

*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 for AlmaLinux and Debian

The screenshot shows a Firefox browser window within an Oracle VM VirtualBox environment. The browser's address bar displays the URL <https://www.mit.edu/topic/climate-change/>. The page content features the MIT logo and navigation links at the top. The main heading is "MIT on Climate Change". Three key statistics are highlighted in large green numbers: "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 with a downward arrow icon and the text "What MIT is doing on climate change" is visible at the bottom of the page. The browser's status bar at the bottom right shows "Right Control".

Windows11-MT [Running] - Oracle VM VirtualBox

Activities Firefox May 20 21:53

Climate Change | MIT - MIT

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

AlmaLinux Documentation Blog Bug tracker GitHub organization

MIT 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

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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

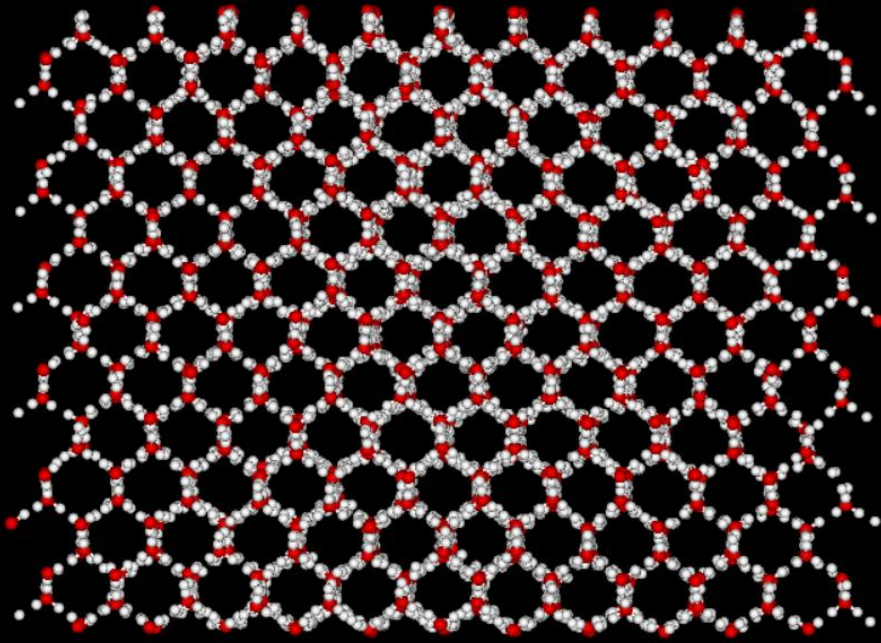
What MIT is doing on climate change

Right Control

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

```
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 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				
0	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. Matsumote, <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 go forward in AlmaLinux-9.

Debian 12

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 perfect.

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 and Debian-12

```
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 /          0.020850000  ev/Ang**3
siesta:          42.98698226          45.67350102  kBar
(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 in AlmaLinux-9.

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