

# *Simulation Tests for AlmaLinux Operating System*

*Motohiko Tanaka, PhD, Japan*

*June 1, 2024*

# *Settings and tests for simulations*

*Installation of AlmaLinux-9, May 2024*

*Use the Windows 11, VirtualBox 7.0.14*

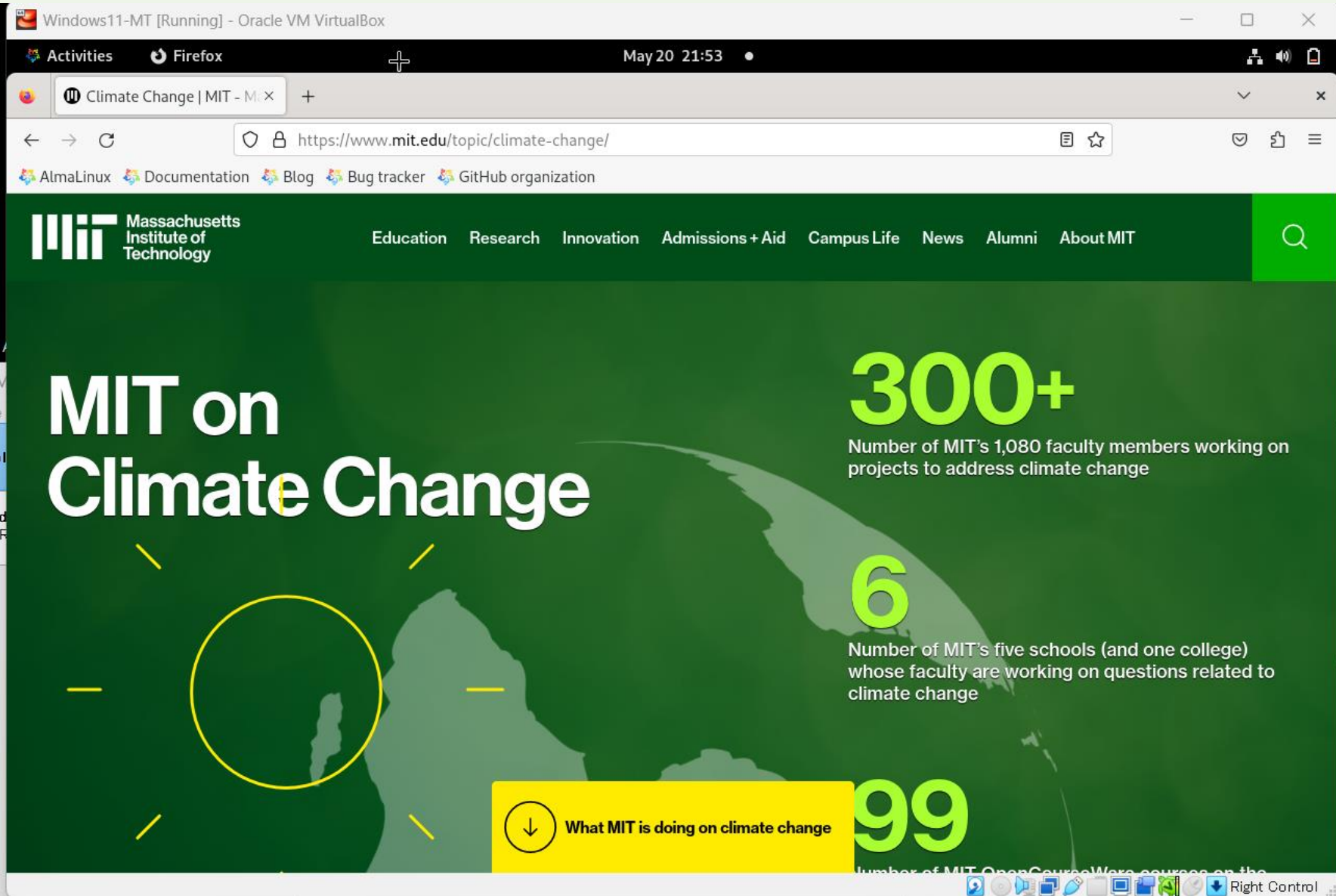
*Open gfortran and pip packages*

## *Simulations*

*>> Three-dimensional electrostatic p3m code,  
with tip5p and Ewald sums*

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

# Firefox works with AlmaLinux and MIT sites



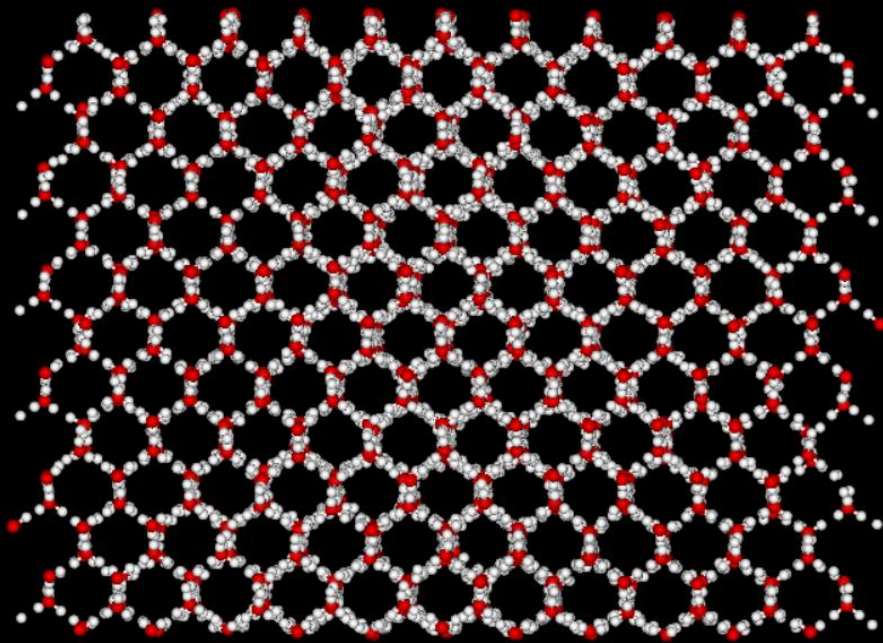
*Terminal showing mpich-4, fftw-3 and Siesta-4.1*

```

[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
[mtanaka@physique ~]$

```

# Test of @p3mtip5p07a.f03, H2O: 5-points with 8640 atoms



*This simulation run is OK, but timing is highly variable in time because the simulation in VirtualBox competes with many tasks of Windows 11. The cpu2 which should be 0.6 sec at least is different with the time steps.*

time:	e_kin.W	e_img.W	e_kin(M)	e_c_r	e_lj	e_p3m	
e_tot	walltm	vm	exc	<ekin>	<eimg>	cpu	
0	cpu1	cpu2	cpu3				
t=	20.0	1.7095E+00	1.9537E-01	0.0000E+00	-1.6974E+02	3.0997E+01	5.1888E
-04	-1.3684E+02	8.656D+02	1.353D-01	0.000D+00	9.893D-04	1.131D-04	1.1
15D+00	4.028D-04	1.106D+00	8.584D-03				
t=	25.0	1.7269E+00	1.9599E-01	0.0000E+00	-1.6972E+02	3.0949E+01	5.3564E
-04	-1.3685E+02	1.076D+03	1.095D-01	0.000D+00	9.993D-04	1.134D-04	1.7
43D+00	3.641D-04	1.734D+00	8.680D-03				
t=	30.0	1.7385E+00	2.0207E-01	0.0000E+00	-1.6976E+02	3.0940E+01	5.4725E
-04	-1.3688E+02	1.295D+03	1.117D-01	0.000D+00	1.006D-03	1.169D-04	5.6
95D-01	3.855D-04	5.607D-01	8.385D-03				

## *Related pip3 packages*

\$ pip3 install genice

*Compilation goes all right for the genice software of CentOS 7. However, it goes with errors in the pairlist package and thus not in the genice software in AlmaLinux-9.*

# Test of Siesta-4.1b

*A keyword -fallow-argument-mismatch in the arch.make file is added for AlmaLinux-9 to avoid non-necessary errors.*

```
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: 2-JUN-2024 10:09:19
```

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

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

```
siesta: 42.98698226 45.67350102 kBar
(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
>> Start of run: 2-JUN-2024 10:09:19
>> End of run: 2-JUN-2024 10:11:55
Job completed
```

```
r**3
**3
```