

# *Simulations of Molecular Dynamics*

## *by Debian-12 v.s. AlmaLinux-9*

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

## *Setting tests for simulations*

*Installation of AlmaLinux-9 and Debian-12*

*Use Windows 11, VirtualBox 7 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 all of 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

# *Windows to Linux terminal: 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

mtanaka@physique:~\$ ls

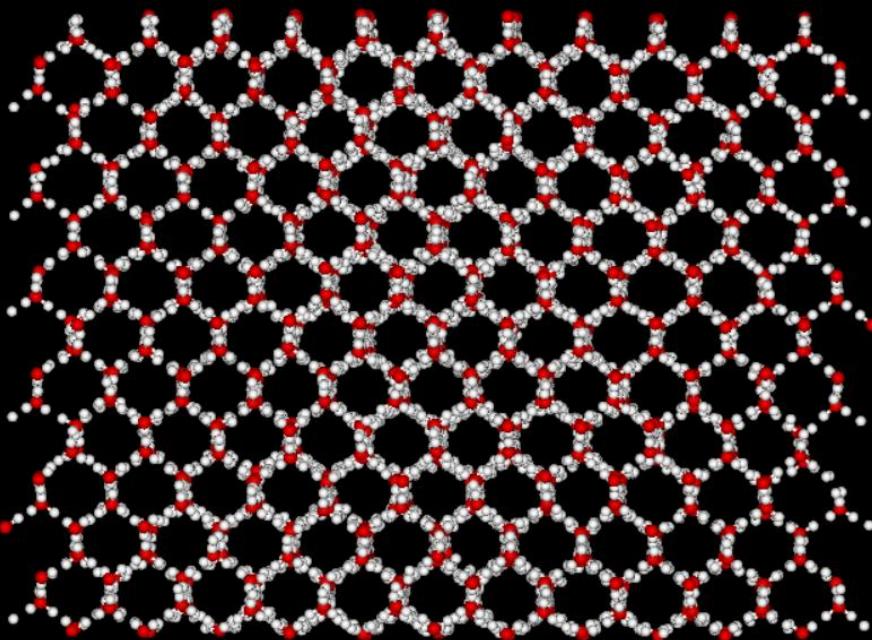
C12H48-MD11	arch0bj	mrg37	siesta7
Genece3-mh3exyz	arch0bjb	p3mtip5	ダウンロード
Genice2Log	bashrc-mtanaka3	sh_obj	テンプレート
Genice3	cnt3-para	siesta-4.1-b4gcc	デスクトップ
GeniceLog	conf-fftw3	siesta-4.1-b4gcc.tar.gz	ドキュメント
MPI_chginv	conf-mpich	siesta-4.1-b4gcc0.tar.gz	ビデオ
OperblasLog	make-BLACS-SRC	siesta-4.1-b4gccA	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 <img&gt;< th=""><th></th><th>cpu</th></img&gt;<>		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				

## *Related pip3 packages*

*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 errors in “genice CS1...” for AlmaLinux-9.6.*

***The Debian-12 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 Ver. 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 for SRC below.*

*Give -fallow-argument-mismatch at Makefile’s \$(FC)  
line in SRC, and type \$ make –k.*

*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*

```
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 12 OS was installed, and gcc, make, mpich, fftw3 were set up on top. It was tested with MD, water code “Genice” (by Dr. Matsumoto), and Siesta-4.1b, all of which were very favorable on Debian.***