編譯器及函式庫

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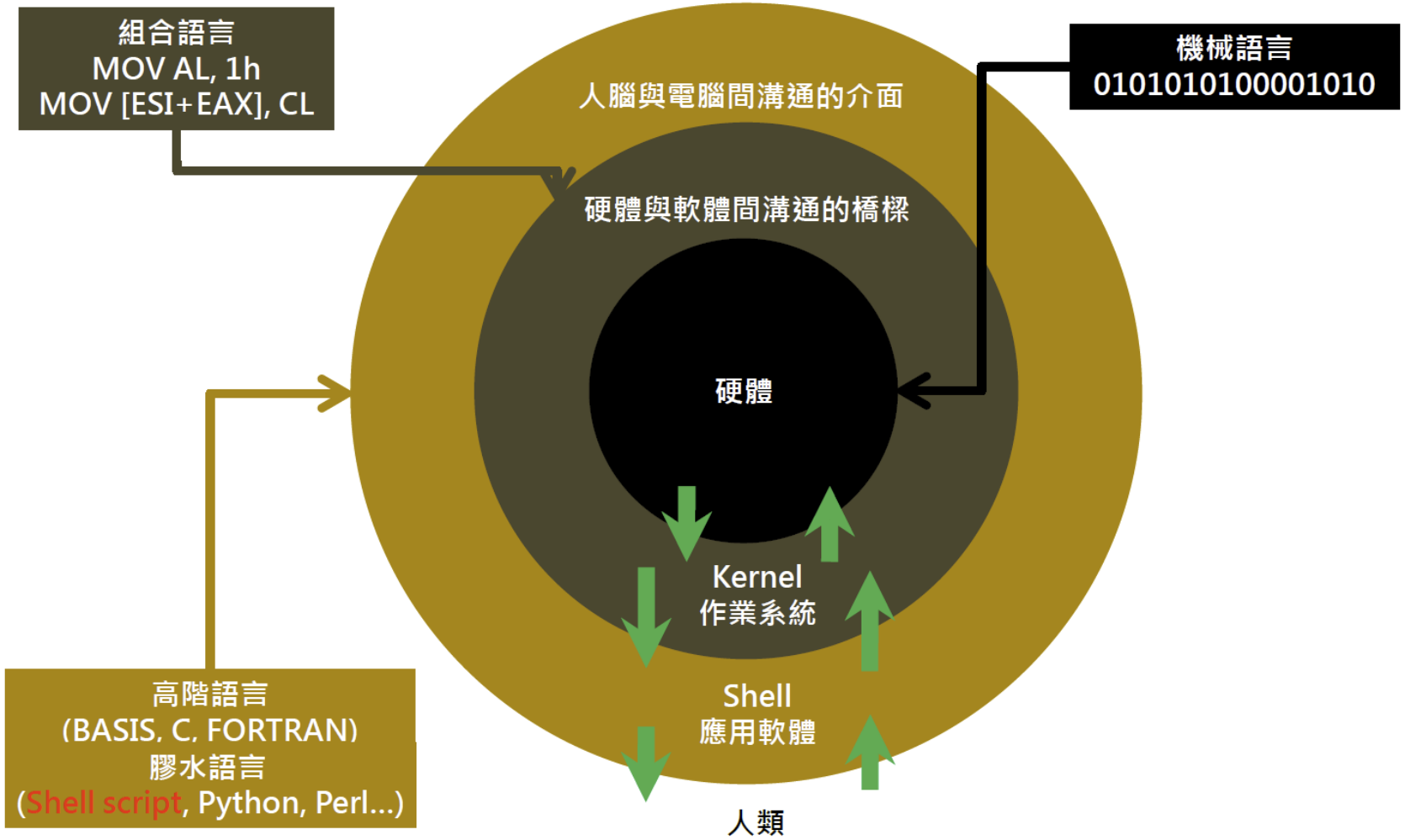
摘要

- 什麼是編譯器？
- 安裝 GNU, Intel, PGI 編譯器
- 分別使用 GNU 跟 Intel 的編譯器安裝 OpenMPI
- 編譯並執行你自己的程式
- 編譯以下的函式庫：
  - FFTW3
  - BLAS
  - LAPACK
  - GSL
  - HDF5
- 使用MKL (Math Kernel Library) 或其它函式庫

什麼是編譯器？


組合語言
MOV AL, 1h
MOV [ESI+EAX], CL
機械語言
0101010100001010
人腦與電腦間溝通的介面
硬體與軟體間溝通的橋樑
硬體
Kernel
作業系統
Shell
應用軟體
人類
高階語言
(BASIS, C, FORTRAN)
膠水語言
(Shell script, Python, Perl...)

常用的編譯器

- GNU Compiler
  依循 GNU License 的編譯器
- Intel Compiler
  由 Intel 開發的編譯器，對 Intel CPU 具最高支援度及效能最佳化
- PGI Compiler
  由 PGI 開發的編譯器，支援 OpenACC
- NVIDIA HPC SDK™

  以PGI Compiler為基礎並整合CUDA開發的編譯器及函式庫，使 HPC 開發人員能夠對從 GPU 基礎到 CPU 以及整個互連的整個 HPC 平台進行編程。

安裝 GNU 編譯器

- 安裝需要的套件

```
[root@master ~]# yum install gcc gcc-gfortran gcc-c++ libtool
```

- 手動編譯 GCC，前往 https://gcc.gnu.org/releases.html 下載編譯，順便安裝需要的套件

```
[root@master ~]# yum install wget bzip2
[root@master ~]# wget http://mirror.linux-ia64.org/gnu/gcc/releases/gcc-13.2.0/gcc-13.2.0.tar.gz
```

- 用 wget 指令下載 gcc-x.y.z.tar.gz，解開程式碼準備進行安裝

```
[root@master ~]# tar zxvf gcc-13.2.0.tar.gz
```

- 進入程式碼並下載 GCC 編譯必要的程式

```
[root@master gcc-13.2.0]# ./contrib/download_prerequisites
```

安裝 GNU 編譯器

- 建立安裝目的目錄

```
[root@master gcc-13.2.0]# mkdir -p /opt/gcc/13.2.0
```

- 組態要安裝的參數

```
[root@master gcc-13.2.0]# ./configure --prefix=/opt/gcc/13.2.0 --enable-checking=release --enable-languages=c,c++,fortran --disable-multilib
```

- 進行編譯，-j 後面的數字視核心數而有所不同

```
[root@master gcc-13.2.0]# make –j (CPU cores)
```

編譯時間大約會花 1 ~ 5 小時

- 進行安裝

```
[root@master gcc-13.2.0]# make install
```

使用 GNU 編譯器

- 使用系統預設的 GCC 不用額外設定，除非要指定其他版本的 GCC 才要設定

```
[root@master ~]# export PATH=/opt/gcc/13.2.0/bin:$PATH
[root@master ~]# export LD_LIBRARY_PATH=/opt/gcc/13.2.0/lib64:$LD_LIBRARY_PATH
```

- 用 gcc , g++, gfortran 指令編譯

```
[root@master ~]# gcc -o test test.c
[root@master ~]# g++ -o test test.cpp
[root@master ~]# gfortran -o test test.f90
```

安裝 Intel 編譯器(Intel® oneAPI Base Toolkit)

- 下載 Intel® oneAPI Base Toolkit：
  https://www.intel.com/content/www/us/en/developer/tools/oneapi/base-toolkit.html

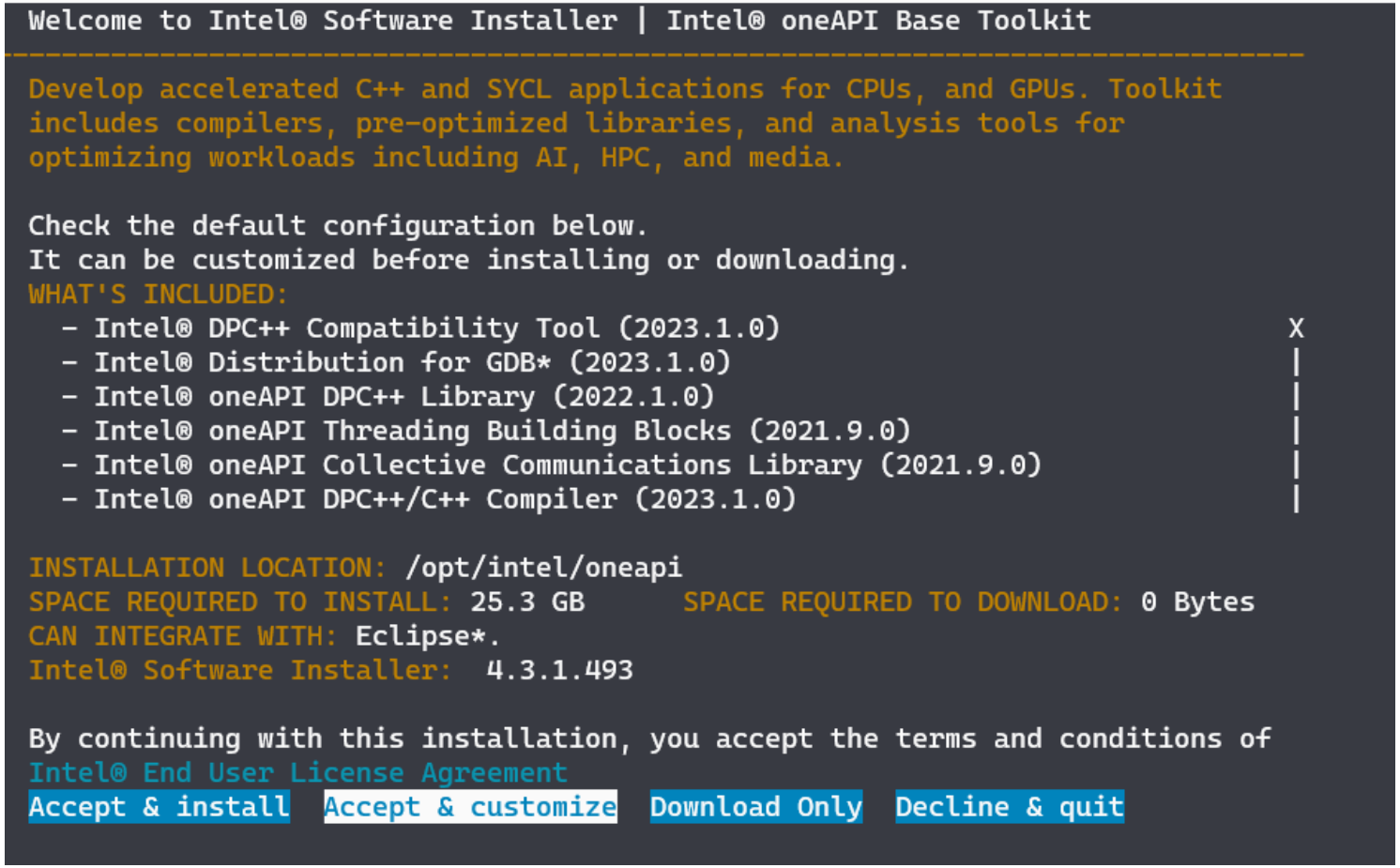
```
[root@master ~]# wget https://registrationcenter-download.intel.com/akdlm/IRC_NAS/7deeaac4-f605-4bcf-a81b-ea7531577c61/l_BaseKit_p_2023.1.0.46401_offline.sh
```

- 進行安裝

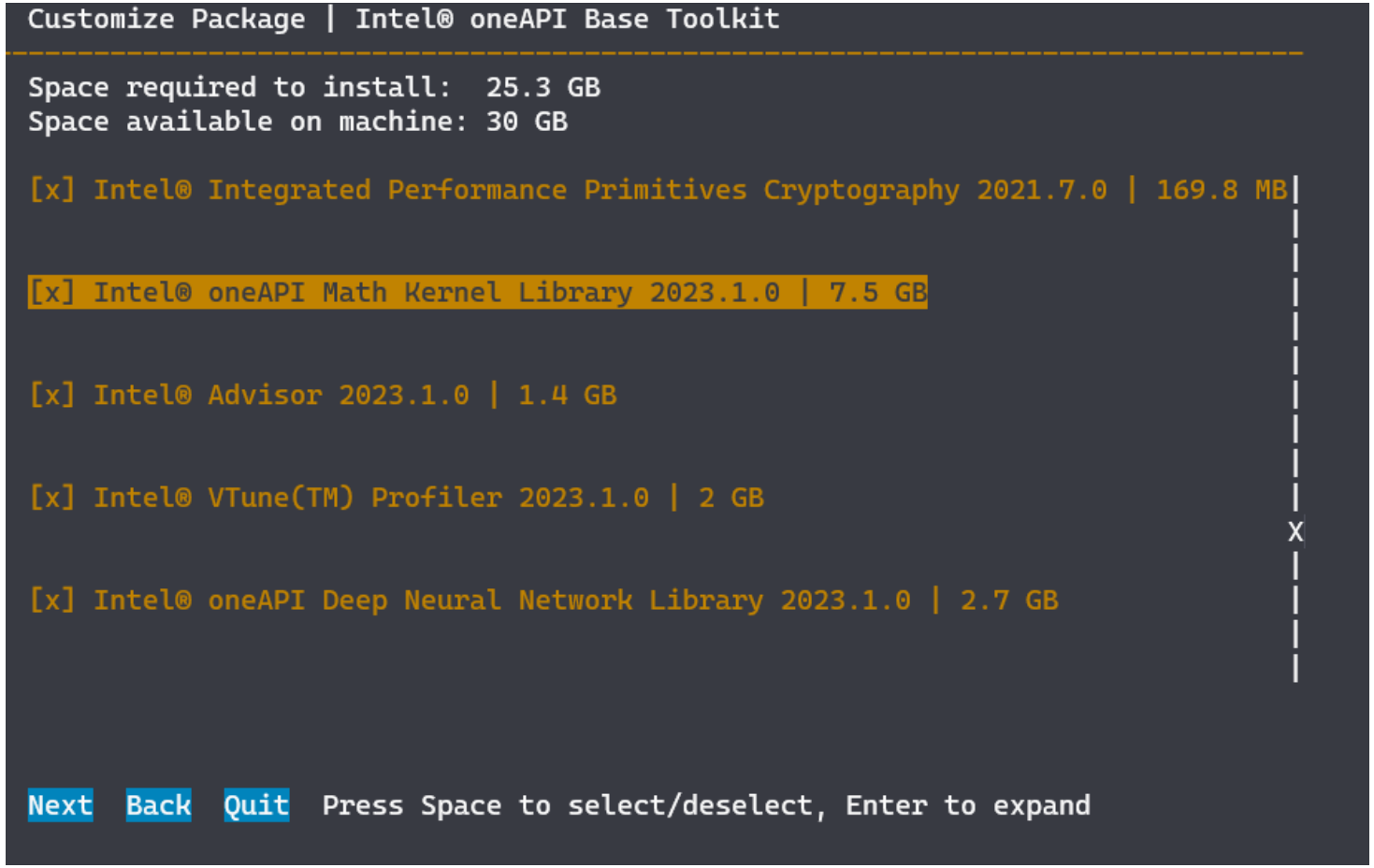
```
[root@master ~]# chmod +x l_BaseKit_p_2023.1.0.46401_offline.sh h
[root@master ~]# ./l_BaseKit_p_2023.1.0.46401_offline.sh
```

標準安裝大約需要 27 GB 空間，參考 VM 調整大小：https://sam.liho.tw/?p=6965

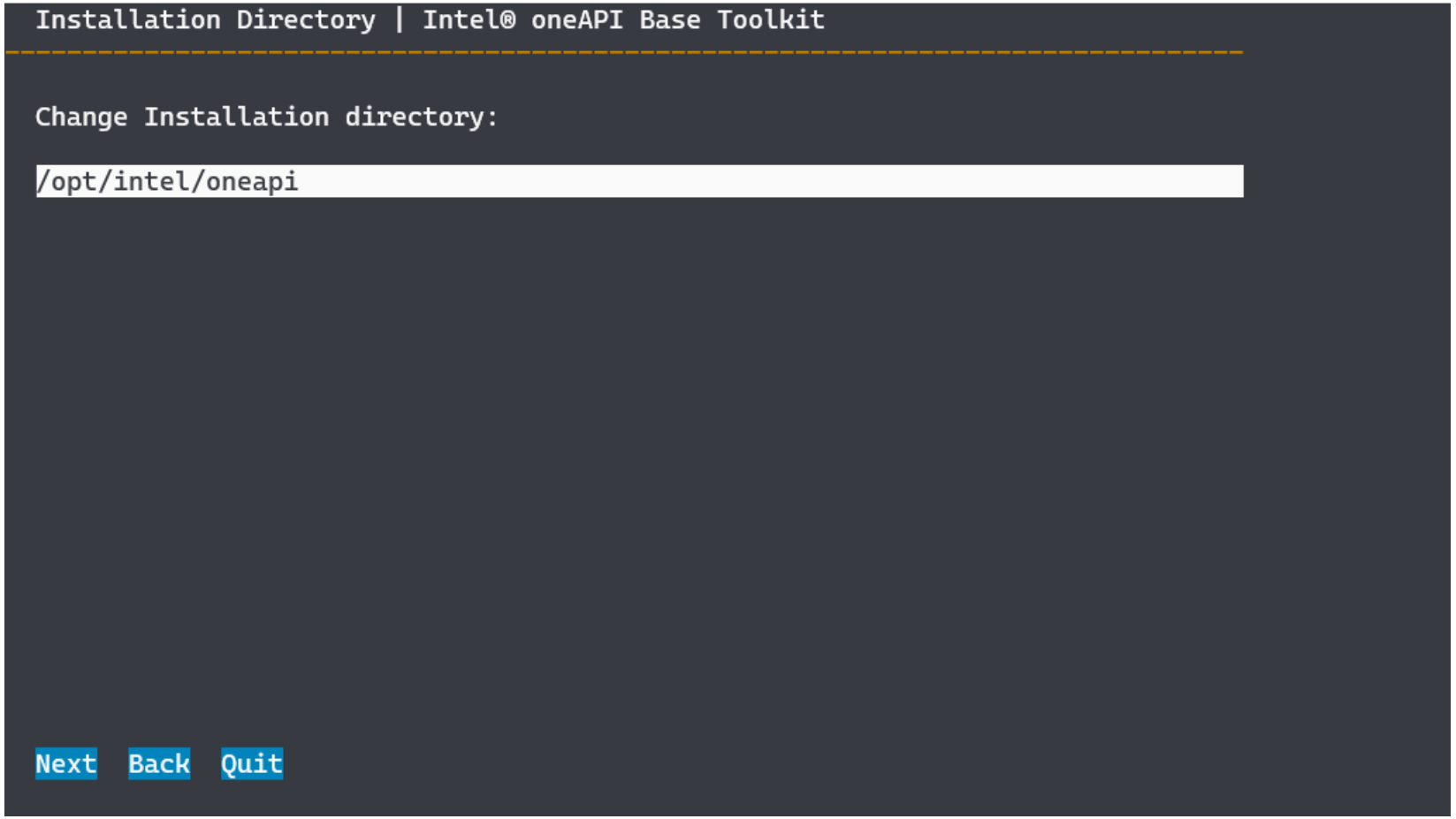
安裝 Intel 編譯器


Welcome to Intel® Software Installer | Intel® oneAPI Base Toolkit
Develop accelerated C++ and SYCL applications for CPUs, and GPUs. Toolkit includes compilers, pre-optimized libraries, and analysis tools for optimizing workloads including AI, HPC, and media.
Check the default configuration below.
It can be customized before installing or downloading.
WHAT'S INCLUDED:
- Intel® DPC++ Compatibility Tool (2023.1.0)
- Intel® Distribution for GDB* (2023.1.0)
- Intel® oneAPI DPC++ Library (2022.1.0)
- Intel® oneAPI Threading Building Blocks (2021.9.0)
- Intel® oneAPI Collective Communications Library (2021.9.0)
- Intel® oneAPI DPC++/C++ Compiler (2023.1.0)
INSTALLATION LOCATION: /opt/intel/oneapi
SPACE REQUIRED TO INSTALL: 25.3 GB
SPACE REQUIRED TO DOWNLOAD: 0 Bytes
CAN INTEGRATE WITH: Eclipse*.
Intel® Software Installer: 4.3.1.493
By continuing with this installation, you accept the terms and conditions of Intel® End User License Agreement
Accept & install
Accept & customize
Download Only
Decline & quit

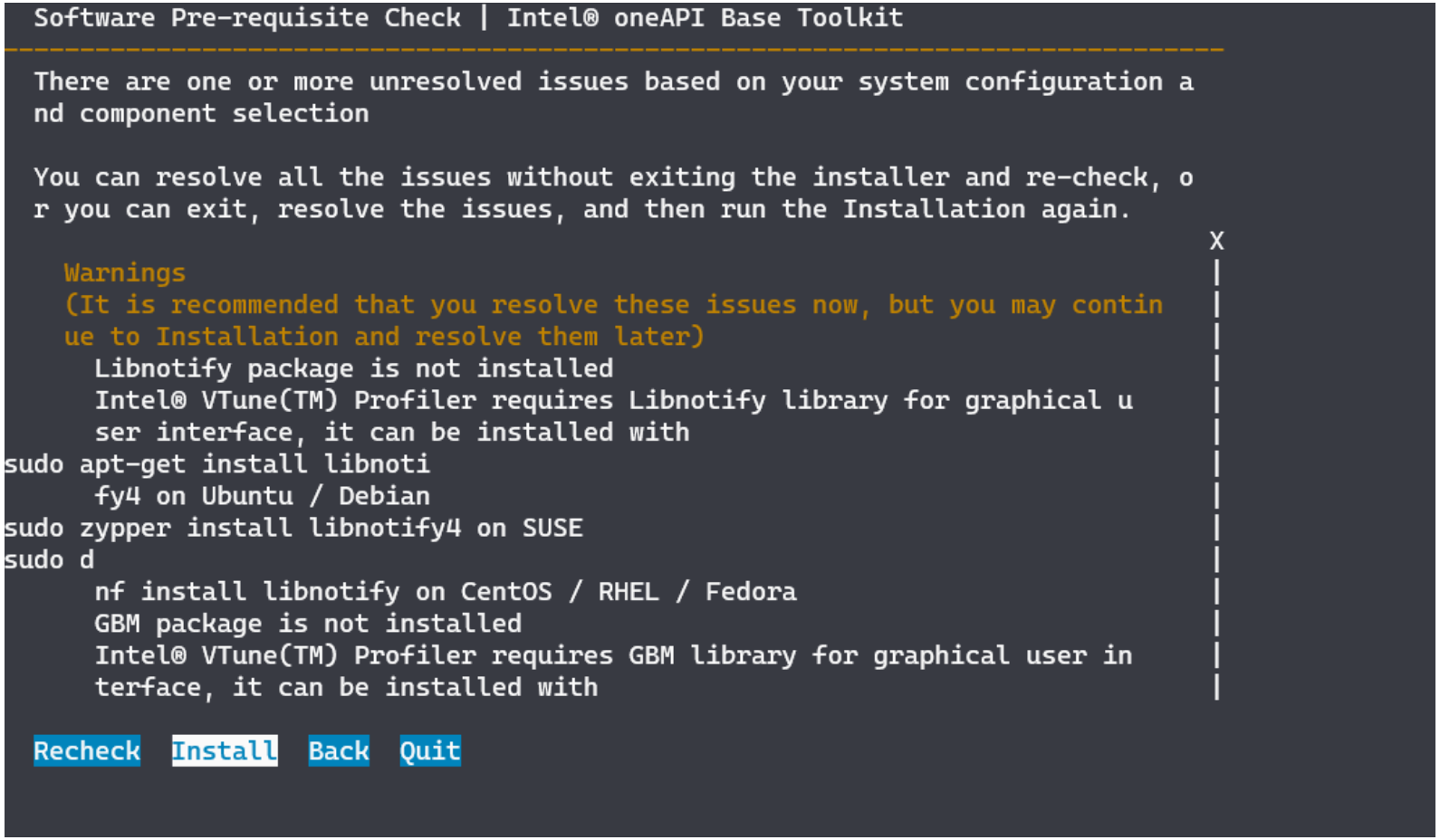
安裝 Intel 編譯器


Customize Package | Intel® oneAPI Base Toolkit
Space required to install: 25.3 GB
Space available on machine: 30 GB
[x] Intel® Integrated Performance Primitives Cryptography 2021.7.0 | 169.8 MB
[x] Intel® oneAPI Math Kernel Library 2023.1.0 | 7.5 GB
[x] Intel® Advisor 2023.1.0 | 1.4 GB
[x] Intel® VTune(TM) Profiler 2023.1.0 | 2 GB
[x] Intel® oneAPI Deep Neural Network Library 2023.1.0 | 2.7 GB
Next Back Quit Press Space to select/deselect, Enter to expand

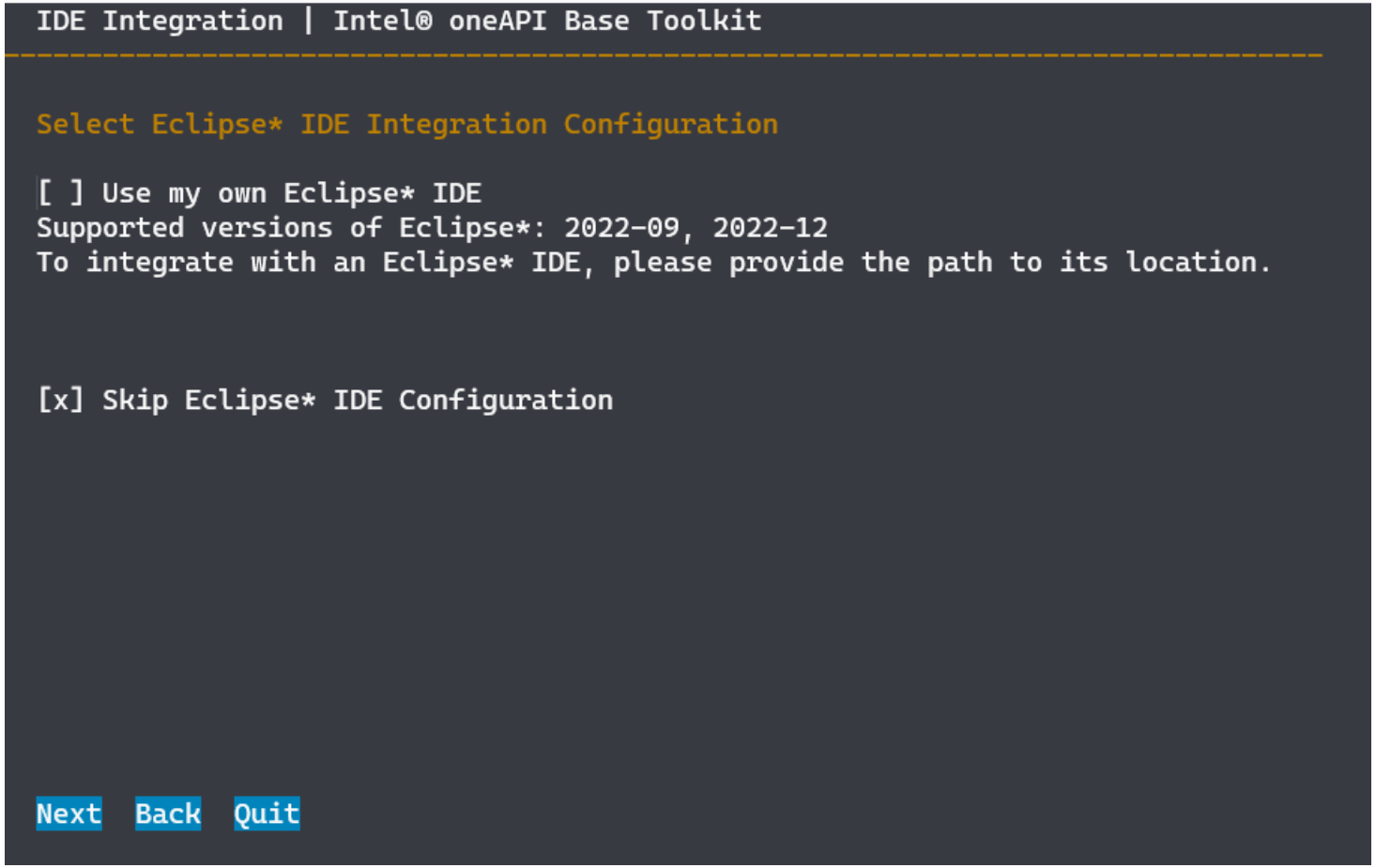
安裝 Intel 編譯器


Installation Directory | Intel® oneAPI Base Toolkit
Change Installation directory:
/opt/intel/oneapi
Next
Back
Quit

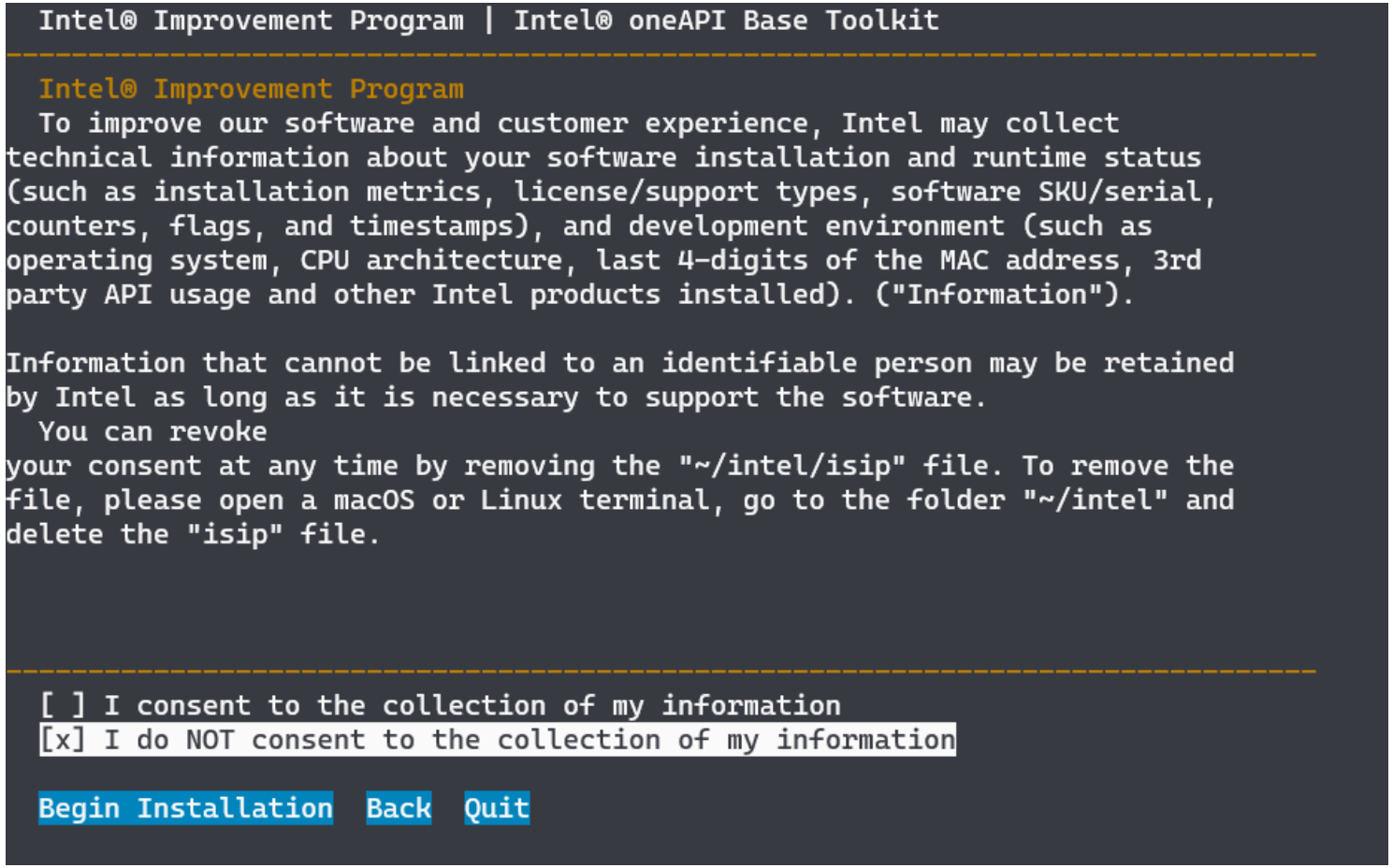
安裝 Intel 編譯器


Software Pre-requisite Check | Intel® oneAPI Base Toolkit
There are one or more unresolved issues based on your system configuration a
nd component selection
You can resolve all the issues without exiting the installer and re-check, o
r you can exit, resolve the issues, and then run the Installation again.
X
Warnings
(It is recommended that you resolve these issues now, but you may contin
ue to Installation and resolve them later)
Libnotify package is not installed
Intel® VTune(TM) Profiler requires Libnotify library for graphical u
ser interface, it can be installed with
sudo apt-get install libnoti
fy4 on Ubuntu / Debian
sudo zypper install libnotify4 on SUSE
sudo d
nf install libnotify on CentOS / RHEL / Fedora
GBM package is not installed
Intel® VTune(TM) Profiler requires GBM library for graphical user in
terface, it can be installed with
Recheck
Install
Back
Quit

安裝 Intel 編譯器


IDE Integration | Intel® oneAPI Base Toolkit
Select Eclipse* IDE Integration Configuration
[ ] Use my own Eclipse* IDE
Supported versions of Eclipse*: 2022-09, 2022-12
To integrate with an Eclipse* IDE, please provide the path to its location.
[x] Skip Eclipse* IDE Configuration
Next
Back
Quit

安裝 Intel 編譯器


Intel® Improvement Program | Intel® oneAPI Base Toolkit
Intel® Improvement Program
To improve our software and customer experience, Intel may 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").
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.
[ ] I consent to the collection of my information
[x] I do NOT consent to the collection of my information
Begin Installation
Back
Quit

安裝 Intel® oneAPI HPC Toolkit

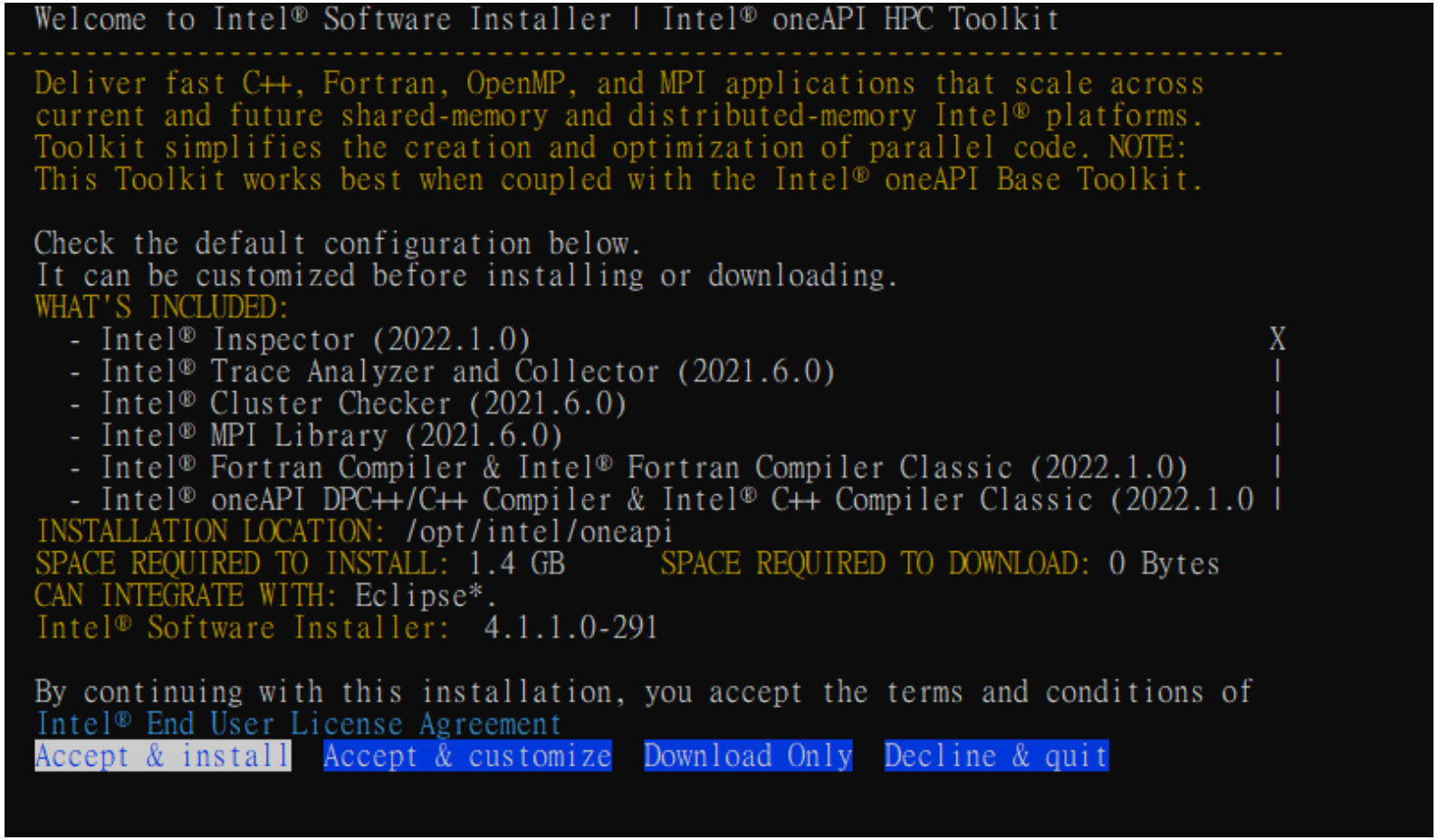
- 下載 Intel® oneAPI Base Toolkit：
  https://www.intel.com/content/www/us/en/developer/tools/oneapi/hpc-toolkit.html

```
[root@master ~]# wget  https://registrationcenter-download.intel.com/akdlm/IRC_NAS/1ff1b38a-8218-4c53-9956-f0b264de35a4/l_HPCKit_p_2023.1.0.46346_offline.sh
```

- 進行安裝

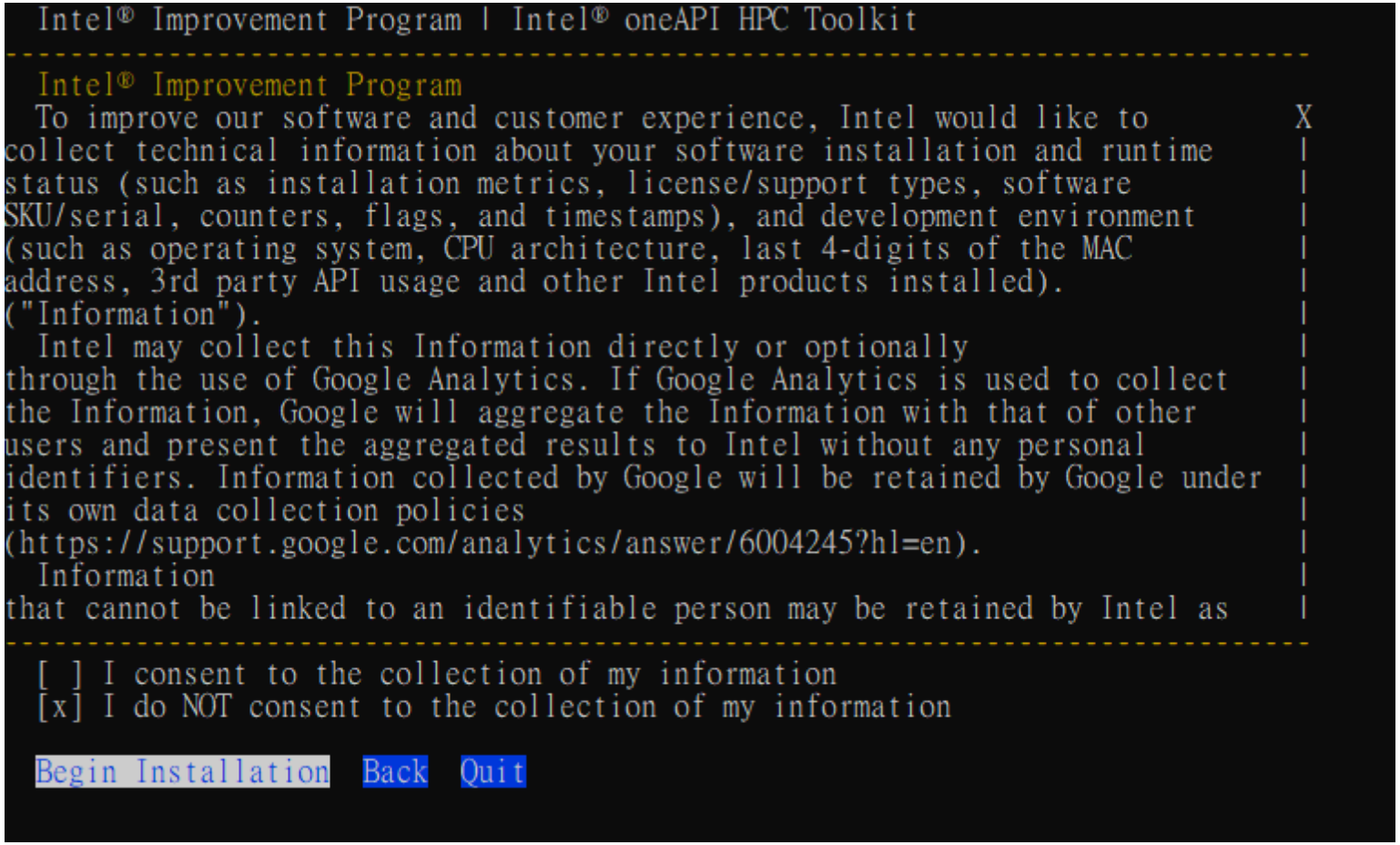
```
[root@master ~]# chmod +x l_HPCKit_p_2023.1.0.46346_offline.sh
[root@master ~]# ./l_HPCKit_p_2023.1.0.46346_offline.sh
```

安装 Intel® oneAPI HPC Toolkit



安装 Intel® oneAPI HPC Toolkit

安裝 Intel® oneAPI HPC Toolkit



使用 Intel 編譯器

- 用 souce 指令載入環境

```
[root@master ~]# source /opt/intel/oneapi/setvars.sh intel64
```

- 用 icc/icx , icpc/icpx, ifort/ifx 指令編譯

```
[root@master ~]# icc -o test test.c
[root@master ~]# icpc -o test test.cpp
[root@master ~]# ifort -o test test.f90
```

PGI 編譯器

- 下載PGI編譯器：https://www.pgroup.com/support/release_archive.php
- 目前已不提供免費下載，改為NVIDIA HPC SDK

安裝 NVIDIA HPC SDK

- NVDIA HPC SDK: https://developer.nvidia.com/hpc-sdk
- 下載「Linux x86_64 Tarball」
- 解壓縮後開始安裝

```
[root@master ~]# wget https://developer.download.nvidia.com/hpc-sdk/23.7/nvhpc_2023_237_Linux_x86_64_cuda_12.2.tar.gz
[root@master ~]# tar xpzf nvhpc_2023_237_Linux_x86_64_cuda_12.2.tar.gz
[root@master ~]# nvhpc_2023_237_Linux_x86_64_cuda_12.2 /install
```

安装 NVIDIA HPC SDK

```
[root@master nvhpc_2023_237_Linux_x86_64_cuda_12.2]# ./install

Welcome to the NVIDIA HPC SDK Linux installer!

You are installing NVIDIA HPC SDK 2023 version 23.7 for Linux_x86_64.
Please note that all Trademarks and Marks are the properties
of their respective owners.

Press enter to continue...


A network installation will save disk space by having only one copy of the
compilers and most of the libraries for all compilers on the network, and
the main installation needs to be done once for all systems on the network.

1  Single system install
2  Network install

Please choose install option:
1
```

安裝 NVIDIA HPC SDK

```
Please specify the directory path under which the software will be installed.
The default directory is /opt/nvidia/hpc_sdk, but you may install anywhere you wish,
assuming you have permission to do so.
Note: directory /opt/nvidia/hpc_sdk was created.
Installation directory? [/opt/nvidia/hpc_sdk]
Installing NVIDIA HPC SDK version 23.7 into /opt/nvidia/hpc_sdk
```

- 用 pgcc , pgc++, pgf90, pgf95, pgfortran 指令編譯

```
[root@master ~]# module load /opt/nvidia/hpc_sdk/modulefiles/nvhpc/22.11
[root@master ~]# pgcc –o test test.c
[root@master ~]# pgc++ -o test test.cpp
[root@master ~]# pgf90 -o test test.f90
```

Compiler 對照表

	GNU	PGI	Intel	Nvidia HPC SDK	OpenMPI	IntelMPI	
						Intel	Other
C	gcc	pgcc	icc/icx	nvc	mpicc	mpiicc	mpicc/ mpigcc
C++	g++	pgc++	icpc/icpx	nvc++	mpiCC/mpic++/mpicxx	mpiicpc	mpicxx/mpigxx
Fortran	gfortran	pgfortran	ifort/ifx	nvcfortran	mpifort/mpif77/mpif90	mpiifort	mpif77/mpif90/mpifc

安裝 OpenMPI - Source Code

- 下載 OpenMPI： https://www.open-mpi.org/
- 解開安裝檔

```
[root@master ~]# wget https://download.open-mpi.org/release/open-mpi/v4.1/openmpi-4.1.5.tar.gz
[root@master ~]# tar zxvf openmpi-4.1.5.tar.gz
```

- 進入解壓縮後的目錄

```
[root@master ~]# cd openmpi-4.1.5
```

- 設定安裝組態

```
[root@master ~]# ./configure --prefix=/path/to/install
```

- 編譯（X 為該台電腦核心數）

```
[root@master ~]# make –j X
```

- 安裝

```
[root@master ~]# make install
```

安裝 OpenMPI - Source Code

- GNU 組態

```
[root@master ~]# ./configure --prefix=/opt/openmpi/4.1.5_gcc_8.5 --enable-mpi-f77 --enable-mpi-f90 --enable-mpi-cxx CC=gcc CXX=c++ FC=gfortran F77=gfortran
```

- Intel 組態

```
[root@master ~]# source /opt/intel/oneapi/setvars.sh intel64
[root@master ~]# ./configure --prefix=/opt/openmpi/4.1.5_intel_2023.1 --enable-mpi-f77 --enable-mpi-f90 --enable-mpi-cxx CC=icx CXX=icpx FC=ifx F77=ifx
```

help選項可以讓你知道更多參數, 如"./configure -h"

編譯函式庫

- 下載編譯函式庫
  - BLAS : http://www.netlib.org/blas/
  - LAPACK : http://www.netlib.org/lapack/
  - FFTW : http://www.fftw.org/
  - GSL : https://www.gnu.org/software/gsl/
  - HDF5 : https://www.hdfgroup.org/solutions/hdf5/
- 解壓縮函式庫原始碼檔

```
tar zxvf library_source.x.y.z.tar.gz
```

- 進入解壓縮後的目錄

```
cd library_source.x.y.z
```

- 先讀 README / INSTALL 檔案，設定組態（./configure --prefix=/path/to/install）或是修改 Makefile / Make.in / Make.XXXX

編譯函式庫

- 編譯

```
[root@master ~]# make
```

- 安裝：有些程式沒有 install 選項，直接複製 *.a 檔案到你要的路徑

```
[root@master ~]# make install 或 # cp *.a /path/to/install
```

- 設定動態及靜態函式庫的環境變數、設定 header files 引入的環境變數

```
[root@master ~]# export LD_LIBRARY_PATH=/path/to/install/lib:$LD_LIBRARY_PATH
[root@master ~]# export LIBRARY_PATH=/path/to/install/lib:$LIBRARY_PATH
[root@master ~]# export INCLUDE=/path/to/install/include:$INCLUDE
[root@master ~]# export C_INCLUDE_PATH=/path/to/install/include:$C_INCLUDE_PATH
```

安裝系統函式庫

記得將計算節點一併設定

- 建議安裝 EPEL

```
[root@master ~]# yum config-manager --set-enabled powertools
[root@master ~]# yum install epel-release
```

- 安裝好 EPEL 才能直接安裝相關系統套件

```
[root@master ~]# yum install blas lapack fftw hdf5 gsl blas-devel lapack-devel fftw-devel hdf5-devel gsl-devel
glibc-static
```

- 檢查系統安裝的套件

```
[root@master ~]# rpm -q blas lapack fftw hdf5
blas-3.8.0-8.el8.x86_64
lapack-3.8.0-8.el8.x86_64
fftw-3.3.5-11.el8.x86_64
hdf5-1.10.5-4.el8.x86_64
```

使用 MKL 或其他函式庫

連結種類	參數	範例
引入 header 檔	-I	-I/opt/openmpi/4.1.5-intel-2023.1/include
動態連結	-L	-L/opt/intel/oneapi/mkl/2023.1.0/lib/intel64 -lmkl_core
靜態連結	libXXX.a	/opt/intel/oneapi/mkl/2023.1.0/lib/intel64/libmkl_core.a

- 動態連結

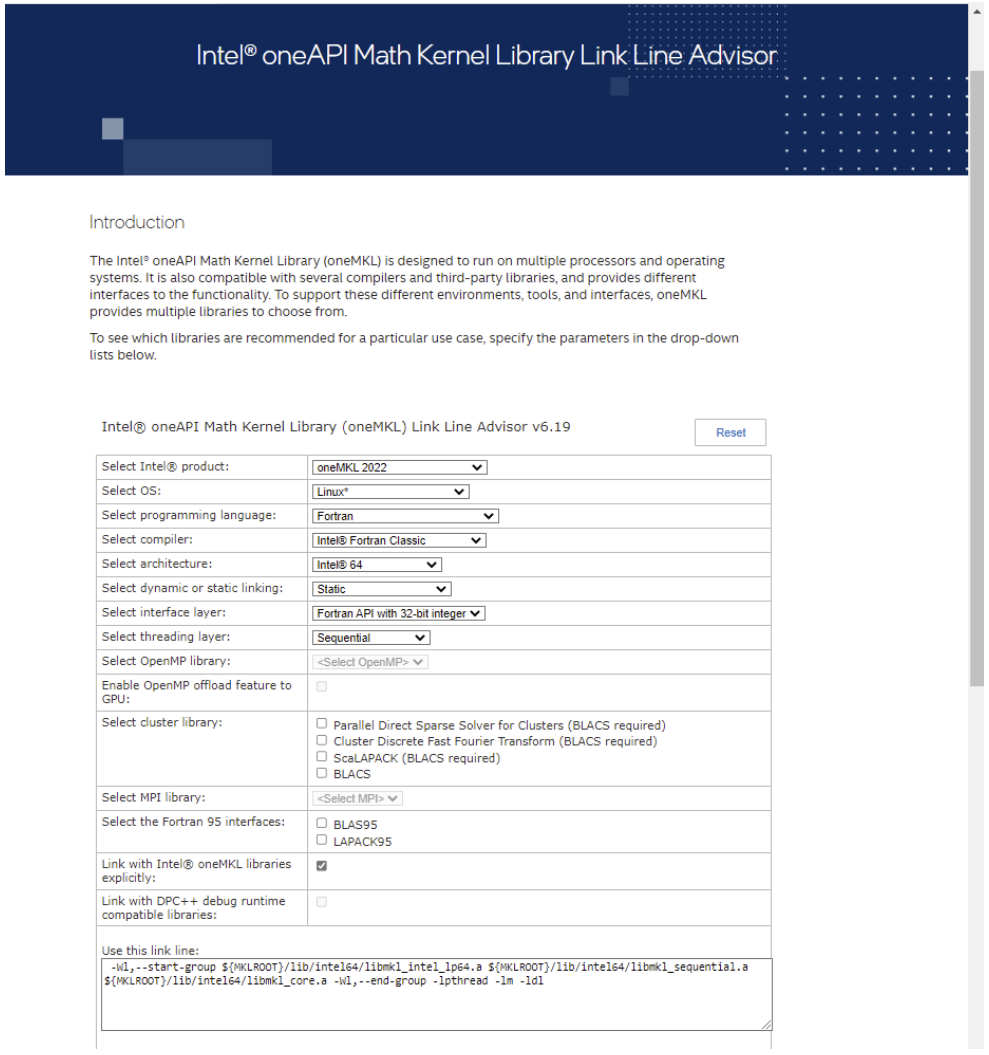
```
[root@master ~]# ifort -o test test.f90 -I/opt/intel/oneapi/mkl/2023.1.0/include -L/opt/intel/oneapi/mkl/2022.1.0/lib/intel64 -lmkl_intel_lp64 -lmkl_sequential -lmkl_core -lpthread -lm -ldl
```

- 靜態連結

```
[root@master ~]# MKLROOT=/opt/intel/oneapi/mkl/2023.1.0/lib/intel64
[root@master ~]# ifort -o test.x test.f90 -I/opt/intel/oneapi/mkl/2023.1.0/include -Wl,--start-group ${MKLROOT}/libmkl_intel_lp64.a ${MKLROOT}/libmkl_sequential.a ${MKLROOT}/libmkl_core.a-Wl,--end-group –lpthread -lm -ldl
```

Intel MKL Link Line Advisor

https://www.intel.com/content/www/us/en/developer/tools/oneapi/onemkl-link-line-advisor.htm



常用最佳化參數

- GNU

```
[root@master ~]# gcc -O2 -ffast-math -ftree-vectorize -funroll-loops
```

- Intel

```
[root@master ~]# icc -O3 -axCORE-AVX2      #### intel 11 or later
[root@master ~]# icc -O3 -axCORE-AVX512    #### intel 15 or later
```

CPU指令集視CPU規格而定，查看 /proc/cpuinfo 檔案

參考：Optimize Options (Using the GNU Compiler Collection (GCC)), Intel® 64 and IA-32 Architectures Optimization Reference Manual,

回家作業

- 練習自行安裝 FFTW3 在自己的 VM（可用 GNU ）
- 編譯 fftw_example.c 程式
  - https://github.com/undees/fftw-example/blob/master/fftw_example.c
  - 參考：

    gcc -o test.exe fftw_example.c -I/opt/gnu-math/fftw-3.3.10/include -L/opt/gnu-math/fftw-3.3.10/lib -lfftw3 -lm
  - 可以嘗試拿掉 -lm 試試看？