

# *Simulations of Molecular Dynamics*

## *by Debian-13 v.s. AlmaLinux-9*

*Motohiko Tanaka, Ph.D., 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 of the browser window has a yellow bar with the text "Firefox works for AlmaLinux and Debian OS. Debian can view internet, but AlmaLinux is limited like FFT3W".

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

What MIT is doing on climate change

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

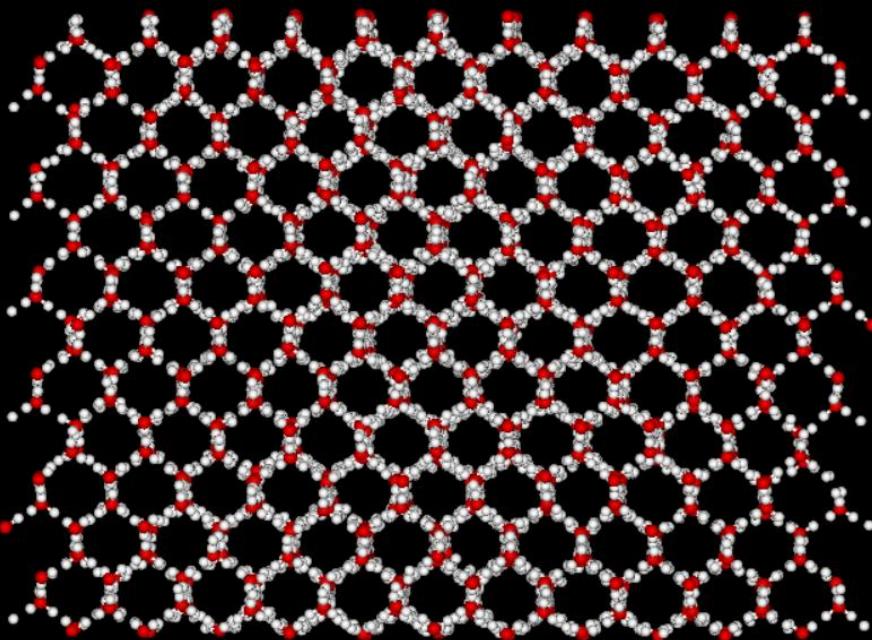
```
ファイル 仮想マシン 表示 入力 デバイス ヘルプ
アクティビティ 端末 12月7日 10:32
+ 端末 検索 ビュー

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 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	<e <sub>kin</sub> >	<e <sub>img</sub> >		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 and*

*-Wno-implicit-function-declaration at \$makefile,*

*of Debian-13. And \$ make in TOOLS, SRC, PBLAS,*

*BLACS, and BLACS/Install directories.*

*It comes with 11 MB of libscalapack.a.*

## (3.b) 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 Debian-13 (Nov. 2025).

```
端末
```

```
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
Libraries      : -lgomp -L/
calapack.a
PARALLEL version          siesta: Pressure (static):
                           siesta:           Solid           Molecule   Units
* Running on 6 nodes in parallel
                           siesta:    0.00029221    0.00031048  Ry/Bohr**3
>> Start of run: 4-DEC-2024 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.f0
>> 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'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 was installed, and gcc, gfortran, mpich, fftw3 were set up on top. It was tested with MD, water code “Genice2” (by Dr. Matsumoto), and Siesta-4.1b, and all of which were very favorable on Debian.***