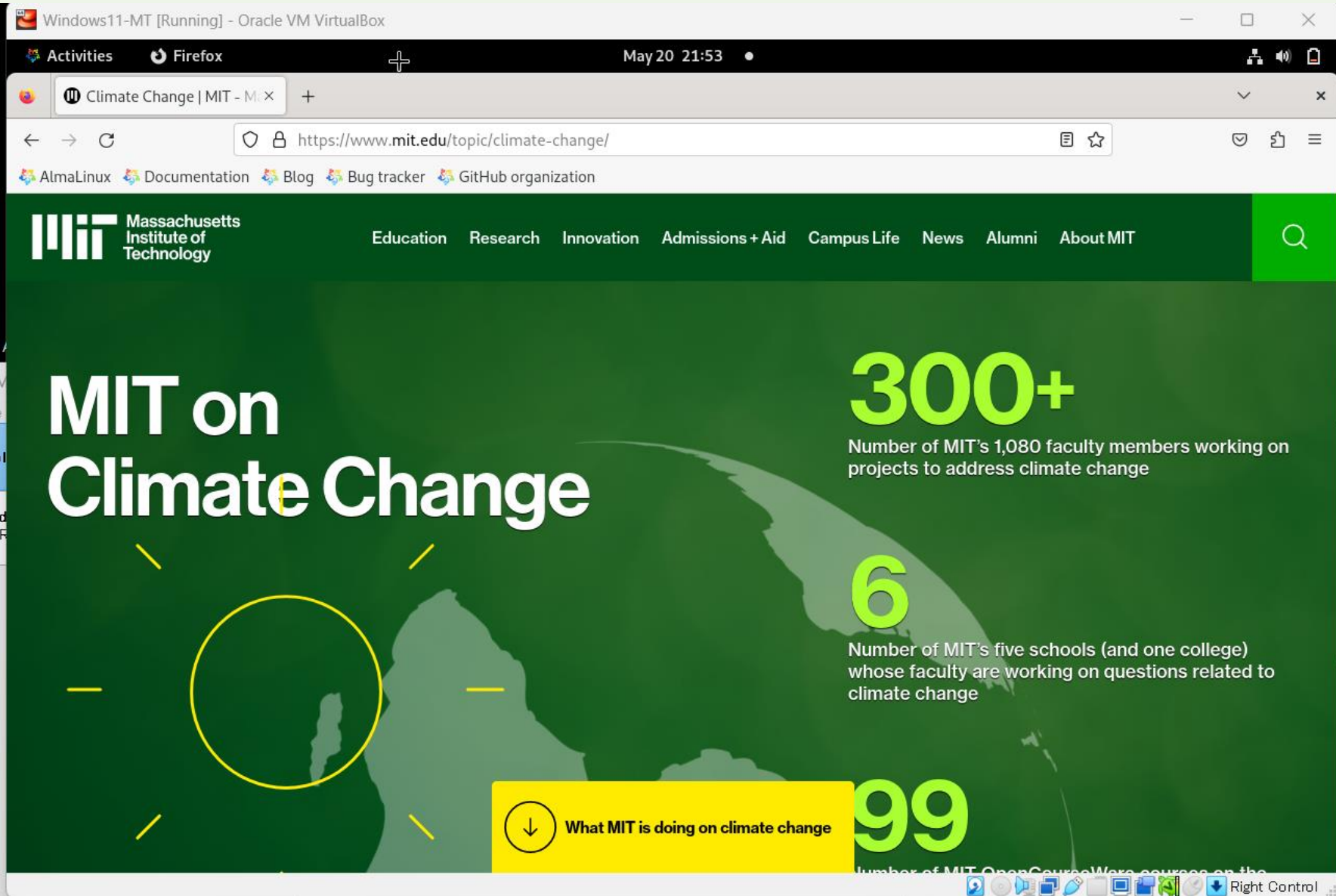
*Open gfortran and pip packages*

## *Simulations*

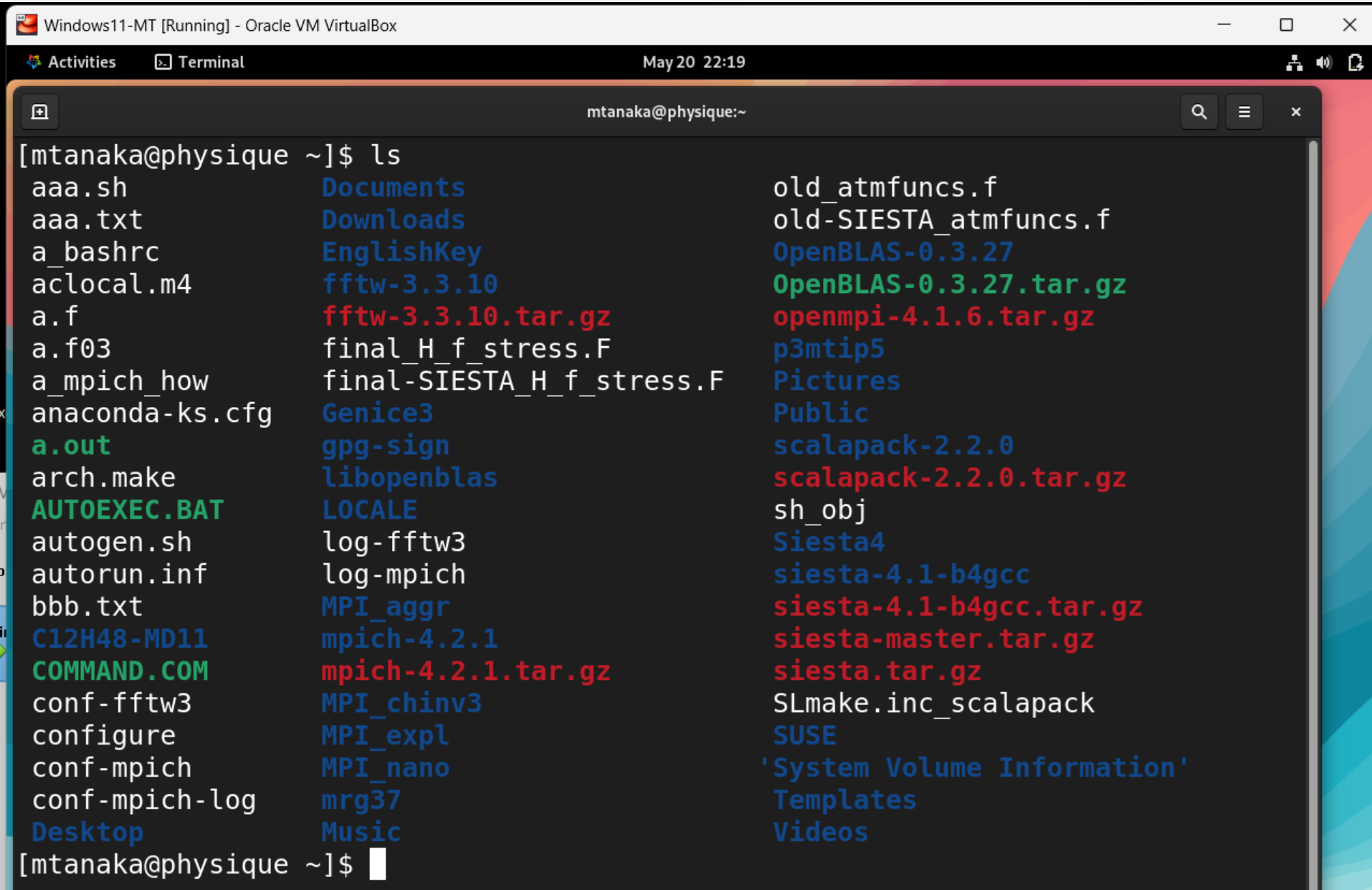
*>> three-dimensional ES p3m code, with tip5,  
Ewald sum*

*>> 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

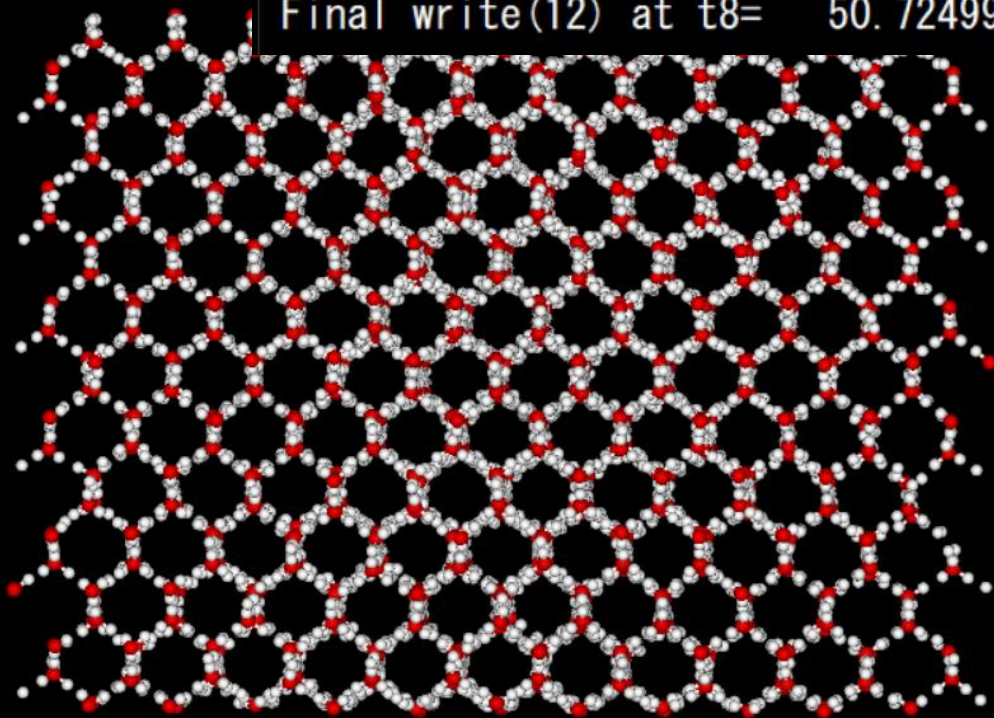


The image shows a terminal window titled "Windows11-MT [Running] - Oracle VM VirtualBox". The terminal is running a Linux environment with the user "mtanaka@physique". The command "ls" has been executed, displaying a list of files and directories in three columns. The files include configuration files, source code, and installation packages for various software like fftw, mpich, and siesta.

```
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, 6 cpu*

```
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= 50.724999999998190 2030 50.5000
000000000000
      Final write(12) at t8= 50.724999999998190
```





# 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
```