Compilation of PHITS using the free Intel Fortran compiler (OneAPI toolkits)

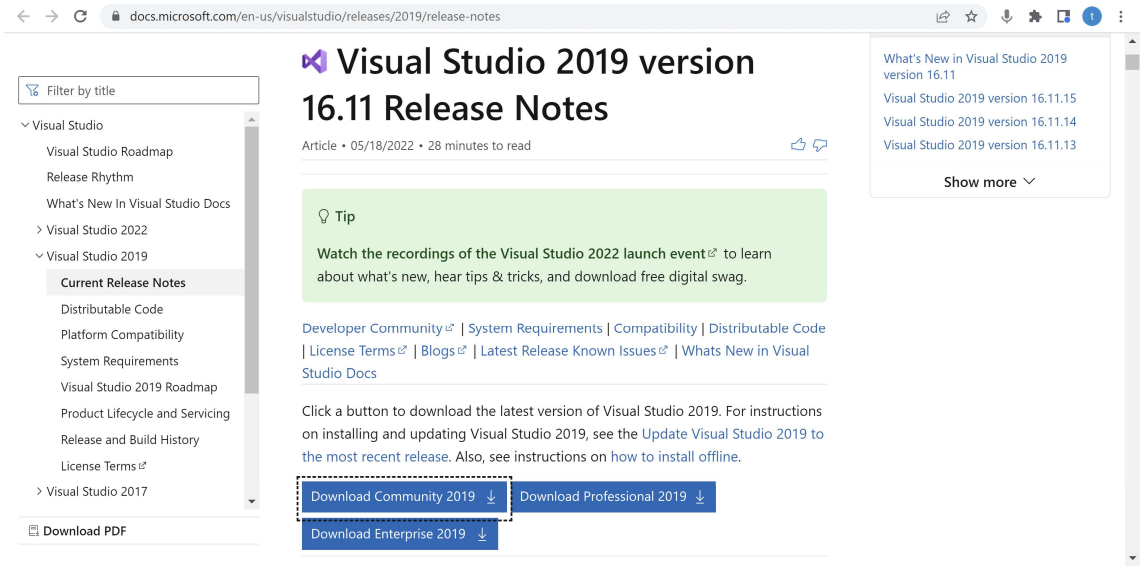
Contents

1. Windows

Phase I: Install Visual Studio IDE (integrated development environment)

I-1

Search “visual studio” or go to https://visualstudio.microsoft.com/



I-2

Download “Visual Studio Community 2019”

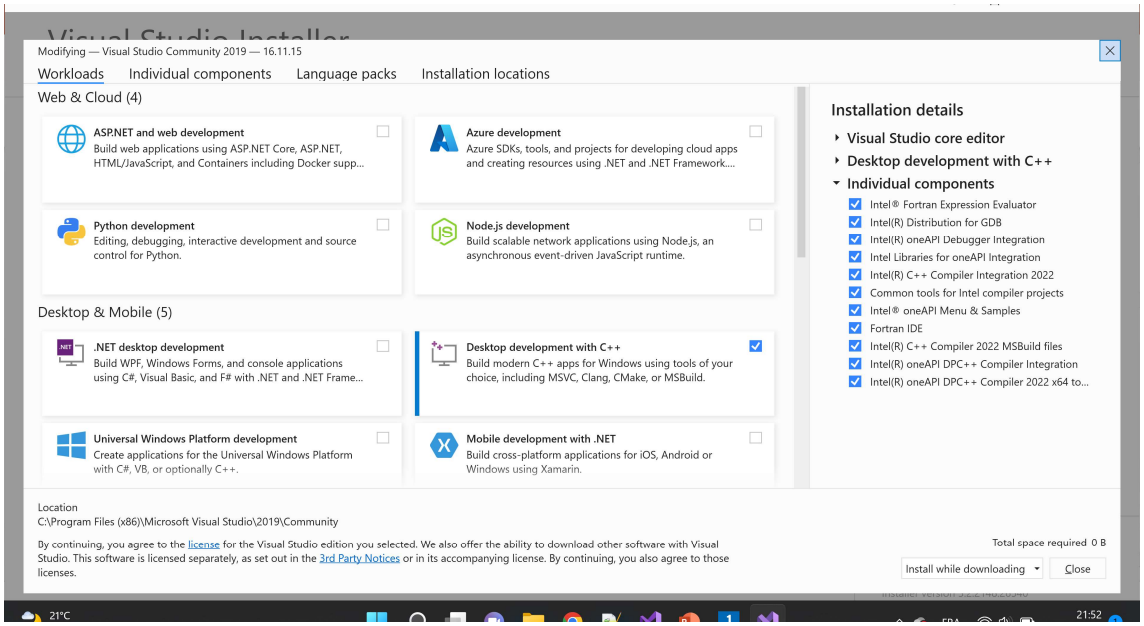
Note : In April 2022, OneAPI and Visual Studio Community/professional/enterprise 2022 are incompatible. Please don’t select 2022 unless the latest OneAPI solves this compatibility problem.

I-3

Install “Visual Studio Community 2019” using the downloaded installer.

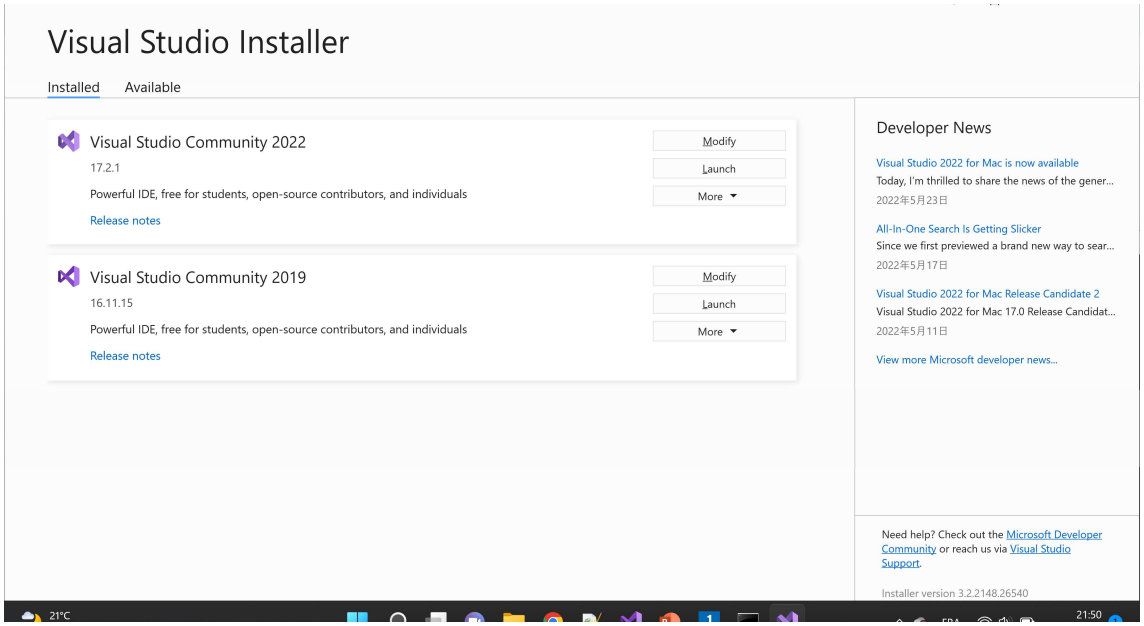
In the window below, please tick “Desktop development with C++”. It says C++ while PHITS is Fortran, but this is OK.

Then click the right bottom button to start installation.



I-4

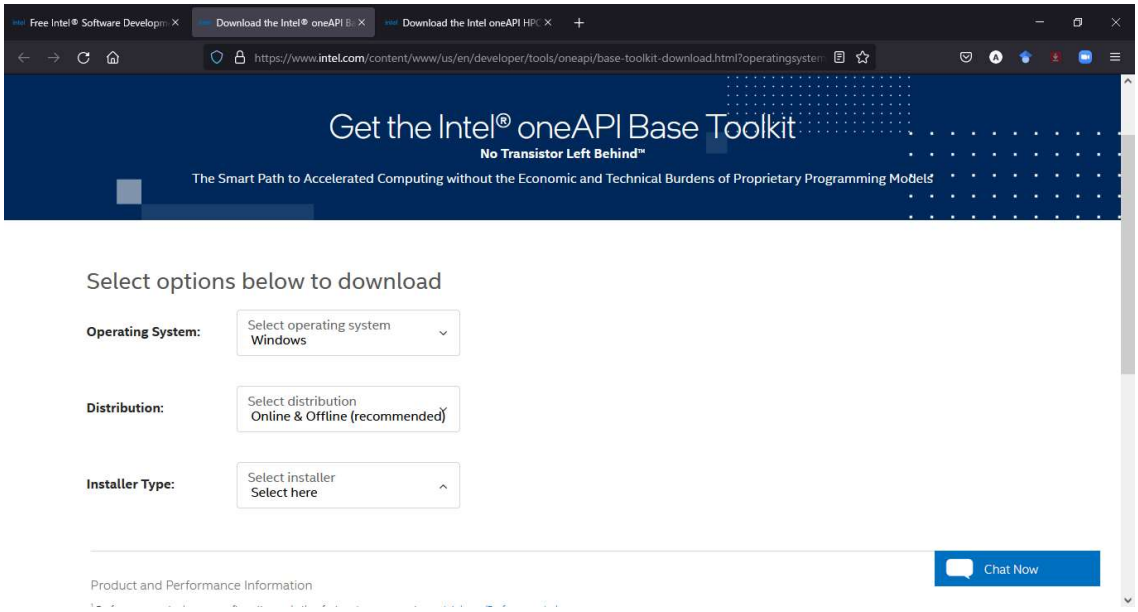
After installation, by launching the installer again, one can see if Visual Studio has been really installed. You will see “Visual Studio Community 2019” installed.



Phase II: Install OneAPI (Fortran compiler and its associated libraries)

II-1

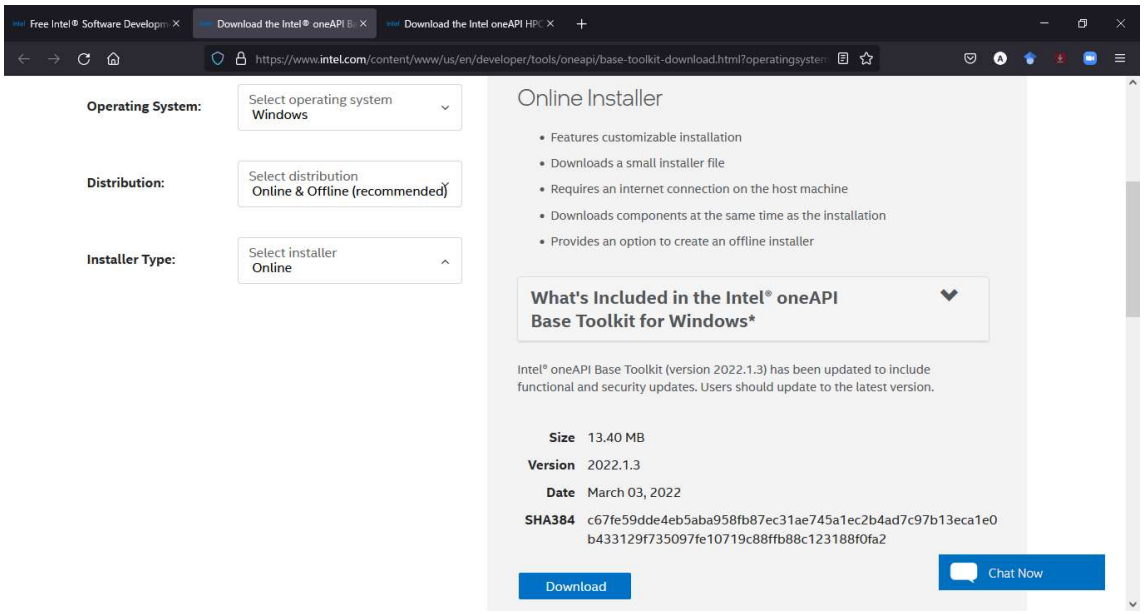
Search “OneAPI BaseToolKit download” or go to https://www.intel.com/content/www/us/en/developer/tools/oneapi/base-toolkit-download.html



II-2

Select your OS, Online & Offline, and Online

(If you fail the installation owing to network access instability, please consider choosing Offline)



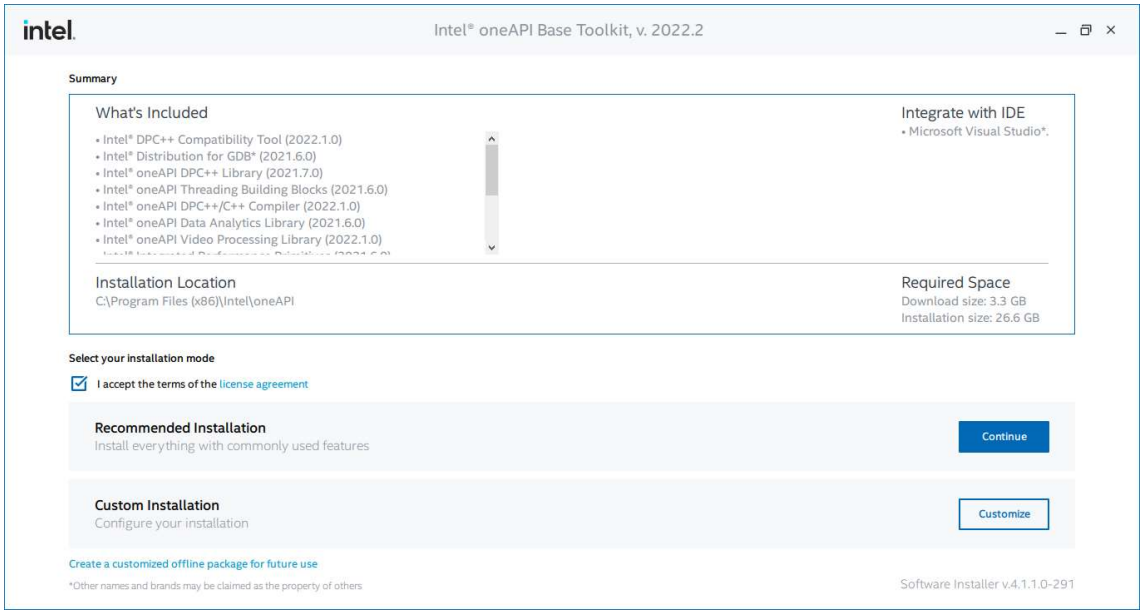
If a pop-up message says “Get Your Download. Sign in to your My Intel account using your existing credentials.”, click “Continue as a Guest (download starts immediately)” to proceed.

II-3

Launch the downloaded installer. Following popup window will show up.

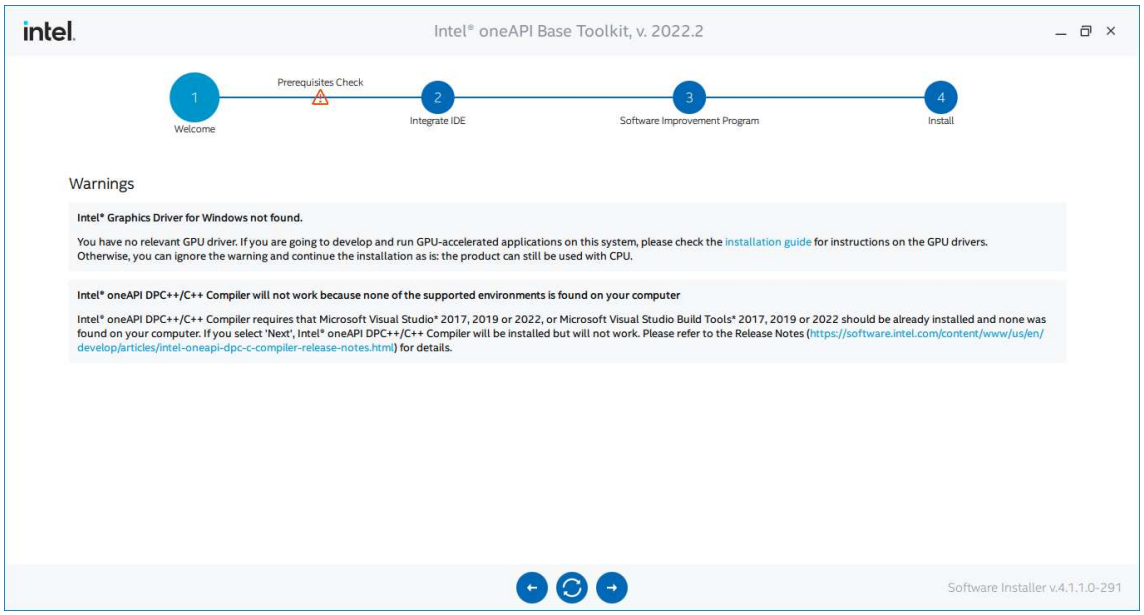
II-4

Tick “I accept the terms of the license agreements” and click “continue” of “Recommended Installation” on the right.



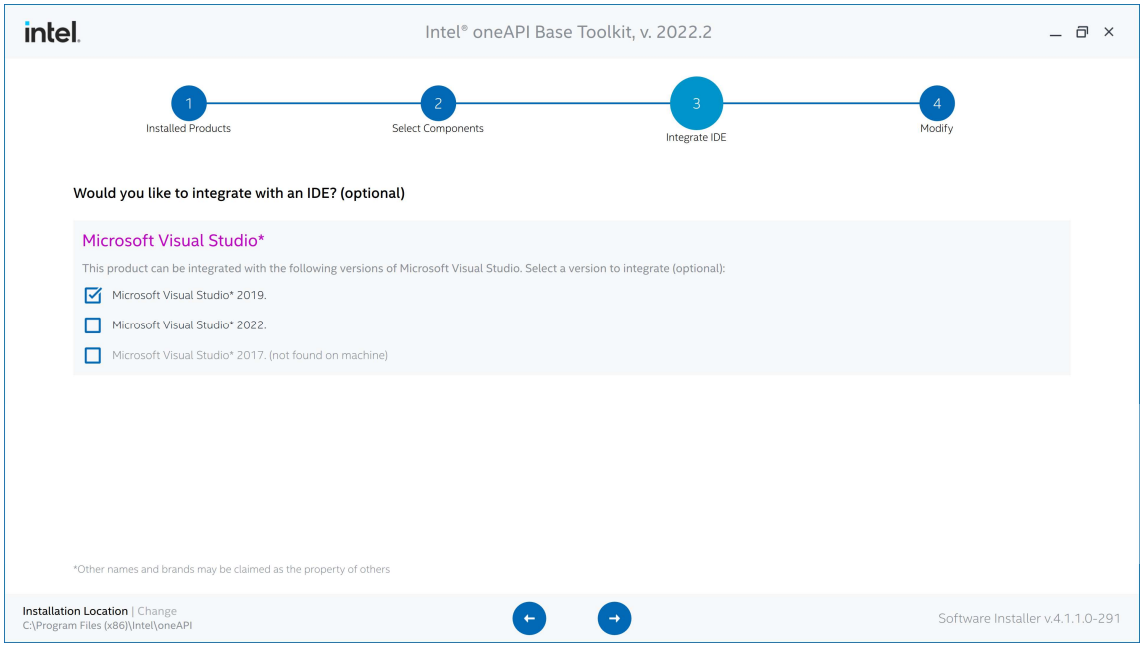
II-5

If you see a warning message below, something is wrong with Visual Studio installation. Please go back to Phase I.



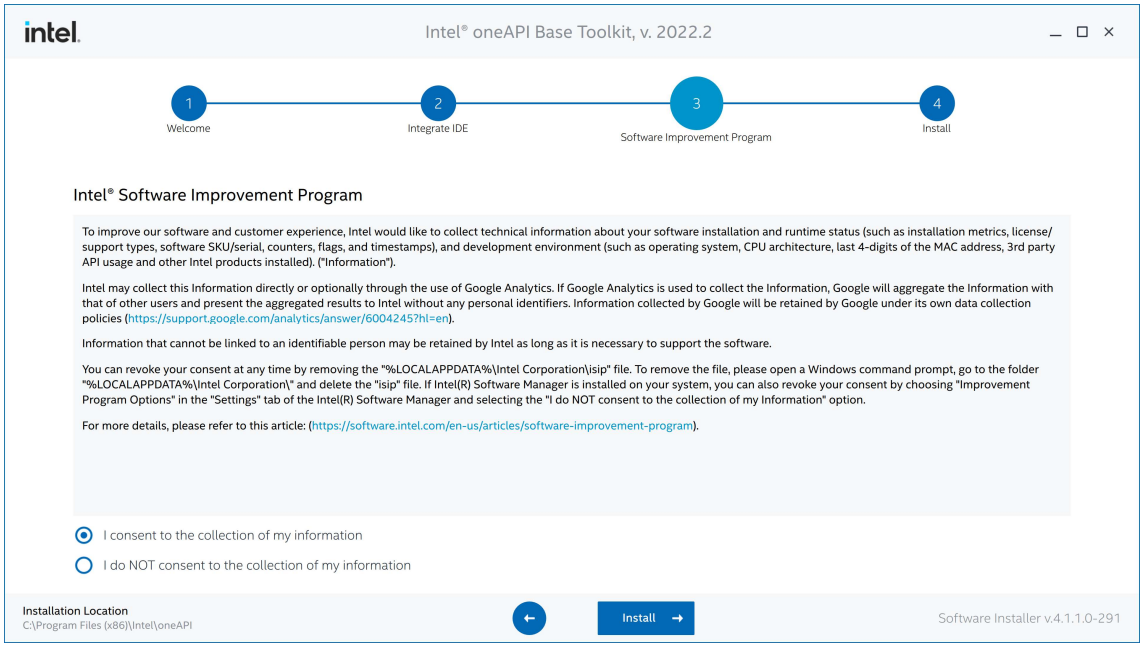
II-6

Tick Microsoft Visual Studio* 2019 and click right arrow button on the bottom.



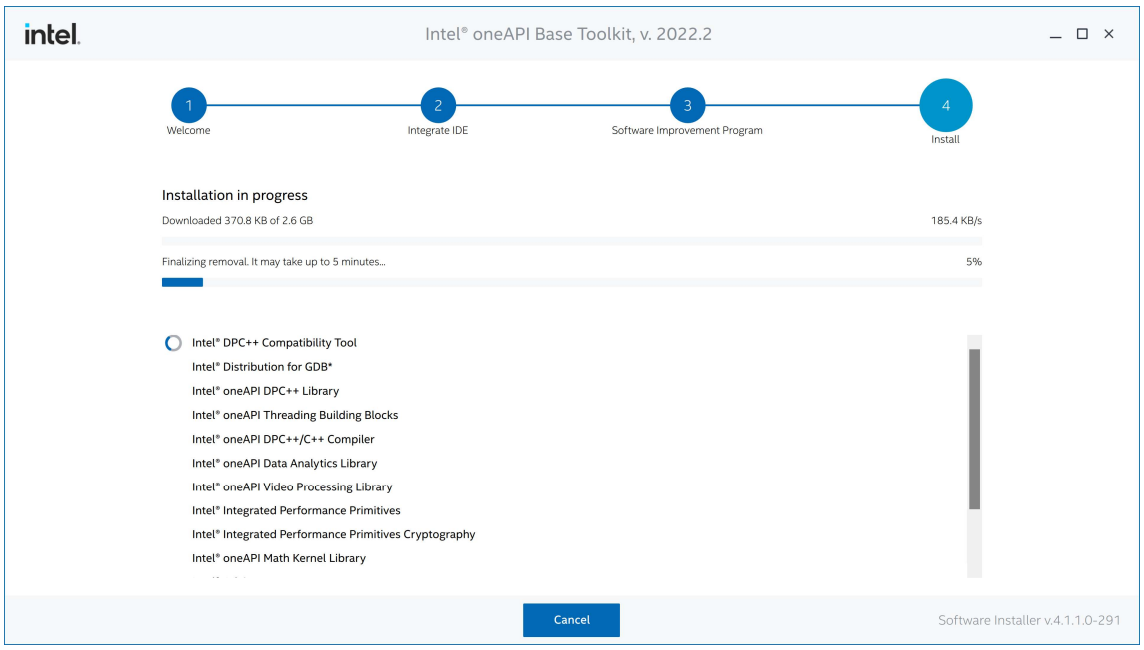
II-7

Tick whichever you prefer and click “Install” button.



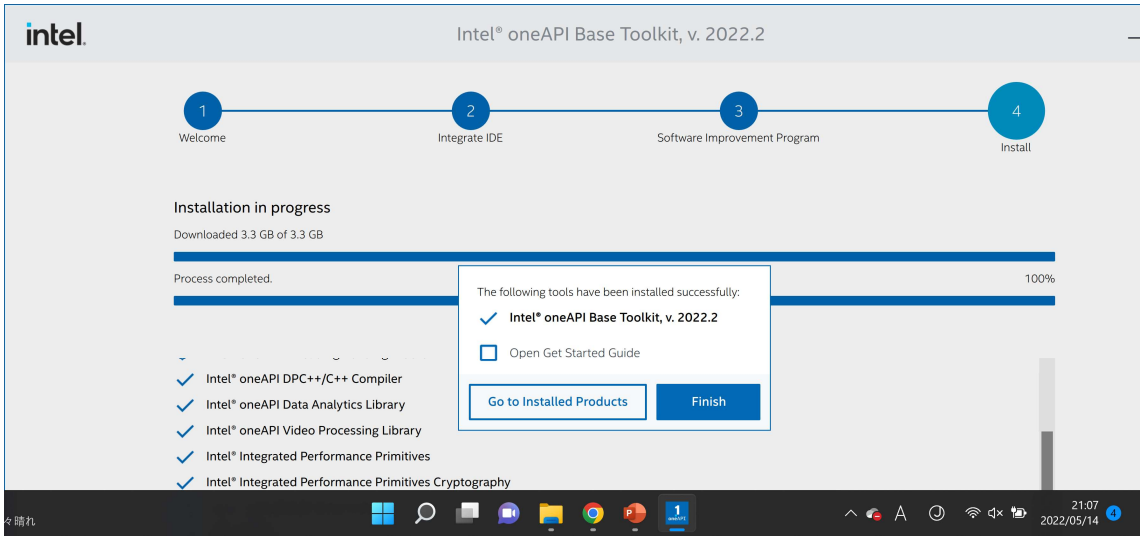
II-8

Wait until the progress bars reach the right edges.



II-9

When installation ends, click “Finish” of the popup window.

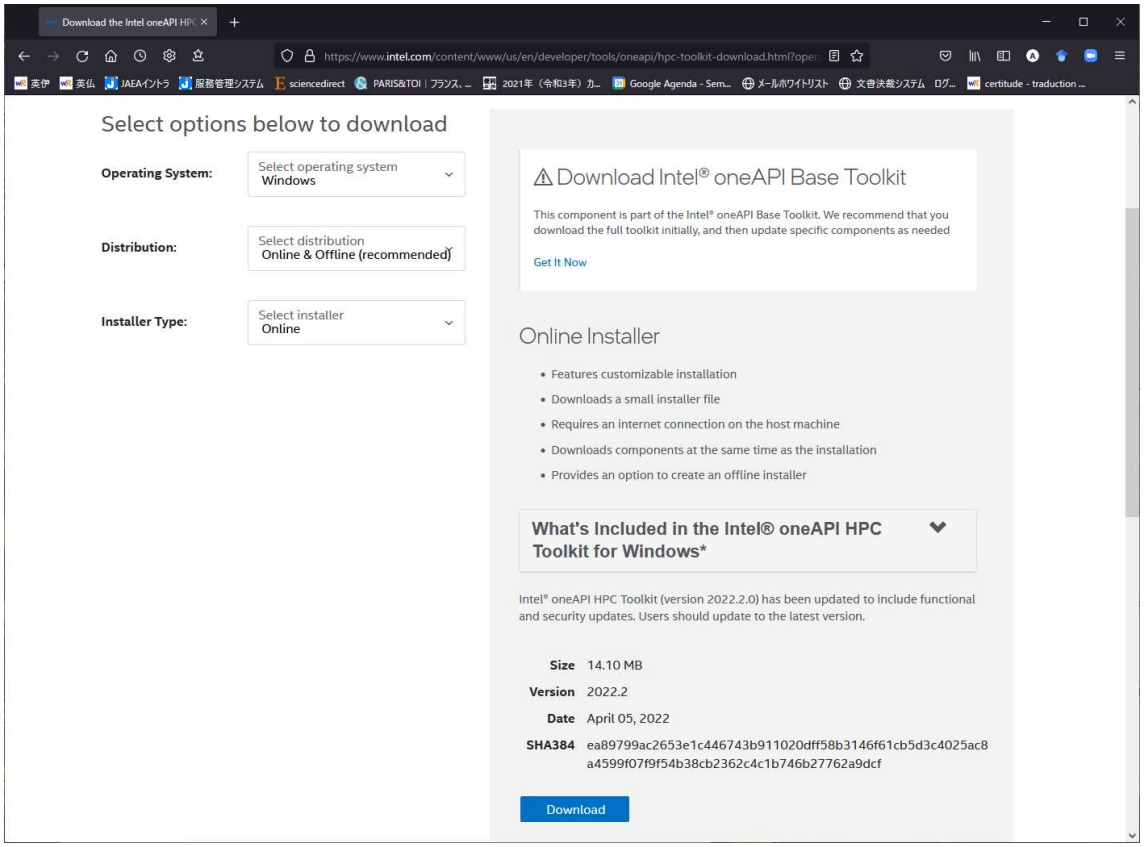

intel
Intel® oneAPI Base Toolkit, v. 2022.2
1
Welcome
2
Integrate IDE
3
Software Improvement Program
4
Install
Installation in progress
Downloaded 3.3 GB of 3.3 GB
Process completed.
100%
Intel® oneAPI DPC++/C++ Compiler
Intel® oneAPI Data Analytics Library
Intel® oneAPI Video Processing Library
Intel® Integrated Performance Primitives
Intel® Integrated Performance Primitives Cryptography
The following tools have been installed successfully:
Intel® oneAPI Base Toolkit, v. 2022.2
Open Get Started Guide
Go to Installed Products
Finish
21:07
2022/05/14

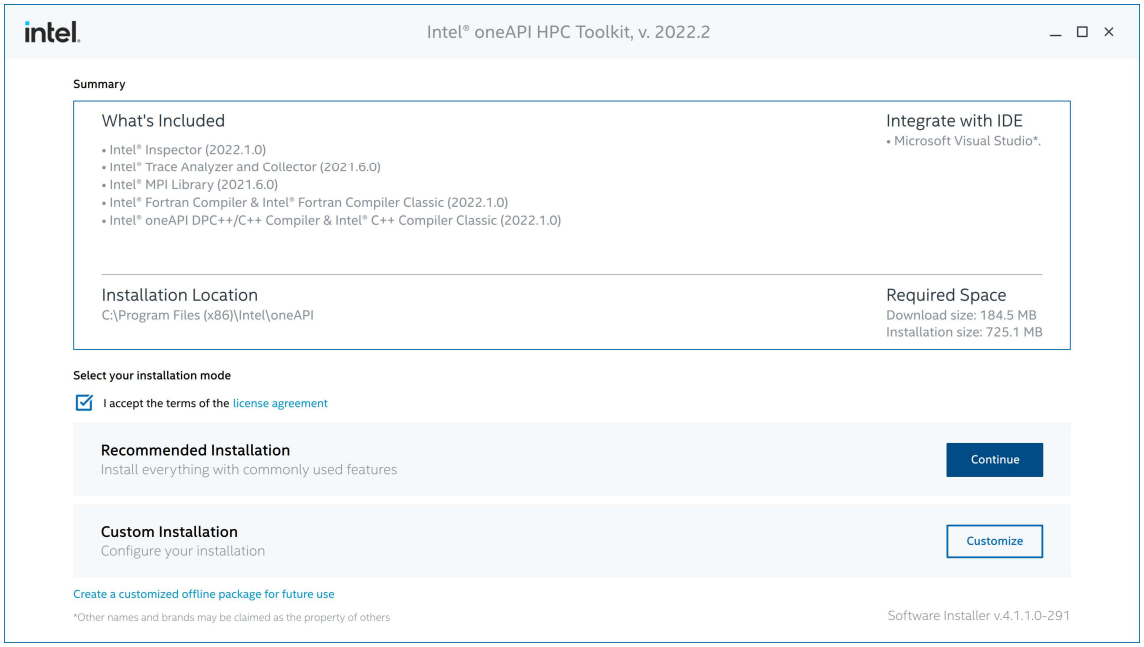
II-10

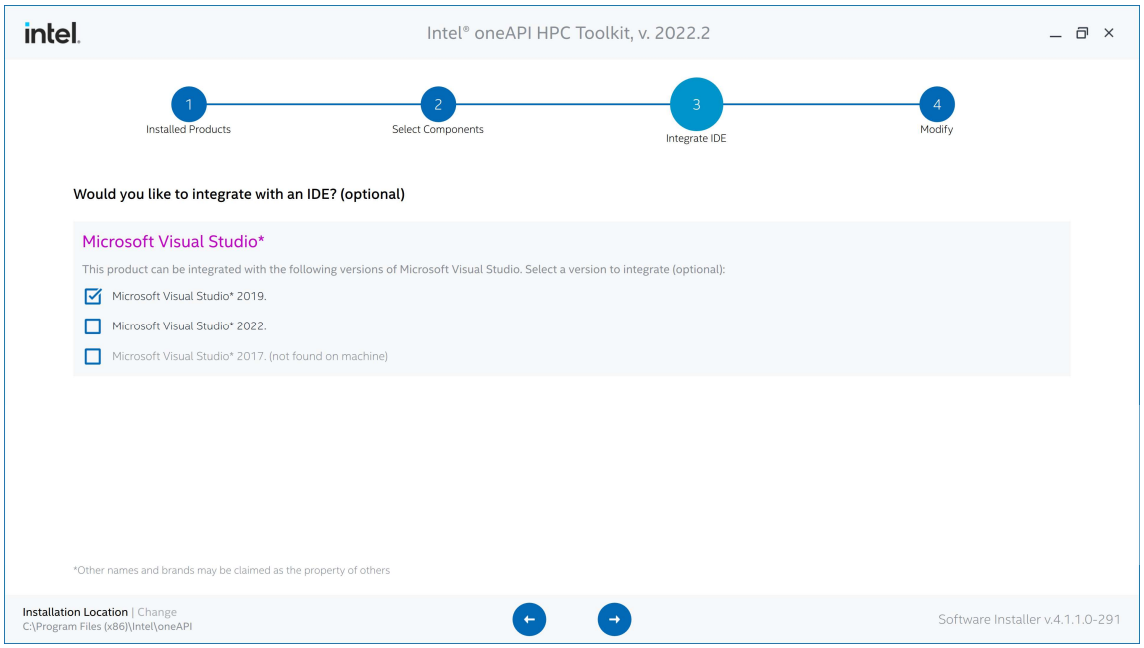
Search “OneAPI HPCToolKit download” or go to https://www.intel.com/content/www/us/en/developer/tools/oneapi/hpc-toolkit-download.html

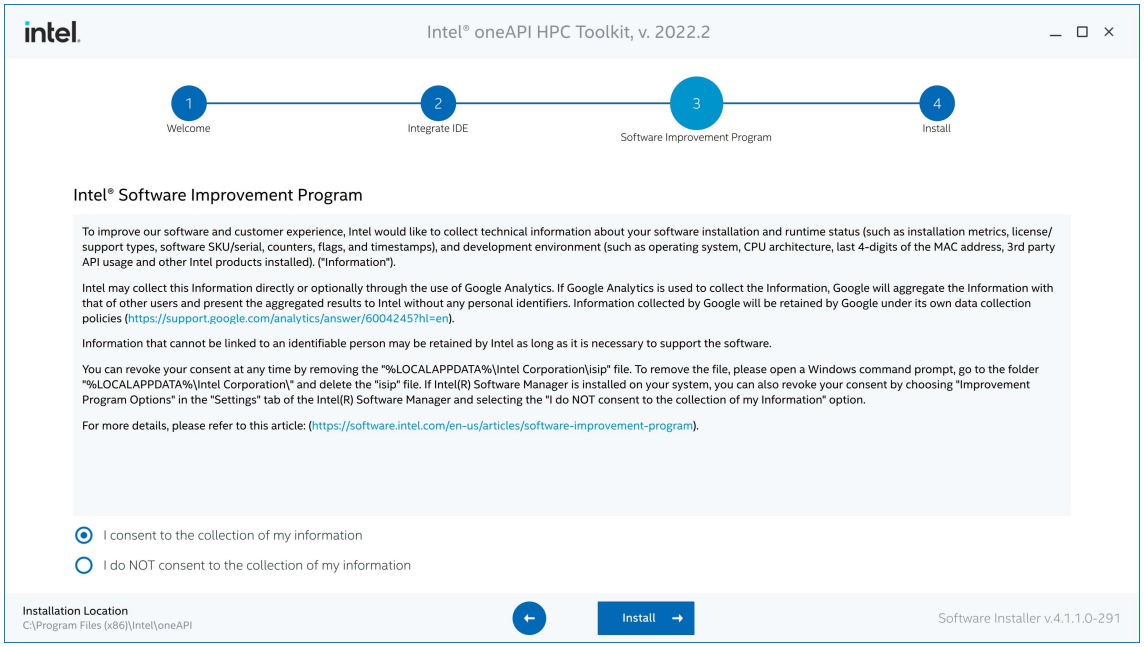
II-11

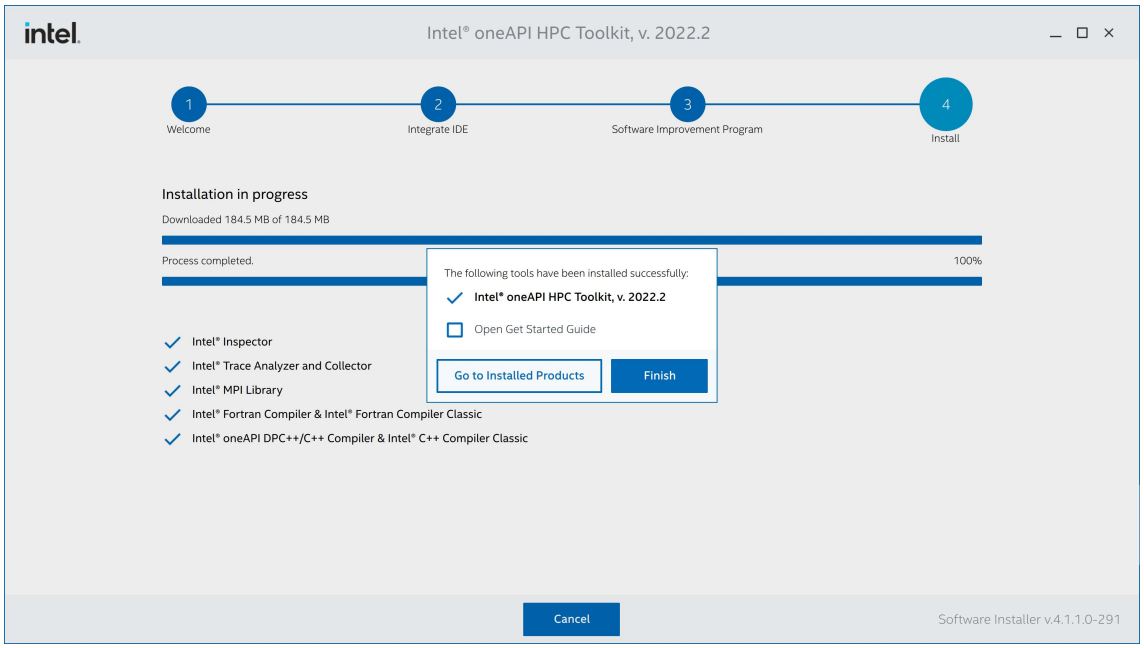
Do the same as BaseToolkit explained above. Below are screenshots during HPCToolKit installation.




intel
Intel® oneAPI HPC Toolkit, v. 2022.2
Summary
What's Included
• Intel® Inspector (2022.1.0)
• Intel® Trace Analyzer and Collector (2021.6.0)
• Intel® MPI Library (2021.6.0)
• Intel® Fortran Compiler & Intel® Fortran Compiler Classic (2022.1.0)
• Intel® oneAPI DPC++/C++ Compiler & Intel® C++ Compiler Classic (2022.1.0)
Integrate with IDE
• Microsoft Visual Studio*.
Installation Location
C:\Program Files (x86)\Intel\oneAPI
Required Space
Download size: 184.5 MB
Installation size: 725.1 MB
Select your installation mode
I accept the terms of the license agreement
Recommended Installation
Install everything with commonly used features
Continue
Custom Installation
Configure your installation
Customize
Create a customized offline package for future use
*Other names and brands may be claimed as the property of others
Software Installer v.4.1.1.0-291


intel
Intel® oneAPI HPC Toolkit, v. 2022.2
1
Installed Products
2
Select Components
3
Integrate IDE
4
Modify
Would you like to integrate with an IDE? (optional)
Microsoft Visual Studio*
This product can be integrated with the following versions of Microsoft Visual Studio. Select a version to integrate (optional):
Microsoft Visual Studio* 2019.
Microsoft Visual Studio* 2022.
Microsoft Visual Studio* 2017. (not found on machine)
*Other names and brands may be claimed as the property of others
Installation Location | Change
C:\Program Files (x86)\Intel\oneAPI
Software Installer v.4.1.1.0-291

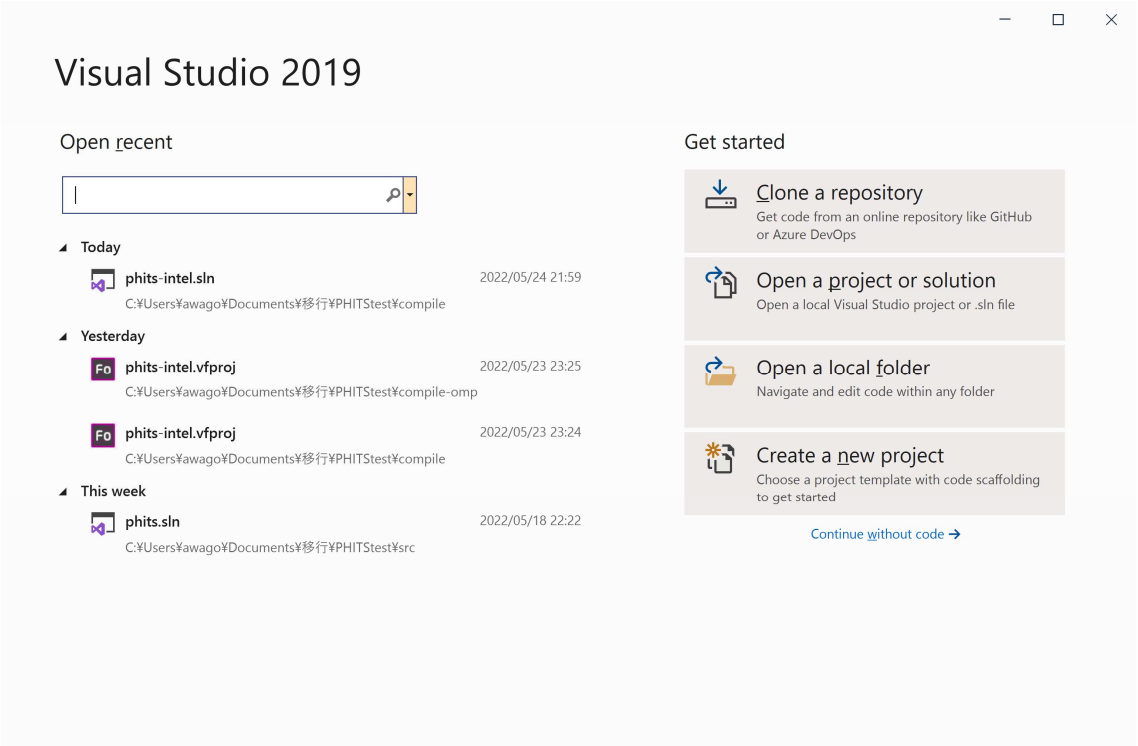

intel
Intel® oneAPI HPC Toolkit, v. 2022.2
1
Welcome
2
Integrate IDE
3
Software Improvement Program
4
Install
Intel® Software Improvement Program
To improve our software and customer experience, Intel would like to collect technical information about your software installation and runtime status (such as installation metrics, license/support types, software SKU/serial, counters, flags, and timestamps), and development environment (such as operating system, CPU architecture, last 4-digits of the MAC address, 3rd party API usage and other Intel products installed). ("Information").
Intel may collect this Information directly or optionally through the use of Google Analytics. If Google Analytics is used to collect the Information, Google will aggregate the Information with that of other users and present the aggregated results to Intel without any personal identifiers. Information collected by Google will be retained by Google under its own data collection policies (https://support.google.com/analytics/answer/6004245?hl=en).
Information that cannot be linked to an identifiable person may be retained by Intel as long as it is necessary to support the software.
You can revoke your consent at any time by removing the "%LOCALAPPDATA%\Intel Corporation\isip" file. To remove the file, please open a Windows command prompt, go to the folder "%LOCALAPPDATA%\Intel Corporation\" and delete the "isip" file. If Intel(R) Software Manager is installed on your system, you can also revoke your consent by choosing "Improvement Program Options" in the "Settings" tab of the Intel(R) Software Manager and selecting the "I do NOT consent to the collection of my Information" option.
For more details, please refer to this article: (https://software.intel.com/en-us/articles/software-improvement-program).
I consent to the collection of my information
I do NOT consent to the collection of my information
Installation Location
C:\Program Files (x86)\Intel\oneAPI
Install
Software Installer v.4.1.1.0-291


intel
Intel® oneAPI HPC Toolkit, v. 2022.2
1
Welcome
2
Integrate IDE
3
Software Improvement Program
4
Install
Installation in progress
Downloaded 184.5 MB of 184.5 MB
Process completed.
100%
The following tools have been installed successfully:
Intel® oneAPI HPC Toolkit, v. 2022.2
Open Get Started Guide
Go to Installed Products
Finish
Intel® Inspector
Intel® Trace Analyzer and Collector
Intel® MPI Library
Intel® Fortran Compiler & Intel® Fortran Compiler Classic
Intel® oneAPI DPC++/C++ Compiler & Intel® C++ Compiler Classic
Cancel
Software Installer v.4.1.1.0-291

Phase III: Compile PHITS

III-0

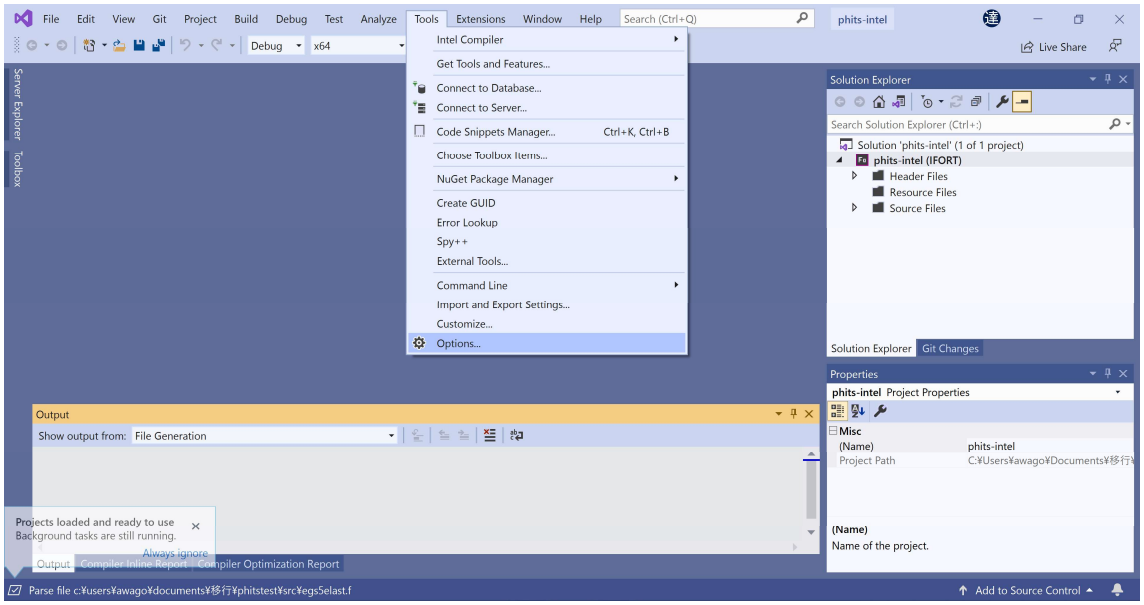
Launch Visual Studio

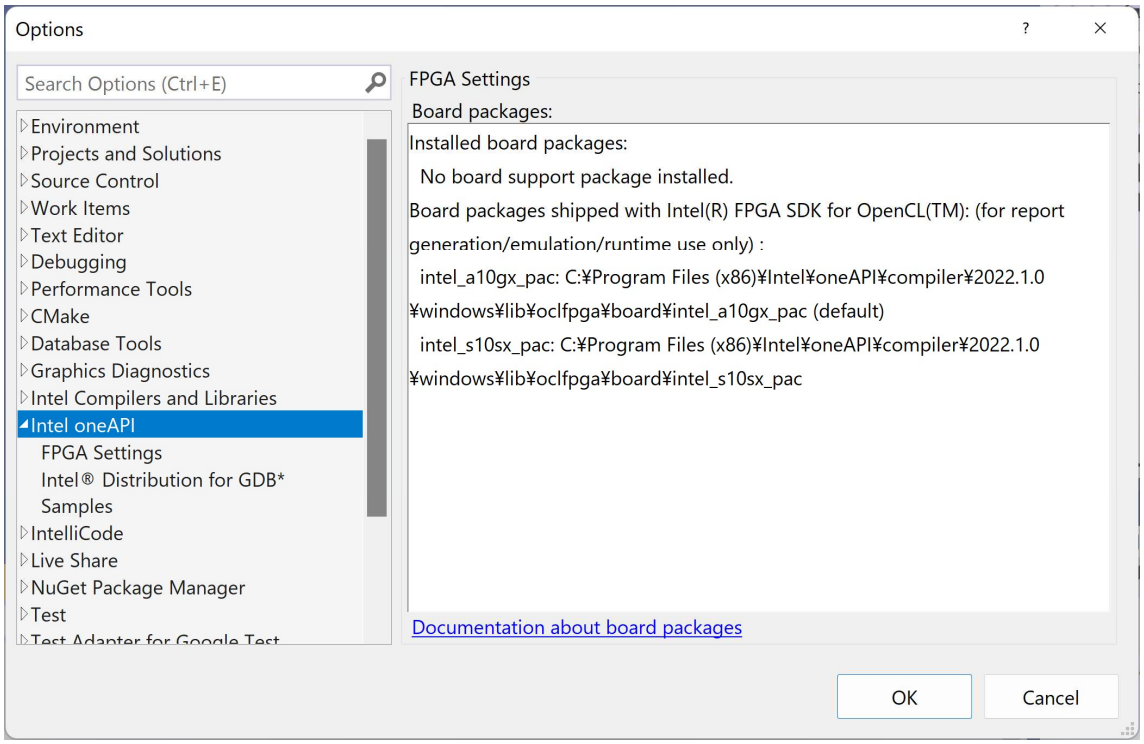


III-1

From “Open a project or solution”, open /phits/bin/phits-intel.vfproj

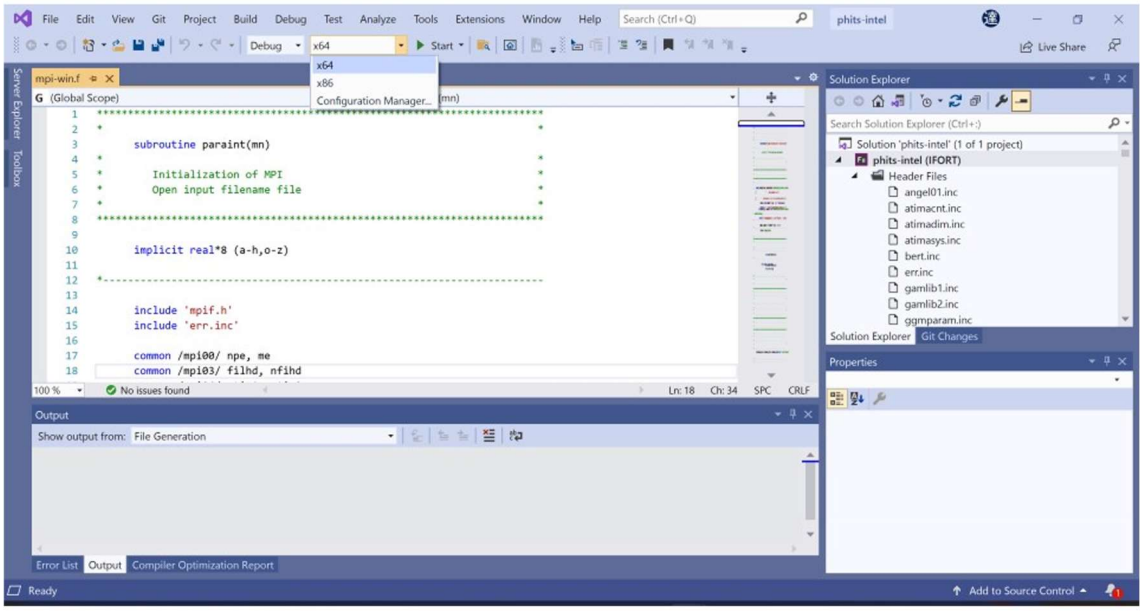
If you cannot select it, please make sure that Intel oneAPI appears in Menu Bar>Tool>Options. If not, oneAPI installation was not successful or you installed Visual Studio 2022.

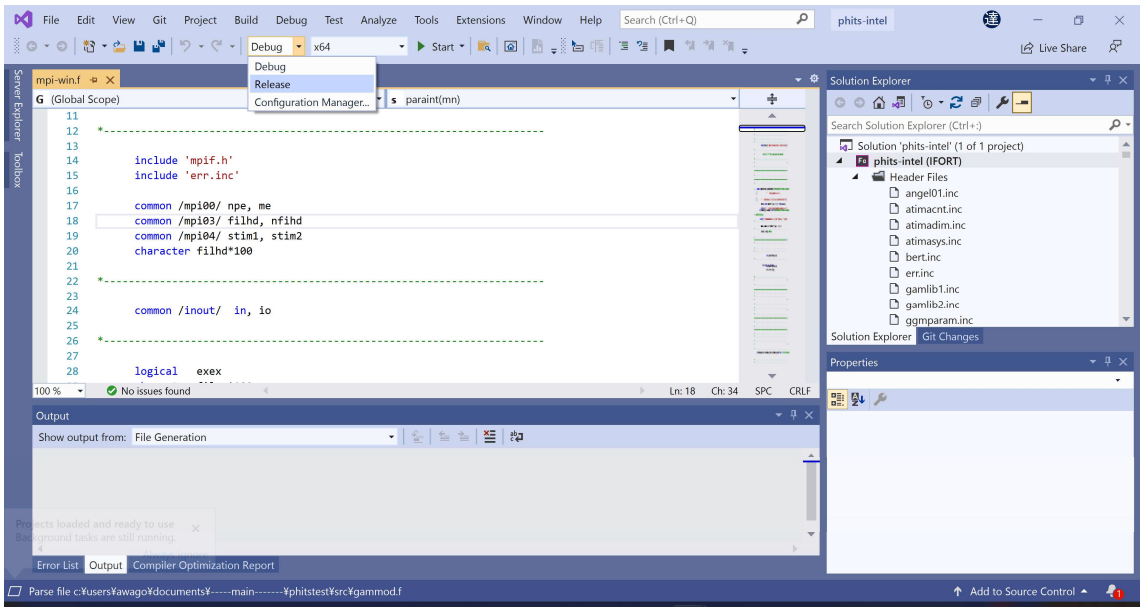




III-2

Select “Release” mode and “x64”. This configuration is the most memory/CPU effective.



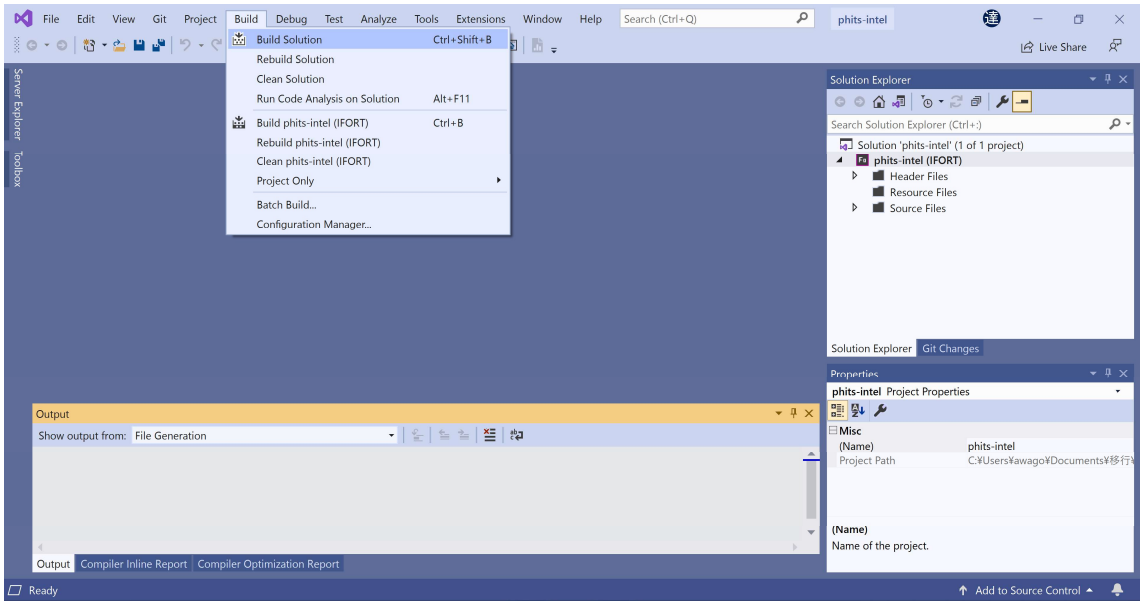


III-3

Create an executable file by

Build > Build Solution

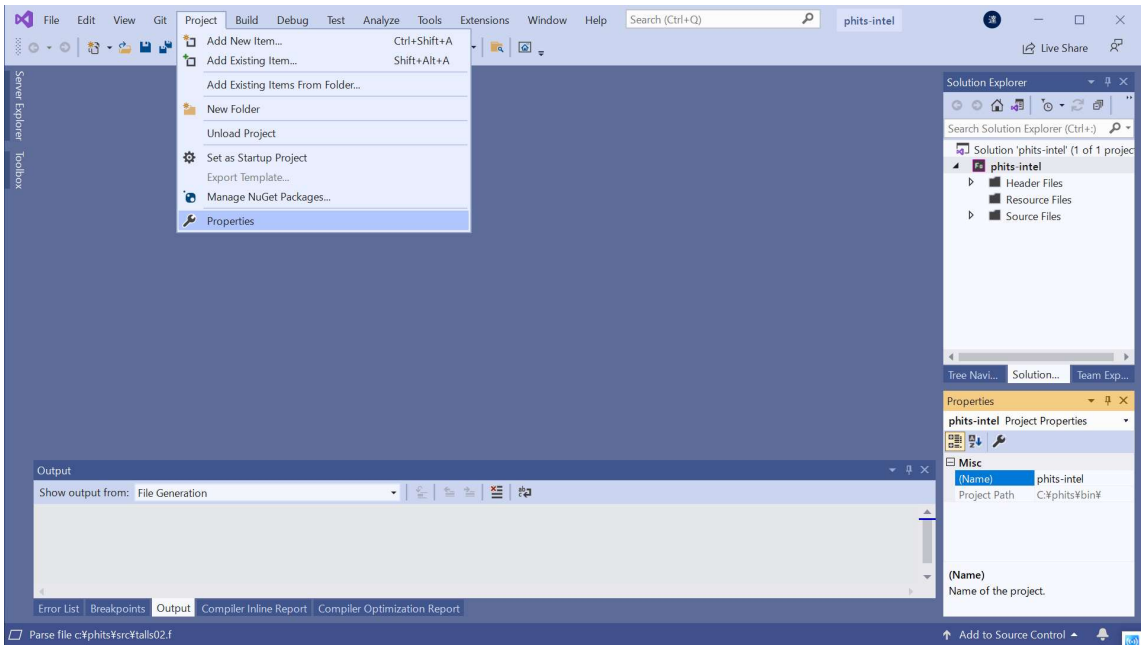
In Windows, please see “Execute via Command Prompt” in the manual on how to launch the executable file.

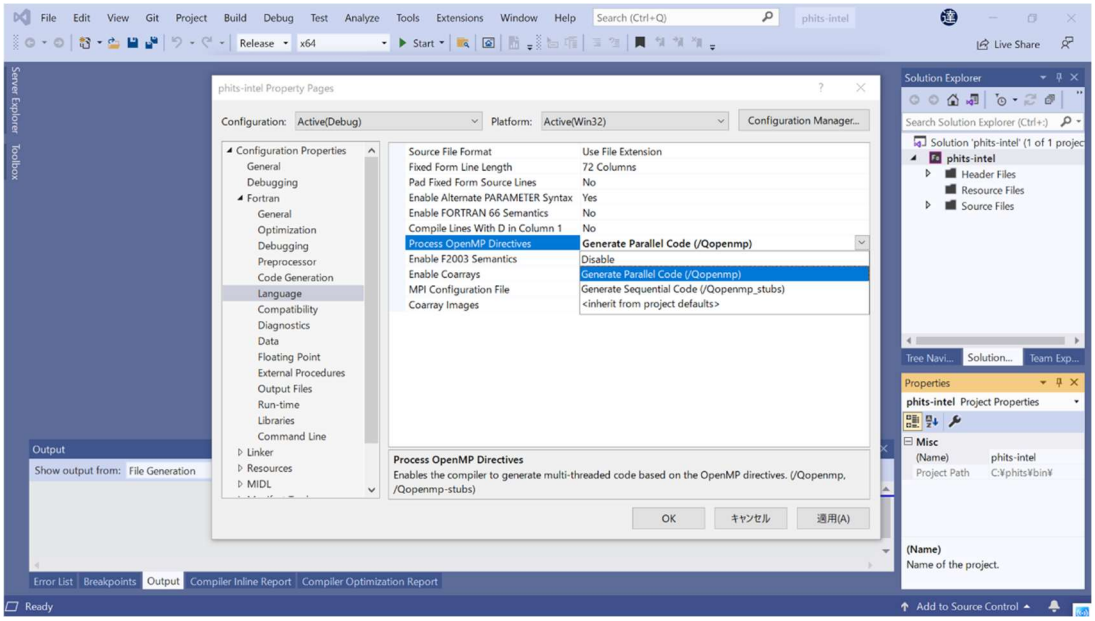


III-3’

To use OpenMP, activate “Qopenmp” option from

Menu bar > Project > Properties > Fortran > Language > Process OpenMP directives > Generate Parallel code





III-3''

III-3''-1

To use MPI, you need to

- Install MS-MPI (not explained in this manual. Please search "MS-MPI install")
- Configure the Build of Visual Studio

To configure the Build of Visual Studio, close Visual Studio and open phits¥bin¥phits-intel.vfproj with a text editor (e.g. notepad++). Then replace a line

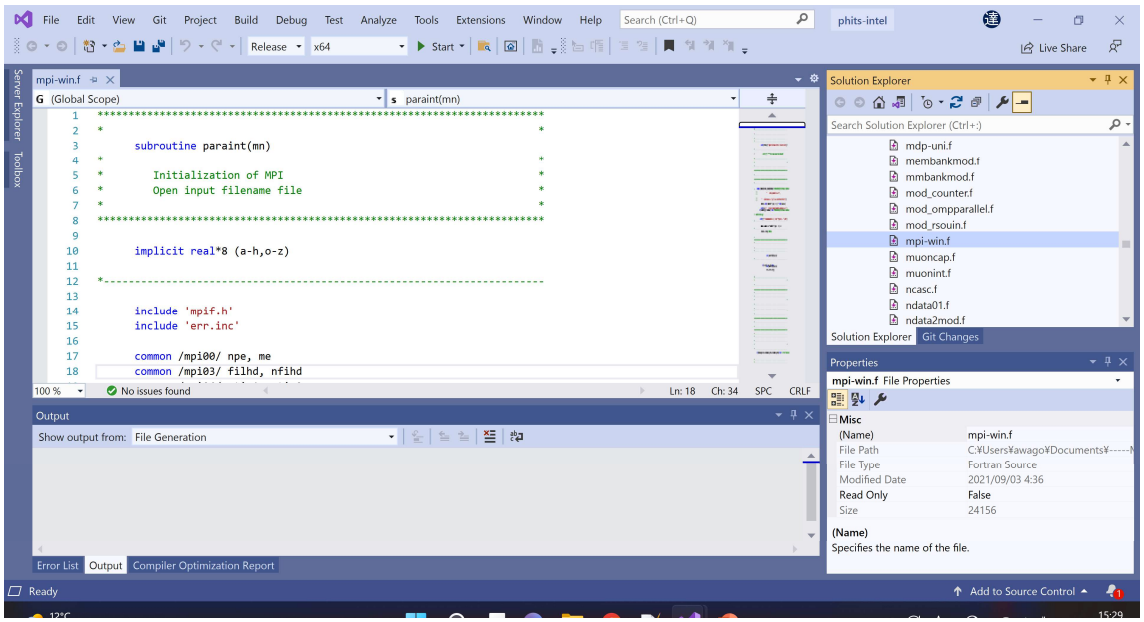
<File RelativePath="..¥src¥mpi-non.f"/>

with

<File RelativePath="..¥src¥mpi-win.f"/>

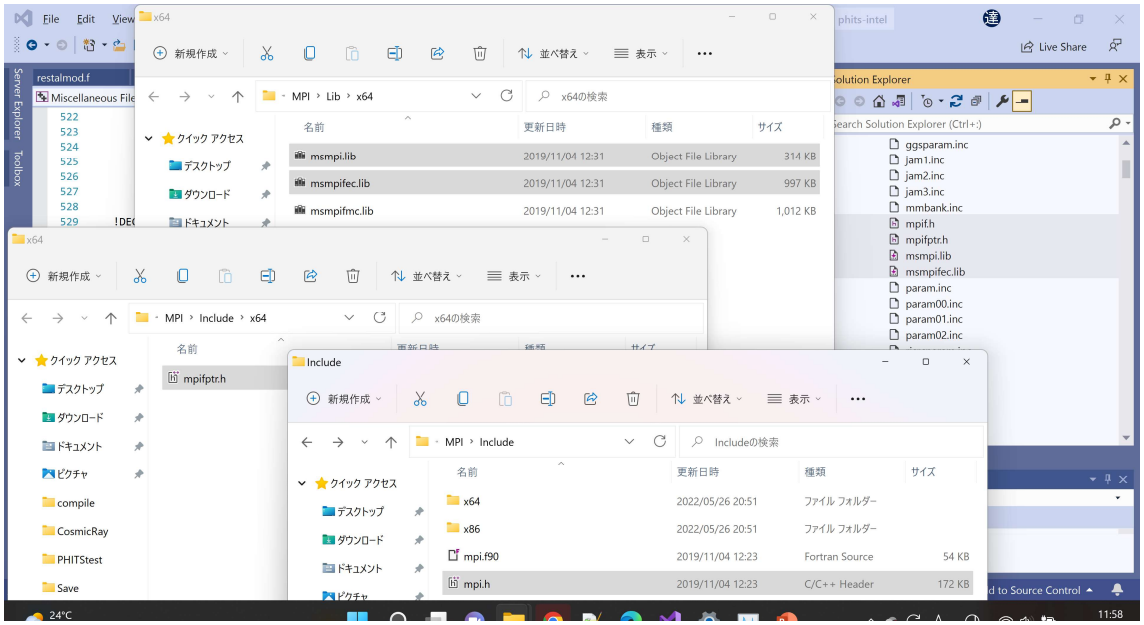
and save, open phits¥bin¥phits-intel.vfproj with Visual Studio again.

Updated project includes mpi-win.f in the solution explorer sub-window.



III-3’’-2

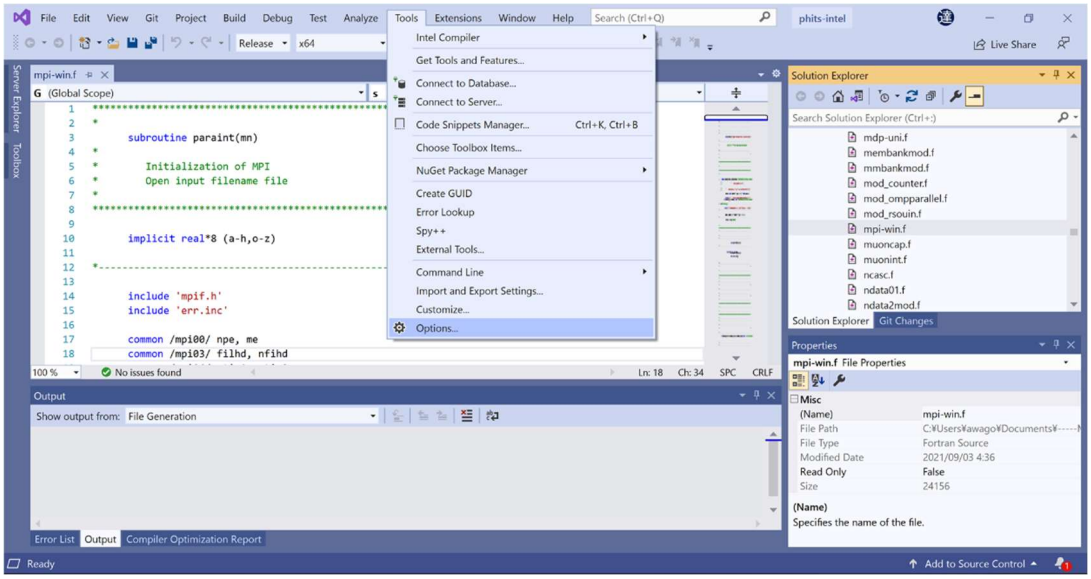
Add library files “msmpi.lib”, “msmpifec.lib”, and header files “mpif.h”, “mpifptr.h” to the solution explorer.

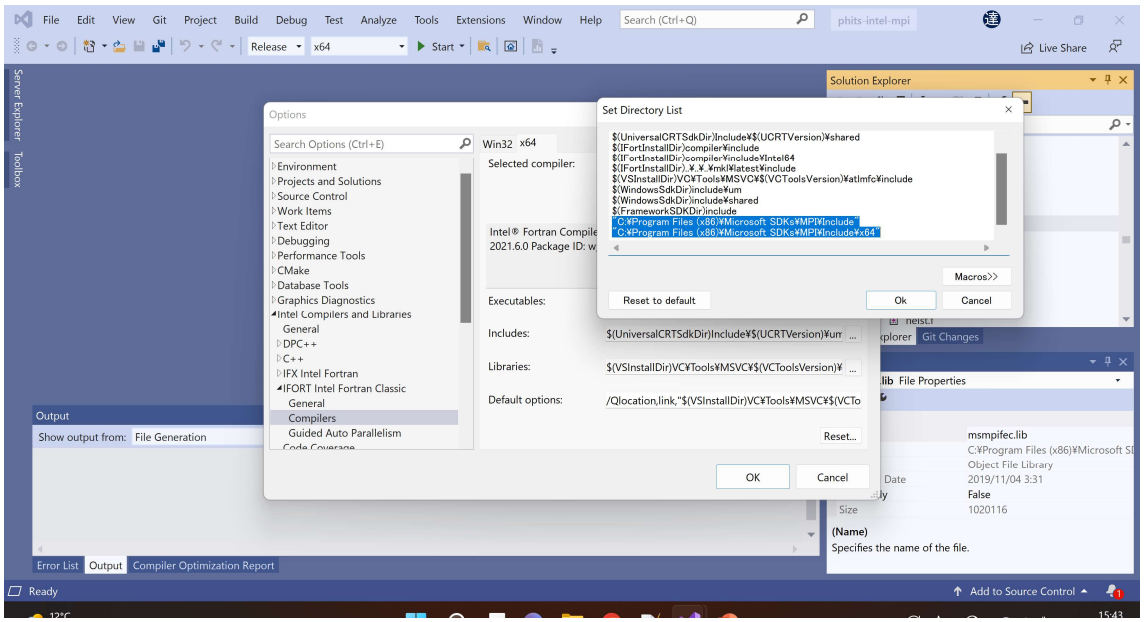


The directory of the files are as follows by default.

C:¥Program Files (x86)¥Microsoft SDKs¥MPI¥Include¥mpif.h
C:¥Program Files (x86)¥Microsoft SDKs¥MPI¥Include¥x64¥mpifptr.h
C:¥Program Files (x86)¥Microsoft SDKs¥MPI¥Lib¥x64¥msmpi.lib
C:¥Program Files (x86)¥Microsoft SDKs¥MPI¥Lib¥x64¥msmpifec.lib

III-3’’-3
Configure the Intel Fortran compiler in Visual studio.
Menu bar -> Tools -> Options -> IFORT Intel Fortran Classic -> Compilers -> x64 (tab) -> “…” of Includes
Add following 2 folders
"C:¥Program Files (x86)¥Microsoft SDKs¥MPI¥Include"
"C:¥Program Files (x86)¥Microsoft SDKs¥MPI¥Include¥x64"





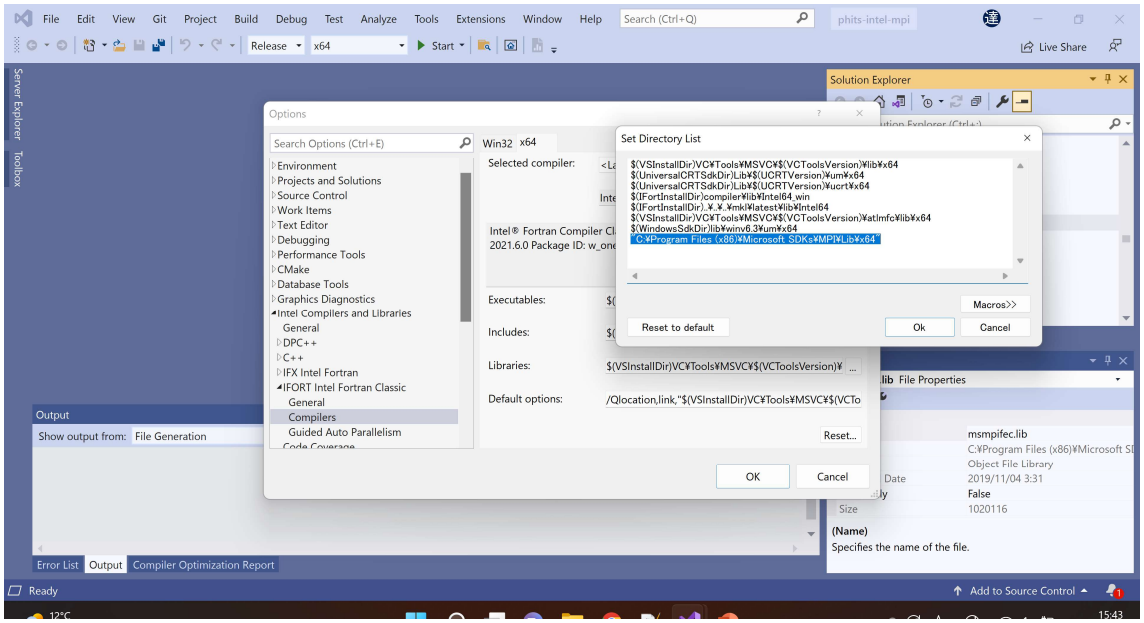
III-3’’-4

Consecutively

In the same tab x64, add a following folder to “…” of Libraries

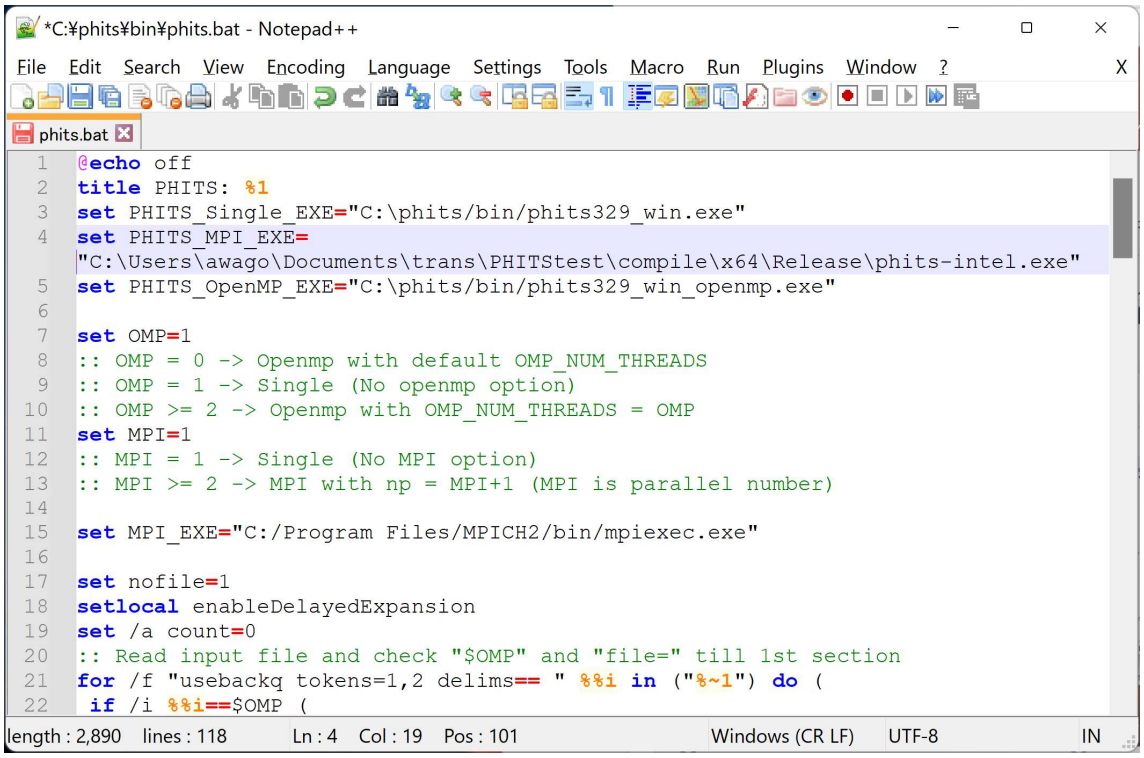
"C:¥Program Files (x86)¥Microsoft SDKs¥MPI¥Lib¥x64"

Then «Build» to create binary executable.

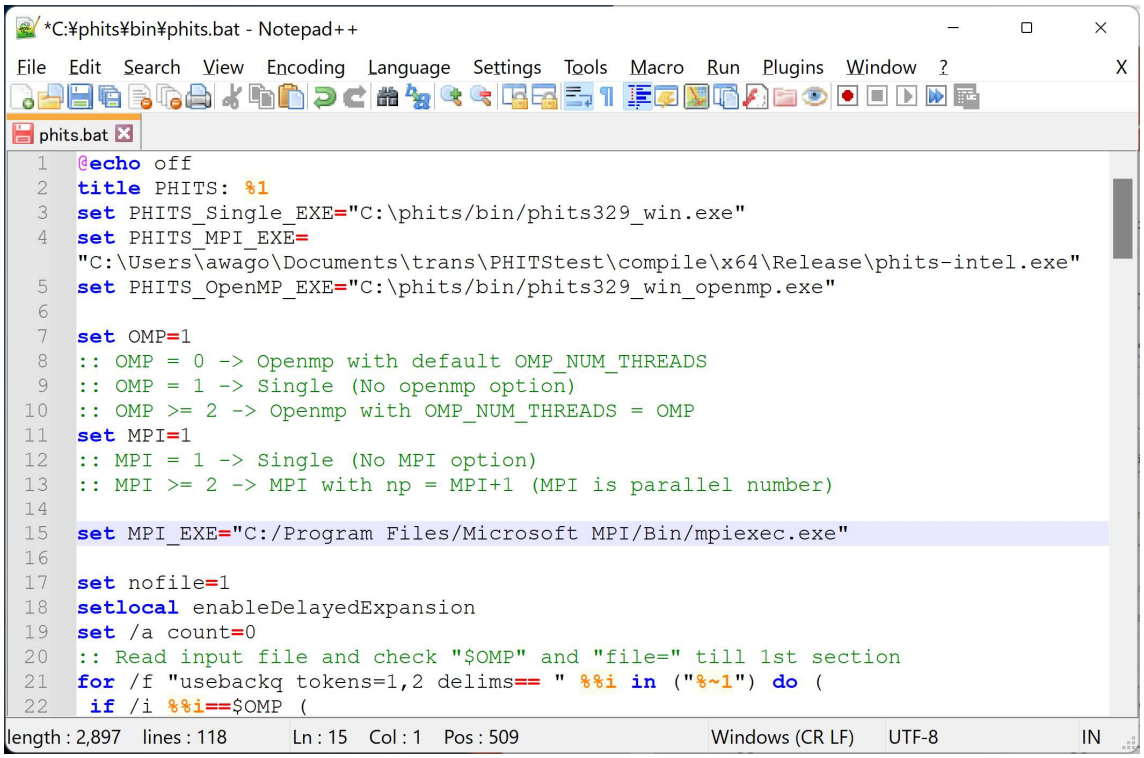


III-3’’-5

Modify phits/bin/phits.bat to use the MPI version of PHITS exe file. If the built executable is at
C:/Users/ogawa/Documents/trans/PHITStest/compile/x64/Release/phits-intel.exe
Change the 4th line of
phits/bin/phits.bat
to be
set PHITS_MPI_EXE = C:
/Users/ogawa/Documents/trans/PHITStest/compile/x64/Release/phits-intel.exe



III-3”-6
Modify another line which specifies MPI_EXE in phits/bin/phits.bat to point the mpi executable (not PHITS executable)
set MPI_EXE=”C:/Program Files/Microsoft MPI/Bin/mpiexec.exe”

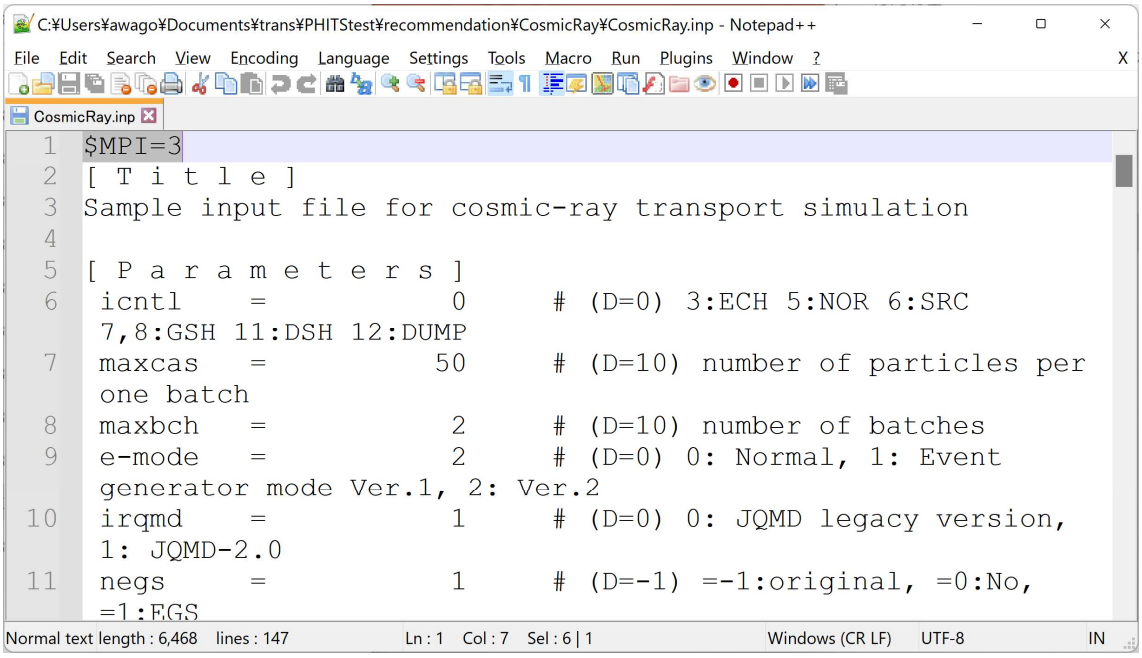


III-3''-7

Insert a line

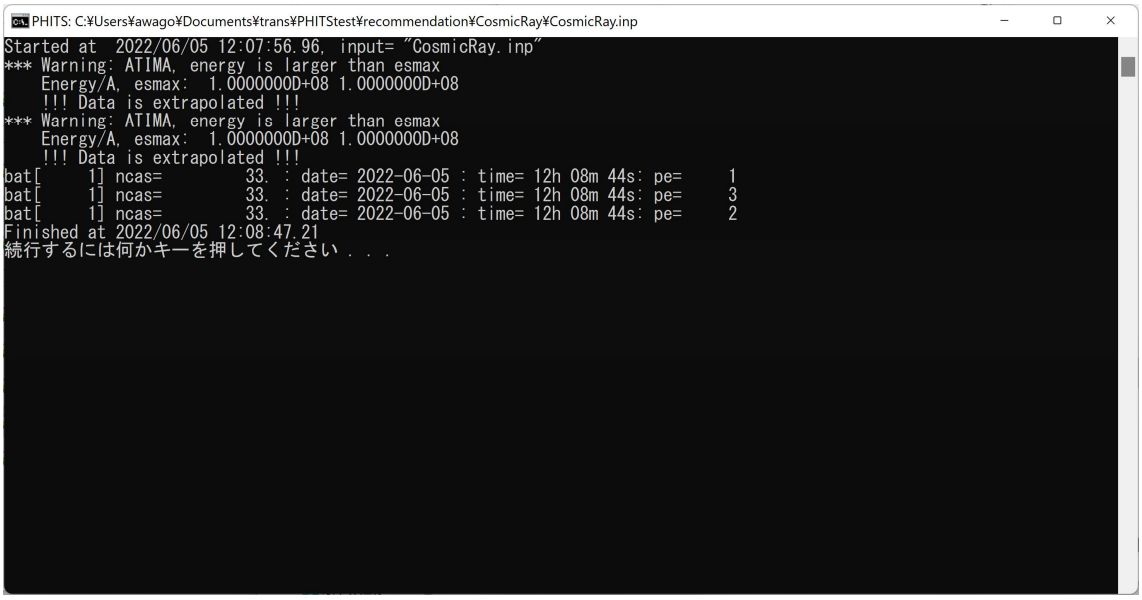
$OMP=**

at the top of PHITS input file where ** is the number of cores you would like to use. Then launch PHITS (e.g. Run shortcut command) with this input file.



III-3’’-8

In the terminal, batch report ends with “pe = ” if MPI works.



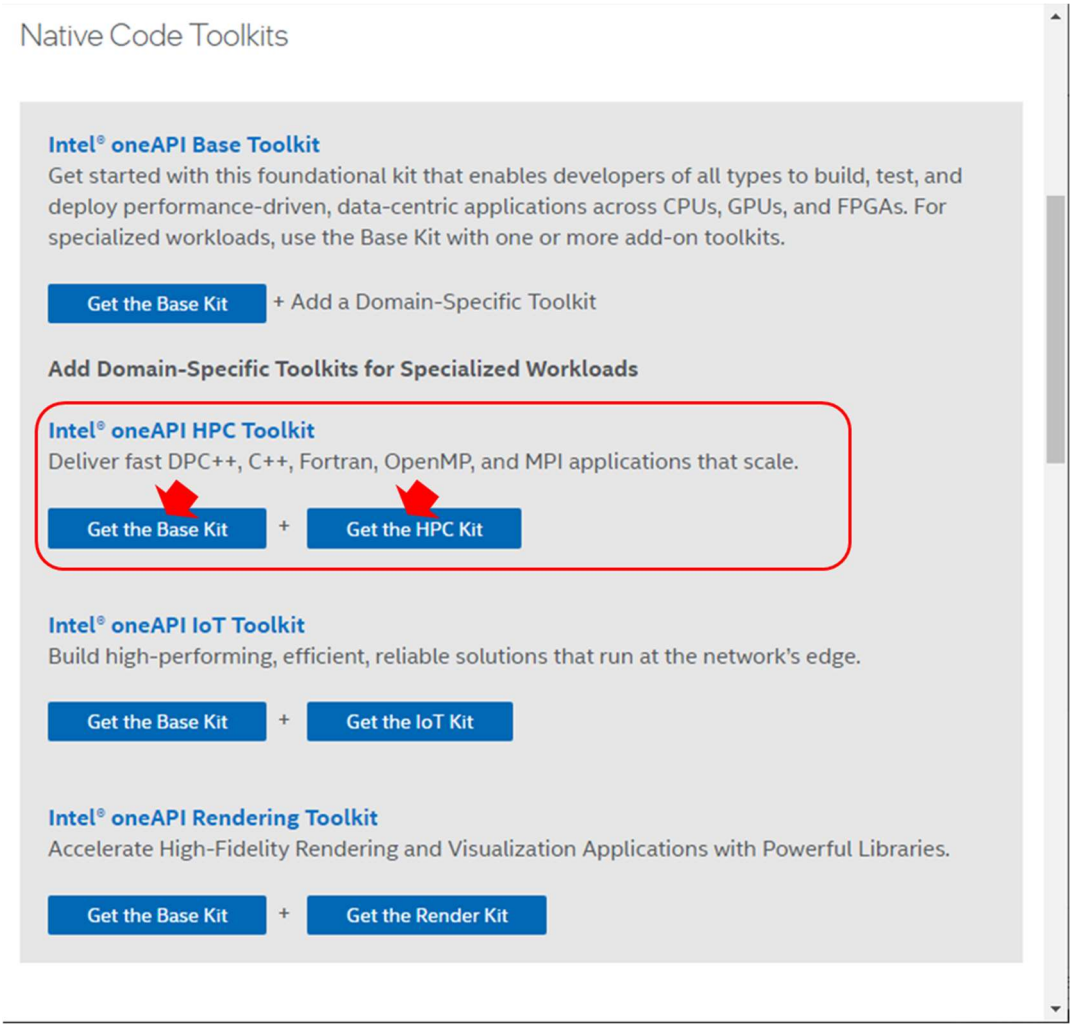
2. Linux

Phase I: Install OneAPI (Fortran compiler and its associated libraries)

I-1

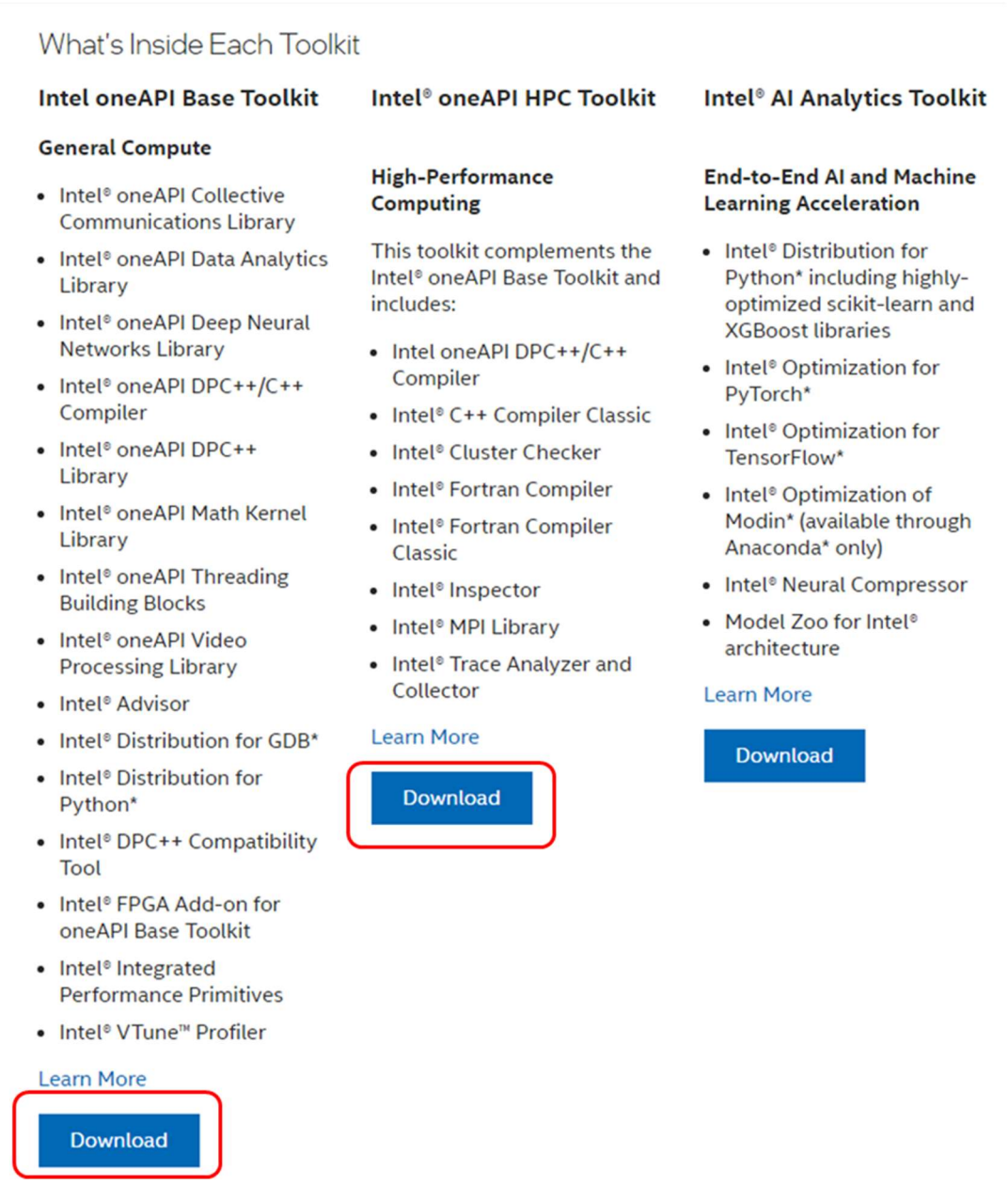
Access to Intel official web site and download toolkits (the Base Kit and the HPC kit are required for the Fortran compiler).

https://www.intel.com/content/www/us/en/developer/articles/news/free-intel-software-developer-tools.html



By clicking either of the above link, it will navigate to the following download page. Then you need to download the “Intel oneAPI Base Toolkit” and “Intel oneAPI HPC Toolkit”. The link

will navigate to the page to choose “Operating System” and “Distribution”. Please choose “Linux” for the “Operating System” and select the distribution choice which is suitable for your distribution. If you are not sure for the choice of “Distribution”, you can choose “Online & Offline”.



I-2

Install the toolkits (the Base Kit and the HPC kit). Please install those toolkits following to the instruction given in the download page. Normally you need to open a terminal and execute

a shell script at the location of the download directory. The super user authorization may be required. Then follow the instruction to continue the installation. The OpenMP and MPI libraries are also included in those toolkits so that parallel computation of PHITS with OpenMP and MPI can be easily performed.

I-3

Environmental setup is required to use the installed oneAPI libraries. The setup shell script is prepared in /opt/intel/oneapi/setvars.sh (for system wide installation) or ~/intel/oneapi/setvars.sh (for private installation). The execution of the setup shell script is required at each time when you open a new terminal window command such as

. /opt/intel/oneapi/setvar.sh (for system wide installation)

or

. ~/intel/oneapi/setvar.sh (for private installation).

If you think it is tedious to do at each opening of new terminal windows, you can add the above command in your setup shell such as ~/.bashrc, ~/.bashrc_profile, or ~/.profile according to your environment. Then the oneAPI setup shell script will be automatically executed when you open a new terminal window.

Phase II: Compile PHITS

II-0

GNU make is required to compile PHITS. So please install GNU make package according to your environment.

II-1

Open a terminal window and change directory to the source code directory of PHITS (phits/src).

II-2

Check (or modify) the makefile located in the source directory. The environmental flag "ENVFLAGS" needs to be changed according to your compilation environment. To use the Intel Fortran compiler for Linux, please set "ENVFLAGS=LinIfort", which should be default option.

If you want to compile PHITS with activating MPI parallelization, please erase "#" before "USEMPI = true". If you want to compile PHITS with activating OpenMP parallelization, please erase "#" before "USEOMP = true".

II-3

Type “make” and return to compile PHITS in the terminal window. You can also parallelize the compilation by typing “make -j **”, where ** is the number of computation cores you want to use for this compilation.

You may see some warning messages but you can ignore those unless you see error messages and the compilation stops. For the parallel compilation, there are cases you see errors by unsolved dependence of the source codes. Please “make” again several times, which may solve the dependence and successfully compile PHITS.

Successful compilation of PHITS will produce the PHITS executable in the parent directory of the source code directory:

phits_LinIfort (without parallelization)
phits_LinIfort_OMP (with OpenMP parallelization)
phits_LinIfort_MPI (with MPI parallelization).

II-4

A setup to use the PHITS shell script as “phits.sh ***.inp” to execute PHITS by overwriting the existing PHITS executables.

Please copy those files into the PHITS binary executable directory (phits/bin) by renaming the file to

phits_LinIfort => phits***_lin.exe
phits_LinIfort_OMP => phits***_lin_openmp.exe
phits_LinIfort_MPI => phits***_lin_mpi.exe

where *** is the PHITS version number.

Using the PHITS shell script, the parallelization can be controlled by the specification in the 1st line of the PHITS input file; “$OMP=**” and “$MPI=**”.

II-4’

A setup to use the PHITS shell script as “phits.sh ***.inp” to execute PHITS with keeping the old PHITS executables.

Please copy the compiled executable files into the PHITS binary executable directory (phits/bin). You can change the file name if you want. Then please modify the PHITS shell script “phits.sh” in the directory according to match the names. The names of executables are specified in “phits.sh” by

PHITS_SINGLE_EXE=phits***_lin.exe (without parallelization)
PHITS_OMP_EXE=phits***_lin_openmp.exe (with OpenMP parallelization)

PHITS_MPI_EXE=phits***_lin_mpi.exe (with MPI parallelization).

So please change the names of executables after "=" to be consistent.

Using the PHITS shell script, the parallelization can be controlled by the specification in the 1st line of the PHITS input file; "$OMP=**" and "$MPI=**".

II-4''

Directly use the executables to perform PHITS execution.

The created PHITS executables can be also used alone such as

```
phits_LinIfort < ***.inp
phits_LinIfort_OMP < ***.inp
mpiexec -n 8 phits_LinIfort_MPI
```

where ***.inp is the PHITS input file. In this MPI execution, the file phits.in with "file=***.inp" at the 1st line is required in the execution directory. The MPI execution command and options may differ by your environment. Here "-n 8" means the 8 MPI process parallelization (7 calculation processes + 1 master process in PHITS).

3. macOS

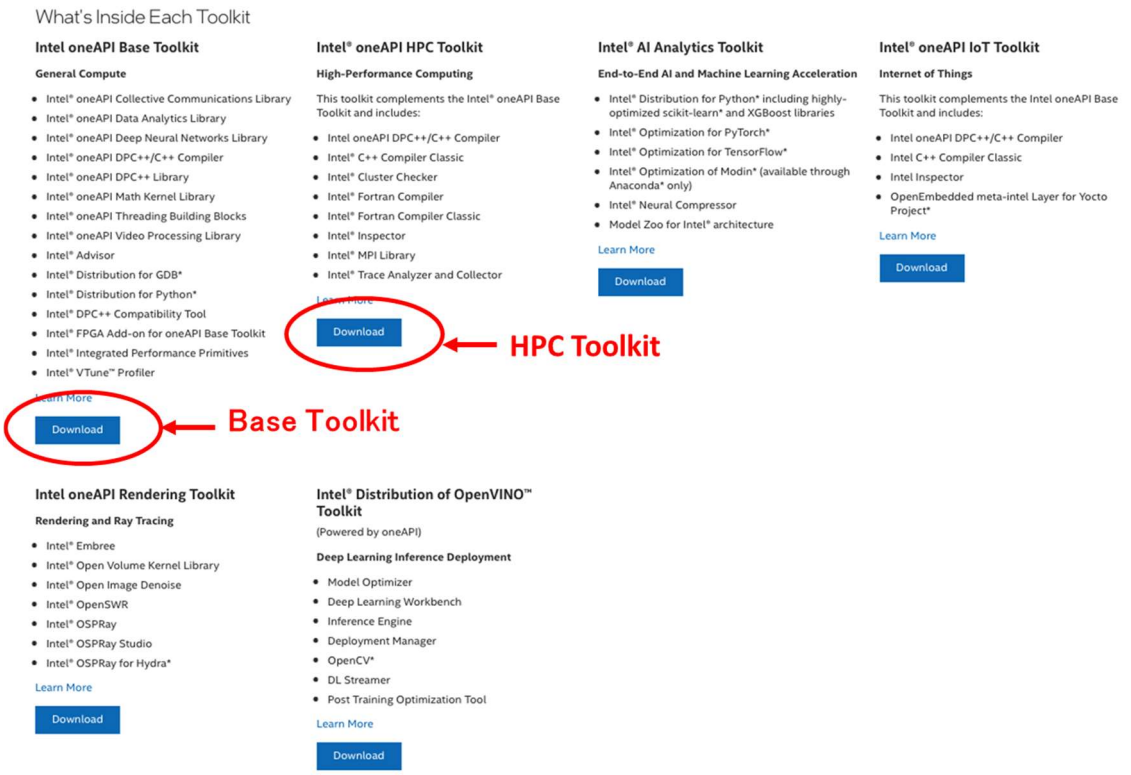
Free use of Intel Fortran (Intel oneAPI Base Toolkit + HPC Toolkit)

Fortran Software:
Intel® oneAPI Base Toolkit (version 2022.2, or later)
Intel® oneAPI HPC Toolkit (version 2022.2, or later)
Please note that the oneAPI for macOS does not include MPI.

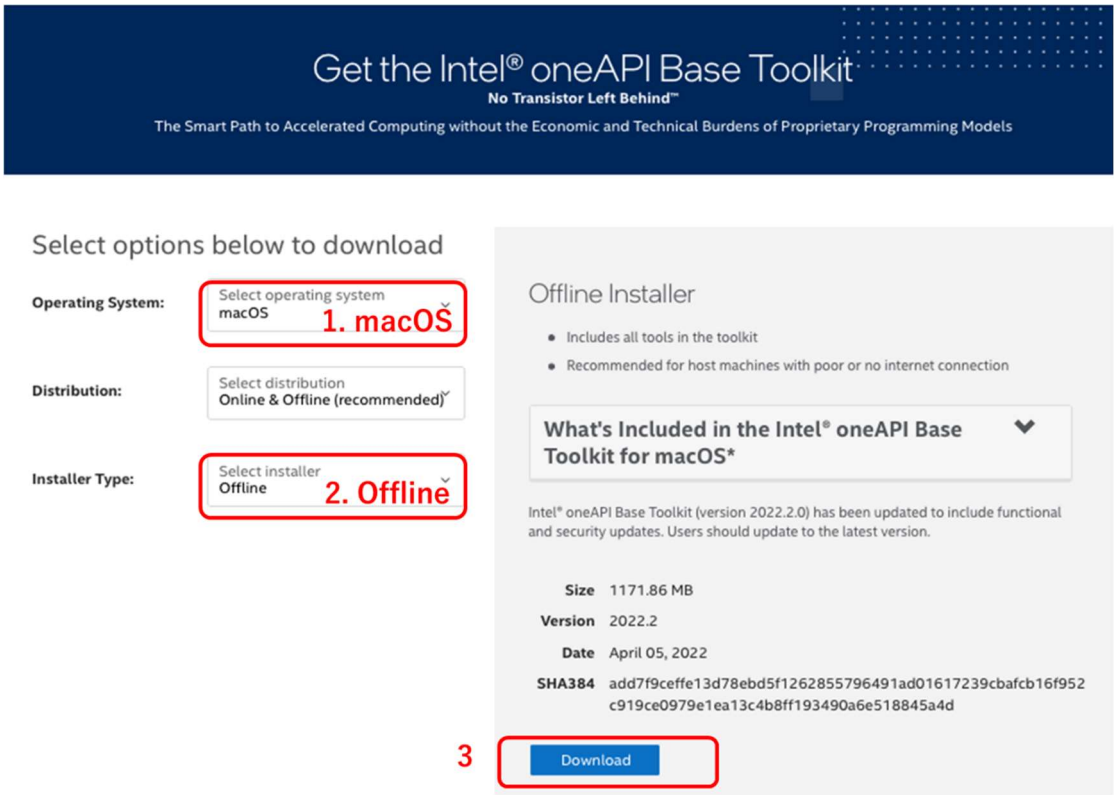
Phase I: Download and installation

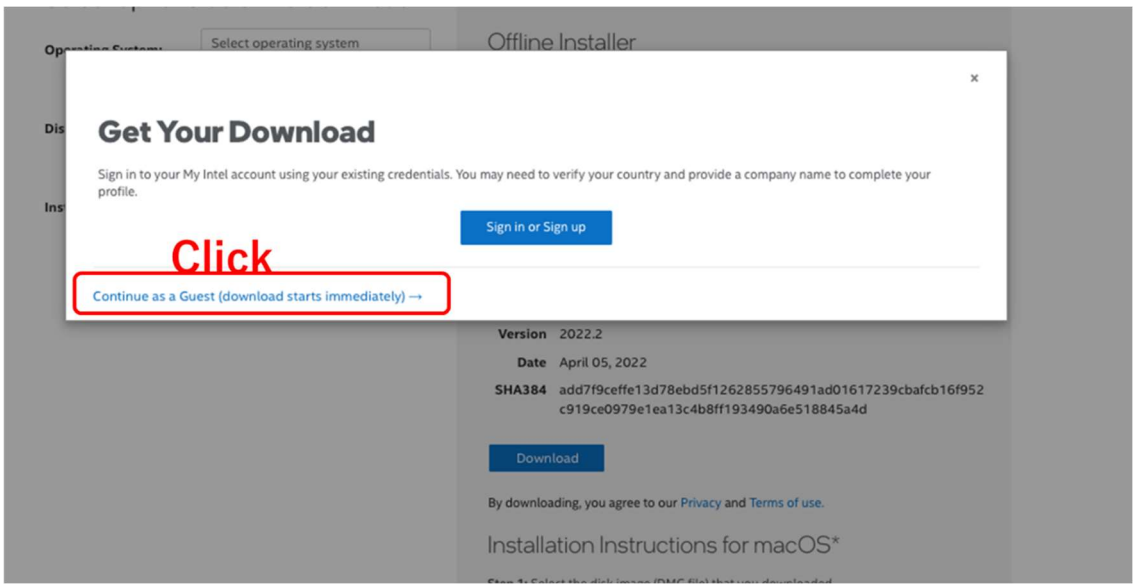
1. Download

1.1 Go to the following and click the download button for Base Toolkit and HPC Toolkit.
https://www.intel.com/content/www/us/en/developer/tools/oneapi/toolkits.html#base-kit

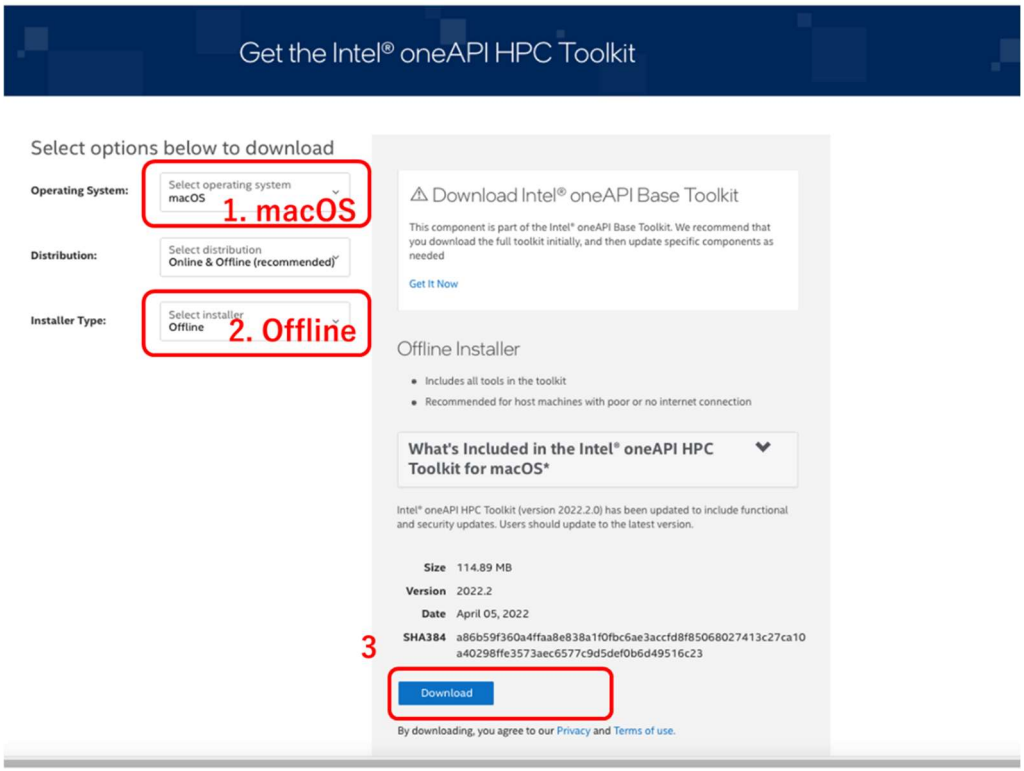


1.2 Download Base Toolkit.



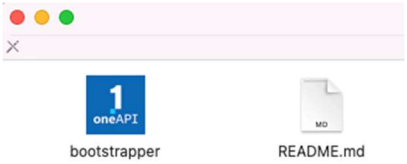


1.3 Download HPC Toolkit.



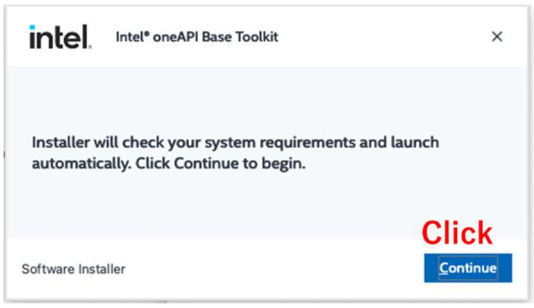
2. Installation of Base Kit

2.1. Expand the dmg file. You will get bootstrapper.app.

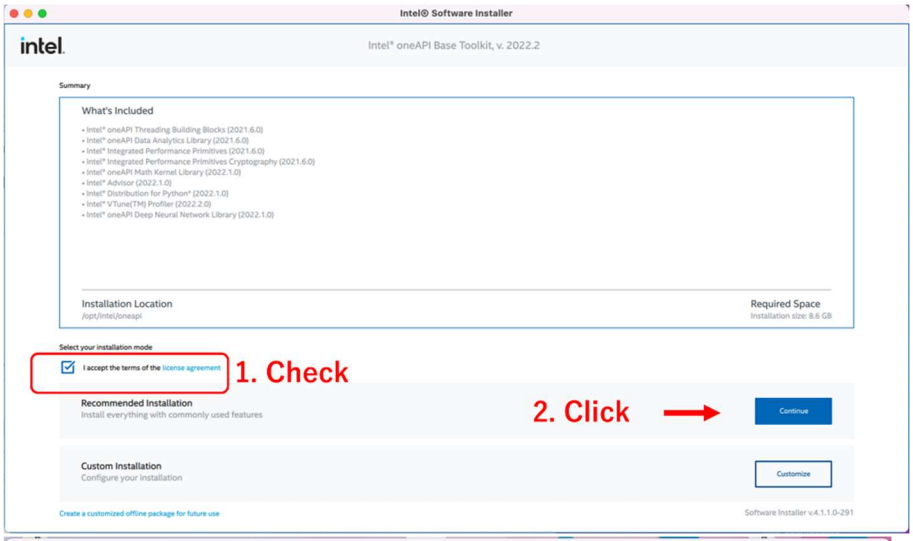


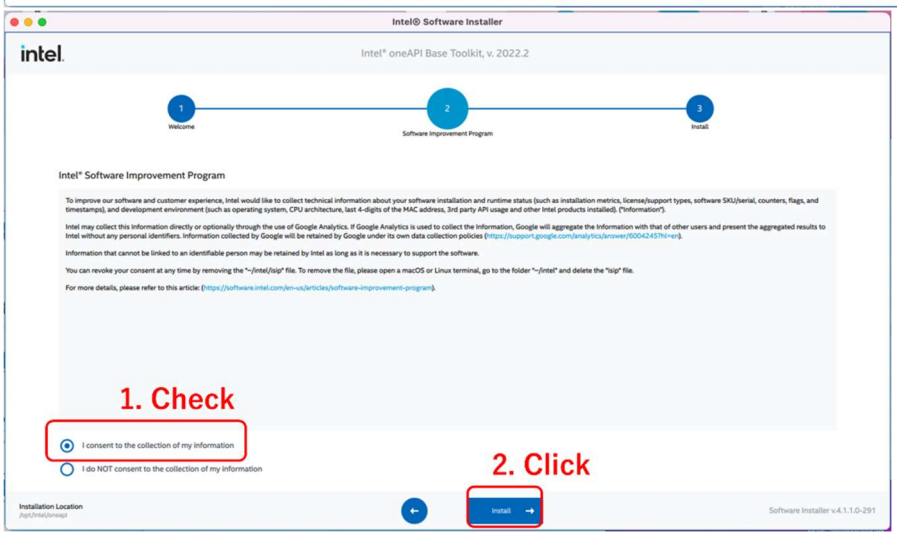
2.2. Double-click bootstrapper.app.

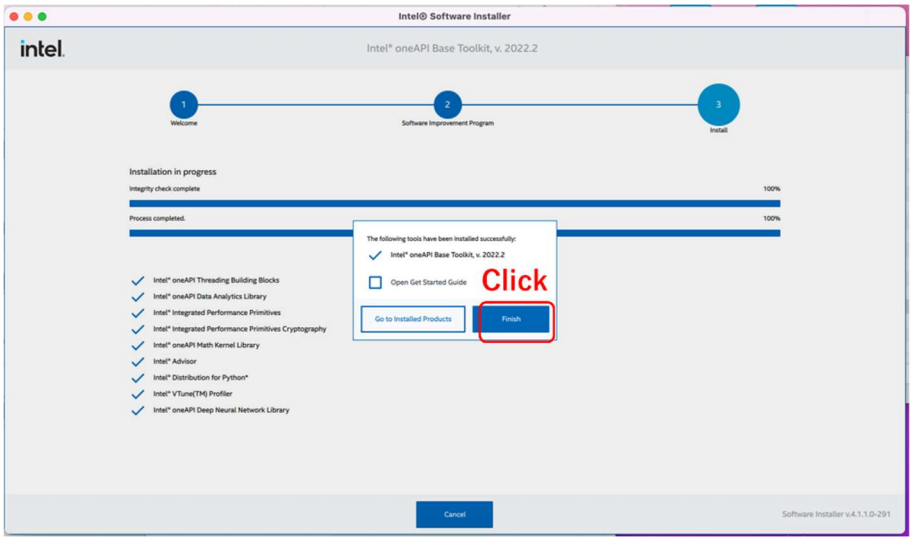
After a few minutes of waiting and a security warning



menu will appear, and "Continue" will take you to the installation screen. (At this point, there are three oneAPI icons lined up in the Dock.)

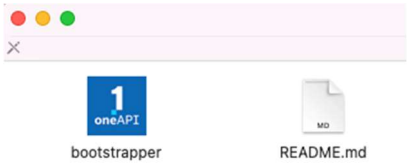

Intel® Software Installer
intel
Intel® oneAPI Base Toolkit, v. 2022.2
Summary
What's Included
• Intel® oneAPI Threading Building Blocks (2021.6.0)
• Intel® oneAPI Data Analytics Library (2021.6.0)
• Intel® Integrated Performance Primitives (2021.6.0)
• Intel® Integrated Performance Primitives Cryptography (2021.6.0)
• Intel® oneAPI Math Kernel Library (2022.1.0)
• Intel® Advisor (2022.1.0)
• Intel® Distribution for Python* (2022.1.0)
• Intel® VTune(TM) Profiler (2022.2.0)
• Intel® oneAPI Deep Neural Network Library (2022.1.0)
Installation Location
/opt/intel/oneapi
Required Space
Installation size: 8.6 GB
Select your installation mode
I accept the terms of the license agreement
1. Check
Recommended Installation
Install everything with commonly used features
2. Click
Continue
Custom Installation
Configure your installation
Customize
Create a customized offline package for future use
Software Installer v.4.1.1.0-291


Intel® Software Installer
intel
Intel® oneAPI Base Toolkit, v. 2022.2
1
Welcome
2
Software Improvement Program
3
Install
Intel® Software Improvement Program
To improve our software and customer experience, Intel would like to collect technical information about your software installation and runtime status (such as installation metrics, license/support types, software SKU/serial, counters, flags, and timestamps), and development environment (such as operating system, CPU architecture, last 4-digits of the MAC address, 3rd party API usage and other Intel products installed). ("Information").
Intel may collect this Information directly or optionally through the use of Google Analytics. If Google Analytics is used to collect the Information, Google will aggregate the Information with that of other users and present the aggregated results to Intel without any personal identifiers. Information collected by Google will be retained by Google under its own data collection policies (https://support.google.com/analytics/answer/6004245?hl=en).
Information that cannot be linked to an identifiable person may be retained by Intel as long as it is necessary to support the software.
You can revoke your consent at any time by removing the "~/intel/isip" file. To remove the file, please open a macOS or Linux terminal, go to the folder "~/intel" and delete the "isip" file.
For more details, please refer to this article: (https://software.intel.com/en-us/articles/software-improvement-program).
1. Check
I consent to the collection of my information
I do NOT consent to the collection of my information
2. Click
Installation Location
/opt/intel/oneapi
Install
Software Installer v.4.1.1.0-291


Intel® Software Installer
intel
Intel® oneAPI Base Toolkit, v. 2022.2
1
Welcome
2
Software Improvement Program
3
Install
Installation in progress
Integrity check complete
100%
Process completed.
100%
The following tools have been installed successfully:
Intel® oneAPI Base Toolkit, v. 2022.2
Open Get Started Guide
Click
Go to Installed Products
Finish
Intel® oneAPI Threading Building Blocks
Intel® oneAPI Data Analytics Library
Intel® Integrated Performance Primitives
Intel® Integrated Performance Primitives Cryptography
Intel® oneAPI Math Kernel Library
Intel® Advisor
Intel® Distribution for Python*
Intel® VTune(TM) Profiler
Intel® oneAPI Deep Neural Network Library
Cancel
Software Installer v.4.1.1.0-291

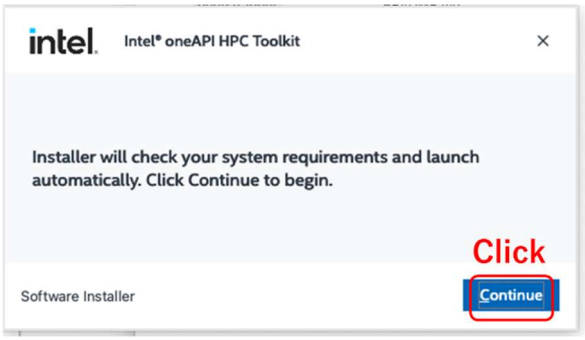
3. Installation of HPC Kit

3.1. Expand the dmg file. You will get bootstrapper.app.

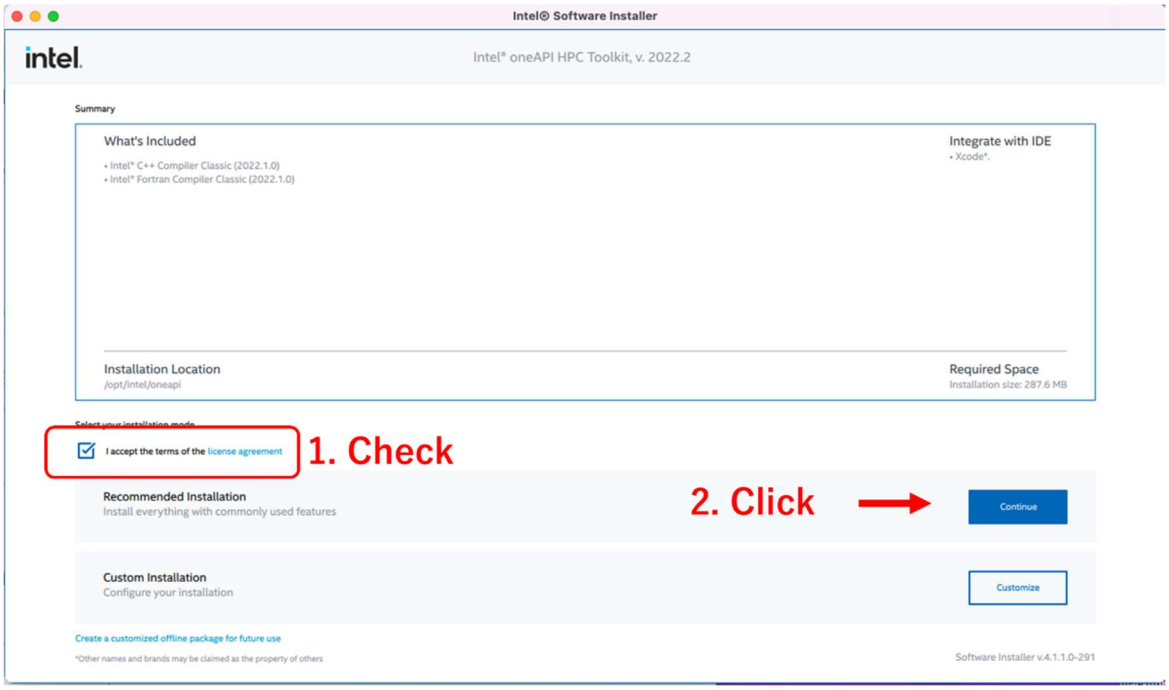


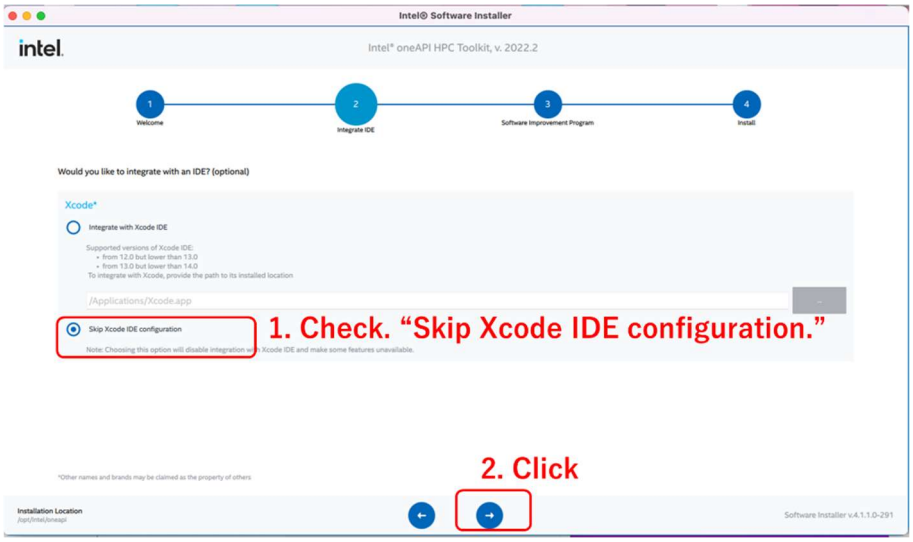
3.2. Double-click bootstrapper.app.

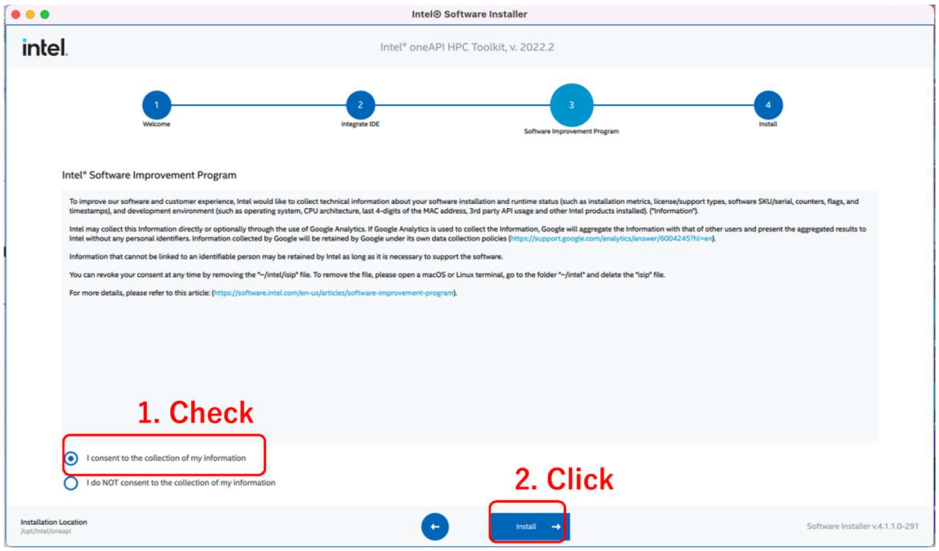
After a few minutes of waiting and a security warning

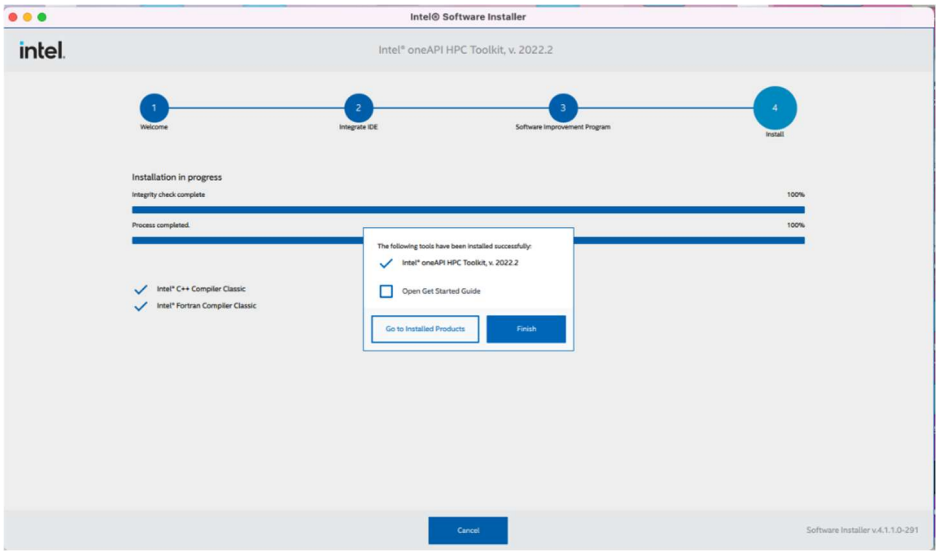


menu will appear, and "Continue" will take you to the installation screen.




Intel® Software Installer
intel.
Intel® oneAPI HPC Toolkit, v. 2022.2
1 Welcome
2 Integrate IDE
3 Software Improvement Program
4 Install
Would you like to integrate with an IDE? (optional)
Xcode*
Integrate with Xcode IDE
Supported versions of Xcode IDE:
• from 12.0 but lower than 13.0
• from 13.0 but lower than 14.0
To integrate with Xcode, provide the path to its installed location
/Applications/Xcode.app
Skip Xcode IDE configuration
1. Check. “Skip Xcode IDE configuration.”
2. Click
Installation Location
Software Installer v.4.1.1.0-291


Intel® Software Installer
intel.
Intel® oneAPI HPC Toolkit, v. 2022.2
1 Welcome
2 Integrate IDE
3 Software Improvement Program
4 Install
Intel® Software Improvement Program
1. Check
I consent to the collection of my information
I do NOT consent to the collection of my information
2. Click
Install
Installation Location
Software Installer v.4.1.1.0-291


Intel® Software Installer
intel.
Intel® oneAPI HPC Toolkit, v. 2022.2
1 Welcome
2 Integrate IDE
3 Software Improvement Program
4 Install
Installation in progress
Integrity check complete
100%
Process completed.
100%
The following tools have been installed successfully:
Intel® oneAPI HPC Toolkit, v. 2022.2
Open Get Started Guide
Go to Installed Products
Finish
Intel® C++ Compiler Classic
Intel® Fortran Compiler Classic
Cancel
Software Installer v.4.1.1.0-291

4. Environment setup

Environment setup is required to use the installed oneAPI libraries. The setup shell script is prepared in /opt/intel/oneapi/setvars.sh (for system wide installation). The execution of the setup shell script is required at each time when you open a new terminal window command such as

source /opt/intel/oneapi/setvars.sh

If you think it is tedious to do at each opening of new terminal windows, you can add the above command in your setup shell such as ~/.zshrc, ~/.bashrc, ~/.bashrc_profile, or ~/.profile according to your environment. Then the oneAPI setup shell script will be automatically executed when you open a new terminal window.

Phase II: Compile PHITS

0

The “make” package is required to compile PHITS. So please install the “make” package with Homebrew or MacPorts.

Homebrew: https://brew.sh/

MacPorts: https://www.macports.org/

1

Open a terminal window and change directory to the source code directory of PHITS (phits/src).

2

Check (or modify) the makefile located in the source directory. The environmental flag “ENVFLAGS” needs to be changed according to your compilation environment. To use the Intel Fortran compiler for Linux, please set “ENVFLAGS=MacIfort”, which should be default option.

If you want to compile PHITS with activating OpenMP parallelization, please erase “#” before “USEOMP = true”.

3

Type “make” and return to compile PHITS in the terminal window. You may see some warning messages but you can ignore those unless you see error messages and the compilation stops. Successful compilation of PHITS will produce the PHITS executable in the parent directory of the source code directory:

phits_MacIfort (without parallelization)

phits_MacIfort_OMP (with OpenMP parallelization)

4

A setup to use the PHITS shell script as “phits.sh ***.inp” to execute PHITS by overwriting the existing PHITS executables.

Please copy those files into the PHITS binary executable directory (phits/bin) by renaming the file to

phits_MacIfort => phits***_mac.exe

phits_MacIfort_OMP => phits***_mac_openmp.exe

where *** is the PHITS version number.

Using the PHITS shell script, the parallelization can be controlled by the specification in the 1st line of the PHITS input file; “$OMP=**”.

4’

Directly use the executables to perform PHITS execution.

The created PHITS executables can be also used alone such as

phits_MacIfort < ***.inp

phits_MacIfort_OMP < ***.inp

where ***.inp is the PHITS input file.