

STEP 1: Install Intel® oneAPI Base Toolkit

- Go to Intel WEB and select the displayed configuration

The screenshot shows the Intel oneAPI Base Toolkit download page. At the top, there's a blue header bar with the Intel logo and navigation links for USA (English), Sign In, and a search icon. Below the header, a large blue banner features the text "Get the Intel® oneAPI Base Toolkit" and a subtext: "No Transistor Left Behind™ The Smart Path to Accelerated Computing without the Economic and Technical Burdens of Proprietary Programming Models". The main content area has a white background. It starts with a section titled "Select options below to download" containing three dropdown menus: "Operating System" (set to Linux), "Distribution" (set to Web & Local (recommended)), and "Installer Type" (set to Local). To the right of these dropdowns is a "Local Installer" section with two bullet points: "Includes all tools in the toolkit" and "Recommended for host machines with poor or no internet connection". Below this is a button labeled "What's Included in the Intel oneAPI Base Toolkit for Linux*". Further down, it shows the download details: "Download size: 3.43 GB", "Version: 2021.3", and "Date: June 24, 2021". At the bottom of the page, there's a "Download" button, a link to "Privacy and Terms of use", and a "Command Line Download" link.

Get the Intel® oneAPI Base Toolkit

No Transistor Left Behind™ The Smart Path to Accelerated Computing without the Economic and Technical Burdens of Proprietary Programming Models

Select options below to download

Operating System: Select operating system
Linux

Distribution: Select distribution
Web & Local (recommended)

Installer Type: Select installer
Local

Local Installer

- Includes all tools in the toolkit
- Recommended for host machines with poor or no internet connection

What's Included in the Intel oneAPI Base Toolkit for Linux*

Download size: 3.43 GB
Version: 2021.3
Date: June 24, 2021

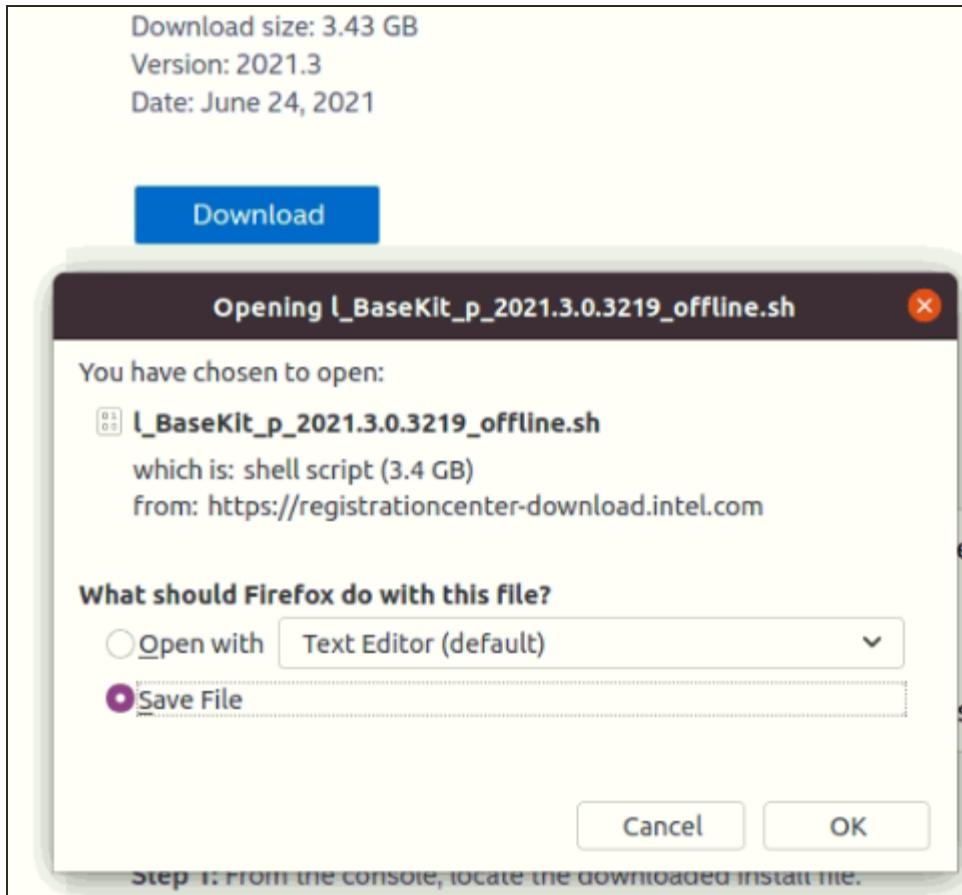
Download

By downloading, you agree to our [Privacy](#) and [Terms of use](#)

Command Line Download

STEP 1: Install Intel® oneAPI Base Toolkit

- Download to hard drive



STEP 1: Install Intel® oneAPI Base Toolkit

- Follow the instructions on the WEB page to install: steps 1 and 2

Installation Instructions

Step 1: From the console, locate the downloaded install file.

Step 2: Use `$ sudo sh <installer>.sh` to launch the GUI Installer as the root.

Optionally, use `$ sh <installer>.sh` to launch the GUI Installer as the current user.

Step 3: Follow the instructions in the installer.

Step 4: Explore the [Get Started Guide](#).

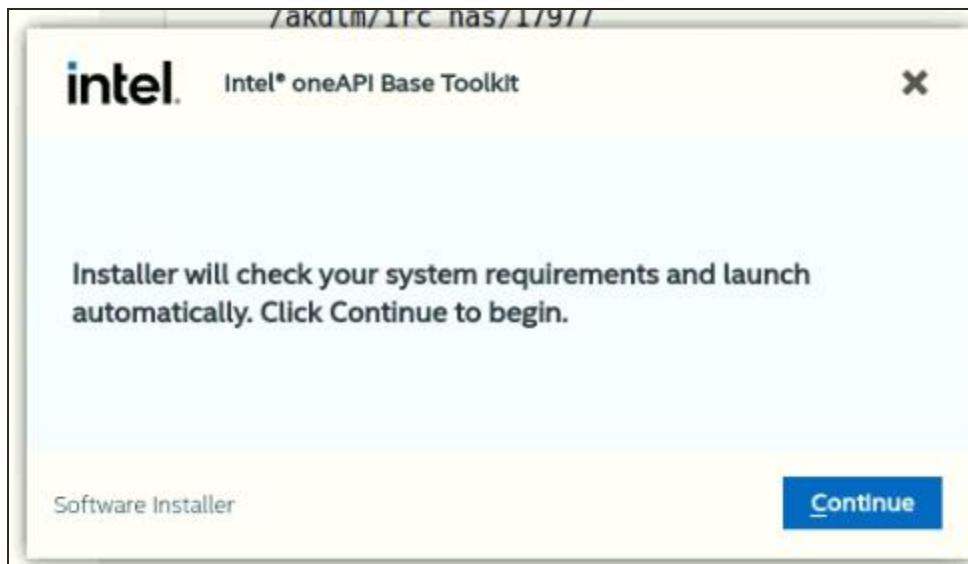


A screenshot of a terminal window titled "pc-1@pc1-Precision-3630-Tower: ~/Downloads". The terminal shows the following command sequence:

```
pc-1@pc1-Precision-3630-Tower:~$ cd Downloads/  
pc-1@pc1-Precision-3630-Tower:~/Downloads$ ls  
l_BaseKit_p_2021.3.0.3219_offline.sh  
pc-1@pc1-Precision-3630-Tower:~/Downloads$ sudo sh ./l_BaseKit_p_2021.3.0.3219_offline.sh
```

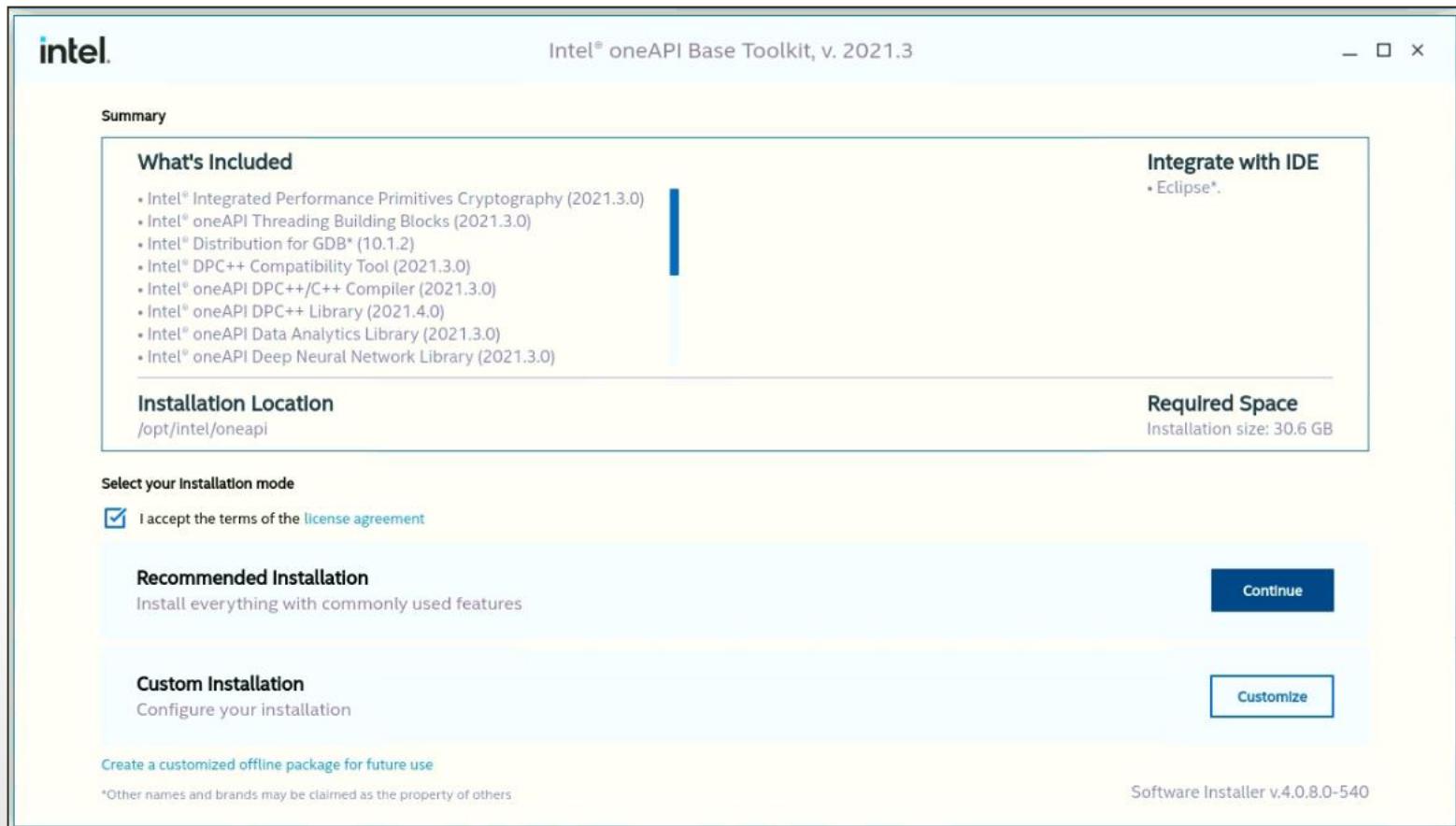
STEP 1: Install Intel® oneAPI Base Toolkit

- Click on "Continue".



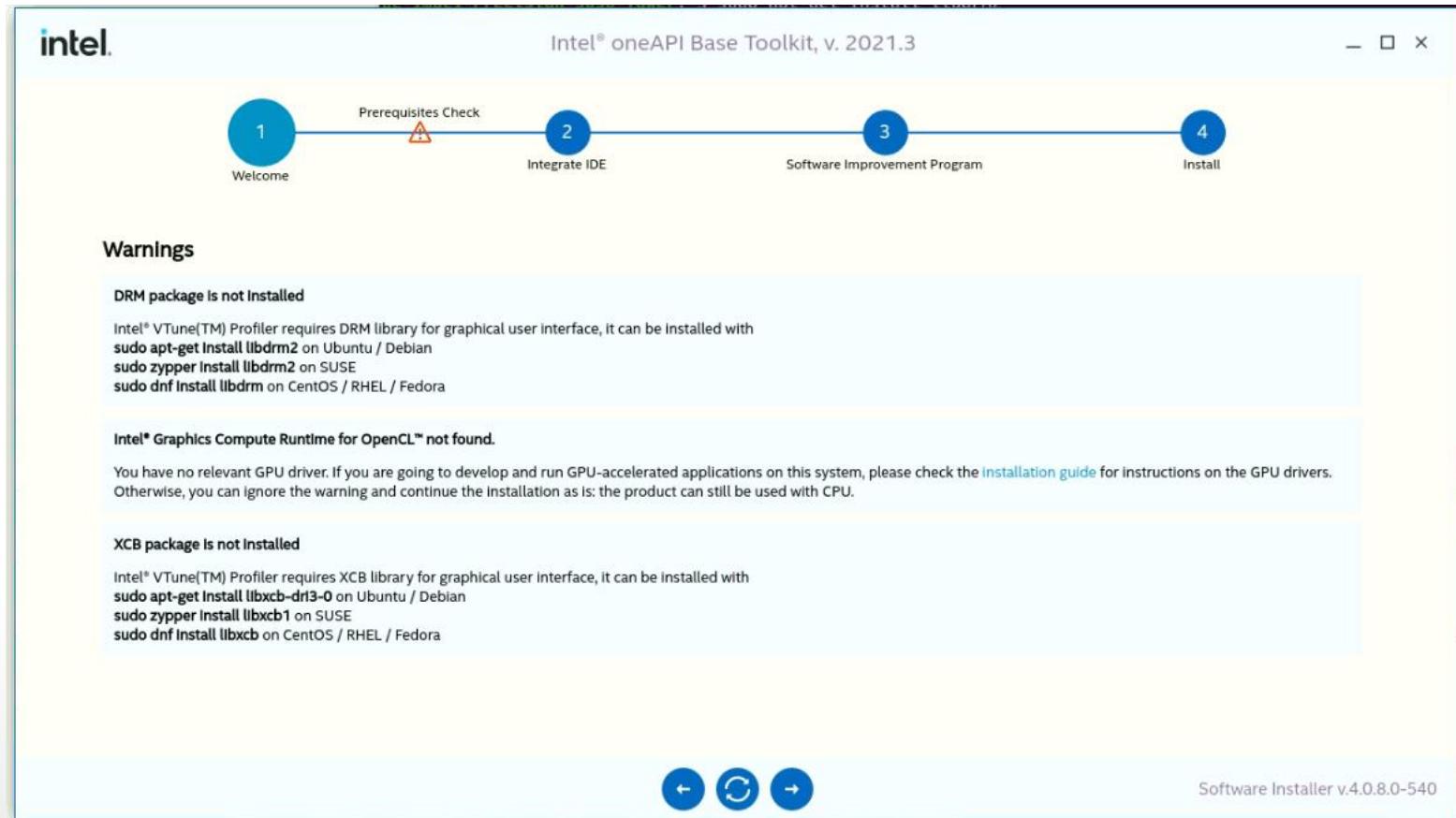
STEP 1: Install Intel® oneAPI Base Toolkit

- Select “I accept the terms ...”
- Click on “Continue” (optional “Recommended Installation”)



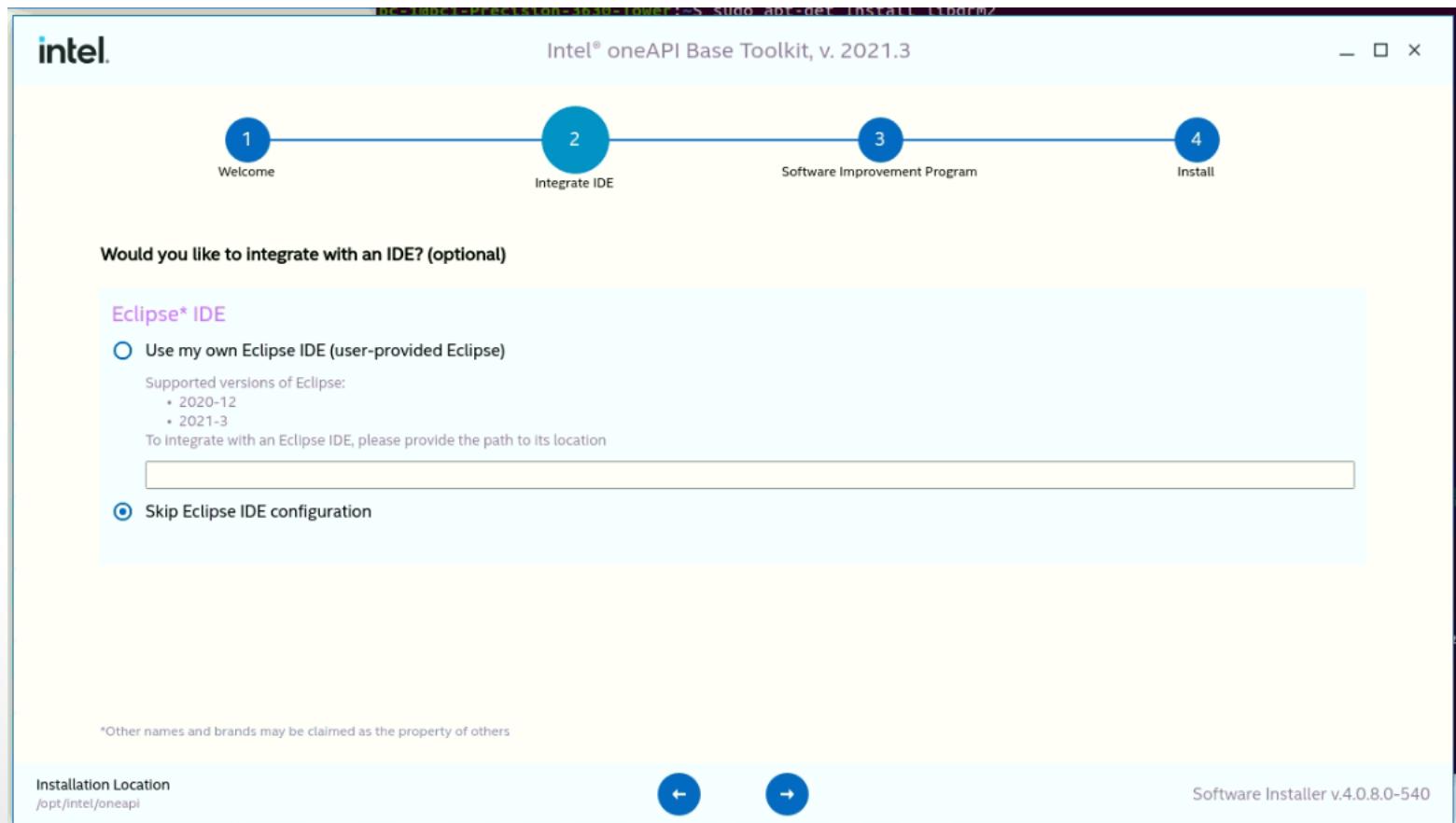
STEP 1: Install Intel® oneAPI Base Toolkit

- Ignore the warnings and click on "right arrow"



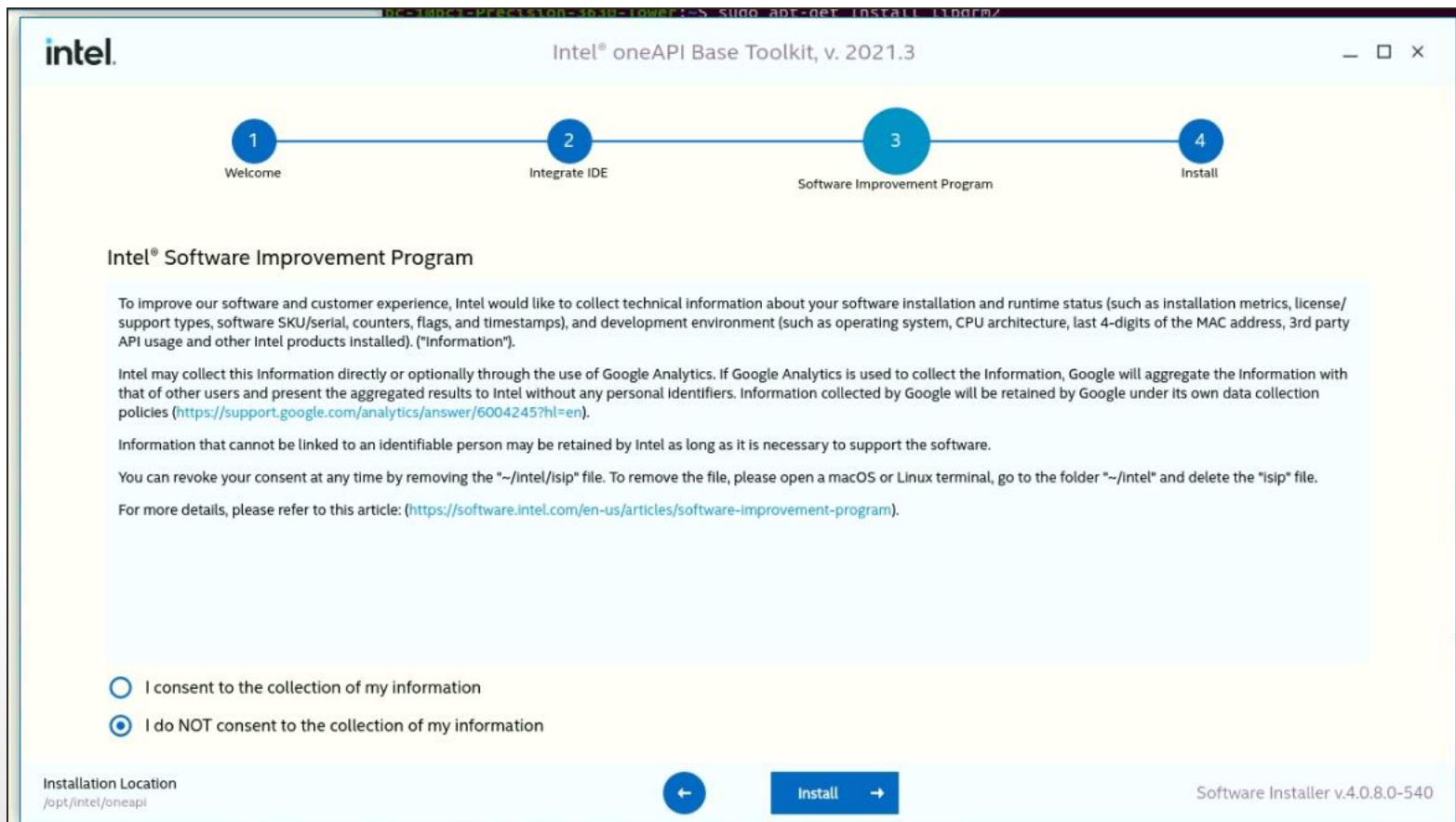
STEP 1: Install Intel® oneAPI Base Toolkit

- Select "Skip Eclipse ..." and click on "right arrow".



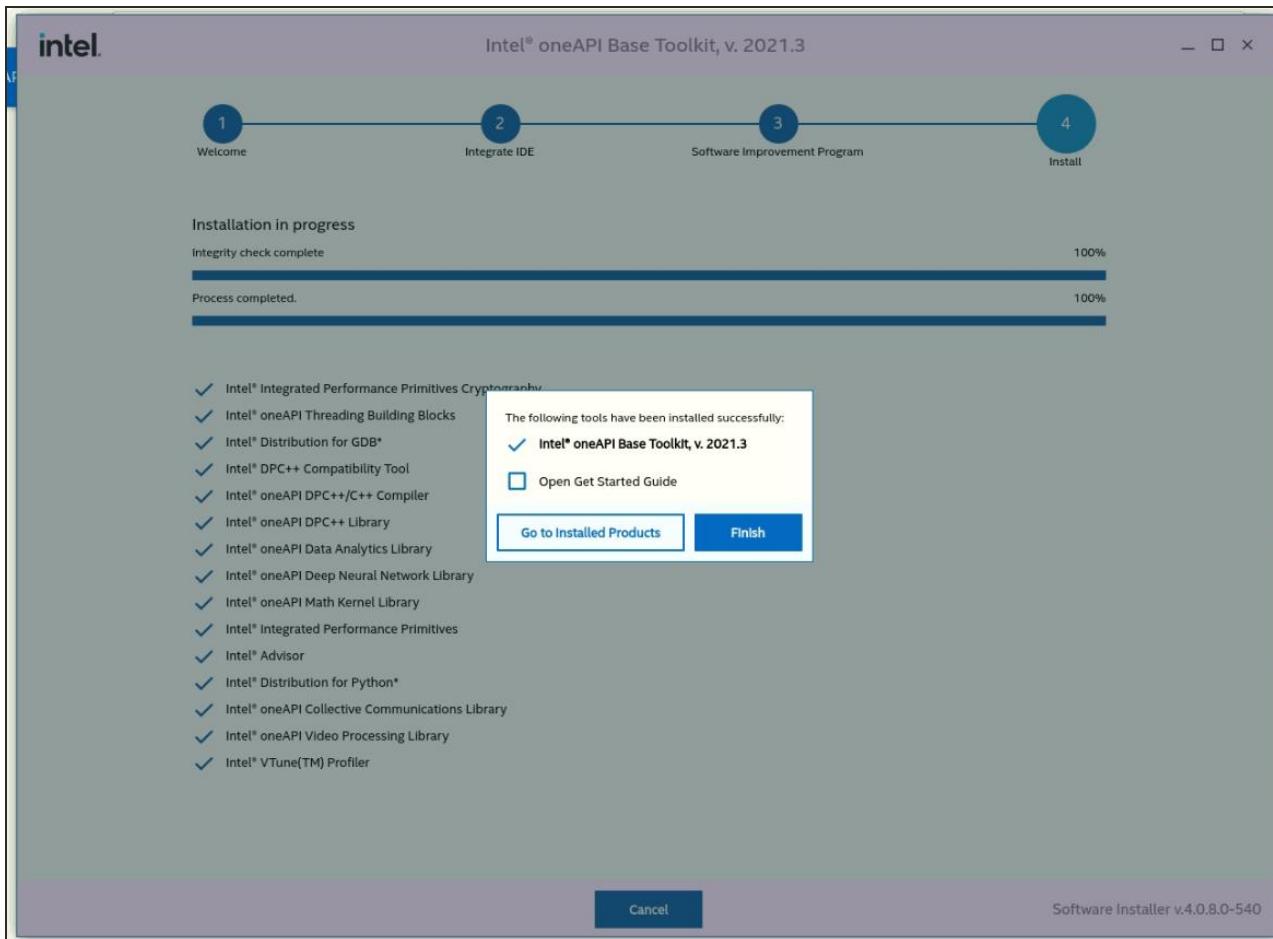
STEP 1: Install Intel® oneAPI Base Toolkit

- Select "I do NOT consent to ..." and click on "Install".



STEP 1: Install Intel® oneAPI Base Toolkit

- The process takes approximately 10 minutes. When all the components are installed click on "Finish."



STEP 2: Install Intel® oneAPI HPC Toolkit

- Go to Intel WEB and select the displayed configuration

The screenshot shows the Intel oneAPI HPC Toolkit download page. At the top, there's a blue header bar with the Intel logo and navigation links for USA (English), My Intel, and a search icon. Below the header, a large blue button says "Get the Intel® oneAPI HPC Toolkit". The main content area has a white background. It starts with a section titled "Select options below to download" containing three dropdown menus: "Operating System" (set to Linux), "Distribution" (set to Web & Local (recommended)), and "Installer Type" (set to Local). To the right of these is a "Toolkit Dependency Notice" box with text about the Base Toolkit and a link to "Download the Base Toolkit". Below this is a "Local Installer" section with two bullet points: "Includes all tools in the toolkit" and "Recommended for host machines with poor or no internet connection". At the bottom, there's a collapsed "What's Included in the Intel® oneAPI HPC Toolkit for Linux*" section and some small text at the very bottom.

Get the Intel® oneAPI HPC Toolkit

Select options below to download

Operating System: Select operating system
Linux

Distribution: Select distribution
Web & Local (recommended)

Installer Type: Select installer
Local

Toolkit Dependency Notice

This toolkit requires that you install the Intel® oneAPI Base Toolkit for full functionality.
[Download the Base Toolkit](#)

Local Installer

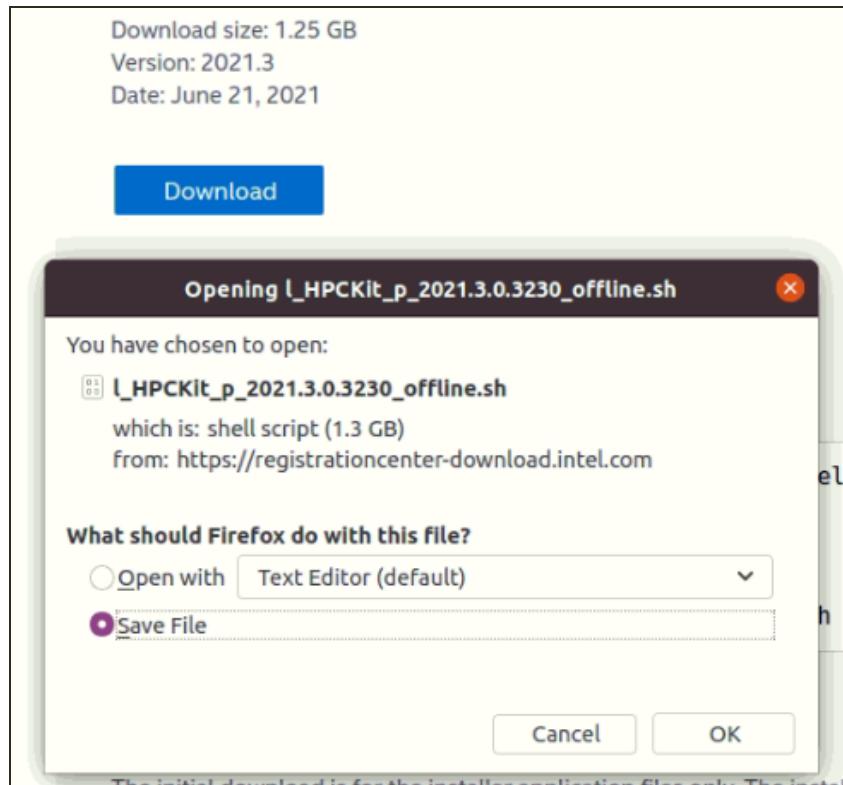
- Includes all tools in the toolkit
- Recommended for host machines with poor or no internet connection

What's Included in the Intel® oneAPI HPC Toolkit for Linux*

Download size: 1.25 GB
Version: 2021.3
Date: June 21, 2021

STEP 2: Install Intel® oneAPI HPC Toolkit

- Download to hard disk



STEP 2: Install Intel® oneAPI HPC Toolkit

- Follow the instructions on the WEB page to install: steps 1 and 2

Installation Instructions

The initial download is for the installer application files only. The installer will acquire all the tools during the installation process.

- Step 1: From the console, locate the downloaded install file.
- Step 2: Use `$ sudo sh ./<installer>.sh` to launch the GUI Installer as root.
- Optional, use `$ sh ./<installer>.sh` to launch the GUI Installer as current user.
- Step 3: Follow the instructions in the installer.
- Step 4: Explore the [Get Started Guide](#).

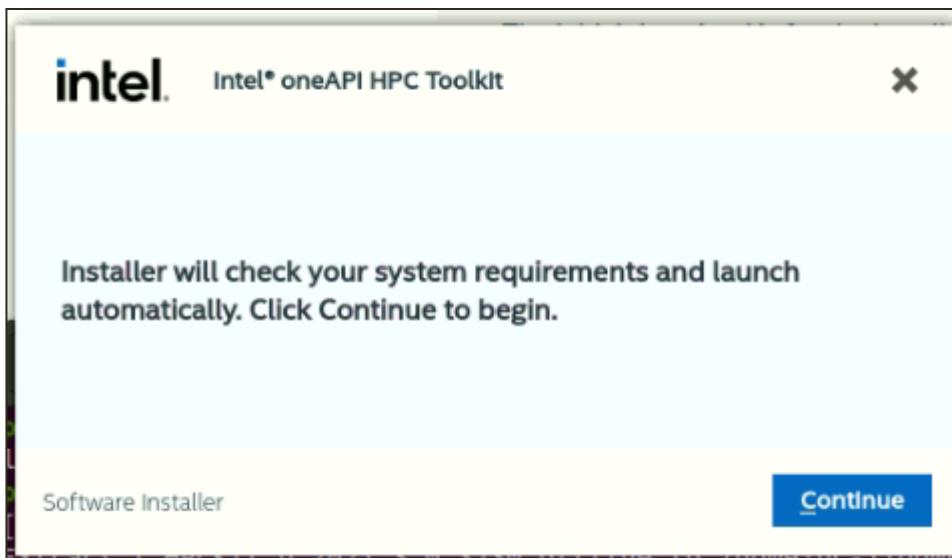


A screenshot of a terminal window titled "pc-1@pc1-Precision-3630-Tower: ~/Downloads". The terminal shows the following command sequence:

```
pc-1@pc1-Precision-3630-Tower:~/Downloads$ ls
l_BaseKit_p_2021.3.0.3219_offline.sh  l_HPCKit_p_2021.3.0.3230_offline.sh
pc-1@pc1-Precision-3630-Tower:~/Downloads$ sudo sh ./l_HPCKit_p_2021.3.0.3230_offline.sh
[sudo] password for pc-1:
Extract l_HPCKit_p_2021.3.0.3230_offline to /home/pc-1/Downloads/l_HPCKit_p_2021.3.0.3230_offline...
[##]
```

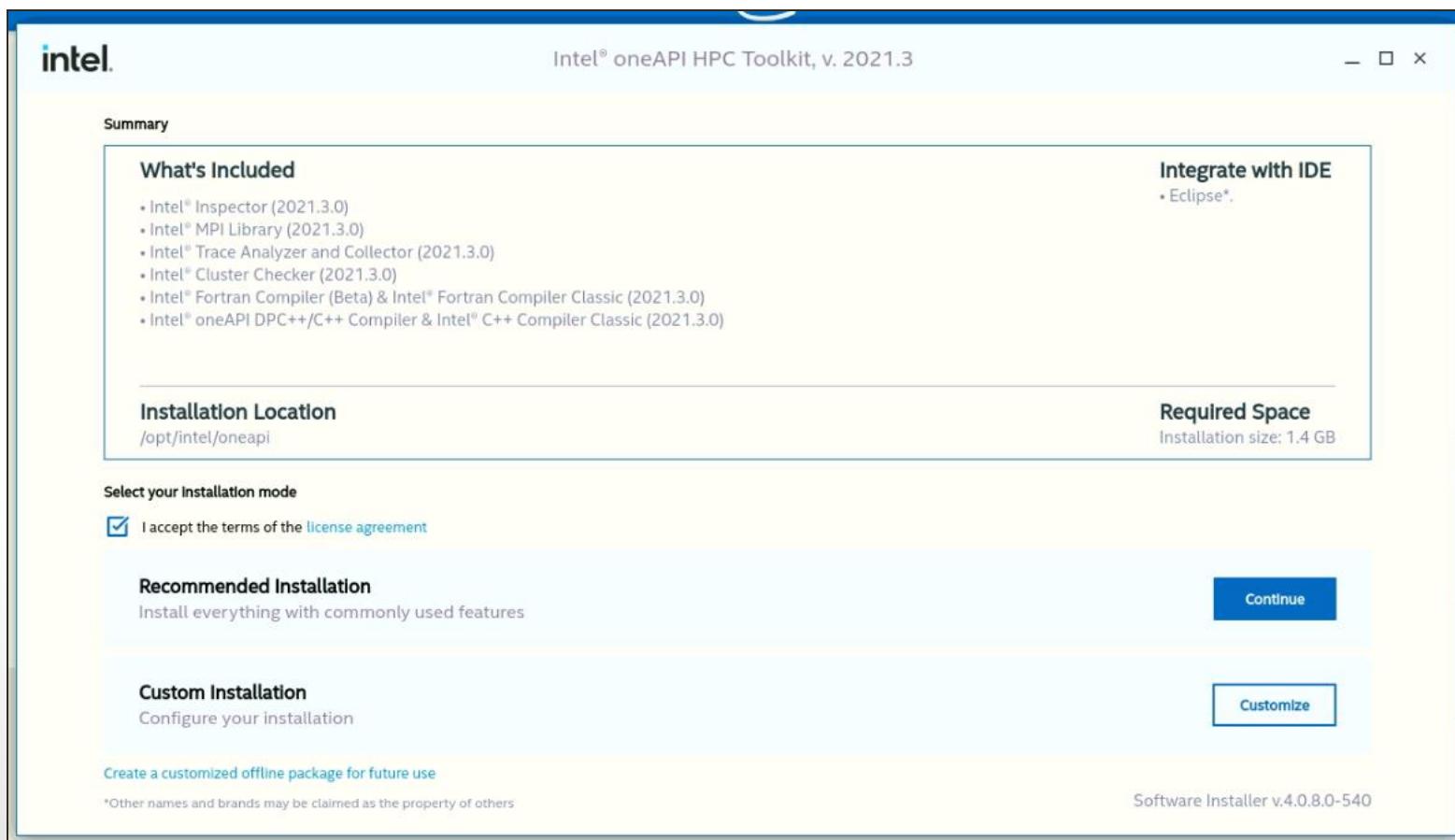
STEP 2: Install Intel® oneAPI HPC Toolkit

- Click on “Continue”



STEP 2: Install Intel® oneAPI HPC Toolkit

- Select “I accept the terms ...”
- Click on “Continue” (option “Recommended Installation”)



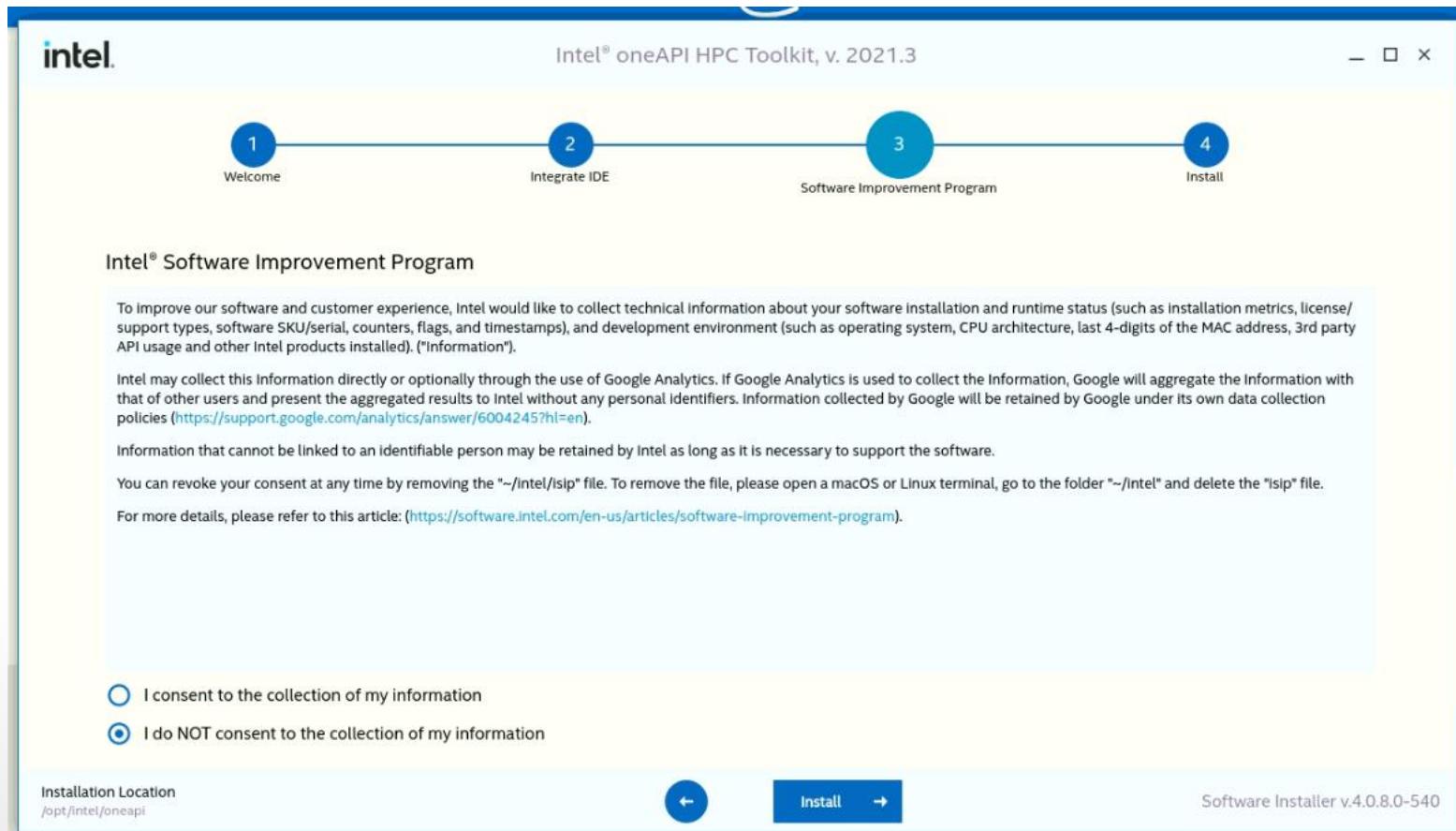
STEP 2: Install Intel® oneAPI HPC Toolkit

- Select “Skip Eclipse ...” and click on “flecha derecha”



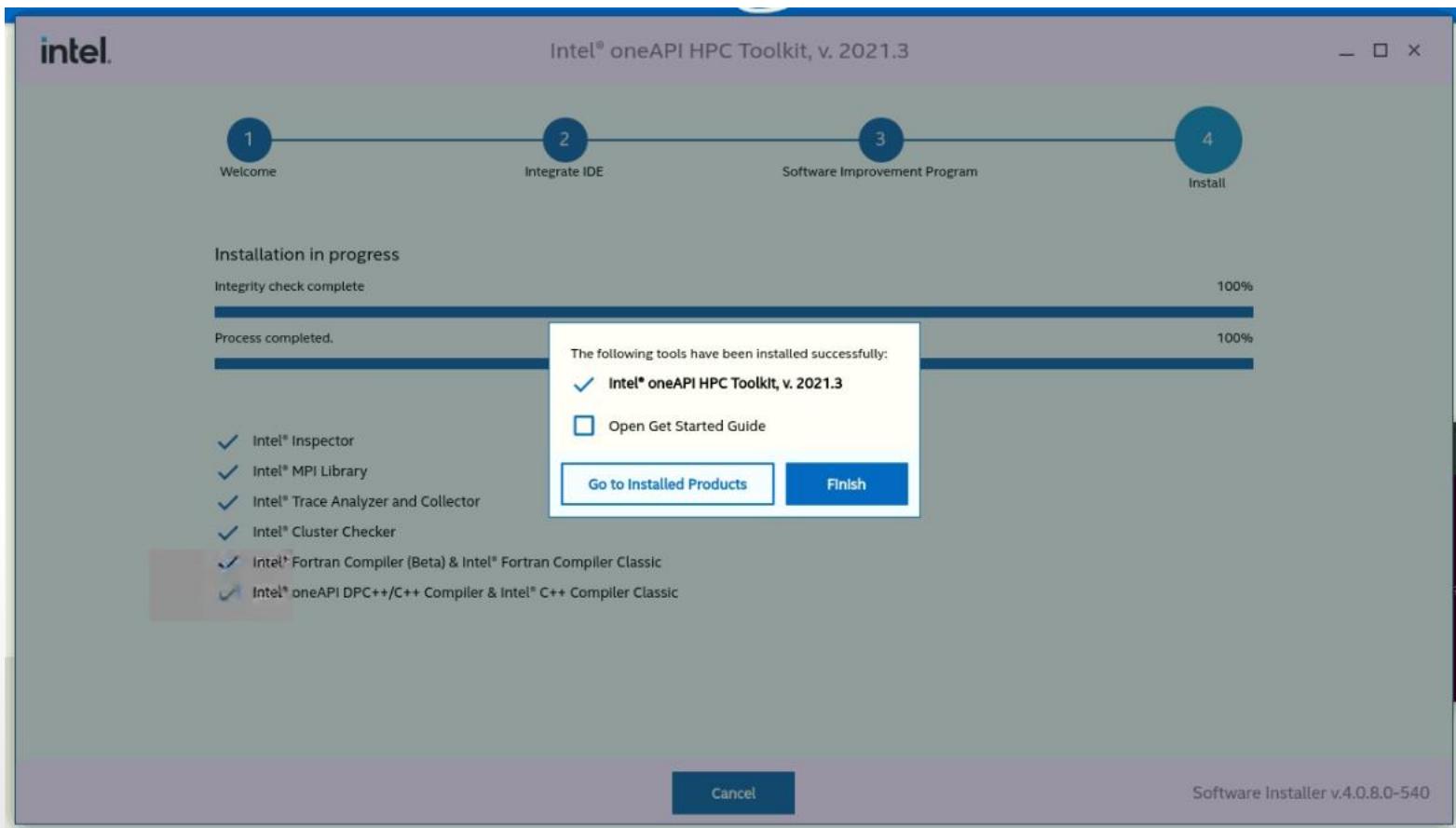
STEP 2: Install Intel® oneAPI HPC Toolkit

- Select “I do NOT consent to ...” and click on “Install”



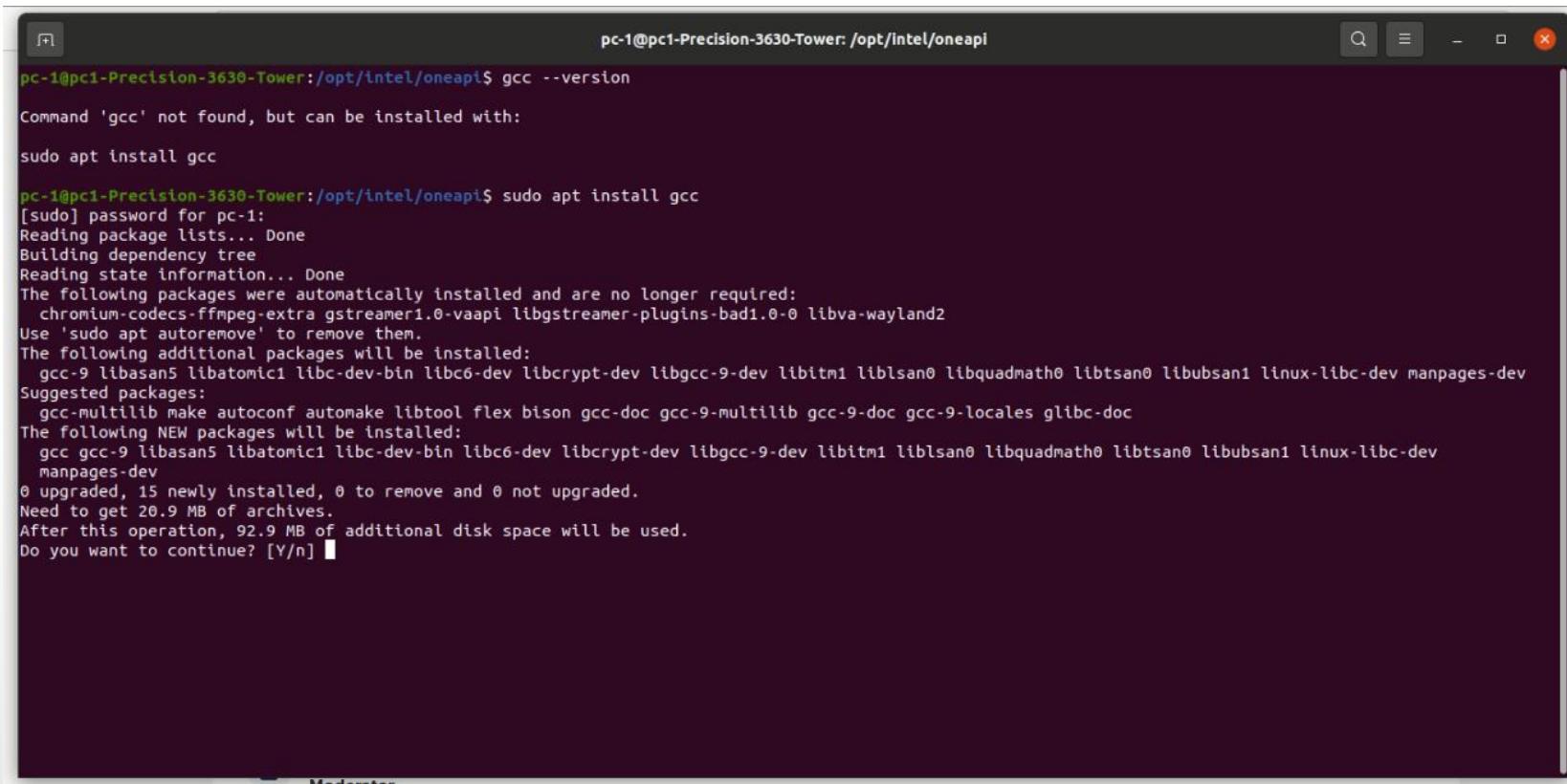
STEP 2: Install Intel® oneAPI HPC Toolkit

- The process takes approximately 5 minutes. When all the components are installed click on "Finish".



Installing gcc

Check if gcc is installed with the "gcc --version" command.
If not, use the command "sudo apt install gcc".



pc-1@pc1-Precision-3630-Tower:/opt/intel/oneapi\$ gcc --version
Command 'gcc' not found, but can be installed with:
sudo apt install gcc
pc-1@pc1-Precision-3630-Tower:/opt/intel/oneapi\$ sudo apt install gcc
[sudo] password for pc-1:
Reading package lists... Done
Building dependency tree
Reading state information... Done
The following packages were automatically installed and are no longer required:
chromium-codecs-ffmpeg-extra gstreamer1.0-vaapi libgstreamer-plugins-bad1.0-0 libvba-wayland2
Use 'sudo apt autoremove' to remove them.
The following additional packages will be installed:
gcc-9 libasan5 libatomic1 libc-dev-bin libcrypt-dev libgcc-9-dev libitm1 liblsan0 libquadmath0 libtsan0 libubsan1 linux-libc-dev manpages-dev
Suggested packages:
gcc-multilib make autoconf automake libtool flex bison gcc-doc gcc-9-multilib gcc-9-doc gcc-9-locales glibc-doc
The following NEW packages will be installed:
gcc gcc-9 libasan5 libatomic1 libc-dev-bin libcrypt-dev libgcc-9-dev libitm1 liblsan0 libquadmath0 libtsan0 libubsan1 linux-libc-dev
manpages-dev
0 upgraded, 15 newly installed, 0 to remove and 0 not upgraded.
Need to get 20.9 MB of archives.
After this operation, 92.9 MB of additional disk space will be used.
Do you want to continue? [Y/n] ■

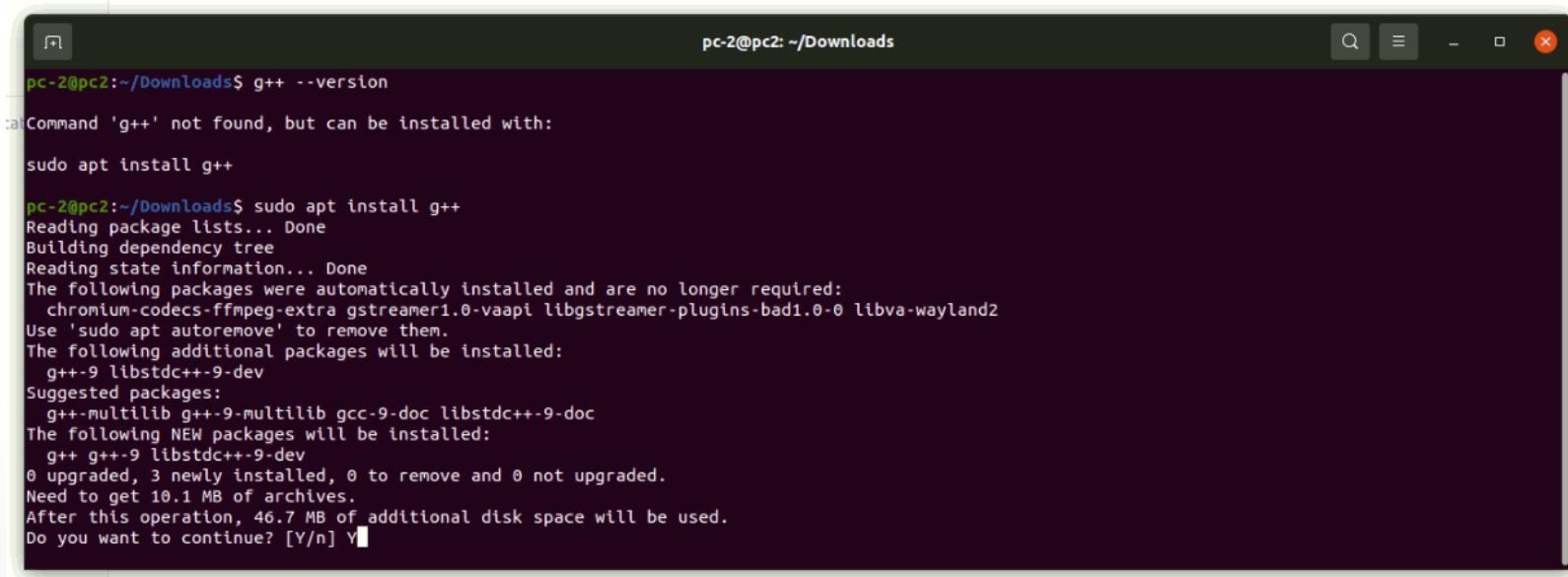
Installing gcc

Use the "gcc -version" command again to verify that it has been installed.

```
pc-1@pc1-Precision-3630-Tower: /opt/intel/oneapi
Selecting previously unselected package linux-libc-dev:amd64.
Preparing to unpack .../11-linu..._dev_5.4.0-77.86_amd64.deb ...
Unpacking linux-libc-dev:amd64 (5.4.0-77.86) ...
Selecting previously unselected package libcrypt-dev:amd64.
Preparing to unpack .../12-libcrypt-dev_1x3a4.4.10-10ubuntu4_amd64.deb ...
Unpacking libcrypt-dev:amd64 (1:4.4.10-10ubuntu4) ...
Selecting previously unselected package libc6-dev:amd64.
Preparing to unpack .../13-libc6-dev_2.31-0ubuntu9.2_amd64.deb ...
Unpacking libc6-dev:amd64 (2.31-0ubuntu9.2) ...
Selecting previously unselected package manpages-dev.
Preparing to unpack .../14-manpages-dev_5.05-1_all.deb ...
Unpacking manpages-dev (5.05-1) ...
Setting up manpages-dev (5.05-1) ...
Setting up linux-libc-dev:amd64 (5.4.0-77.86) ...
Setting up libasan5:amd64 (9.3.0-17ubuntu1~20.04) ...
Setting up libquadmath0:amd64 (10.3.0-1ubuntu1~20.04) ...
Setting up libatomic1:amd64 (10.3.0-1ubuntu1~20.04) ...
Setting up libubsan1:amd64 (10.3.0-1ubuntu1~20.04) ...
Setting up libcrypt-dev:amd64 (1:4.4.10-10ubuntu4) ...
Setting up libc-dev-bin (2.31-0ubuntu9.2) ...
Setting up liblsan0:amd64 (10.3.0-1ubuntu1~20.04) ...
Setting up libitm1:amd64 (10.3.0-1ubuntu1~20.04) ...
Setting up libtsan0:amd64 (10.3.0-1ubuntu1~20.04) ...
Setting up libgcc-9-dev:amd64 (9.3.0-17ubuntu1~20.04) ...
Setting up libc6-dev:amd64 (2.31-0ubuntu9.2) ...
Setting up gcc-9 (9.3.0-17ubuntu1~20.04) ...
Setting up gcc (4:9.3.0-1ubuntu2) ...
Processing triggers for man-db (2.9.1-1) ...
Processing triggers for libc-bin (2.31-0ubuntu9.2) ...
pc-1@pc1-Precision-3630-Tower:/opt/intel/oneapi$ gcc --version
gcc (Ubuntu 9.3.0-17ubuntu1~20.04) 9.3.0
Copyright (C) 2019 Free Software Foundation, Inc.
This is free software; see the source for copying conditions. There is NO
warranty; not even for MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE.
pc-1@pc1-Precision-3630-Tower:/opt/intel/oneapi$ Moderator
```

Installing g++

Use the command "g++ --version" to find out which version is installed.
If no version is installed, use the command "sudo apt install g++".



```
pc-2@pc2:~/Downloads$ g++ --version
Command 'g++' not found, but can be installed with:
sudo apt install g++

pc-2@pc2:~/Downloads$ sudo apt install g++
Reading package lists... Done
Building dependency tree
Reading state information... Done
The following packages were automatically installed and are no longer required:
  chromium-codecs-ffmpeg-extra gstreamer1.0-vaapi libgstreamer-plugins-bad1.0-0 libva-wayland2
Use 'sudo apt autoremove' to remove them.
The following additional packages will be installed:
  g++-9 libstdc++-9-dev
Suggested packages:
  g++-multilib g++-9-multilib gcc-9-doc libstdc++-9-doc
The following NEW packages will be installed:
  g++ g++-9 libstdc++-9-dev
0 upgraded, 3 newly installed, 0 to remove and 0 not upgraded.
Need to get 10.1 MB of archives.
After this operation, 46.7 MB of additional disk space will be used.
Do you want to continue? [Y/n] Y
```

Installing Cmake

Download the Cmake source file for Linux



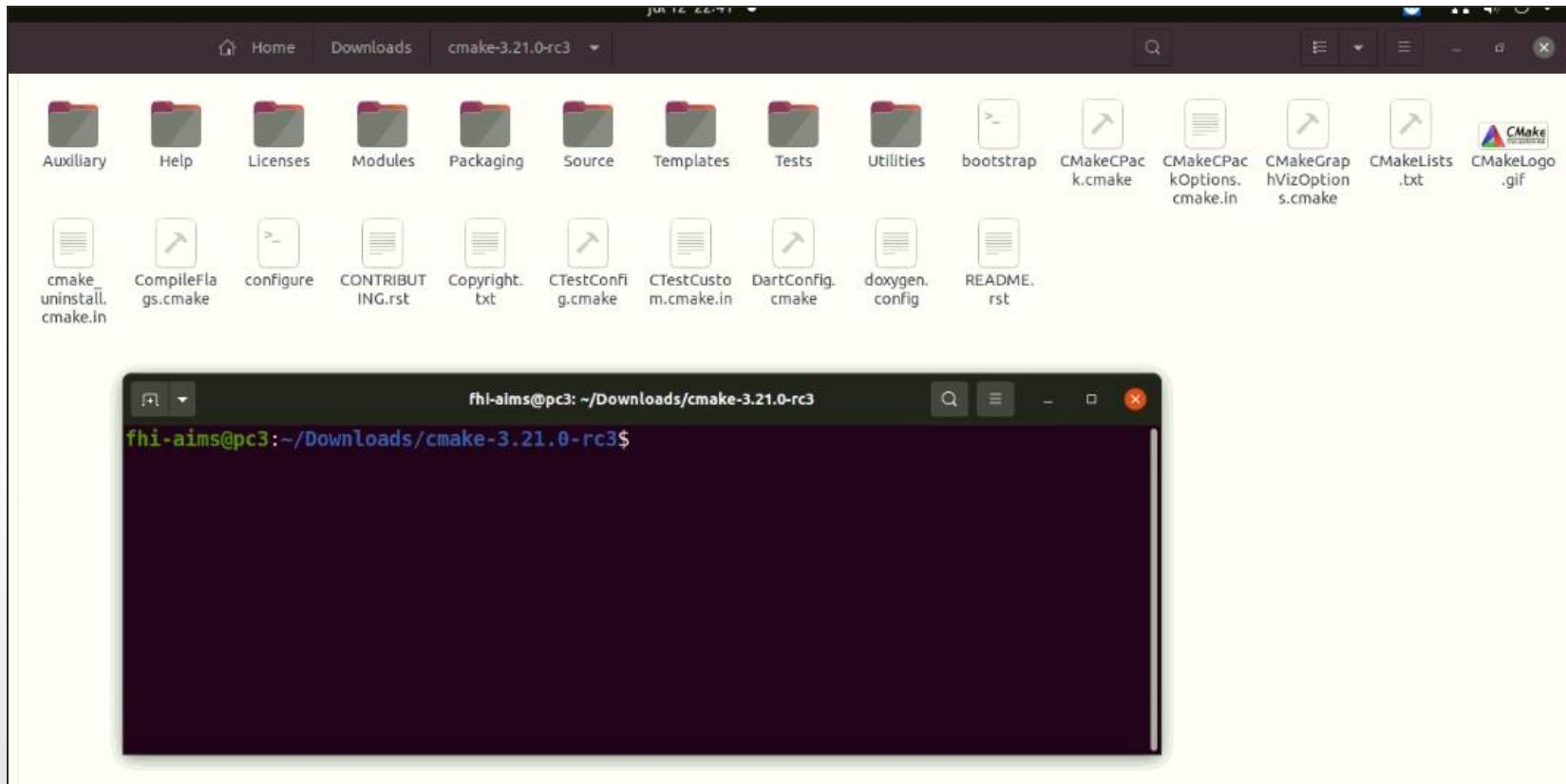
The screenshot shows a web browser window with the URL `cmake.org/download/` in the address bar. The page displays the CMake download section. On the left, there's a table with two rows: the first row has "Platform" and "Files" headers; the second row lists "Unix/Linux Source (has \n line feeds)" and a link to "cmake-3.21.0-rc3.tar.gz". The third row lists "Windows Source (has \r\n line feeds)" and a link to "cmake-3.21.0-rc3.zip". To the right of the table, there's a "KITWARE IS HIRING" banner featuring a magnifying glass icon. The browser's toolbar and menu bar are visible at the top.

Platform	Files
Unix/Linux Source (has \n line feeds)	cmake-3.21.0-rc3.tar.gz
Windows Source (has \r\n line feeds)	cmake-3.21.0-rc3.zip

KITWARE
IS HIRING

Installing Cmake

- Unzip Cmake
- Enter the unzipped folder
- Open a terminal inside the folder



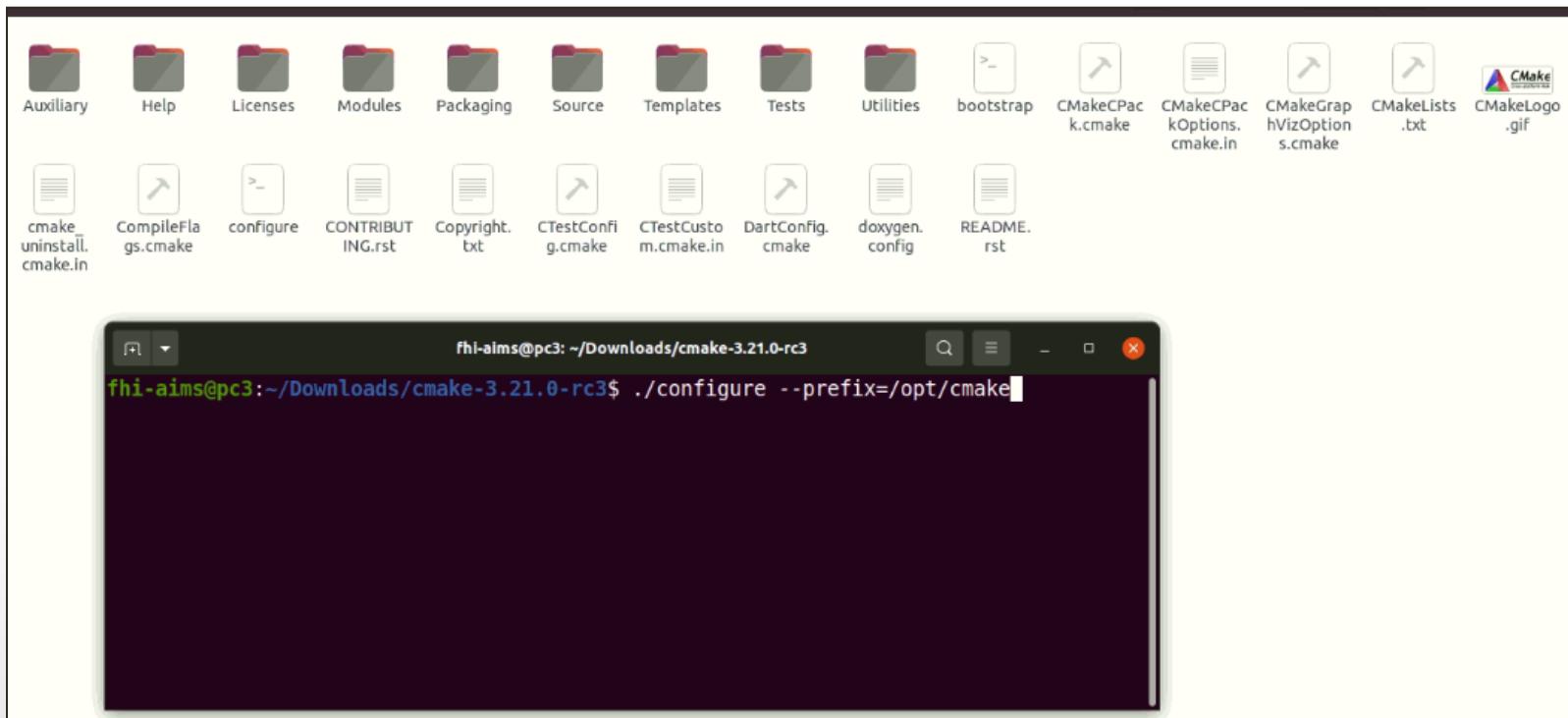
Installing Cmake

- Type the command:

```
./configure --prefix=/opt/cmake
```

***If this step fails, capture this command:
sudo apt-get install build-essential
Then try again*

Enter

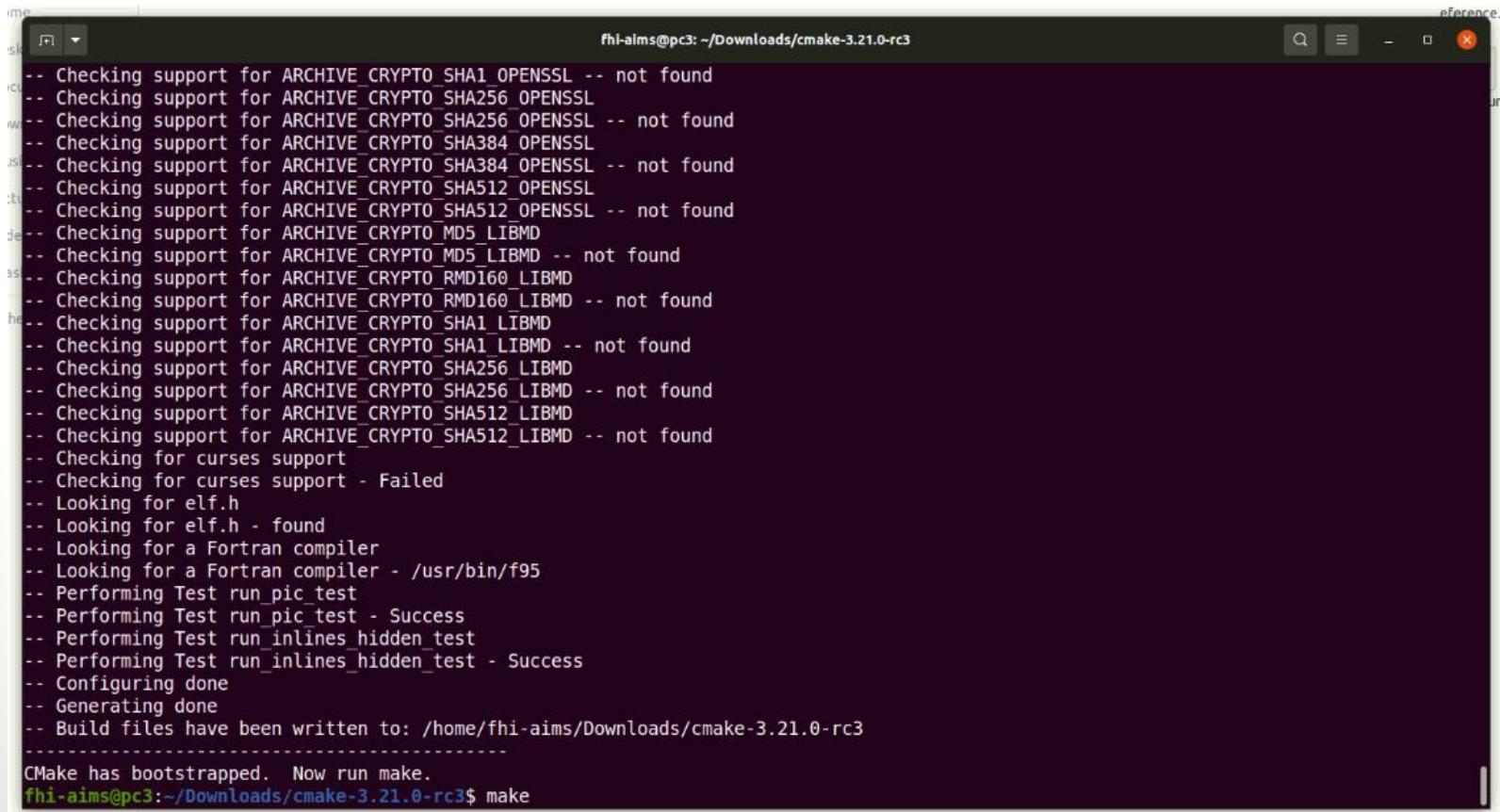


Installing Cmake

- Type the command:

make

- Enter



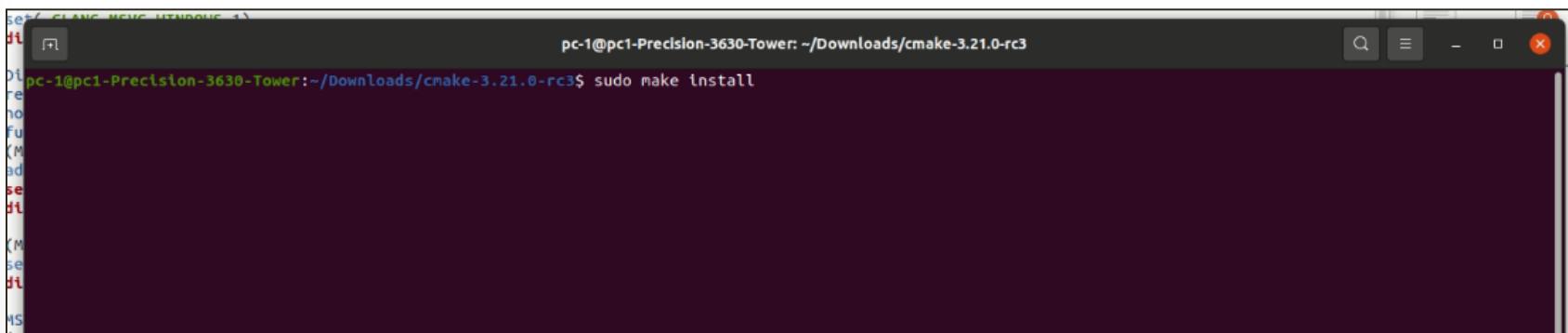
```
fhi-aims@pc3: ~/Downloads/cmake-3.21.0-rc3
-- Checking support for ARCHIVE_CRYPTO_SHA1_OPENSSL -- not found
-- Checking support for ARCHIVE_CRYPTO_SHA256_OPENSSL
-- Checking support for ARCHIVE_CRYPTO_SHA256_OPENSSL -- not found
-- Checking support for ARCHIVE_CRYPTO_SHA384_OPENSSL
-- Checking support for ARCHIVE_CRYPTO_SHA384_OPENSSL -- not found
-- Checking support for ARCHIVE_CRYPTO_SHA512_OPENSSL
-- Checking support for ARCHIVE_CRYPTO_SHA512_OPENSSL -- not found
-- Checking support for ARCHIVE_CRYPTO_MD5_LIBMD
-- Checking support for ARCHIVE_CRYPTO_MD5_LIBMD -- not found
-- Checking support for ARCHIVE_CRYPTO_RMD160_LIBMD
-- Checking support for ARCHIVE_CRYPTO_RMD160_LIBMD -- not found
-- Checking support for ARCHIVE_CRYPTO_SHA1_LIBMD
-- Checking support for ARCHIVE_CRYPTO_SHA1_LIBMD -- not found
-- Checking support for ARCHIVE_CRYPTO_SHA256_LIBMD
-- Checking support for ARCHIVE_CRYPTO_SHA256_LIBMD -- not found
-- Checking support for ARCHIVE_CRYPTO_SHA512_LIBMD
-- Checking support for ARCHIVE_CRYPTO_SHA512_LIBMD -- not found
-- Checking for curses support
-- Checking for curses support - Failed
-- Looking for elf.h
-- Looking for elf.h - found
-- Looking for a Fortran compiler
-- Looking for a Fortran compiler - /usr/bin/f95
-- Performing Test run_pic_test
-- Performing Test run_pic_test - Success
-- Performing Test run_inlines_hidden_test
-- Performing Test run_inlines_hidden_test - Success
-- Configuring done
-- Generating done
-- Build files have been written to: /home/fhi-aims/Downloads/cmake-3.21.0-rc3
-----
CMake has bootstrapped. Now run make.
fhi-aims@pc3:~/Downloads/cmake-3.21.0-rc3$ make
```

Installing Cmake

- Type the command:

```
sudo make install
```

Enter



A screenshot of a terminal window titled "pc-1@pc1-Precision-3630-Tower: ~/Downloads/cmake-3.21.0-rc3". The terminal shows the command "sudo make install" being typed at the prompt. The background of the terminal is dark, and the text is white.

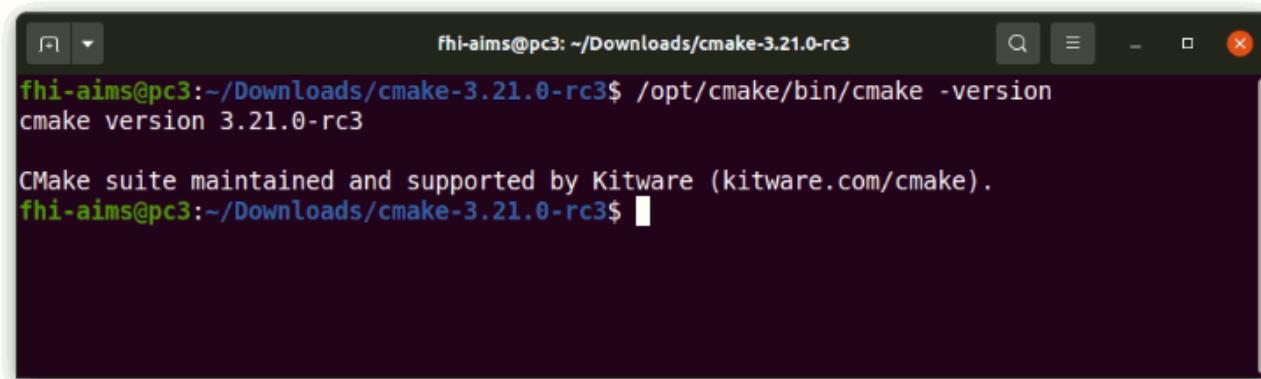
```
pc-1@pc1-Precision-3630-Tower:~/Downloads/cmake-3.21.0-rc3$ sudo make install
```

Installing Cmake

- Write the command :

/opt/cmake/bin/cmake -version

Enter



A screenshot of a terminal window titled "fhi-aims@pc3: ~/Downloads/cmake-3.21.0-rc3". The window contains the following text:

```
fhi-aims@pc3:~/Downloads/cmake-3.21.0-rc3$ /opt/cmake/bin/cmake -version
cmake version 3.21.0-rc3

CMake suite maintained and supported by Kitware (kitware.com/cmake).
fhi-aims@pc3:~/Downloads/cmake-3.21.0-rc3$ █
```

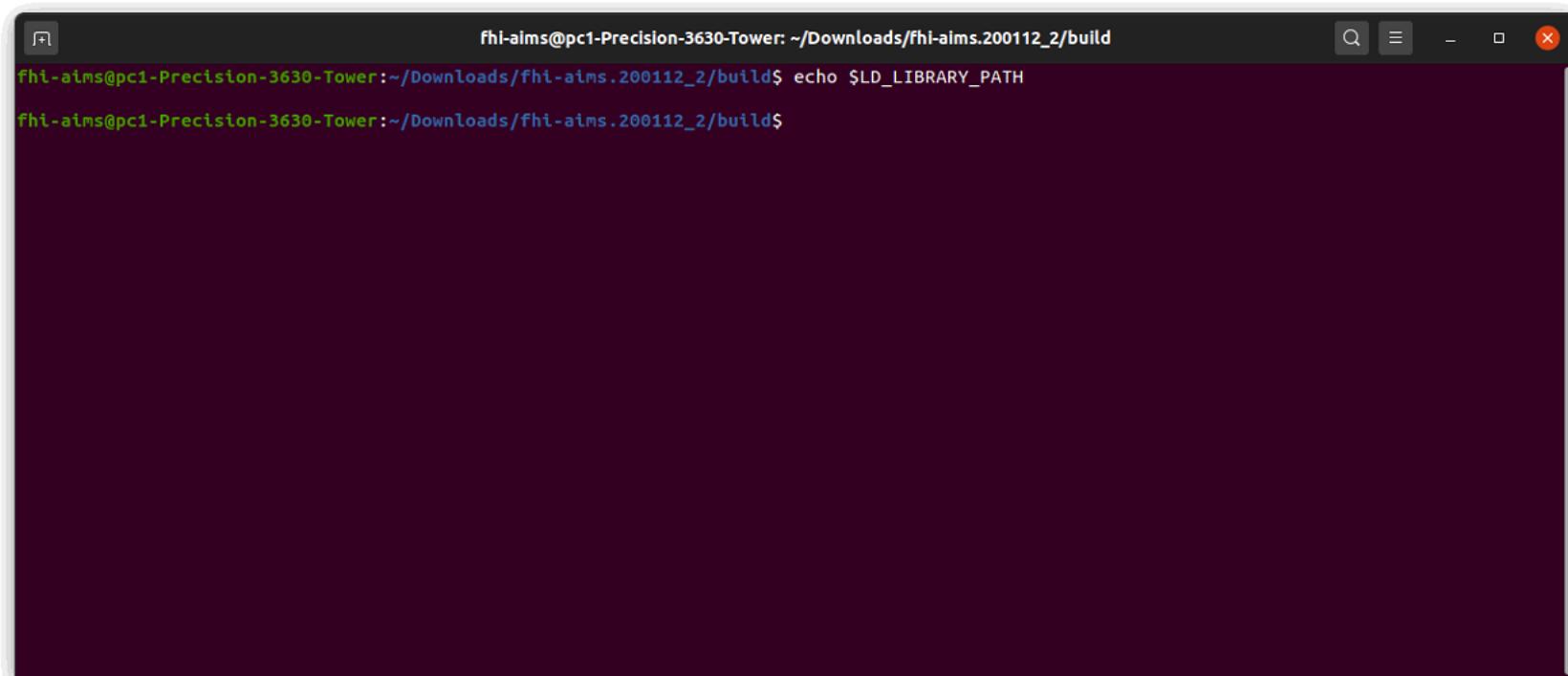
Installing Fhi-aims

Check the content of the following variable “ \$LD_LIBRARY_PATH”: executing the command:

```
echo $LD_LIBRARY_PATH
```

Enter

*if the result is too short or even empty you have to assign the values of oneAPI again to that variable as shown in the following page



A screenshot of a terminal window titled "fhi-aims@pc1-Precision-3630-Tower: ~/Downloads/fhi-aims.200112_2/build". The window shows the command "echo \$LD_LIBRARY_PATH" being typed and executed. The output is empty, indicating that the variable has not been assigned yet.

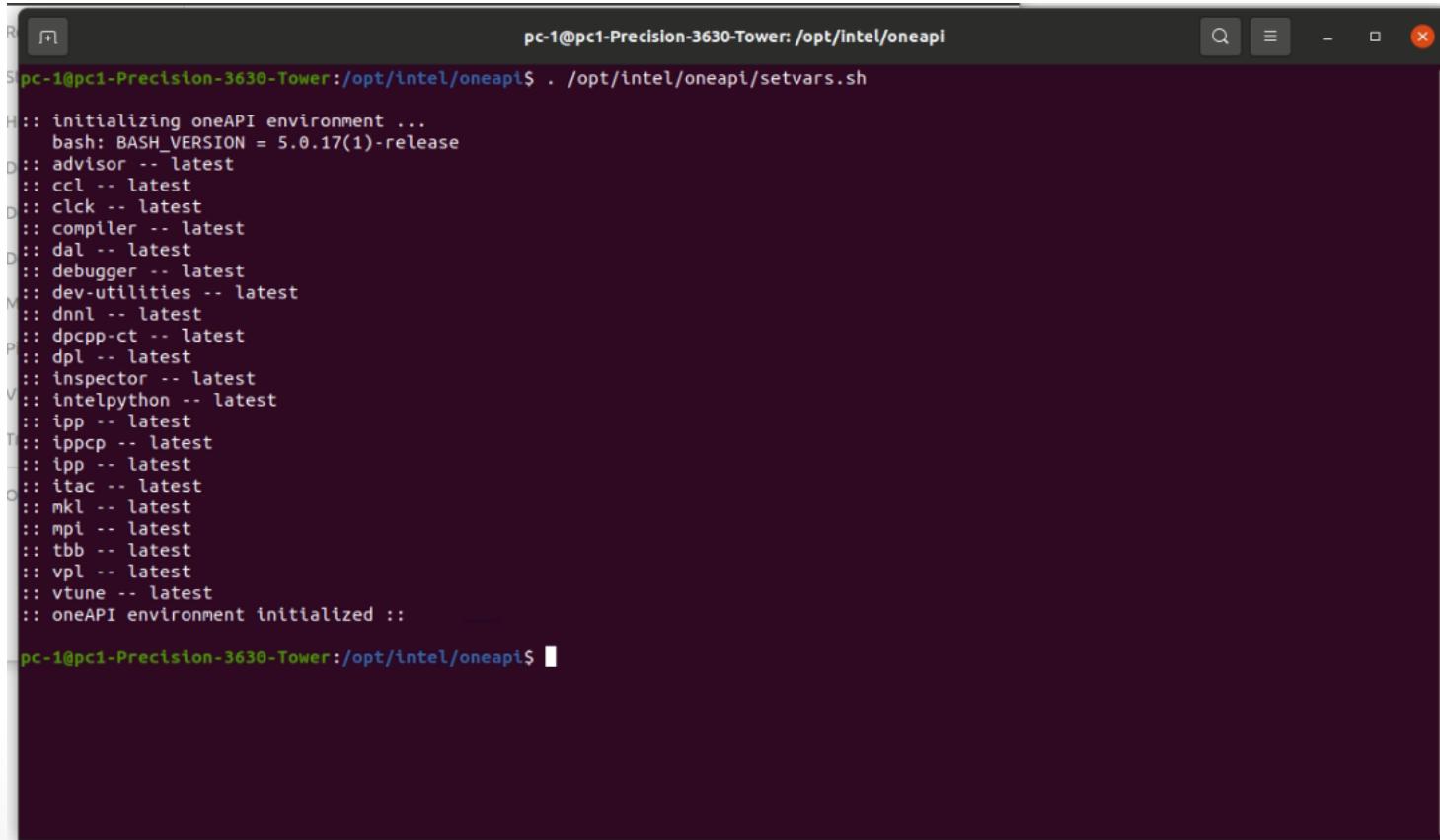
```
fhi-aims@pc1-Precision-3630-Tower:~/Downloads/fhi-aims.200112_2/build$ echo $LD_LIBRARY_PATH
fhi-aims@pc1-Precision-3630-Tower:~/Downloads/fhi-aims.200112_2/build$
```

Installing Fhi-aims

Run the command:

. /opt/intel/oneapi/setvars.sh

Enter



A screenshot of a terminal window titled "pc-1@pc1-Precision-3630-Tower: /opt/intel/oneapi". The window shows the command ". /opt/intel/oneapi/setvars.sh" being run and its output. The output is a series of environment variable assignments for various Intel oneAPI components, each preceded by a colon and followed by "latest". The components listed include advisor, ccl, clk, compiler, dal, debugger, dev-utilities, dnln, dcpp-ct, dpl, inspector, intelpython, ipp, ippcp, itac, mkl, mpi, tbb, vpl, and vtune. The final line of output is ": oneAPI environment initialized :". The terminal window has a dark background and light-colored text.

```
pc-1@pc1-Precision-3630-Tower: /opt/intel/oneapi$ . /opt/intel/oneapi/setvars.sh

:: initializing oneAPI environment ...
bash: BASH_VERSION = 5.0.17(1)-release
:: advisor -- latest
:: ccl -- latest
:: clk -- latest
:: compiler -- latest
:: dal -- latest
:: debugger -- latest
:: dev-utilities -- latest
:: dnln -- latest
:: dcpp-ct -- latest
:: dpl -- latest
:: inspector -- latest
:: intelpython -- latest
:: ipp -- latest
:: ippcp -- latest
:: ipp -- latest
:: itac -- latest
:: mkl -- latest
:: mpi -- latest
:: tbb -- latest
:: vpl -- latest
:: vtune -- latest
:: oneAPI environment initialized ::

pc-1@pc1-Precision-3630-Tower: /opt/intel/oneapi$
```

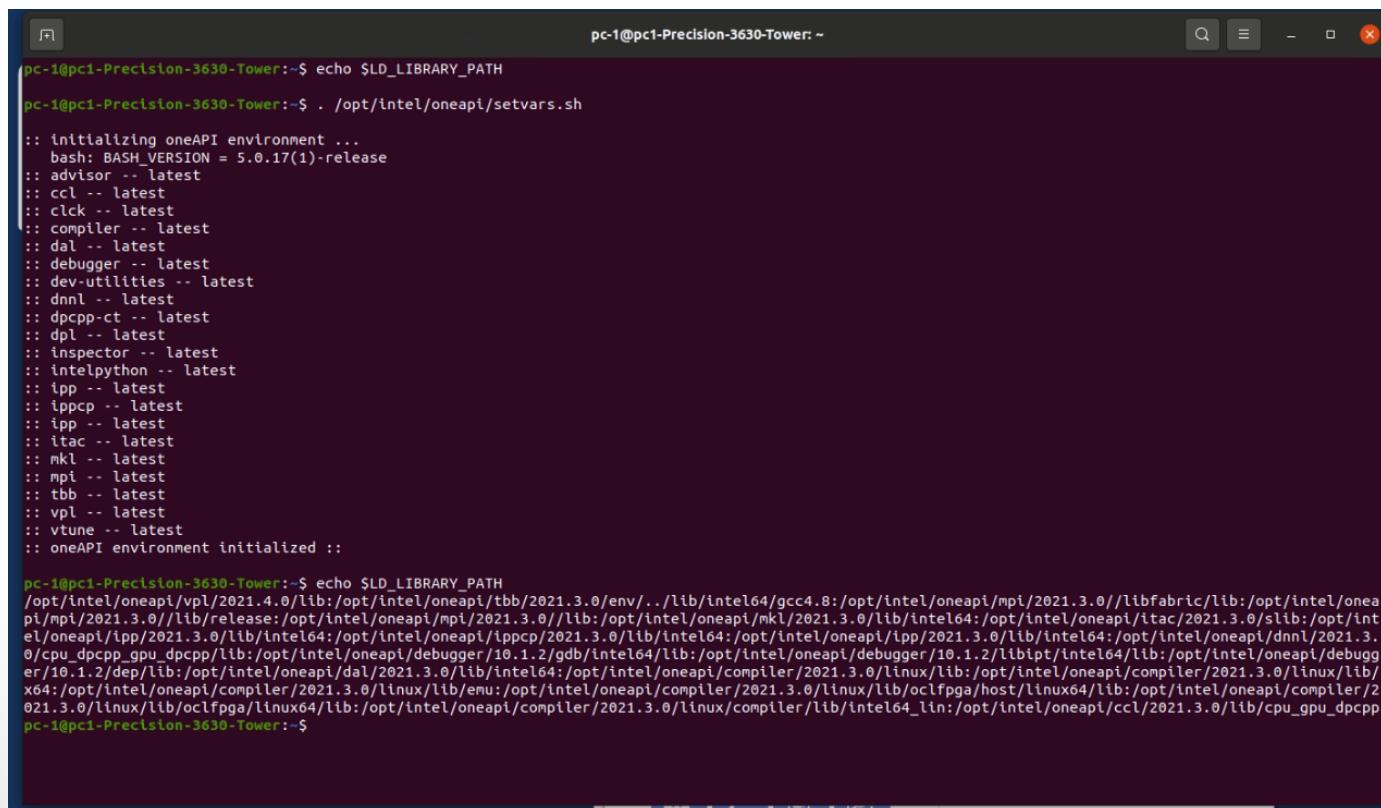
Installing Fhi-aims

Use again the command:

```
echo $LD_LIBRARY_PATH
```

Enter

*The variable has this value only for this window, if a new Terminal is opened it is necessary to load values to the variable

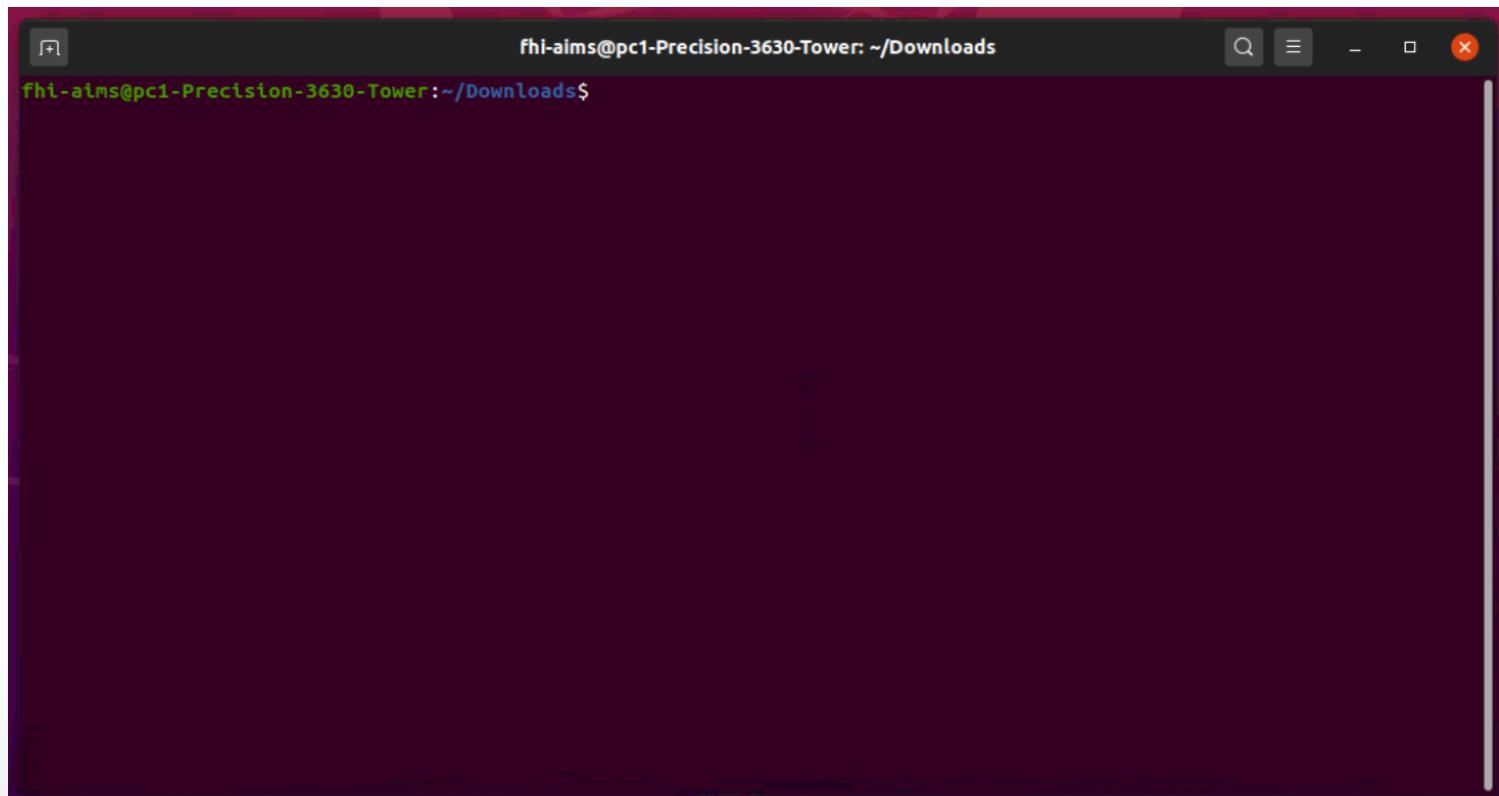


```
pc-1@pc1-Precision-3630-Tower:~$ echo $LD_LIBRARY_PATH
pc-1@pc1-Precision-3630-Tower:~$ . /opt/intel/oneapi/setvars.sh
:: initializing oneAPI environment ...
bash: BASH_VERSION = 5.0.17(1)-release
:: advisor -- latest
:: ccl -- latest
:: clk -- latest
:: compiler -- latest
:: dal -- latest
:: debugger -- latest
:: dev-utilities -- latest
:: dnnl -- latest
:: dpcpp-ct -- latest
:: dpl -- latest
:: inspector -- latest
:: intelpython -- latest
:: ipp -- latest
:: ippcc -- latest
:: ipp -- latest
:: itac -- latest
:: mkl -- latest
:: mpi -- latest
:: tbb -- latest
:: vpl -- latest
:: vtune -- latest
:: oneAPI environment initialized ::

pc-1@pc1-Precision-3630-Tower:~$ echo $LD_LIBRARY_PATH
/opt/intel/oneapi/vpl/2021.4.0/lib:/opt/intel/oneapi/tbb/2021.3.0/env/../lib/intel64/gcc4.8:/opt/intel/oneapi/mpi/2021.3.0//libfabric/lib:/opt/intel/oneapi/mpi/2021.3.0//lib/release:/opt/intel/oneapi/mpi/2021.3.0//lib:/opt/intel/oneapi/mkl/2021.3.0/lib/intel64:/opt/intel/oneapi/itac/2021.3.0/slib:/opt/intel/oneapi/ipp/2021.3.0/lib/intel64:/opt/intel/oneapi/ipp/2021.3.0/lib/dep/lib:/opt/intel/oneapi/ipp/2021.3.0/lib/intel64:/opt/intel/oneapi/ipp/2021.3.0/lib/intel64:/opt/intel/oneapi/dnnl/2021.3.0/cpu_dpcpp_gpu_dpcpp/lib:/opt/intel/oneapi/debugger/10.1.2/gdb/intel64/lib:/opt/intel/oneapi/debugger/10.1.2/liblpt/intel64/lib:/opt/intel/oneapi/debugger/10.1.2/dep/lib:/opt/intel/oneapi/dal/2021.3.0/lib/intel64:/opt/intel/oneapi/compiler/2021.3.0/linux/lib:/opt/intel/oneapi/compiler/2021.3.0/linux/lib/x64:/opt/intel/oneapi/compiler/2021.3.0/linux/lib/emu:/opt/intel/oneapi/compiler/2021.3.0/linux/lib/oclpga/host/linux64/lib:/opt/intel/oneapi/compiler/2021.3.0/linux/lib/oclpga/linux64/lib:/opt/intel/oneapi/compiler/2021.3.0/linux/compiler/lib/intel64_lin:/opt/intel/oneapi/ccl/2021.3.0/lib/cpu_dpcpp
pc-1@pc1-Precision-3630-Tower:~$
```

Installing Fhi-aims

Go to Download folder



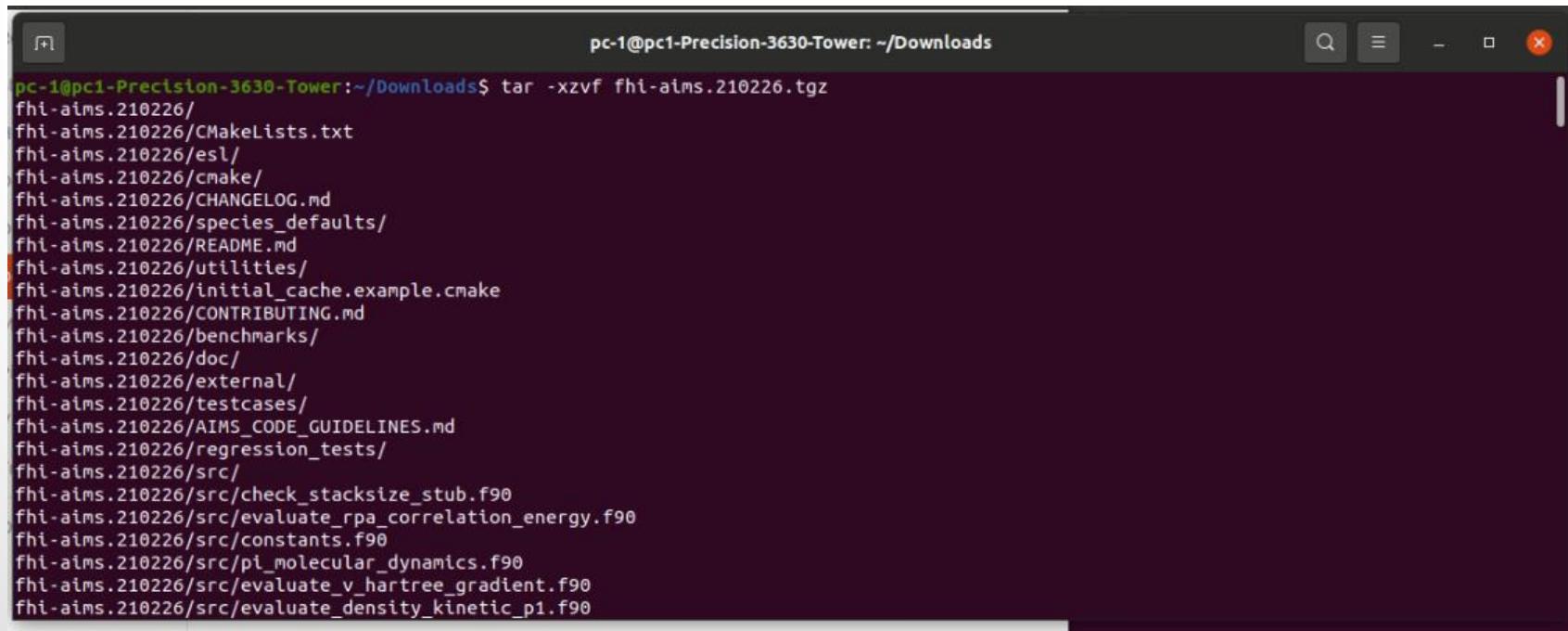
```
fhi-aims@pc1-Precision-3630-Tower: ~/Downloads$
```

Installing Fhi-aims

Unzip the fhi-aims with the following command

```
tar -xzvf fhi-aims.210226.tgz
```

Enter



A screenshot of a terminal window titled "pc-1@pc1-Precision-3630-Tower: ~/Downloads". The window shows the command "tar -xzvf fhi-aims.210226.tgz" being run, followed by a list of files extracted from the archive. The files listed include: fhi-aims.210226/, fhi-aims.210226/CMakeLists.txt, fhi-aims.210226/esl/, fhi-aims.210226/cmake/, fhi-aims.210226/CHANGELOG.md, fhi-aims.210226/species_defaults/, fhi-aims.210226/README.md, fhi-aims.210226/utilities/, fhi-aims.210226/initial_cache.example.cmake, fhi-aims.210226/CONTRIBUTING.md, fhi-aims.210226/benchmarks/, fhi-aims.210226/doc/, fhi-aims.210226/external/, fhi-aims.210226/testcases/, fhi-aims.210226/AMIS_CODE_GUIDELINES.md, fhi-aims.210226/regression_tests/, fhi-aims.210226/src/, fhi-aims.210226/src/check_stacksize_stub.f90, fhi-aims.210226/src/evaluate_rpa_correlation_energy.f90, fhi-aims.210226/src/constants.f90, fhi-aims.210226/src/pi_molecular_dynamics.f90, fhi-aims.210226/src/evaluate_v_hartree_gradient.f90, fhi-aims.210226/src/evaluate_density_kinetic_p1.f90.

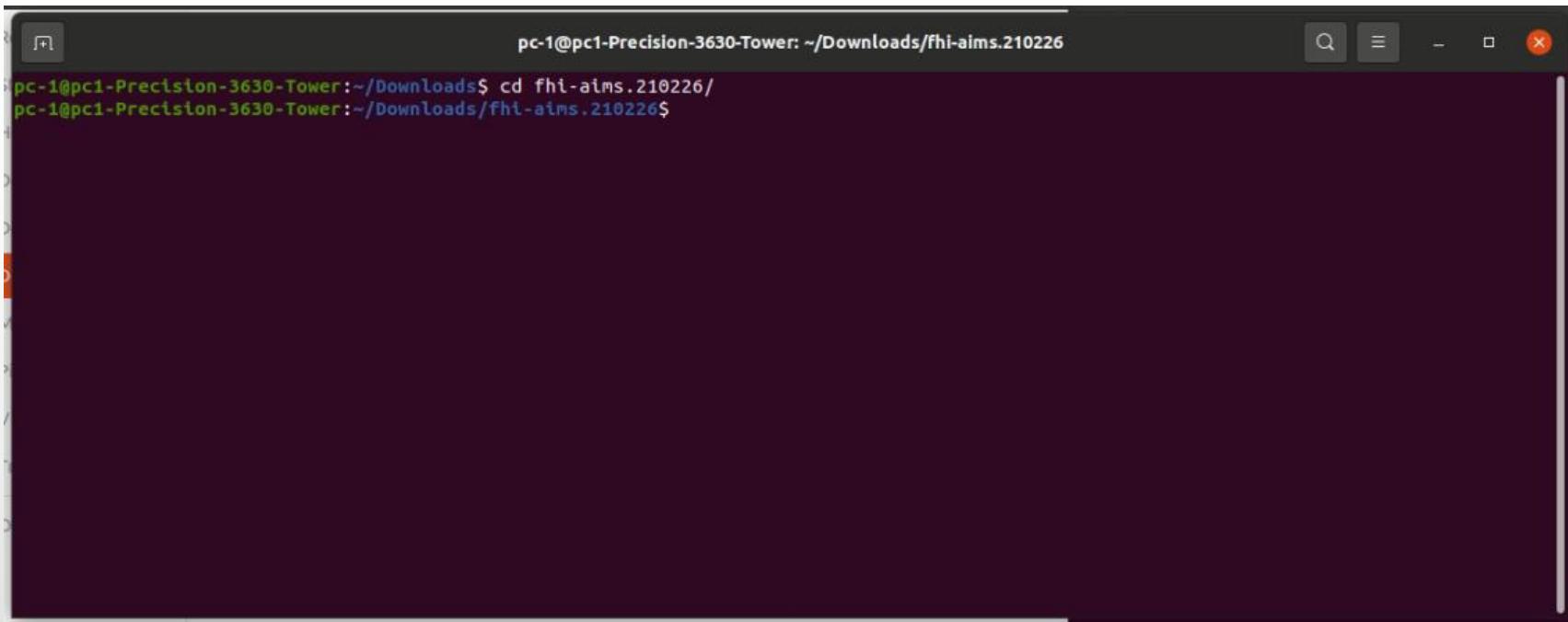
```
pc-1@pc1-Precision-3630-Tower:~/Downloads$ tar -xzvf fhi-aims.210226.tgz
fhi-aims.210226/
fhi-aims.210226/CMakeLists.txt
fhi-aims.210226/esl/
fhi-aims.210226/cmake/
fhi-aims.210226/CHANGELOG.md
fhi-aims.210226/species_defaults/
fhi-aims.210226/README.md
fhi-aims.210226/utilities/
fhi-aims.210226/initial_cache.example.cmake
fhi-aims.210226/CONTRIBUTING.md
fhi-aims.210226/benchmarks/
fhi-aims.210226/doc/
fhi-aims.210226/external/
fhi-aims.210226/testcases/
fhi-aims.210226/AMIS_CODE_GUIDELINES.md
fhi-aims.210226/regression_tests/
fhi-aims.210226/src/
fhi-aims.210226/src/check_stacksize_stub.f90
fhi-aims.210226/src/evaluate_rpa_correlation_energy.f90
fhi-aims.210226/src/constants.f90
fhi-aims.210226/src/pi_molecular_dynamics.f90
fhi-aims.210226/src/evaluate_v_hartree_gradient.f90
fhi-aims.210226/src/evaluate_density_kinetic_p1.f90
```

Installing Fhi-aims

Enter the unzipped folder with the following command

```
cd fhi-aims.210226/
```

Enter



A screenshot of a terminal window titled "pc-1@pc1-Precision-3630-Tower: ~/Downloads/fhi-aims.210226". The window shows the command "cd fhi-aims.210226/" being typed at the prompt. The terminal has a dark background with light-colored text. The title bar and window controls are visible at the top.

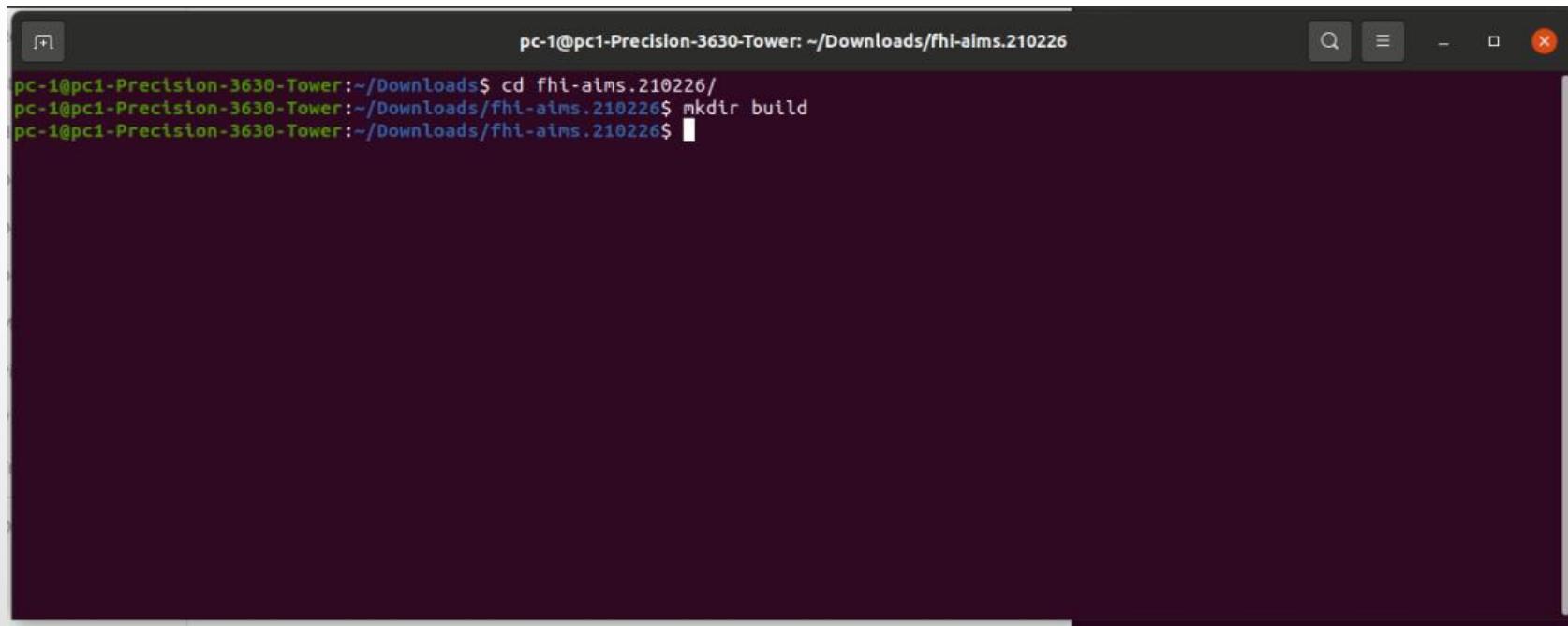
```
pc-1@pc1-Precision-3630-Tower:~/Downloads/fhi-aims.210226$ cd fhi-aims.210226/
pc-1@pc1-Precision-3630-Tower:~/Downloads/fhi-aims.210226$
```

Installing Fhi-aims

Create a folder called "build" with the command

`mkdir build`

Enter



A screenshot of a Linux terminal window titled "pc-1@pc1-Precision-3630-Tower: ~/Downloads/fhi-aims.210226". The terminal shows the following command being run:

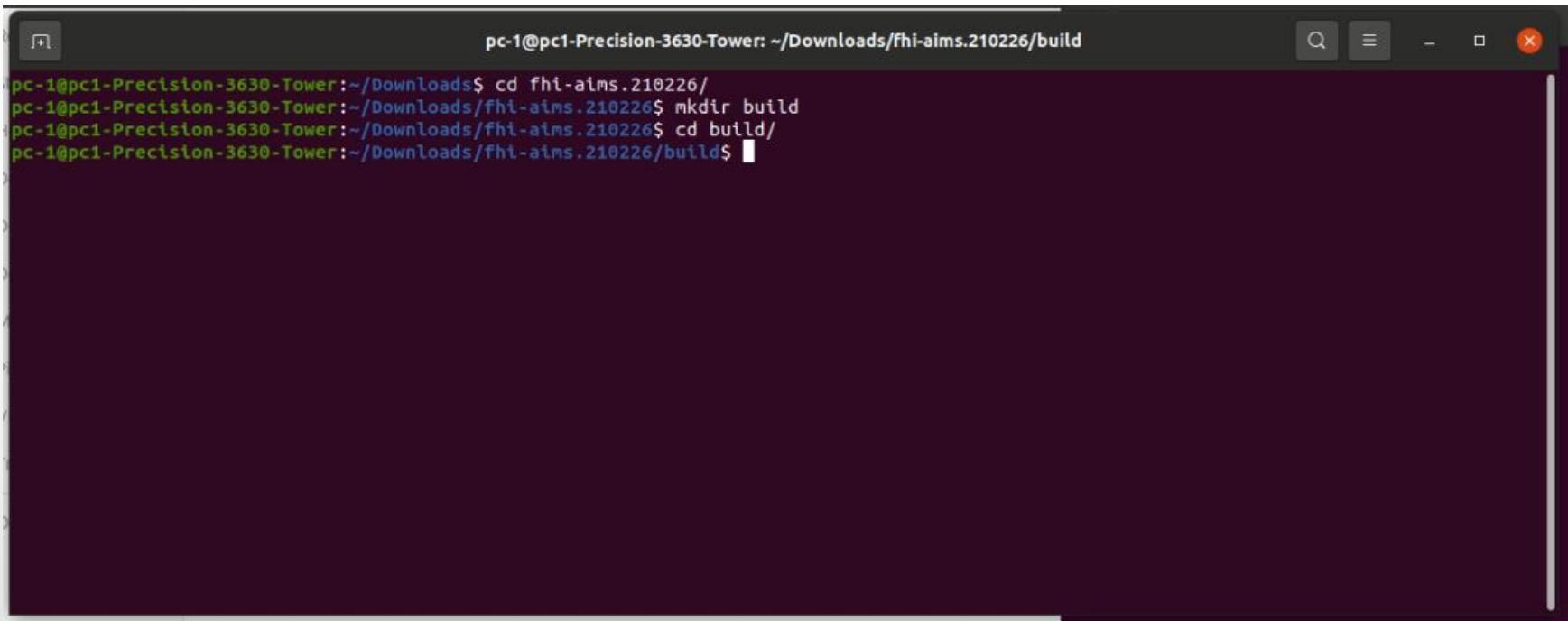
```
pc-1@pc1-Precision-3630-Tower:~/Downloads$ cd fhi-aims.210226/
pc-1@pc1-Precision-3630-Tower:~/Downloads/fhi-aims.210226$ mkdir build
pc-1@pc1-Precision-3630-Tower:~/Downloads/fhi-aims.210226$ █
```

Installing Fhi-aims

Enter the "build" folder with the following command

cd build

Enter



A screenshot of a terminal window titled "pc-1@pc1-Precision-3630-Tower: ~/Downloads/fhi-aims.210226/build". The window shows a command-line interface with a dark background and light-colored text. The user has typed the command "cd build" and is awaiting the system's response.

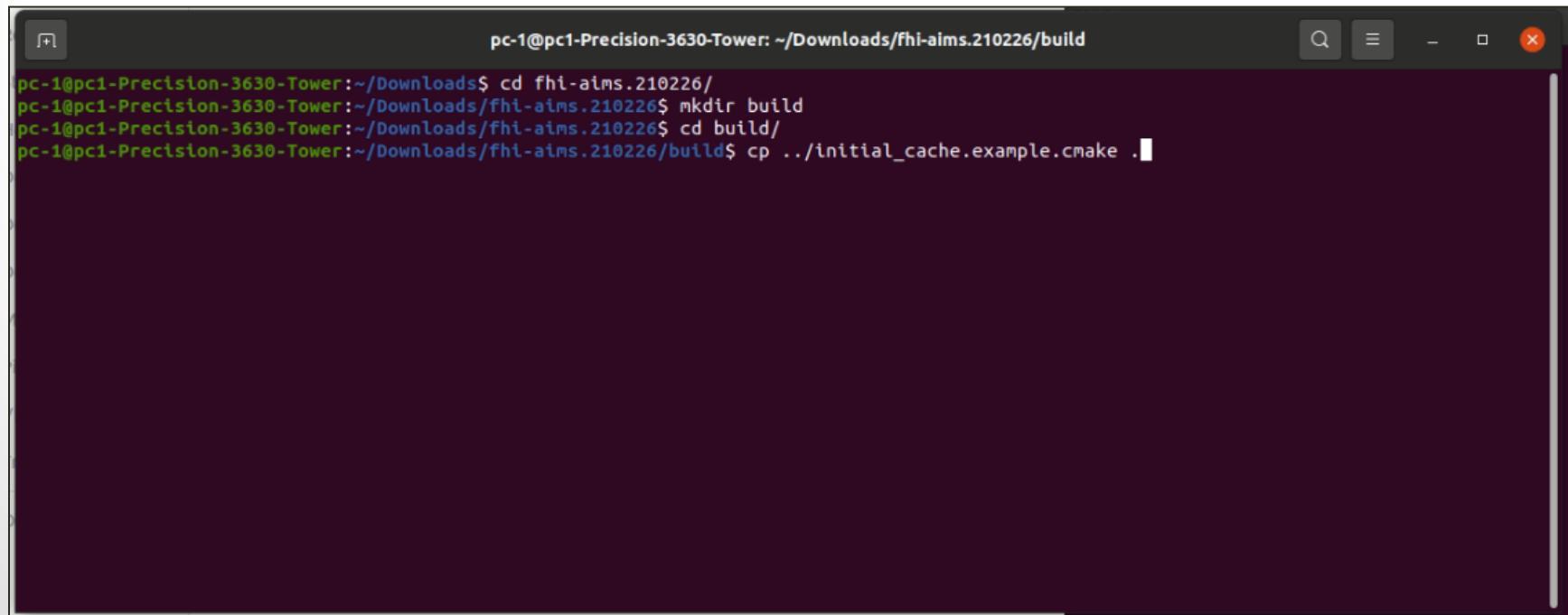
```
pc-1@pc1-Precision-3630-Tower:~/Downloads/fhi-aims.210226/build
pc-1@pc1-Precision-3630-Tower:~/Downloads/fhi-aims.210226$ mkdir build
pc-1@pc1-Precision-3630-Tower:~/Downloads/fhi-aims.210226$ cd build/
pc-1@pc1-Precision-3630-Tower:~/Downloads/fhi-aims.210226/build$ █
```

Installing Fhi-aims

Copy from the above folder the example file named "initial_cache.example.cmake" with the command:

```
cp ./initial_cache.example.cmake .
```

Enter



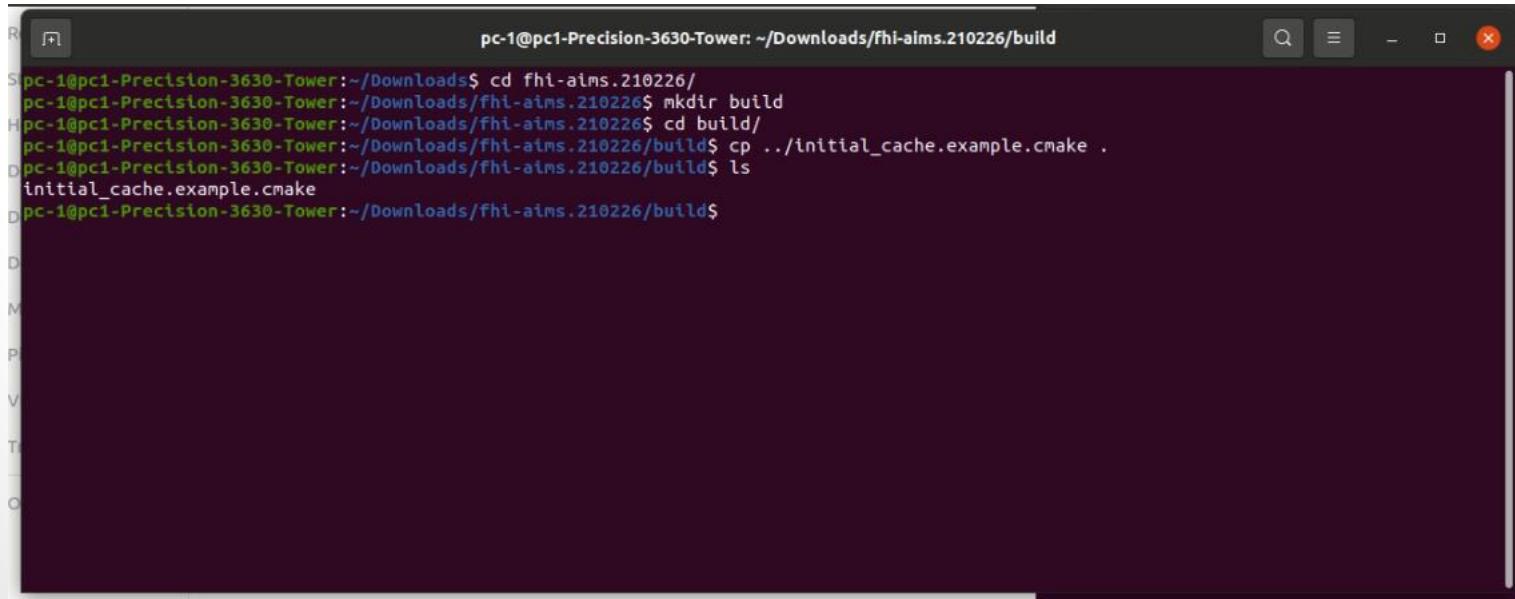
```
pc-1@pc1-Precision-3630-Tower: ~/Downloads/fhi-aims.210226/build
pc-1@pc1-Precision-3630-Tower:~/Downloads/fhi-aims.210226$ cd fhi-aims.210226/
pc-1@pc1-Precision-3630-Tower:~/Downloads/fhi-aims.210226$ mkdir build
pc-1@pc1-Precision-3630-Tower:~/Downloads/fhi-aims.210226$ cd build/
pc-1@pc1-Precision-3630-Tower:~/Downloads/fhi-aims.210226/build$ cp ../initial_cache.example.cmake .
```

Installing Fhi-aims

Verify that the file is in our folder with the command

ls

Enter



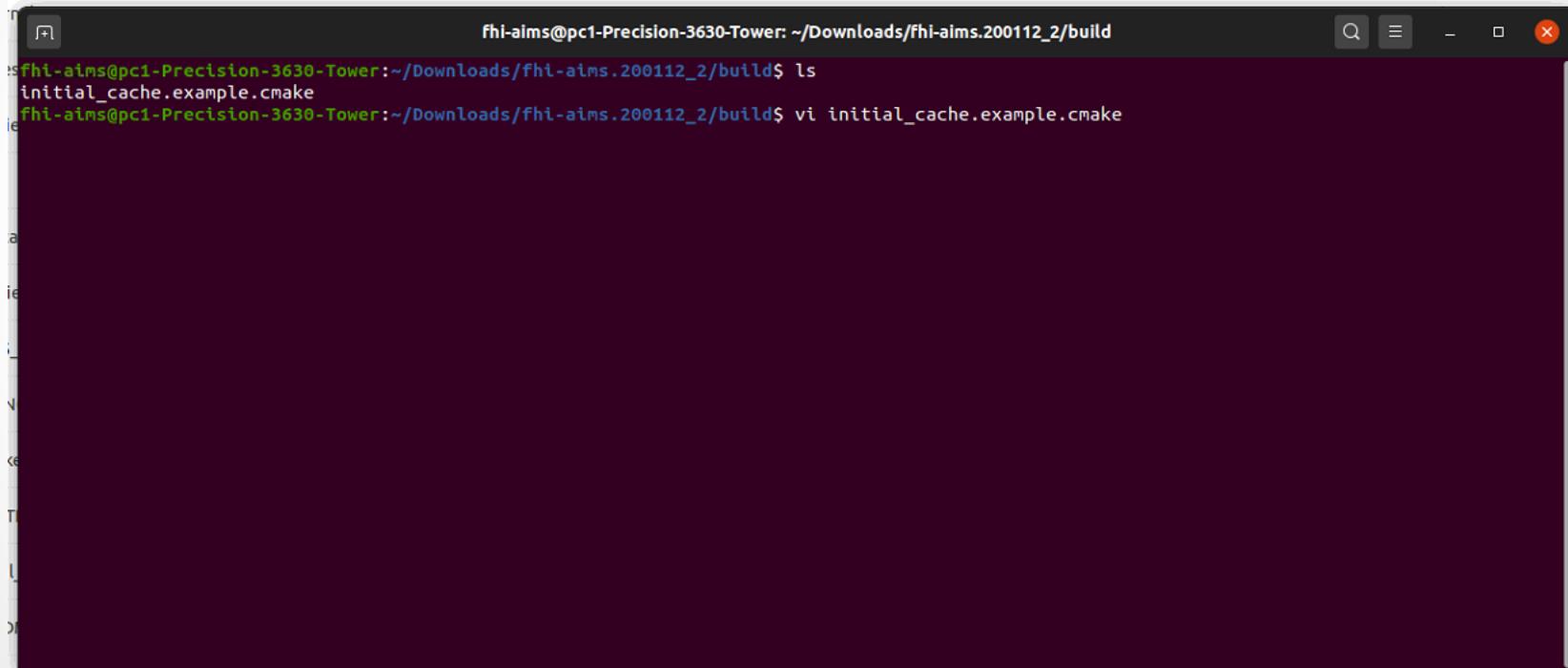
```
pc-1@pc1-Precision-3630-Tower: ~/Downloads/fhi-aims.210226/build
pc-1@pc1-Precision-3630-Tower:~/Downloads/fhi-aims.210226$ mkdir build
pc-1@pc1-Precision-3630-Tower:~/Downloads/fhi-aims.210226$ cd build/
pc-1@pc1-Precision-3630-Tower:~/Downloads/fhi-aims.210226/build$ cp ../initial_cache.example.cmake .
pc-1@pc1-Precision-3630-Tower:~/Downloads/fhi-aims.210226/build$ ls
initial_cache.example.cmake
pc-1@pc1-Precision-3630-Tower:~/Downloads/fhi-aims.210226/build$
```

Installing Fhi-aims

Enter the copied file with the "vi" editor which is native to all Linux kernels.

vi initial_cache.example.cmake

Enter



```
fhi-aims@pc1-Precision-3630-Tower: ~/Downloads/fhi-aims.200112_2/build$ ls  
initial_cache.example.cmake  
fhi-aims@pc1-Precision-3630-Tower:~/Downloads/fhi-aims.200112_2/build$ vi initial_cache.example.cmake
```

Installing Fhi-aims

```
#####
# Fortran Flags      #
#####
set(CMAKE_Fortran_COMPILER "mpiifort" CACHE STRING "")
set(CMAKE_Fortran_FLAGS "-O3 -ip -fp-model precise" CACHE STRING "")

#####
# Library Flags      #
#####
set(LIB_PATHS "/opt/intel/oneapi/mkl/2021.3.0/lib/intel64" CACHE STRING "")
set(LIBS "mkl_intel_lp64 mkl_sequential mkl_core mkl_blacs_intelmpi_lp64 mkl_scalapack_lp64" CACHE STRING "")

#####
# C Flags      #
#####
set(CMAKE_C_COMPILER "mpiicc" CACHE STRING "")
set(CMAKE_C_FLAGS "-O3 -ip -fp-model precise" CACHE STRING "")
set(USE_C_FILES ON CACHE BOOL "")

#####
# C++ Flags      #
#####
set(CMAKE_CXX_COMPILER "mpiicpc" CACHE STRING "")
set(CMAKE_CXX_FLAGS "-O3 -ip -fp-model precise" CACHE STRING "")
set(USE_CXX_FILES ON CACHE BOOL "")

#####
# Parallelization Library Flags      #
#####
set(USE_MPI ON CACHE BOOL "")
set(USE_SCALAPACK ON CACHE BOOL "")

#####
# Optional Library Flags      #
#####
set(USE_SPGLIB ON CACHE BOOL "")
set(USE_LIBXC ON CACHE BOOL "")
set(USE_RLSY ON CACHE BOOL "")
set(USE_HDF5 OFF CACHE BOOL "")

#####
# Experimental      #
#####
# GPU Acceleration Flags      #
#####
#set(USE_CUDA ON CACHE BOOL "")
#set(CMAKE_CUDA_COMPILER nvcc CACHE STRING "")
#set(CMAKE_CUDA_FLAGS "-O3 -DAdd_ -arch=sm_60 -lcublas" CACHE STRING "")
#set(ENABLE_CUDA_BY_DEFAULT ON CACHE BOOL "")
```

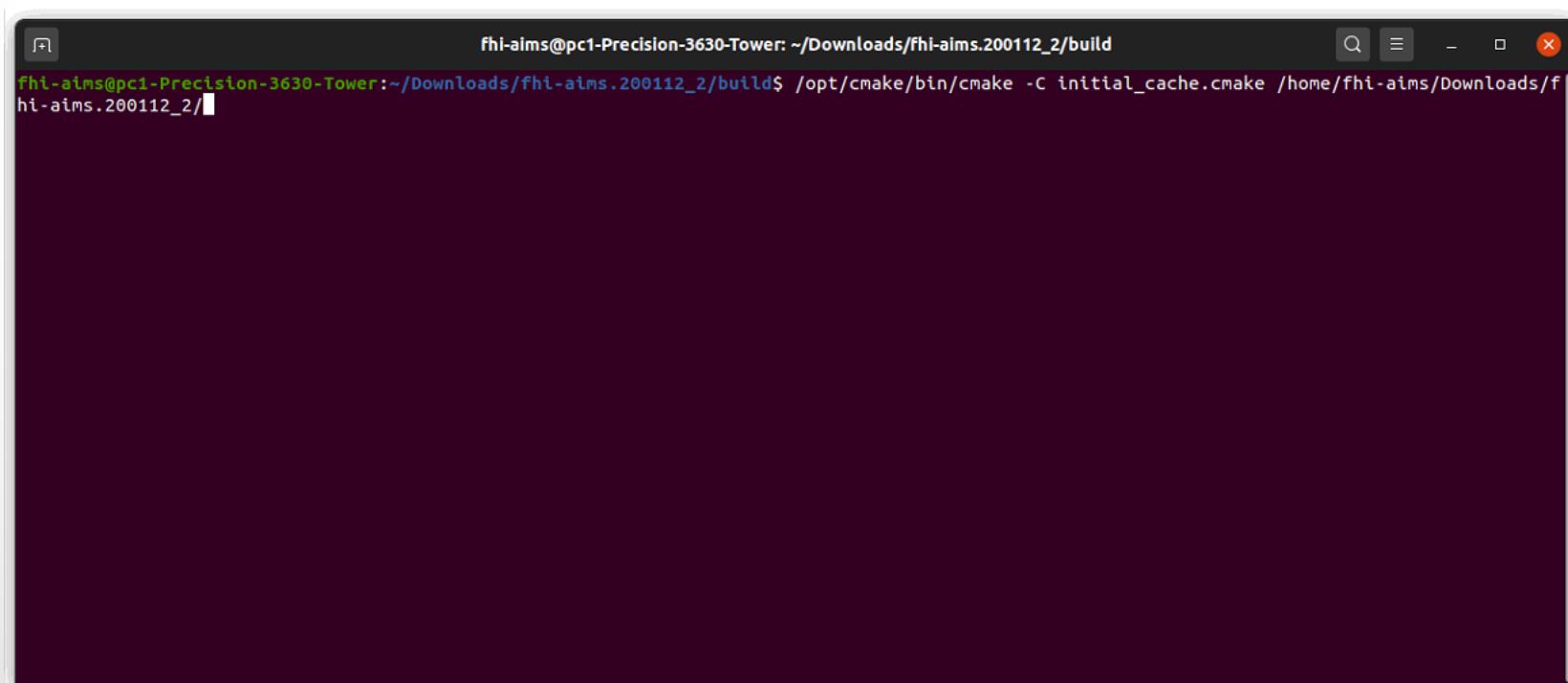
Load the displayed values
into the file and save.

Installing Fhi-aims

Collect the information to be used by the fhi-aims software with the command:

```
/opt/cmake/bin/cmake -C initial_cache.example.cmake /home/fhi-aims/Downloads/fhi-aims.200112_2/
```

Enter

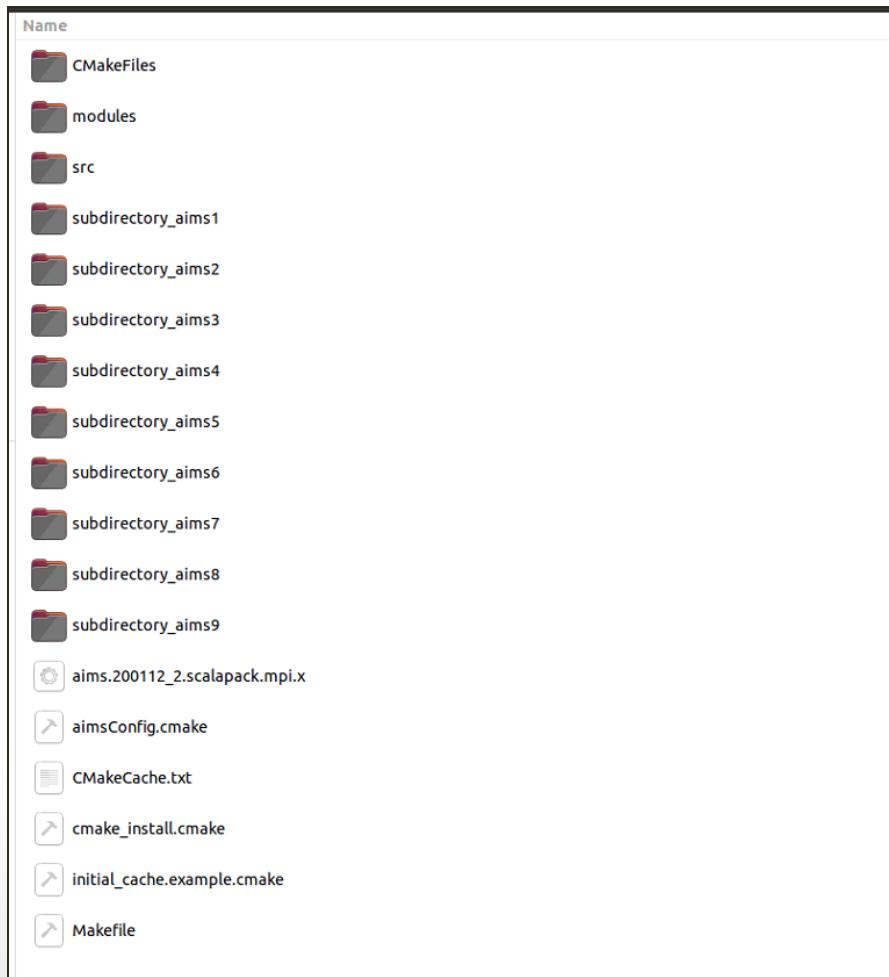


A screenshot of a terminal window titled "fhi-aims@pc1-Precision-3630-Tower: ~/Downloads/fhi-aims.200112_2/build". The terminal is dark-themed. The command entered is "/opt/cmake/bin/cmake -C initial_cache.example.cmake /home/fhi-aims/Downloads/fhi-aims.200112_2/". The cursor is visible at the end of the command line.

```
fhi-aims@pc1-Precision-3630-Tower:~/Downloads/fhi-aims.200112_2/build$ /opt/cmake/bin/cmake -C initial_cache.example.cmake /home/fhi-aims/Downloads/fhi-aims.200112_2/
```

Installing Fhi-aims

The .make file configuration must have created the following folders



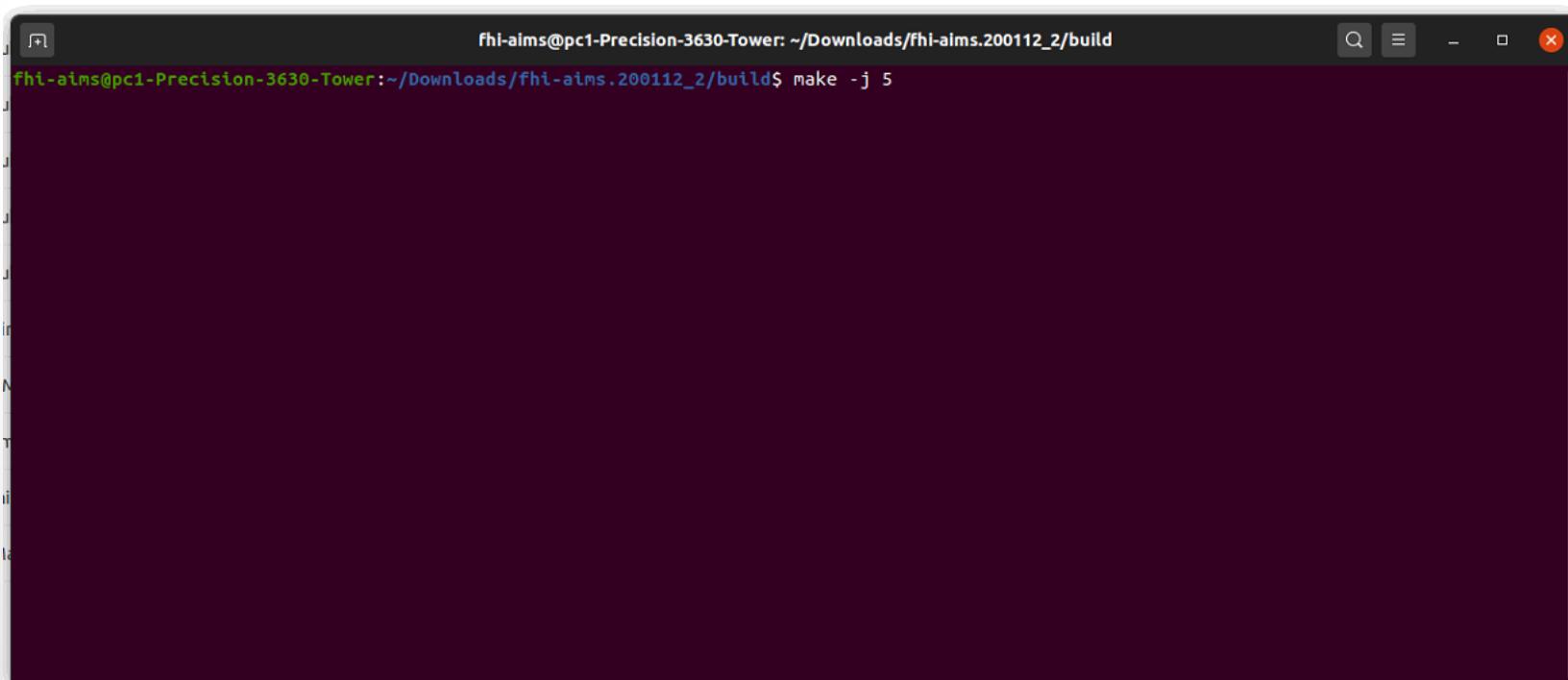
Installing Fhi-aims

Compile the software with the command:

make -j 5

*** NOT run "sudo make -j 5" because it fails

* 5 means that it will use 5 cores. It can be varied from 1 to the total cores of the PC or node.



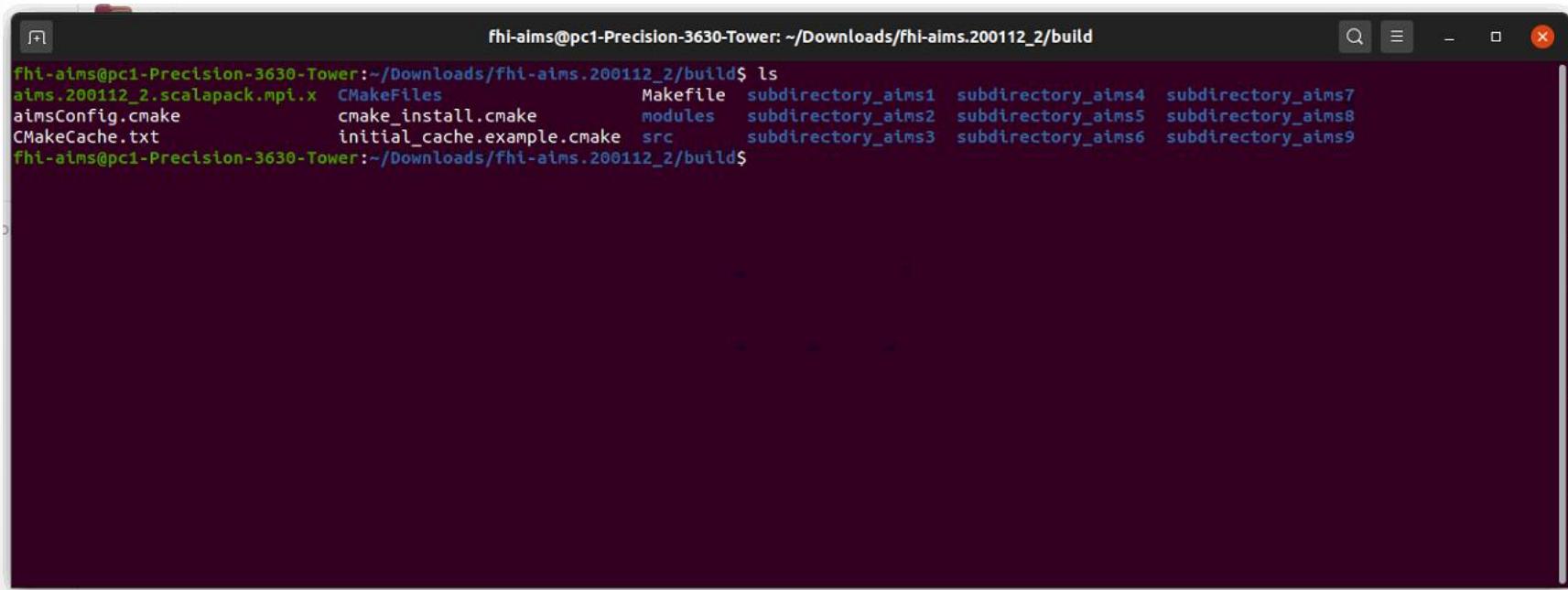
A screenshot of a terminal window titled "fhi-aims@pc1-Precision-3630-Tower: ~/Downloads/fhi-aims.200112_2/build". The terminal shows the command "make -j 5" being typed at the prompt. The window has a dark background and a light-colored title bar. The terminal text is white on a dark background.

```
fhi-aims@pc1-Precision-3630-Tower:~/Downloads/fhi-aims.200112_2/build$ make -j 5
```

Installing Fhi-aims

The compilation process created an executable file named

aims.200112_2.scalapack.mpi.x



```
fhi-aims@pc1-Precision-3630-Tower:~/Downloads/fhi-aims.200112_2/build$ ls
aims.200112_2.scalapack.mpi.x  CMakeFiles           Makefile  subdirectory_aims1  subdirectory_aims4  subdirectory_aims7
aimsConfig.cmake                cmake_install.cmake  modules   subdirectory_aims2  subdirectory_aims5  subdirectory_aims8
CMakeCache.txt                  initial_cache.example.cmake  src      subdirectory_aims3  subdirectory_aims6  subdirectory_aims9
fhi-aims@pc1-Precision-3630-Tower:~/Downloads/fhi-aims.200112_2/build$
```

Installing Fhi-aims

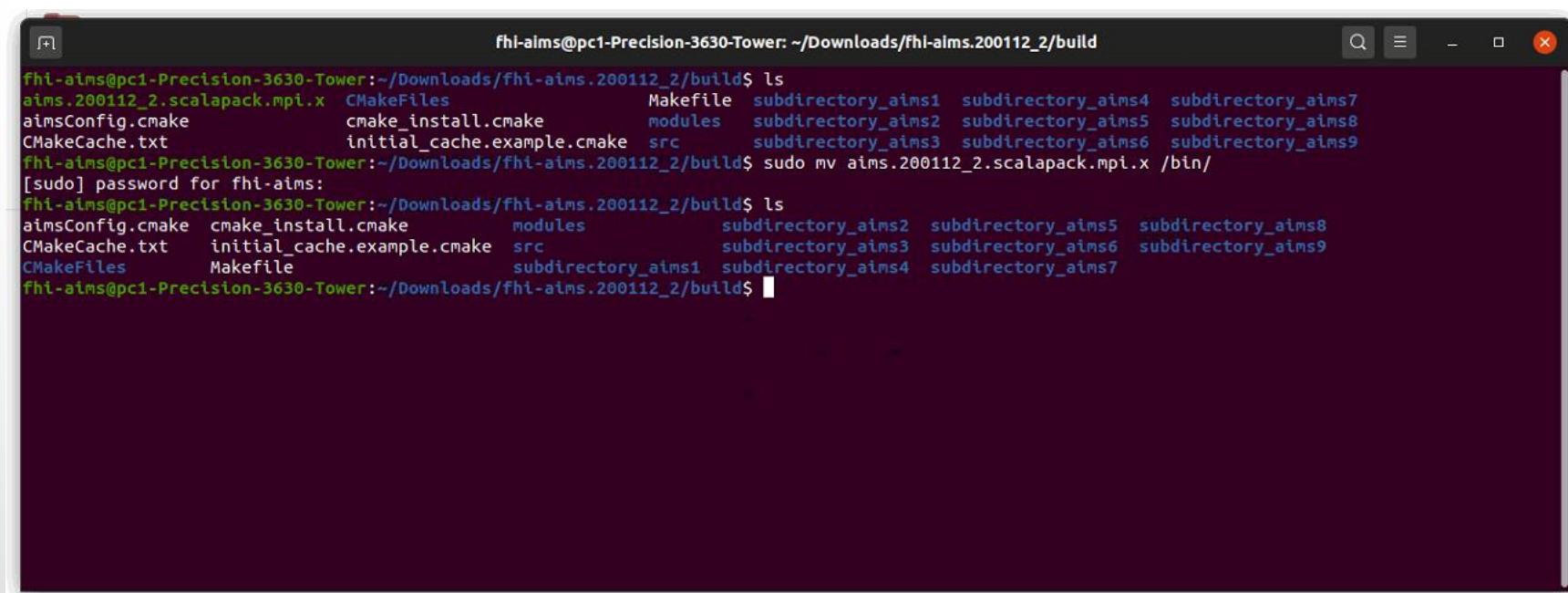
Move it to the /bin folder of the operating system with the command

```
sudo mv aims.210226.scalapack.mpi.x /bin/
```

Enter

Administrator Password

Enter



The screenshot shows a terminal window titled "fhi-aims@pc1-Precision-3630-Tower: ~/Downloads/fhi-aims.200112_2/build". The terminal displays the following commands and output:

```
fhi-aims@pc1-Precision-3630-Tower:~/Downloads/fhi-aims.200112_2/build$ ls
aims.200112_2.scalapack.mpi.x  CMakeFiles          Makefile    subdirectory_aims1  subdirectory_aims4  subdirectory_aims7
aimsConfig.cmake                cmake_install.cmake  modules     subdirectory_aims2  subdirectory_aims5  subdirectory_aims8
CMakeCache.txt                  initial_cache.example.cmake  src        subdirectory_aims3  subdirectory_aims6  subdirectory_aims9
fhi-aims@pc1-Precision-3630-Tower:~/Downloads/fhi-aims.200112_2/build$ sudo mv aims.200112_2.scalapack.mpi.x /bin/
[sudo] password for fhi-aims:
fhi-aims@pc1-Precision-3630-Tower:~/Downloads/fhi-aims.200112_2/build$ ls
aimsConfig.cmake    cmake_install.cmake      modules           subdirectory_aims2  subdirectory_aims5  subdirectory_aims8
CMakeCache.txt      initial_cache.example.cmake  src            subdirectory_aims3  subdirectory_aims6  subdirectory_aims9
CMakeFiles          Makefile              subdirectory_aims1  subdirectory_aims4  subdirectory_aims7
fhi-aims@pc1-Precision-3630-Tower:~/Downloads/fhi-aims.200112_2/build$
```

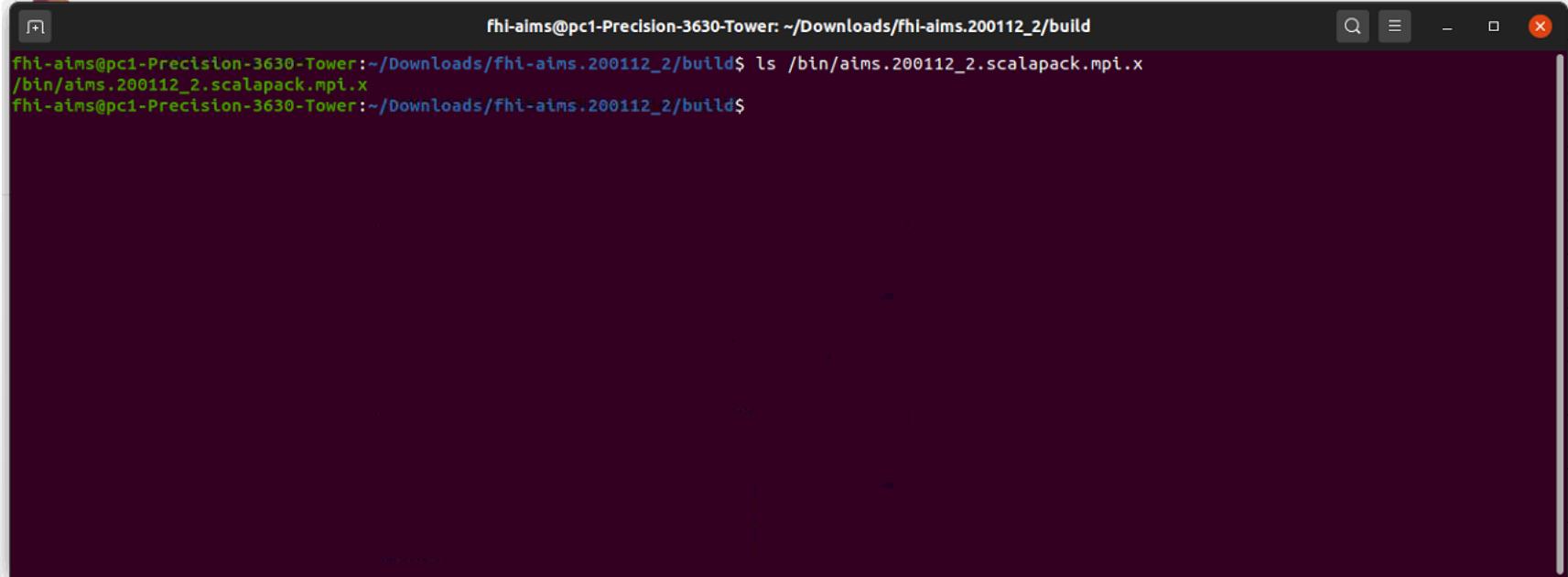
Installing Fhi-aims

Check that the executable is in the /bin folder.

```
ls /bin/aims.200112_2.scalapack.mpi.x
```

Enter

The application must appear in the requested list.



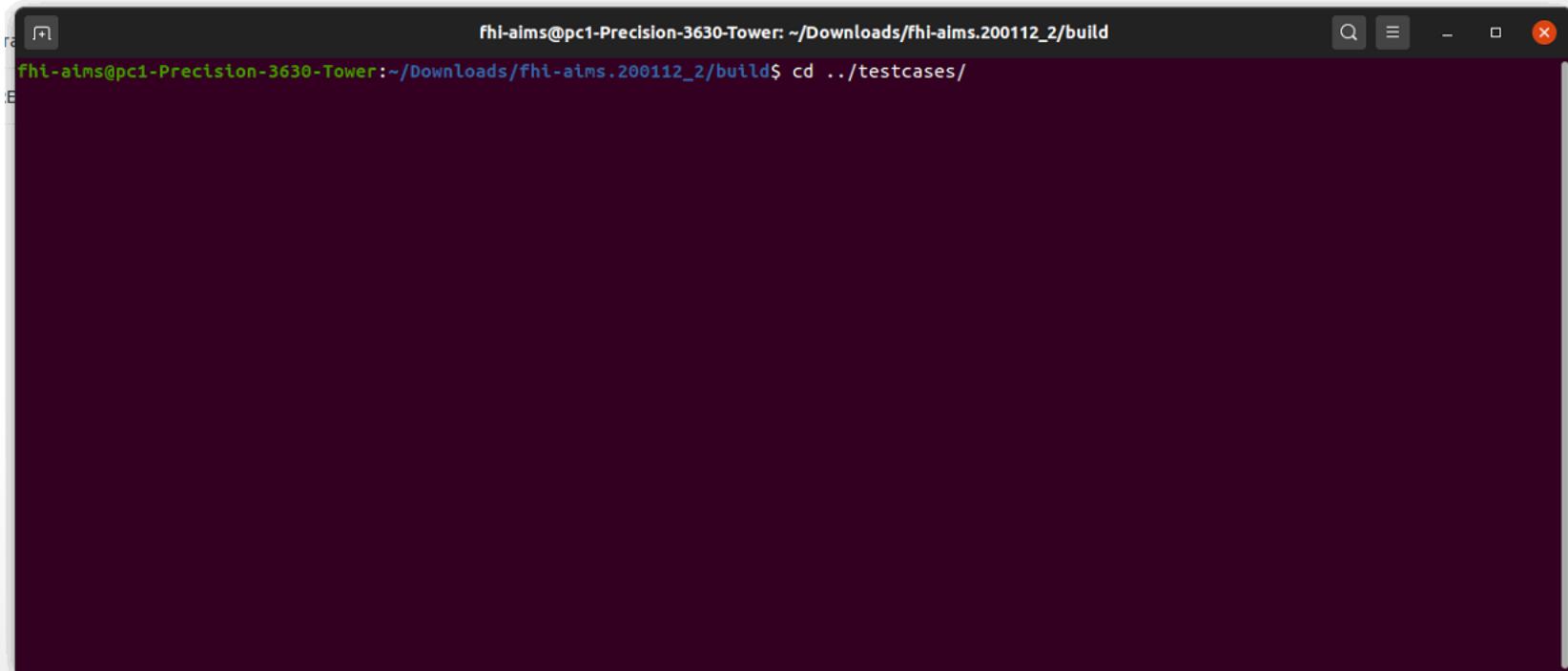
```
fhi-aims@pc1-Precision-3630-Tower: ~/Downloads/fhi-aims.200112_2/build
fhi-aims@pc1-Precision-3630-Tower:~/Downloads/fhi-aims.200112_2/build$ ls /bin/aims.200112_2.scalapack.mpi.x
/bin/aims.200112_2.scalapack.mpi.x
fhi-aims@pc1-Precision-3630-Tower:~/Downloads/fhi-aims.200112_2/build$
```

Fhi-aims: test case

Go from the "build" folder to the "testcases" folder with the following command:

```
cd ../testcases/
```

Enter



A screenshot of a terminal window titled "ra". The title bar shows the path: "fhi-aims@pc1-Precision-3630-Tower: ~/Downloads/fhi-aims.200112_2/build". The main area of the terminal shows the command "cd ..testcases/" being typed. The terminal has a dark background with light-colored text.

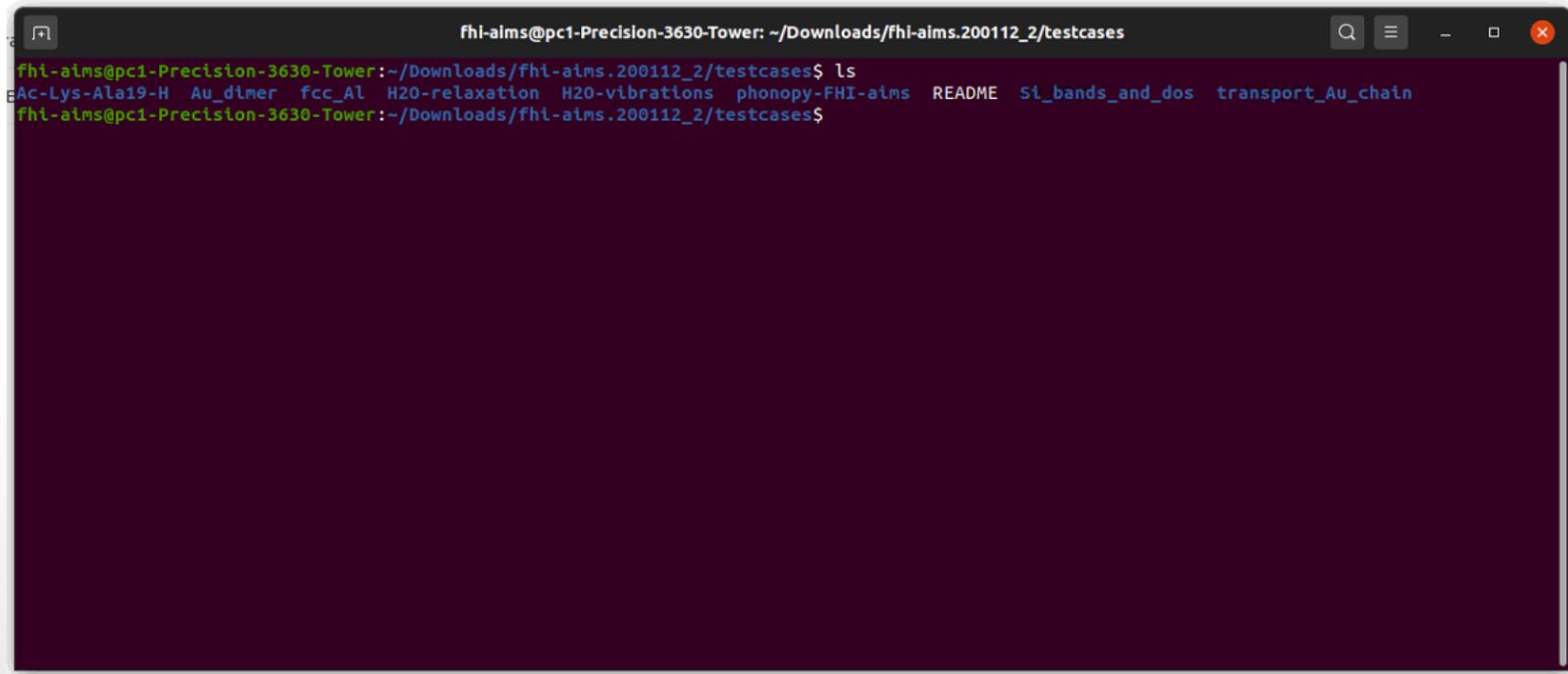
```
fhi-aims@pc1-Precision-3630-Tower:~/Downloads/fhi-aims.200112_2/build$ cd ..testcases/  
E
```

Fhi-aims: test case

Check the contents of the folder with the command:

ls

Enter



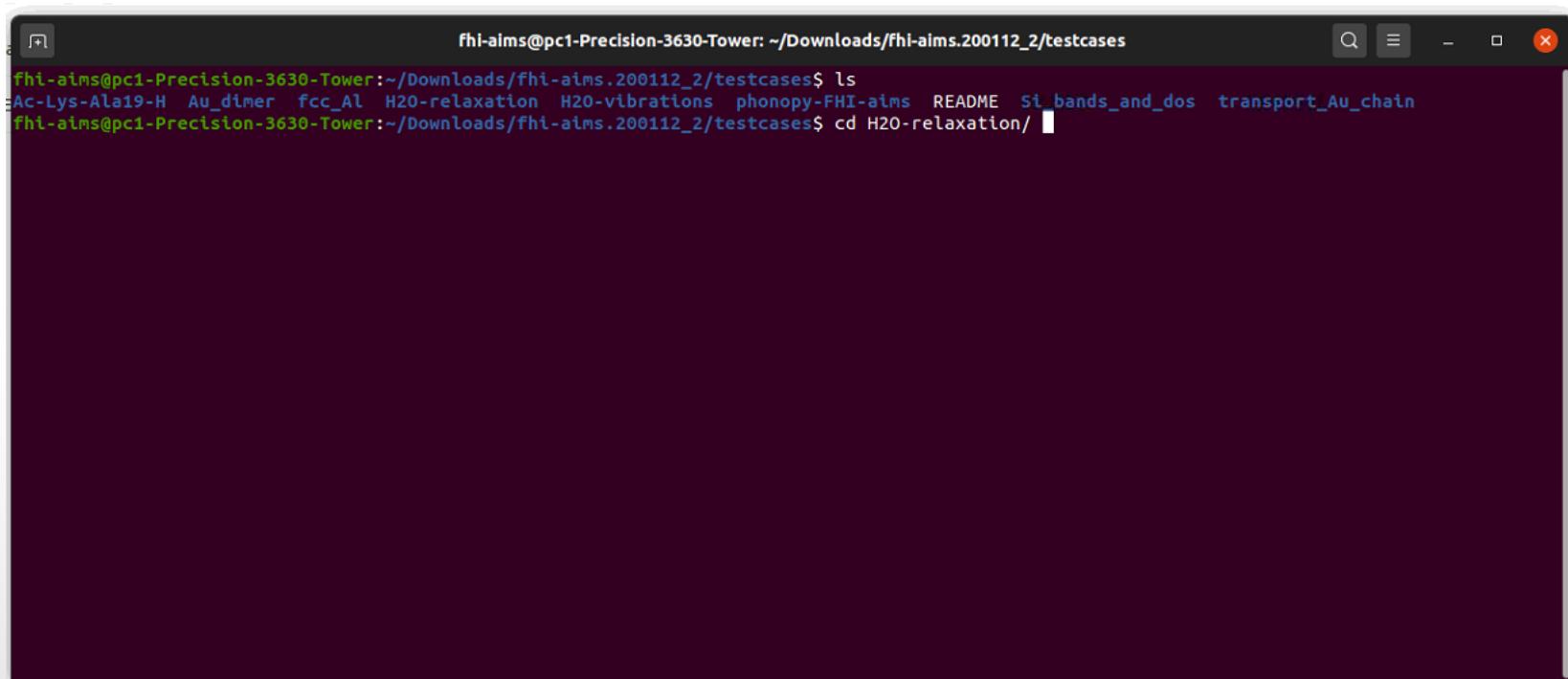
```
fhi-aims@pc1-Precision-3630-Tower: ~/Downloads/fhi-aims.200112_2/testcases$ ls
Ac-Lys-Ala19-H Au_dimer fcc_Al H2O-relaxation H2O-vibrations phonopy-FHI-aims README si_bands_and_dos transport_Au_chain
fhi-aims@pc1-Precision-3630-Tower:~/Downloads/fhi-aims.200112_2/testcases$
```

Fhi-aims: test case

As a first example, enter the H2O-relaxation folder with the following command

```
cd H2O-relaxation
```

Enter

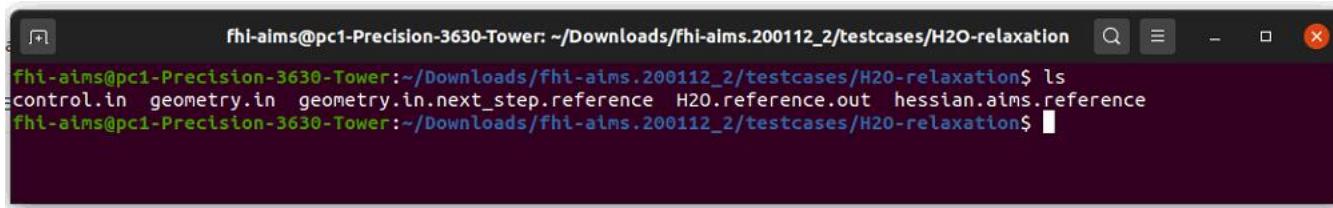


A screenshot of a terminal window titled "fhi-aims@pc1-Precision-3630-Tower: ~/Downloads/fhi-aims.200112_2/testcases". The window shows the output of the "ls" command, listing several directories and files: "Ac-Lys-Ala19-H", "Au_dimer", "fcc_Al", "H2O-relaxation", "H2O-vibrations", "phonopy-FHI-aims", "README", "Si_bands_and_dos", and "transport_Au_chain". Below this, the command "cd H2O-relaxation/" is entered at the prompt. The terminal has a dark background with light-colored text and standard Linux-style window controls.

```
fhi-aims@pc1-Precision-3630-Tower:~/Downloads/fhi-aims.200112_2/testcases$ ls
Ac-Lys-Ala19-H  Au_dimer  fcc_Al   H2O-relaxation  H2O-vibrations  phonopy-FHI-aims  README  Si_bands_and_dos  transport_Au_chain
fhi-aims@pc1-Precision-3630-Tower:~/Downloads/fhi-aims.200112_2/testcases$ cd H2O-relaxation/
```

Fhi-aims: test case

- This folder contains input and output files, which were calculated by the team programming the fhi-aims software.
- The intention is to run our own calculation and compare against theirs.

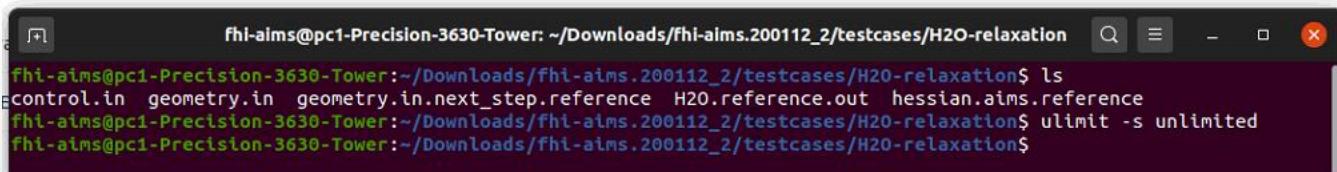


```
fhi-aims@pc1-Precision-3630-Tower: ~/Downloads/fhi-aims.200112_2/testcases/H2O-relaxation$ ls
control.in  geometry.in  geometry.in.next_step.reference  H2O.reference.out  hessian.aims.reference
fhi-aims@pc1-Precision-3630-Tower:~/Downloads/fhi-aims.200112_2/testcases/H2O-relaxation$
```

Before running the calculation it is necessary to execute the following command

ulimit -s unlimited

Enter



```
fhi-aims@pc1-Precision-3630-Tower: ~/Downloads/fhi-aims.200112_2/testcases/H2O-relaxation$ ls
control.in  geometry.in  geometry.in.next_step.reference  H2O.reference.out  hessian.aims.reference
fhi-aims@pc1-Precision-3630-Tower:~/Downloads/fhi-aims.200112_2/testcases/H2O-relaxation$ ulimit -s unlimited
fhi-aims@pc1-Precision-3630-Tower:~/Downloads/fhi-aims.200112_2/testcases/H2O-relaxation$
```

Fhi-aims: test case

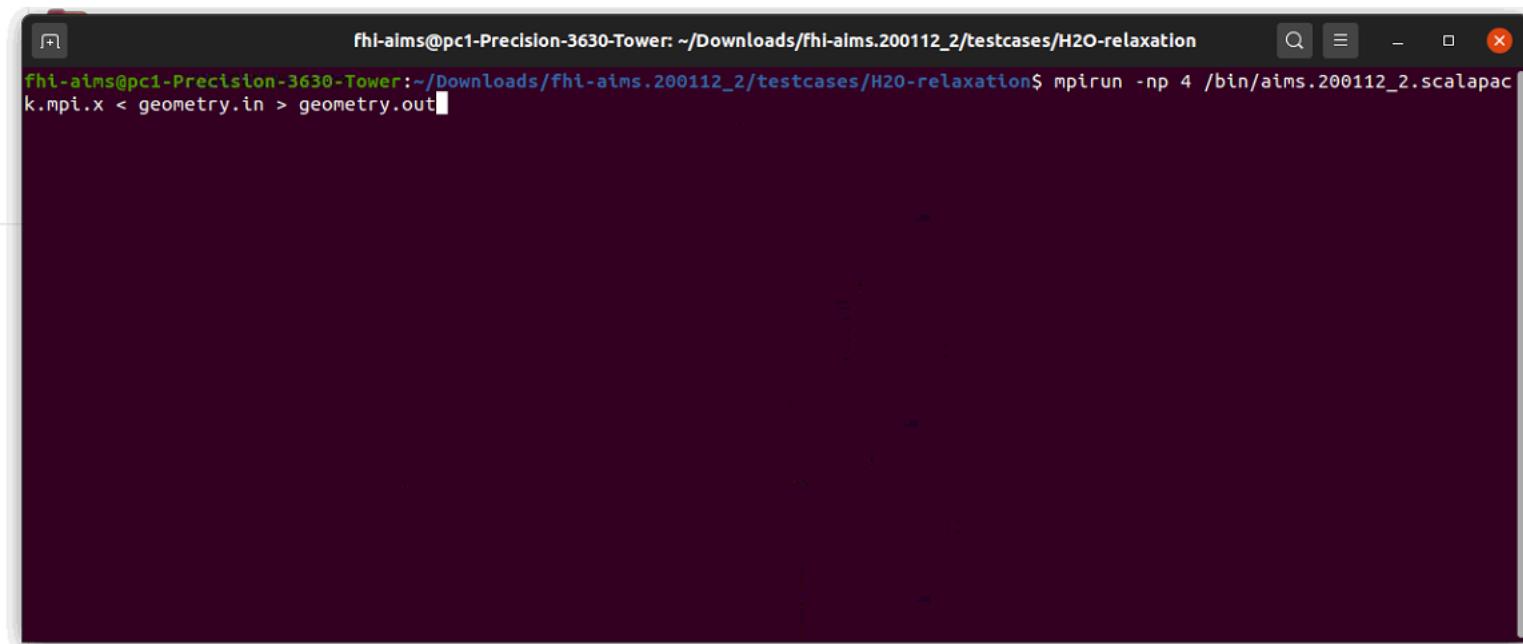
Execute the command:

```
mpirun -np 4 /bin/aims.200112_2.scalapack.mpi.x < geometry.in > geometry.out
```

Enter

This is the input file provided
by the software

It is the output file after
calculating



A screenshot of a terminal window titled "fhi-aims@pc1-Precision-3630-Tower: ~/Downloads/fhi-aims.200112_2/testcases/H2O-relaxation". The window shows a command being entered: "mpirun -np 4 /bin/aims.200112_2.scalapack.mpi.x < geometry.in > geometry.out". The terminal has a dark background and light-colored text. The title bar and window frame are visible.

Fhi-aims: test case

Comparing our output file (left side) against the output file that the fhi-aims programmers (right side), we can see the number of cores used in both cases = 4.

```
geometry.out
~/Downloads/fhi-aims.200112.2/testcases/H2O-relaxation Save Open +1
16
17
18
19 Date : 20200623, Time : 174453.960
20 Time zero on CPU 1 : 0.6354400000000000-01 s.
21 Internal wall clock time zero : 362166293.960 s.
22
23 FHI-aims created a unique identifier for this run for later identification
24 aims_uid : 311E117D-142F-4B83-AF91-762ACD8099A9
25
26 Build configuration of the current instance of FHI-aims
27 -----
28 FHI-aims version : 200112.2
29 Commit number : GITDIR-NOTFOUND
30 CMake host system : Linux-5.4.0-37-generic
31 CMake version : 3.17.3
32 Fortran compiler : /opt/intel/compilers_and_libraries_2020.1.217/linux/mpi/intel64/bin/mpifort (Intel) version 19.1.0.20200306
33 Fortran compiler flags: -O3 -ip -fp-model precise
34 C compiler : /opt/intel/compilers_and_libraries_2020.1.217/linux/mpi/intel64/bin/mpicc (Intel) version 19.1.0.20200306
35 C compiler flags : -O3 -ip -fp-model precise
36 Architecture :
37 Using MPI
38 Using Scalapack
39 Using C files
40 Using LibXC
41 Using SPGLib
42 Using i-PI
43 Using RLSY
44 Linking against: /opt/intel/mkl/lib/intel64/libmkl_intel_lp64.so
45 /opt/intel/mkl/lib/intel64/libmkl_sequential.so
46 /opt/intel/mkl/lib/intel64/libmkl_core.so
47 /opt/intel/mkl/lib/intel64/libmkl_bla_c_intelmp1_lp64.so
48 /opt/intel/mkl/lib/intel64/libmkl_scalapack_lp64.so
49
50 Using 4 parallel tasks.
51 Task 0 on host pci-Precision-3630-Tower reporting.
52 Task 1 on host pci-Precision-3630-Tower reporting.
53 Task 2 on host pci-Precision-3630-Tower reporting.
54 Task 3 on host pci-Precision-3630-Tower reporting.
55
56 Performing system and environment tests:
57 *** Environment variable OMP_NUM_THREADS is not set
58 *** For performance reasons you might want to set it to 1
59 | Maximum stacksize for task 0: unlimited
60 | Maximum stacksize for task 1: unlimited
61 | Maximum stacksize for task 2: unlimited
62 | Maximum stacksize for task 3: unlimited
63 | Current stacksize for task 0: unlimited
64 | Current stacksize for task 1: unlimited
65 | Current stacksize for task 2: unlimited
66
67 H2O.reference.out
~/Downloads/fhi-aims.200112.2/testcases/H2O-relaxation Save Open +1
68 Setting configuration of the current instance of H2O-aims
69
70 FHI-aims version : 200112
71 Commit number : See1177b9
72 CMake host system : Linux-4.12.14-95.40-default
73 CMake version : 3.5.2
74 Fortran compiler : /mpcdf/soft/SLE_12_SP4/packages/x86_64/intel_parallel_studio/2018.4/compilers_and_libraries_2018.5.274/linux/mpi/bin64/mpifort (Intel) version 18.0.5.20180823
75 Fortran compiler flags: -O3 -ip -fp-model precise
76 C compiler : /mpcdf/soft/SLE_12_SP4/packages/x86_64/intel_parallel_studio/2018.4/compilers_and_libraries_2018.5.274/linux/mpi/bin64/mpicc (Intel) version 18.0.5.20180823
77 C compiler flags : -O3 -ip -fp-model precise
78 C++ compiler : /mpcdf/soft/SLE_12_SP4/packages/skylake/intel/18.0.5/bin/cpp (Intel) version 18.0.5.20180823
79 C++ compiler flags : -O3 -ip -fp-model precise
80 Architecture :
81 Using MPI
82 Using Scalapack
83 Using C files
84 Using LibXC
85 Using SPGLib
86 Using i-PI
87 Using RLSY
88 Linking against: /mpcdf/soft/SLE_12_SP4/packages/x86_64/intel_parallel_studio/2018.4/mkl/lib/intel64/libmkl_intel_lp64.so
89 /mpcdf/soft/SLE_12_SP4/packages/x86_64/intel_parallel_studio/2018.4/mkl/lib/intel64/libmkl_sequential.so
90 /mpcdf/soft/SLE_12_SP4/packages/x86_64/intel_parallel_studio/2018.4/mkl/lib/intel64/libmkl_core.so
91 /mpcdf/soft/SLE_12_SP4/packages/x86_64/intel_parallel_studio/2018.4/mkl/lib/intel64/libmkl_bla_c_intelmp1_lp64.so
92 /mpcdf/soft/SLE_12_SP4/packages/x86_64/intel_parallel_studio/2018.4/mkl/lib/intel64/libmkl_scalapack_lp64.so
93
94 Using 4 parallel tasks.
95 Task 0 on host c06523 reporting.
96 Task 1 on host c06523 reporting.
97 Task 2 on host c06523 reporting.
98 Task 3 on host c06523 reporting.
99
100 Performing system and environment tests:
101 *** Environment variable OMP_NUM_THREADS is not set
102 *** For performance reasons you might want to set it to 1
103 | Maximum stacksize for task 0: unlimited
104 | Maximum stacksize for task 1: unlimited
105 | Maximum stacksize for task 2: unlimited
106 | Maximum stacksize for task 3: unlimited
107 | Current stacksize for task 0: unlimited
108 | Current stacksize for task 1: unlimited
109 | Current stacksize for task 2: unlimited
110 | Current stacksize for task 3: unlimited
```

Fhi-aims: test case

The calculated energies in both cases are the same.

```
geometry.out          H2O.reference.out
-----          -----
6430 -----          6432 -----
6431 Start decomposition of the XC Energy          6433 Start decomposition of the XC Energy
6432 -----          6434 -----
6433 X and C from original XC functional choice          6435 X and C from original XC functional choice
6434 Hartree-Fock Energy : 0.000000000 Ha          0.000000000 eV
6435 X Energy : -8.905291046 Ha          -242.325298746 eV
6436 C Energy : -0.325048723 Ha          -8.845025782 eV
6437 Total XC Energy : -9.230339769 Ha          -251.170324527 eV
6438 -----
6439 LDA X and C from self-consistent density          6440 -----
6440 X Energy LDA : -8.090652398 Ha          -220.157853253 eV
6441 C Energy LDA : -0.659246390 Ha          -17.939006999 eV
6442 -----
6443 End decomposition of the XC Energy          6444 -----
6444 -----
6445 -----
6446 -----
6447 Relaxation / MD: End force evaluation. : max(cpu_time) wall_clock(cpu1)
6448 | Time for this force evaluation : 0.107 s          0.107 s
6449 -----
6450 | Time for this force evaluation : 0.203 s          0.203 s
```

Fhi-aims: test case

The atomic structure is the same in both cases

```
6463 Present geometry is converged.  
6464  
6465 -----  
6466 Final atomic structure:  
6467          x [A]      y [A]      z [A]  
6468    atom   -0.0000000  -0.07327020  -0.00000000  O  
6469    atom    0.76741277  -0.67036490  -0.00000000  H  
6470    atom   -0.76741277  -0.67036490  -0.00000000  H  
6471 -----  
6472  
6473 -----  
6474 Final output of selected total energy values:  
6475
```

```
6465 Present geometry is converged.  
6466  
6467 -----  
6468 Final atomic structure:  
6469          x [A]      y [A]      z [A]  
6470    atom   0.0000000  -0.07327020  0.00000000  O  
6471    atom    0.76741277  -0.67036490  -0.00000000  H  
6472    atom   -0.76741277  -0.67036490  -0.00000000  H  
6473 -----  
6474  
6475 -----  
6476 Final output of selected total energy values:  
6477
```

Fhi-aims: test case

The two calculations used the same number of self-consistent cycles, initiations and relaxation steps.

*With these three points we can conclude that the installation was carried out correctly.

The image shows two terminal windows side-by-side. The left window is titled "geometry.out" and the right window is titled "H2O.reference.out". Both windows have a header with "Open", "Save", and other file operations. The "geometry.out" window contains the following text:

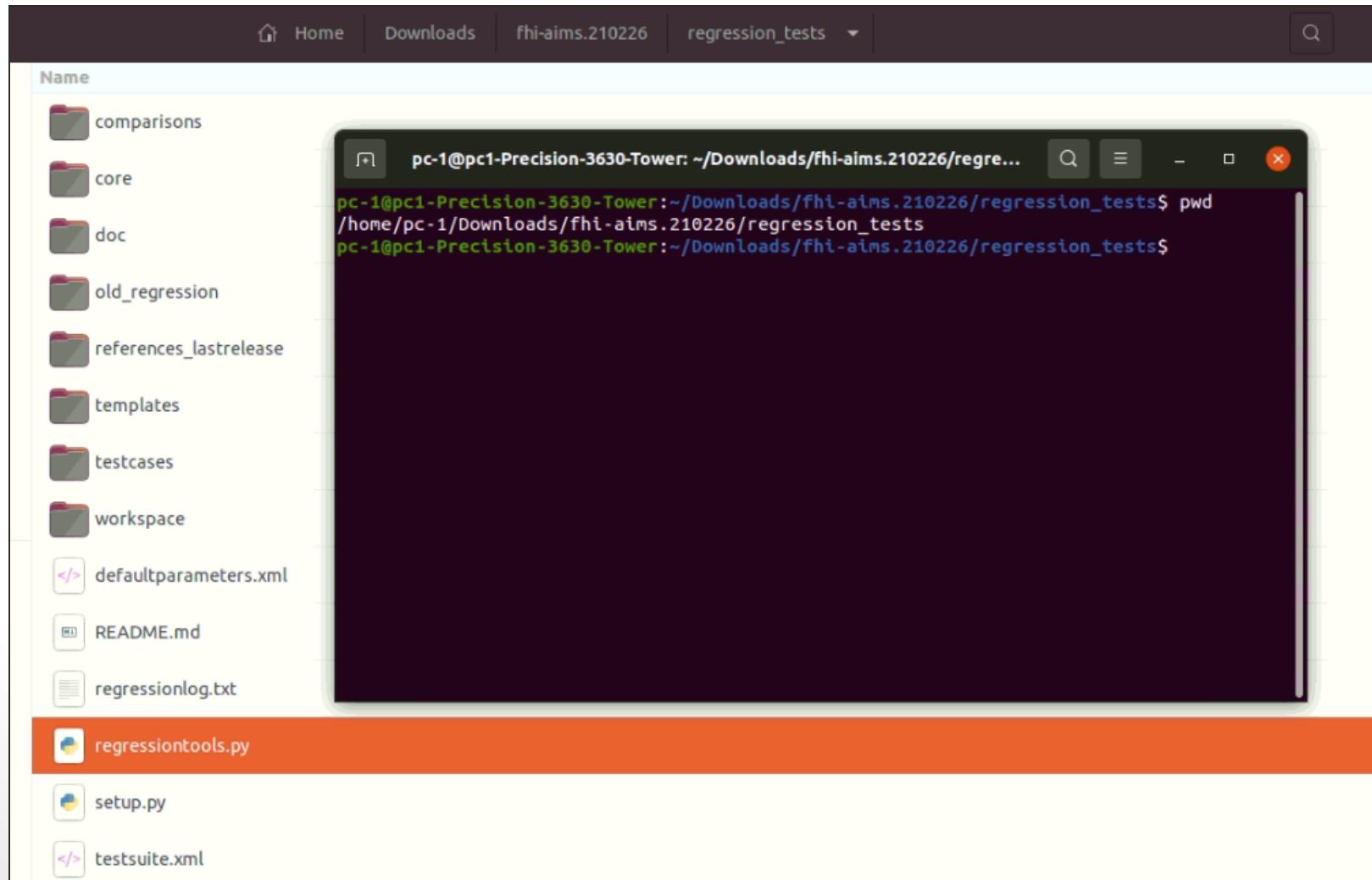
```
Implementations in the
6535 FHI-aims code. The reason is purely practical (length of this list) - please
credit others as well.
6536
6537 -----
6538 Leaving FHI-aims.
6539 Date : 20200623, Time : 174454.821
6540
6541 Computational steps:
6542 | Number of self-consistency cycles : 49
6543 | Number of SCF (re)initializations : 5
6544 | Number of relaxation steps : 4
6545
6546 Detailed time accounting : max(cpu_time)
   wall_clock(cpu1)
6547 | Total time : 0.830 s
```

The "H2O.reference.out" window contains the following text:

```
Implementations in the
6537 FHI-aims code. The reason is purely practical (length of this list) - please
credit others as well.
6538
6539 -----
6540 Leaving FHI-aims.
6541 Date : 20200114, Time : 132204.380
6542
6543 Computational steps:
6544 | Number of self-consistency cycles : 49
6545 | Number of SCF (re)initializations : 5
6546 | Number of relaxation steps : 4
6547
6548 Detailed time accounting : max(cpu_time)
   wall_clock(cpu1)
6549 | Total time : 1.606
   s           1.618 s
```

Fhi-aims: Regression test

To run the regression test automatically, go to the "regression_test" folder where you can find the python 3 script called "regressiontools.py".



Fhi-aims: Regression test

The calculation series starts with the command:

```
./regressiontools.py full references_lastrelease/ /bin/aims.210226.scalapack.mpi.x
```

Enter

```
pc-1@pc1-Precision-3630-Tower:~/Downloads/fhi-aims.210226/regression_tests$ ./regressiontools.py full references_lastrelease/ /bin/aims.210226.scalapack.mpi.x
Overriding Parameter "SCF HOMO occupation number" for TestCase "ScN, PW_LDA+U, Band Structure output"
Overriding Parameter "SCF HOMO occupation number" for TestCase "ScN, spin, band output"
overriding Parameter "Residual memory (MB)" for TestCase "He, PBE with postprocess Laplacian"
overriding Parameter "Residual memory (MB)" for TestCase "He w/ spin, PBE with postprocess Laplacian"
overriding Parameter "Residual memory (MB)" for TestCase "Si2 crystal, PBE with postprocess Laplacian"
overriding Parameter "Residual memory (MB)" for TestCase "Si2 crystal w/ spin, PBE with postprocess Laplacian"
Now running: H2+_boys_1A
Now running: H2+_boys_5A
Now running: H2, IR
Now running: H2, IR, reduce memory
Now running: H2, polarizability
Now running: H2-line, dielectric
Now running: H2-line, phonon
Now running: H2-line, phonon_reduce_memory
Now running: Au, frozen core, cluster
Now running: Br2_Q4C, fully relativistic, VWN
Now running: CH3, M06-L SCF calculation with forces and TPSS post-processing
Now running: CO, COHSEX
Now running: H2 (x3), HSE06, (product) basis output
Now running: H2 ACKS2
Now running: H2, minimal basis, spin-collinear PBE
Now running: H20, PBE, 2nd iteration forces
Now running: H20, ESP-charges, PBE
Now running: H20, M11 Long-range corrected hybrid meta-GGA SCF calculation
Now running: H20, PBE, ill-conditioning
Now running: H20^+1, ESP-charges, PBE
Now running: Hg atom, PBE with spin-orbit coupling
Now running: Hg atom, PBE with spin-orbit coupling and packed_matrix_format none
Now running: Kr Ion, VWN (test of on-site orthonormalization)
Now running: N2, PW-LDA
Now running: NaCl, QMMM embedding, PBE
Now running: NaCl, spin-constrained, relativistic PBE
Now running: Pd50, spin-collinear, PW-LDA, DOS-output
Now running: V3 +1, PBE0, no relativity, spin-collinear
Now running: Zn, atom_sphere solver
Now running: Al, PBE, Methfessel-Paxton broadening
Now running: Al, fcc phase, PW_LDA, stress tensor
Now running: Au, frozen core, periodic
Now running: CO on Cu, cube files
Now running: Cu, fcc phase, PW_LDA
Now running: GaAs, PBE with spin-orbit coupling
Now running: GaAs, PBE with spin-orbit coupling, Gamma point only
Now running: GaAs, TPSS functional, Analytic Stress Tensor, Gamma Point only
Now running: GaAs, TPSS functional, Numerical Stress Tensor
Now running: GaAs, spin texture, LAPACK, SR + SOC
Now running: GaAs_Q4C, fully relativistic, PBE
Now running: H20, ESP-charges, PBE
Now running: MgS, PBE, Mulliken Analysis and Projected DOS
Now running: MgS, PBE, Mulliken Analysis and Projected DOS, Gamma point only
```

Fhi-aims: Regression test

```
Now running: ScN, PW_LDA+U, Band Structure output
Now running: ScN, spin, band output
Now running: Si, HSE06, test xc_pre
Now running: Si, PBE, ill-conditioning
Now running: Si, PBE, ill-conditioning, full spectrum
Now running: Si, libxc interface (PBE)
Now running: TiCl, PBE+U, total energy test
Now running: He w/ spin, PBE with postprocess Laplacian
Now running: He, PBE with postprocess Laplacian
Now running: Si2 crystal w/ spin, PBE with postprocess Laplacian
Now running: Si2 crystal, PBE with postprocess Laplacian
Now running: PbS2, PBE dielectric function with spin-orbit coupling
Now running: PbS2, PBE dielectric function without spin-orbit coupling
Now running: FO-DFT GGA molecule
Now running: FO-DFT Hybrid basic
Now running: CO, load-balancing
Now running: N2, BSE-TDA singlet
Now running: N2, BSE-TDA singlet reduce matrix
Now running: N2, BSE-TDA triplet
Now running: N2, BSE-TDA triplet reduce matrix
Now running: N2, LR-TDDFT
Now running: N2, LR-TDDFT-TDA
Now running: H2 crystal
Now running: H2 dimer
Now running: Al, molecular dynamics, periodic thermodynamic integration
Now running: H2O, molecular dynamics, GLE thermostat
Now running: H5O2, molecular dynamics, Nose-Hoover thermostat
Now running: NH3, molecular dynamics, NVE ensemble
Now running: NH3, molecular dynamics, including force correction, NVE ensemble
Now running: MPB-DFT cl=0 MERM_atom_wise=true.
Now running: MPB-DFT cl=0 MERM_atom_wise=true. density_update_method=density_matrix
Now running: MPB-DFT cl=0 MERM_in_SPE_solver=false.
Now running: MPB-DFT cl=0 MERM_in_SPE_solver=true.
Now running: MPB-DFT cl=0 MERM_in_SPE_solver=true. density_update_method=density_matrix
Now running: MPB-DFT c=0 MERM_atom_wise=true.
Now running: MPB-DFT c=0 MERM_in_SPE_solver=false.
Now running: CH3F in water, cavity overlapping_spheres rho, factorization type QR+SVD
Now running: CH3F in water, cavity rho_free with kill ratio, factorization type QR+SVD
Now running: CH3F in water, cavity rho_free, factorization type QR+SVD
Now running: CH3F in water, cavity rho_free, factorization type QR+SVD, cavity restart
Now running: CH3F in water, cavity rho_free, factorization type SVD
Now running: CH3F in water, cavity rho_free, factorization type SVD, cavity restart
Now running: CH3F in water, cavity rho_free, try restore convergence, factorization type QR+SVD
Now running: CH3F in water, cavity rho_multipole_dynamic with kill ratio, factorization type QR+SVD
Now running: CH3F in water, cavity rho_multipole_dynamic with kill ratio, factorization type QR+SVD
Now running: CH3F in water, cavity rho_multipole_dynamic, factorization type QR+SVD, full restart
Now running: CH3F in water, cavity rho_multipole_static, factorization type QR+SVD
Now running: RPA@PBE relaxation
Now running: H2: RT-TDDFT+Ehrenfest, Ekin_H(0)=0.26 eV, CFM4, length gauge, write trajectory
Now running: H2: RT-TDDFT, read restart, delta kick, Crank-Nicolson, velocity gauge
Now running: H2: RT-TDDFT, write restart, sinus-gaussian, Exponential Midpoint, length gauge
```

```
Now running: Si-bulk: RT-TDDFT, scaling + squaring, step-kick, velocity gauge, calculate current
Now running: Si: it-TDDFT
Now running: restart, cluster, spin collinear, LAPACK with DENSMAT
Now running: restart, cluster, spin collinear, LAPACK with ORBITAL
Now running: restart, cluster, spin collinear, hybrid, LAPACK with DENSMAT
Now running: restart, cluster, spin collinear, hybrid, LAPACK with ORBITAL
Now running: restart, cluster, spin none, LAPACK with DENSMAT
Now running: restart, cluster, spin none, LAPACK with ORBITAL
Now running: restart, forced_singlefile, periodic, spin none, LAPACK with DENSMAT
Now running: restart, periodic, spin collinear, LAPACK with DENSMAT
Now running: restart, periodic, spin collinear, hybrid, LAPACK with DENSMAT
Now running: restart, periodic, spin none, LAPACK with DENSMAT
Now running: restart, cluster, spin collinear, SCALAPACK/ELPA with DENSMAT
Now running: restart, cluster, spin collinear, SCALAPACK/ELPA with ORBITAL
Now running: restart, cluster, spin collinear, hybrid, SCALAPACK/ELPA with DENSMAT
Now running: restart, cluster, spin none, SCALAPACK/ELPA with DENSMAT
Now running: restart, cluster, spin none, SCALAPACK/ELPA with ORBITAL
Now running: restart, forced_singlefile, periodic, spin none, SCALAPACK/ELPA with DENSMAT
Now running: restart, periodic, spin collinear, SCALAPACK/ELPA with DENSMAT
Now running: restart, periodic, spin collinear, hybrid, SCALAPACK/ELPA with DENSMAT
Now running: restart, periodic, spin none, SCALAPACK/ELPA with DENSMAT
Now running: CH4, GW0 with contour deformation and manual pre relativistic correction, QPs
Now running: CH4, Restart GW0 with contour deformation, QPs
Now running: Density matrix, ELSI ELPA, complex case
Now running: Density matrix, ELSI ELPA, real case
Now running: Density matrix, ELSI NTPoly, complex case
Now running: Density matrix, ELSI NTPoly, real case
Now running: Density matrix, ELSI libOMM, complex case
Now running: Density matrix, ELSI libOMM, real case
Now running: GaAs, load_balancing, complex case
Now running: GaAs, load_balancing, real case
Now running: GaAs, use_local_index, complex case
Now running: GaAs, use_local_index, real case
Now running: H2O, GW0 with Hedin shift (AO and CO)
Now running: H2O, GW0 with contour deformation, QPs
Now running: H2O, ev-scGW with contour deformation, spectral function
Now running: H2O, ev-scGW0 with CD and post relativistic corr., QPs
Now running: O2, GW0-Zshot with contour deformation, QPs
Now running: Si kpont 444, symmetry
Now running: Si kpont 444, symmetry refine
Now running: Si PBE sglib kpoints
Now running: CH4, GW0@LDA (analytic continuation: Pade approximation)
Now running: CO, RPA@PBE
Now running: Cu2, MP2@HF
Now running: H2, self-consistent GW
Now running: H2 dimer, MP2/RPA@HF, RI-LVL_full
Now running: H2O magnetic response
Now running: H2O magnetic response (ZORA)
Now running: H2O, GW0@PBE, Z-shot (analytic continuation: Pade approximation)
Now running: N2, MP2@HF with Gaussians
Now running: Na4, GW0@LDA (analytic continuation: two-pole fitting)
Now running: Al2Zn54, SCR_periodic relaxation, PW-LDA
```

Fhi-aims: Regresion test

- With each Enter you can see the result of each test.
- Most of the "FAILED" are because our calculated value was done in less time than the reference.
- In other cases, the "FAILED" value is because the whole calculation was done in fewer iterations.

```
TestSuite DFPT:  
  
TestCase H2, IR: [folder 'H2_DFPT_IR']  
Property | Ref-Value | Test-Value | Status | Importance | Details  
-----|-----|-----|-----|-----|-----  
DFT/HF total energy (eV) | -30.94112010 | -30.94112010 | PASSED | mandatory | abs diff = 0.000E+00 (tol = 1.000E-05)  
HOMO-LUMO gap | 11.86482317 | 11.86482317 | PASSED | consistent | abs diff = 0.000E+00 (tol = 2.000E-05)  
Initialization Energy (eV) | -31.70638840 | -31.70638840 | PASSED | mandatory | abs diff = 0.000E+00 (tol = 1.000E-05)  
Number of SCF steps | 17 | 17 | PASSED | optional | abs diff = 0 (tol = 0)  
Post-SCF total energy (eV) | ----- | ----- | PASSED | consistent | ref: 0/1 matches found, test: 0/1 matches found  
Residual memory (MB) | 0.000000 | 0.000000 | PASSED | mandatory | abs diff = 0.000E+00 (tol = 1.000E-07)  
SCF HOMO energy (eV) | -10.31780739 | -10.31780739 | PASSED | mandatory | abs diff = 0.000E+00 (tol = 1.000E-05)  
SCF HOMO occupation number | 2.00000000 | 2.00000000 | PASSED | mandatory | abs diff = 0.000E+00 (tol = 1.000E-05)  
Total calculation time (sec) | 1.812 | 1.002 | FAILED | informative | rel diff = 44.70% (tol = 5.00%)  
Vibrational Frequencies | <TABLE> | <TABLE> | PASSED | mandatory | 6/6 rows equal - max diff: 3.771E-05 (abs tol = 2...  
TestCase H2, IR: PASSED  
  
Press enter to proceed to the next test case...  
TestCase H2, IR, reduce memory: [folder 'H2_DFPT_IR_reduce_memory']  
Property | Ref-Value | Test-Value | Status | Importance | Details  
-----|-----|-----|-----|-----|-----  
DFT/HF total energy (eV) | -30.94112010 | -30.94112010 | PASSED | mandatory | abs diff = 0.000E+00 (tol = 1.000E-05)  
HOMO-LUMO gap | 11.86482317 | 11.86482317 | PASSED | consistent | abs diff = 0.000E+00 (tol = 2.000E-05)  
Initialization Energy (eV) | -31.70638840 | -31.70638840 | PASSED | mandatory | abs diff = 0.000E+00 (tol = 1.000E-05)  
Number of SCF steps | 7 | 7 | PASSED | optional | abs diff = 0 (tol = 0)  
Post-SCF total energy (eV) | ----- | ----- | PASSED | consistent | ref: 0/1 matches found, test: 0/1 matches found  
Residual memory (MB) | 0.000000 | 0.000000 | PASSED | mandatory | abs diff = 0.000E+00 (tol = 1.000E-07)  
SCF HOMO energy (eV) | -10.31780739 | -10.31780739 | PASSED | mandatory | abs diff = 0.000E+00 (tol = 1.000E-05)  
SCF HOMO occupation number | 2.00000000 | 2.00000000 | PASSED | mandatory | abs diff = 0.000E+00 (tol = 1.000E-05)  
Total calculation time (sec) | 5.517 | 4.045 | FAILED | informative | rel diff = 26.68% (tol = 5.00%)  
Vibrational Frequencies | <TABLE> | <TABLE> | PASSED | mandatory | 6/6 rows equal - max diff: 3.683E-05 (abs tol = 2...  
TestCase H2, IR, reduce memory: PASSED  
  
Press enter to proceed to the next test case...  
TestCase H2, polarizability: [folder 'H2_DFPT_polarizability']  
Property | Ref-Value | Test-Value | Status | Importance | Details  
-----|-----|-----|-----|-----|-----  
DFT/HF total energy (eV) | -30.94112010 | -30.94112010 | PASSED | mandatory | abs diff = 0.000E+00 (tol = 1.000E-05)  
HOMO-LUMO gap | 11.86482317 | 11.86482317 | PASSED | consistent | abs diff = 0.000E+00 (tol = 2.000E-05)  
Initialization Energy (eV) | -31.70638840 | -31.70638840 | PASSED | mandatory | abs diff = 0.000E+00 (tol = 1.000E-05)  
Number of SCF steps | 13 | 13 | PASSED | optional | abs diff = 0 (tol = 0)  
Post-SCF total energy (eV) | ----- | ----- | PASSED | consistent | ref: 0/1 matches found, test: 0/1 matches found  
Residual memory (MB) | 0.000000 | 0.000000 | PASSED | mandatory | abs diff = 0.000E+00 (tol = 1.000E-07)  
SCF HOMO energy (eV) | -10.31780739 | -10.31780739 | PASSED | mandatory | abs diff = 0.000E+00 (tol = 1.000E-05)  
SCF HOMO occupation number | 2.00000000 | 2.00000000 | PASSED | mandatory | abs diff = 0.000E+00 (tol = 1.000E-05)  
Total calculation time (sec) | 0.380 | 0.278 | FAILED | informative | rel diff = 26.84% (tol = 5.00%)  
polarizability | <TABLE> | <TABLE> | PASSED | mandatory | 3/3 rows equal - max diff: 3.651E-08 (abs tol = 1...  
TestCase H2, polarizability: PASSED
```

Fhi-aims: Regression test

- In addition, a summary of the 158 tests is shown.

TestSuite	Status	passed	optfails	failed
Boys localization	PASSED	2	0	0
DFPT	PASSED	6	0	0
DFT, isolated molecules	FAILED	20	1	0
DFT, periodic systems	FAILED	21	1	0
DFT, postprocess output Laplacian	PASSED	4	0	0
Dielectric function	PASSED	2	0	0
FO-DFT	PASSED	2	0	0
Infrastructure	PASSED	1	0	0
LRTDDFT	PASSED	6	0	0
MBD	PASSED	2	0	0
MD	PASSED	5	0	0
MPB-DFT	PASSED	8	0	0
MPE implicit solvation	PASSED	12	0	0
Post-DFT, relaxation	PASSED	1	0	0
RT-TDDFT	PASSED	6	0	0
Restarts, LAPACK	PASSED	10	0	0
Restarts, ScaLAPACK/ELPA	PASSED	9	0	0
ScaLAPACK only	PASSED	18	0	0
Symmetry-RLSY	PASSED	2	0	0
Symmetry-SPGlib	PASSED	1	0	0
beyond DFT	PASSED	10	0	0
relaxation	PASSED	10	0	0