

Simulation Tests of AlmaLinux-9 Operating System

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Settings and tests of simulations

Installation of AlmaLinux-9, March 2024

Use the Windows 11, VirtualBox 7.0.14

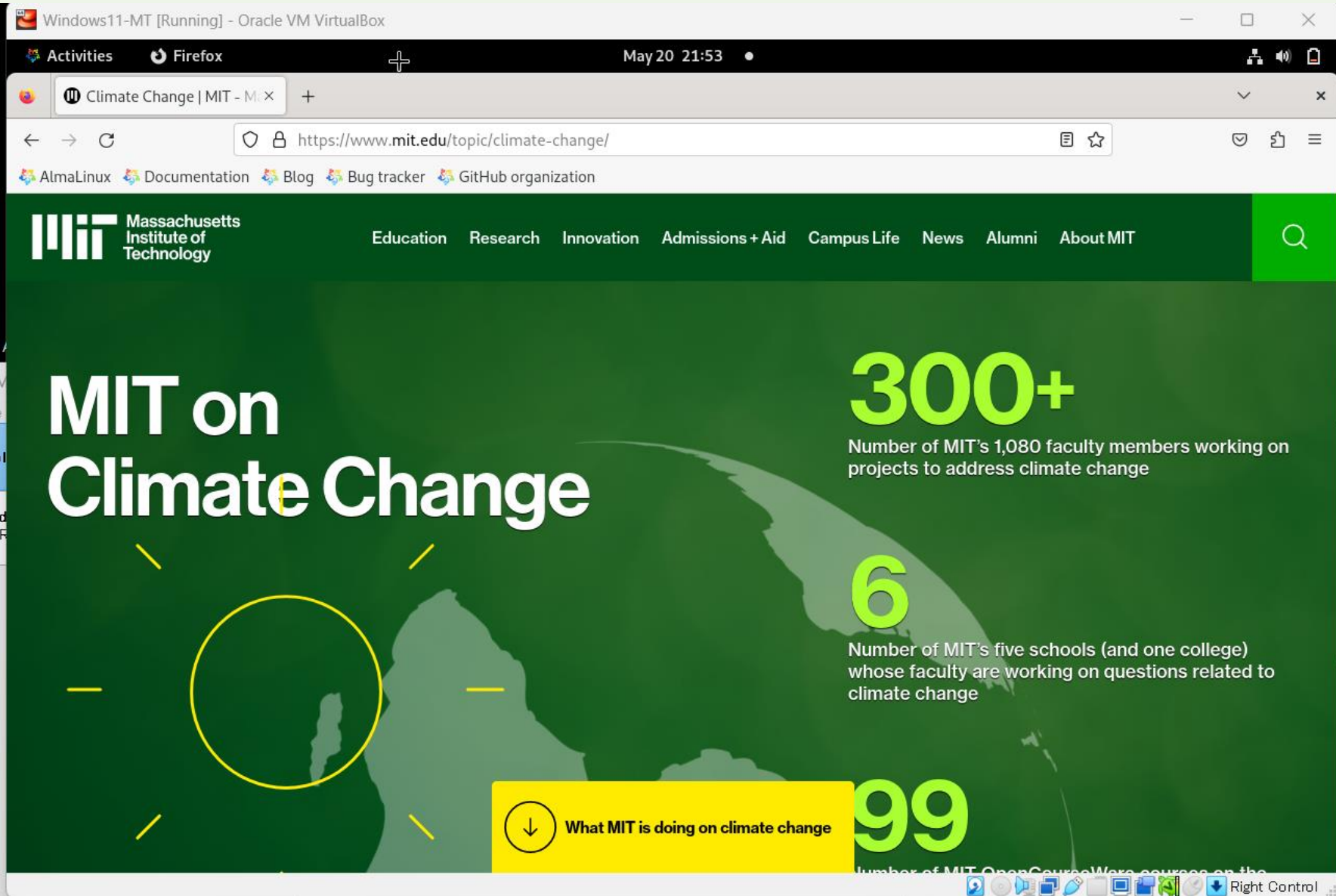
Open gfortran and pip packages

Simulations

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

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

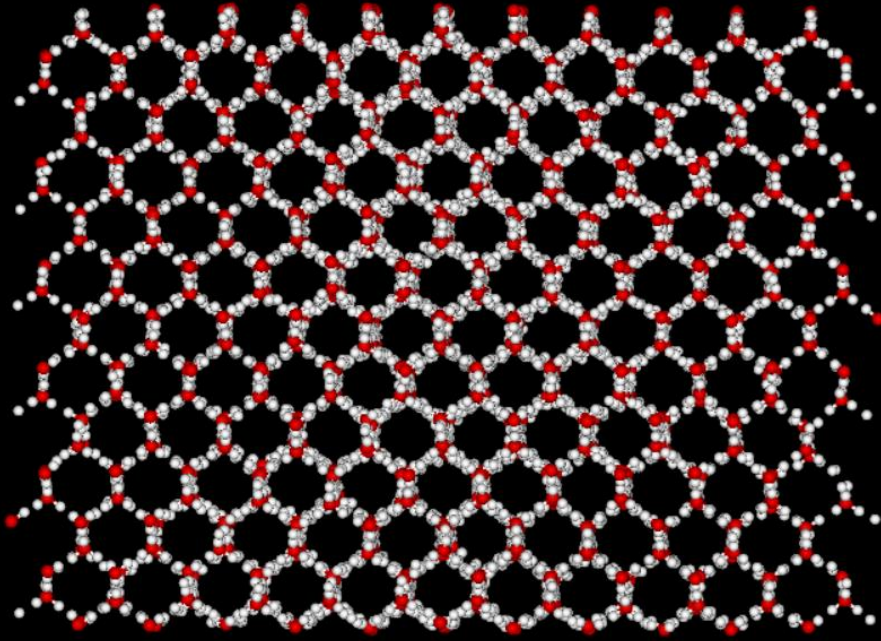
Firefox works with AlmaLinux and MIT sites



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

```
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
a.f03           final_H_f_stress.F
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
conf-fftw3      MPI_chinv3    siesta-master.tar.gz
configure       MPI_expl      siesta.tar.gz
conf-mpich      MPI_nano      SLmake.inc_scalapack
conf-mpich-log  mrg37         SUSE
Desktop         Music         'System Volume Information'
               Templates
               Videos
[mtanaka@physique ~]$
```

Test of @p3mtip5p07a.f03 H2O: 5-points, 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 is very different in 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				

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
```