

Simulations of Molecular Dynamics

by Debian-13 v.s. AlmaLinux-9

Motohiko Tanaka, PhD., Nagoya, Japan
<https://github.com/Mtanaka77/>

Setting tests for simulations

Installation of AlmaLinux-9 and Debian-13

*Use Windows 11, and VirtualBox 7.5 to login Linux
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 internet, but AlmaLinux is limited like FFT3W

A screenshot of a Firefox browser window displaying the MIT Climate Change website. The page has a dark green background featuring a stylized globe graphic. On the left, the text "MIT on Climate Change" is displayed in large white letters. On the right, there are three prominent statistics: "300+" (Number of MIT's 1,080 faculty members working on projects to address climate change), "6" (Number of MIT's five schools (and one college) whose faculty are working on questions related to climate change), and "99" (Number of MIT OpenCourseWare courses on the topic). A yellow button at the bottom left says "What MIT is doing on climate change". The browser's address bar shows the URL <https://www.mit.edu/topic/climate-change/>. The top navigation bar includes links for AlmaLinux, Documentation, Blog, Bug tracker, GitHub organization, and various MIT departments.

Climate Change | MIT - Mozilla Firefox

https://www.mit.edu/topic/climate-change/

AlmaLinux Documentation Blog Bug tracker GitHub organization

Massachusetts Institute of Technology

Education Research Innovation Admissions + Aid Campus Life News Alumni About MIT

MIT on Climate Change

300+

Number of MIT's 1,080 faculty members working on projects to address climate change

6

Number of MIT's five schools (and one college) whose faculty are working on questions related to climate change

99

Number of MIT OpenCourseWare courses on the topic

(1) Linux terminal from Windows: Installation of mpich4, fftw3. Tests of p3mtip5, and Siesta-4.1b codes

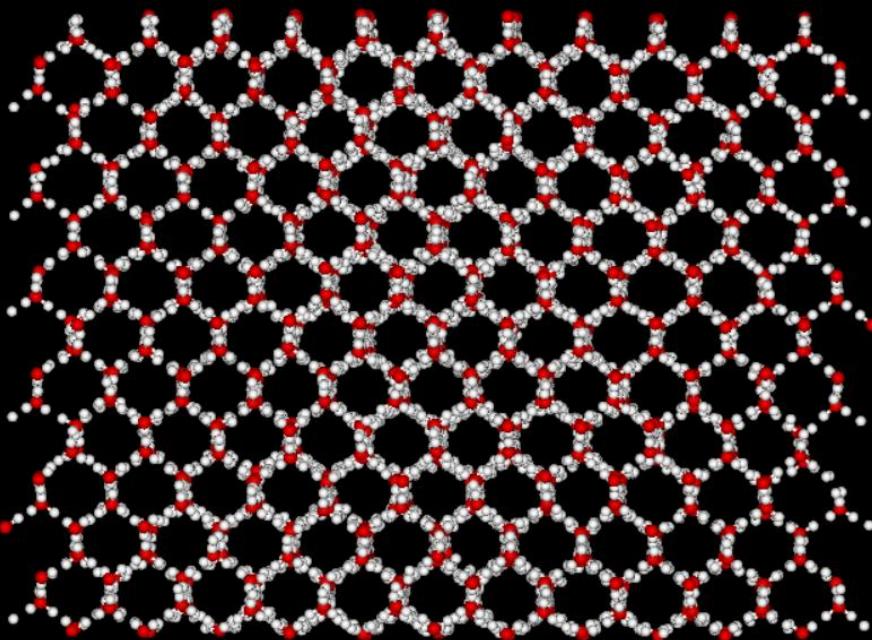
```
ファイル 仮想マシン 表示 入力 デバイス ヘルプ
アクティビティ 端末 12月7日 10:32
+ 端末 検索 ビュー

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
ファイルシステム 1K-ブロック 使用 可用 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	<e _{kin} >	<e _{img} >		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	
-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	
-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	
-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				

(2) Related pip3 packages, Genice2

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

Compilation goes well in genice2 software for Debian. However, it goes with strange errors in “genice CS1...” for AlmaLinux-9.6.

The Debian-13 has been installed, and is tested by “mrg37” which is quite OK. The pip3 packages and ‘pip3 install genice2’ is successfully installed. “genice CS1...” generates water molecules which is perfect.

(3.a) To compile Scalapack Ver. 2

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

*One downloads scalapack-2.2.2.tgz and expands it.
Give -fallow-argument-mismatch (FC) and
-Wno-implicit-function-declaration (GCC) at
SLmake.make of Debian-13. Do \$ make in TOOLS,
SRC, PBLAS, BLACS, and BLACS/Install directories.
It generates libscalapack.a with 11 MB.*

(3.b) Test of Ab-initio Siesta-4.1b code

A keyword `-fallow-argument-mismatch` is added in the `arch.make` of Siesta-4.1b for Debian-13 (Nov. 2025).

```
Siesta Version   : v4.1-b4
Architecture     : gfortran-MPI
Compiler version: GNU Fortran (Debian 14.2.0-19) 14.2.0
Compiler flags   : mpifort -O2 -fPIC -ftree-vectorize -march=native -fallow-argument-mismatch
PP flags        : -DMPI -DFC HAVE_ABORT
Libraries       : -lgomp -L/opt/openblas/lib -lopenblasomp -L/opt/scalapack/lib -lscalapack
PARALLEL version

* Running on 8 nodes in parallel
>> Start of run: 2-DEC-2025 10:00:06

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


reinit: Reading from iceA841.fdf

reinit: -----
reinit: System Name: ice non-periodic Verlet w/MW w/o spin
reinit: ---
reinit: Sys Setting up quadratic distribution...
reinit: --- ExtMesh (bp) on 0 = 100 x 88 x 65 = 572000
reinit: --- PhiOnMesh: Number of (b)points on node 0 = 72000
reinit: --- PhiOnMesh: nlist on node 0 = 1021031

          iscf      Eharris(eV)      E_KS(eV)      FreeEng(eV)      dDmax      Ef(eV)      dHmax(eV)
scf: at      scf:    1  -60126.087499  -60126.165752  -60126.165752  0.003535  -2.063753  0.020507
10 step      scf:    2  -60126.165089  -60126.165603  -60126.165603  0.000435  -2.061038  0.037459
                  scf:    3  -60126.165932  -60126.165832  -60126.165832  0.000259  -2.062652  0.003224
                  scf:    4  -60126.165842  -60126.165838  -60126.165838  0.000045  -2.062701  0.000656
                  scf:    5  -60126.165838  -60126.165838  -60126.165838  0.000000  -2.062702  0.000647
```

Overall Results of AlmaLinux and Debian OS's

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 errors at “genice CS1 ...” in AlmaLinux-9.6.

Debian 13 OS is installed, and gcc, gfortran, mpich, fftw3 are set up on top. It is tested with MD, water code “Genice2” (by Dr. Matsumoto), and Siesta-4.1b, and all of which are very favorable on Debian.