

Simulations of Molecular Dynamics by AlmaLinux v.s. Debian-12 OS

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<https://github.com/Mtanaka77/>

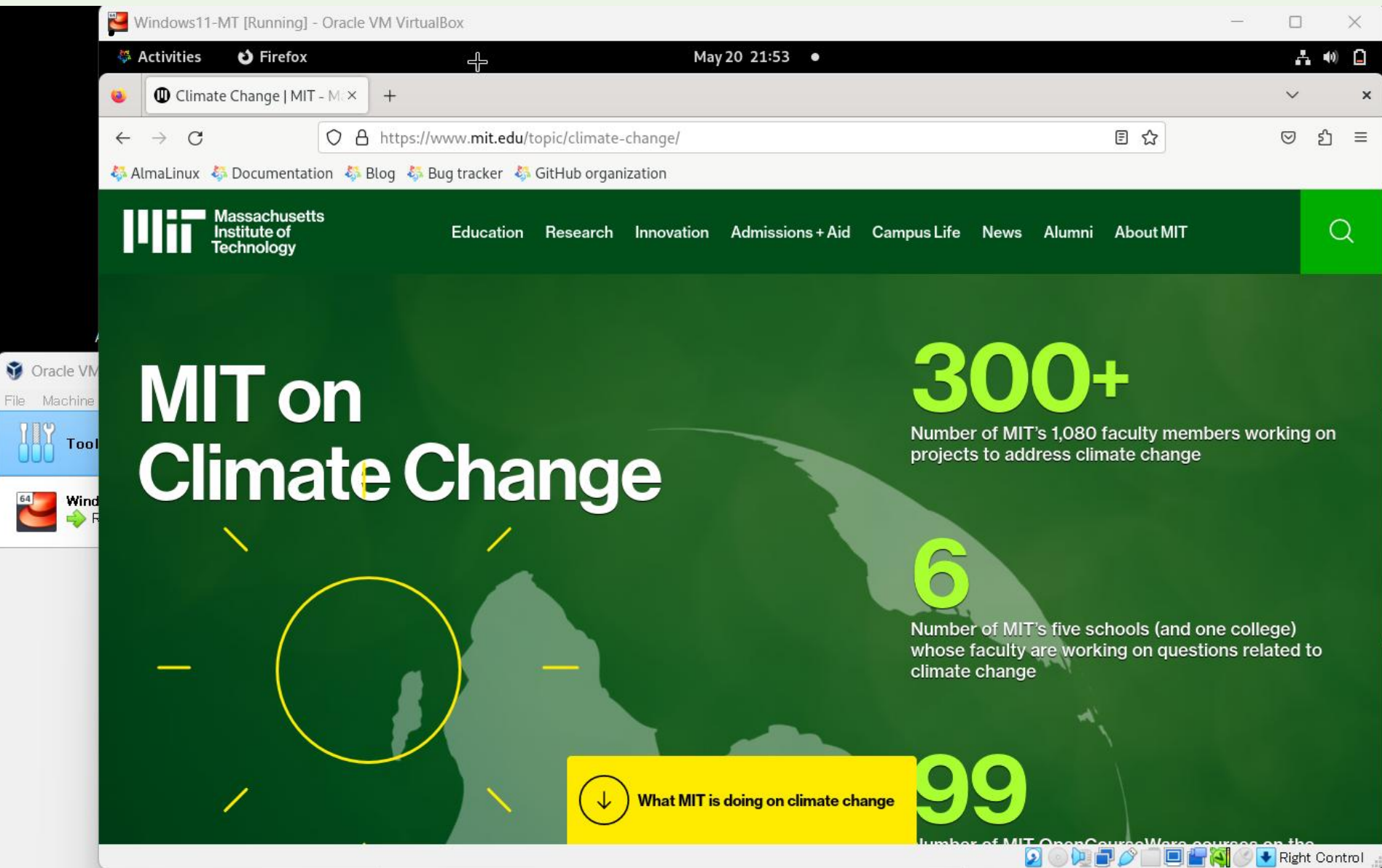
Settings and tests for simulations

*Installation of AlmaLinux-9, May 2024, and
Debian 12, Nov. 2024*

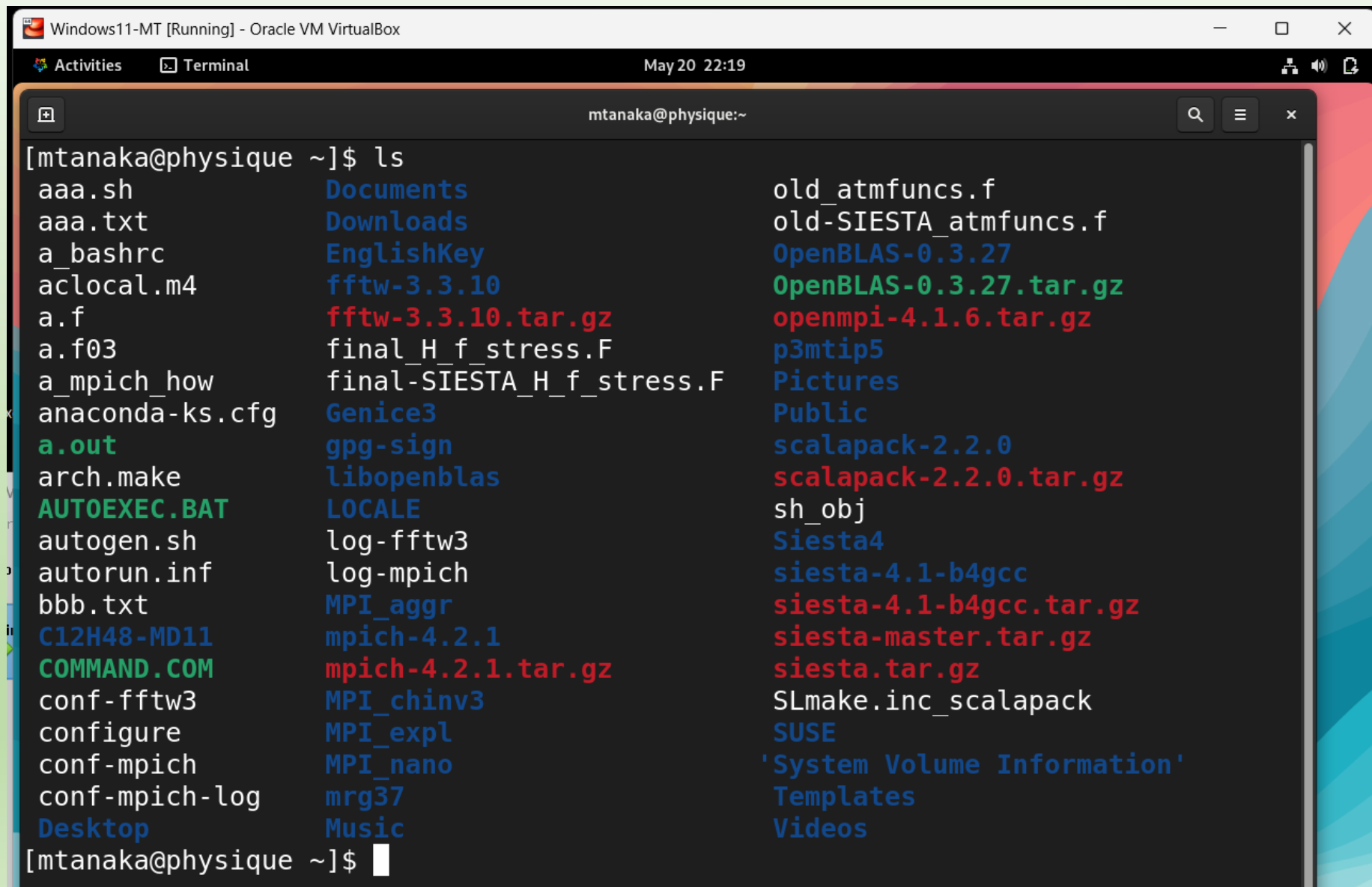
*Use Windows 11, VirtualBox 7
Linux gfortran and pip packages*

*Simulations, <https://github.com/Mtanaka77/>
>> 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

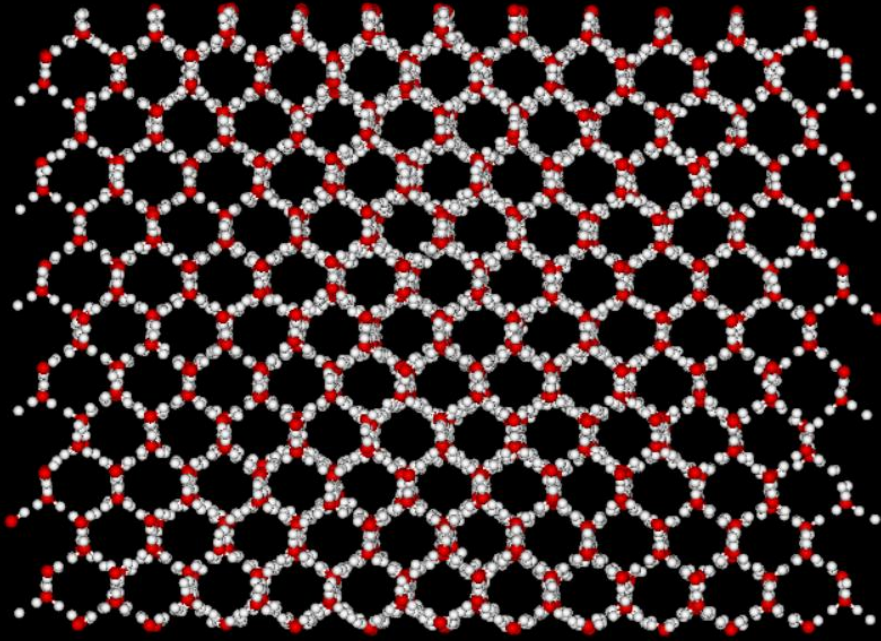


Linux terminal shows installation of mpich-4, fftw-3, p3mtip5 and Siesta-4.1



```
Windows11-MT [Running] - Oracle VM VirtualBox
Activities Terminal 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 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 MD @p3mtip5p07a.f03, 5-points water 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

*The initial states of water and hydrate are constructed
(Dr. Matsumoto, <https://github.com/vitroid/>).*

\$ pip3 install genice

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

Debian 12 OS

***The Debian OS has been installed, and is tested by /mrg37
which is quite OK. Pip3 packages and 'pip3 install genice2' is
successfully installed. The initial water configuration is OK.***

To compile Scalapack v.2

Download scalapack.2-2-0 and expand it.

In BLACS, PBLAS, SRC, TOOLS, do \$ make (no option), except one difference is SRC.

Give `-fallow-argument-mismatch` at Makefile's \$ (FC) line of SRC, and type \$ make `-k` when errors are shown.

Scalapack is 10.7 MB for libscalapack.a

Test of *ab-initio* Siesta-4.1b code

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: 0.0208500 / 0.020850085 ev/Ang**3
siesta: 42.98698226 45.67350102 kBar**3
(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
```


Overall results

The tests of classic and ab-initio molecular dynamics on AlmaLinux-9 OS are successful. Some alterations must be necessary on this specific operating system.

However, other sites including FFTW3 software fail by busy signal. The scalapack software is on unresolved errors. The pip3 of pairlist goes wrong, while it is all right on CentOS 7 OS.

Debian 12 OS is installed, and gcc, make, mpich are set up. It is tested with MD and water initial configuration of pip3 (by Dr. Matsumoto), which are quite fine