

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

*Motohiko Tanaka, Ph.D., Japan
June, Nov.-Dec., 2024*

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

Settings and tests of simulations

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

*Use Windows 11, VirtualBox 7 to login Linux OS
Linux gfortran and pip3 packages*

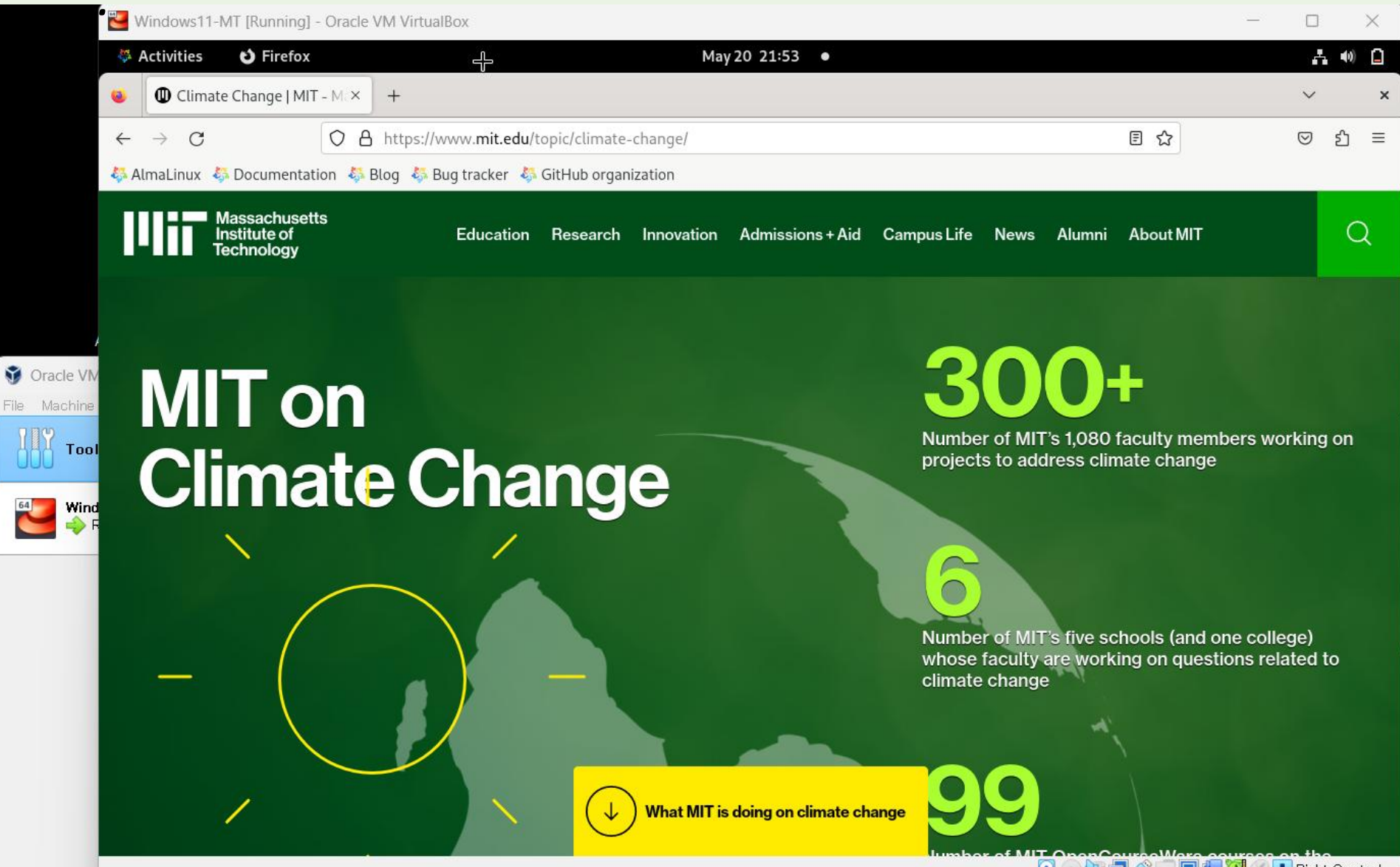
Simulations, cf. <https://github.com/Mtanaka77/>

*>> Three-dimensional electrostatic p3mtip5 code,
with tip5p and Ewald sums*

*>> Siesta-4.1b, with mpich4 fft3w, OpenBLAS,
and Scalapack*

Firefox works for AlmaLinux and Debian OS

Debian can view all of internet, but AlmaLinux is quite limited



Windows to Linux terminal: Installation of mpich4, fftw3 Tests of p3mtip5, and Siesta-4.1b codes

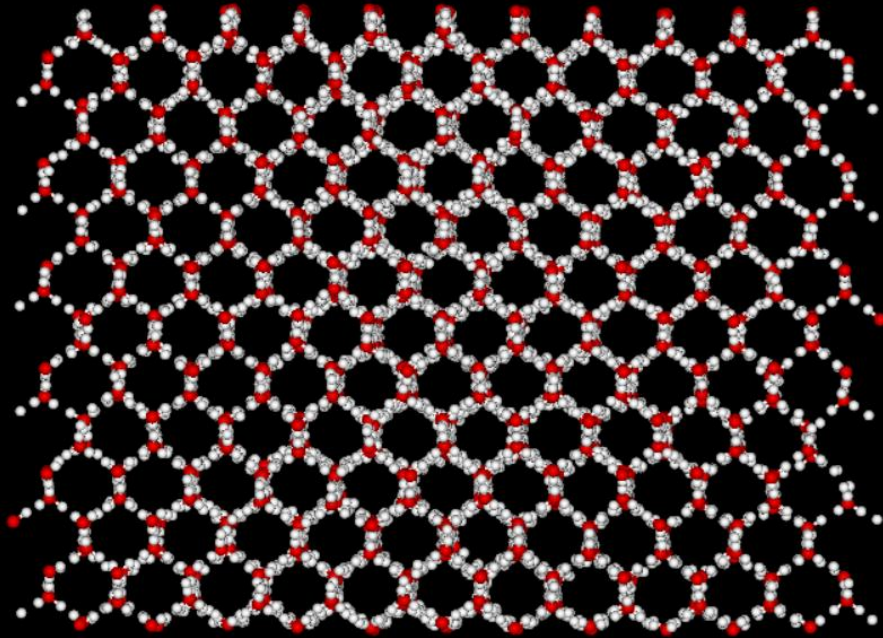
```
アクティビティ  端末  12月7日 10:32

+  端末  検索  三

mtanaka@physique:~$ ls
C12H48-MD11      arch0bjja      mrg37          siesta7
Genece3-mh3exyz arch0bjb       p3mtip5        ダウンロード
Genice2Log       bashrc-mtanaka3 sh_obj         テンプレート
Genice3          cnt3-para      siesta-4.1-b4gcc デスクトップ
GeniceLog        conf-fftw3     siesta-4.1-b4gcc.tar.gz ドキュメント
MPI_chginv       conf-mpich     siesta-4.1-b4gcc0.tar.gz ビデオ
OperblasLog      make-BLACS-SRC siesta-4.1-b4gccA 音楽
aaa-p3m.sh       make-PBLAS-SRC siesta-4.1-b4gccA.tar.gz 画像
arch.make-MPIOMP make-SRC       siesta4.1-MPI     公開
arch.make-OMP    make-TOOLS     siesta4.1-MPI-OMP

mtanaka@physique:~$ df
ファイルシス  1K-ブロック  使用  使用可  使用%  マウント位置
udev          1971352      0    1971352    0%  /dev
tmpfs         400732      1252    399480    1%  /run
/dev/sda1     30018340 10344732 18123428   37%  /
tmpfs         2003640      0    2003640    0%  /dev/shm
tmpfs         5120         8      5112      1%  /run/lock
tmpfs         400728      100    400628    1%  /run/user/1000
mtanaka@physique:~$
```

Test of MD: @p3mtip5p07a.f03, by 5-points water model



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	
	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 configuration of water and hydrate are constructed (Dr. Matsumoto, <https://github.com/vitroid/>)
\$ pip3 install genice2

Compilation goes OK in genice2 software of CentOS 7. However, it goes errors in the pairlist package and thus not go forward in AlmaLinux-9.

Debian 12

The Debian OS has been installed, and is tested by “mrg37” which is quite OK. The pip3 packages and ‘pip3 install genice2’ is successfully installed. The initial water configuration turns to be perfect.

To compile Scalapack Version 2

“This is the inside story of Scalapack’s make.”

*One downloads scalapack-2.2.0.tgz and expands it.
In BLACS, PBLAS, SRC, TOOLS, do \$ make (no option),
except one difference in SRC.*

*Give -fallow-argument-mismatch at Makefile’s \$(FC)
line in SRC, then type \$ make -k when one meets errors.
Scalapack is 10.7 MB for libscalapack.a*

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

A keyword -fallow-argument-mismatch is added in the arch.make file of Siesta-4.1b for AlmaLinux-9 and Debian-12

```
Siesta Version   : v4.1-b4
Architecture    : mpifort-MPI
Compiler version: GNU Fortran (Debian 12.2.0-14) 12.2.0
Compiler flags  : mpifort -O2 -ftree-vectorize -fprefetch-loop-arrays -march=native -fallow-argument-mismatch -fPIE
PP flags        : -DMPI -DFC_LAPACK -DSCF
Libraries       : -lgomp -L/...
calapack.a
PARALLEL version

>> Start of run: 4-DEC-2024

siesta: Cell volume = 720.000000 Ang**3

siesta: Pressure (static):
siesta: Solid Molecule Units
siesta: 0.00029221 0.00031048 Ry/Bohr**3
siesta: 0.02683002 0.02850685 eV/Ang**3
siesta: 42.98689824 45.67350469 kBar
**:(Free)E+ p_basis*V_orbitals = -2615.811581
* (Free)Eharris+ p_basis*V_orbitals = -2615.811581
**:
dhscf: Vacuum level (max, mean) = -0.569552 -0.682007 eV

reinit: Reading from c12h48.f
>> Start of run: 4-DEC-2024 17:38:16
>> End of run: 4-DEC-2024 17:39:58
1:42 min./10 cycles/6-MPI
Job completed
```


Overall Results of AlmaLinux and Debian OS

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

Many internet sites including FFTW3 failed by busy signal, the pip3 compilation of pairlist was wrong in AlmaLinux-9.

Debian 12 OS was installed, and gcc, make, mpich, fftw3 were set up on top. It was tested with MD and water initial cof pip3 (by Dr. Matsumoto) and Siesta-4.1b, all of which were quite fine on Debian.