Usage instructions for Intel Ponte Vecchio nodes



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1 Introduction

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This document serves as a basic installation and usage guide for the Intel Data Center GPU Max compute nodes at the Lichtenberg II high-performance cluster at TU-Darmstadt. There are five nodes available with four accelerators (i.e., GPUs) each. This guide applies to Red Hat Enterprise Linux version 9.4¹. You can check the release with "cat /etc/redhat-release".

At the time of writing, there are frequent updates and changes in many different contexts: in the PyTorch and Tensorflow frameworks, in the Intel GPU support and in how we manage the software stack. Therefore, we recommend to always check and use the latest version of this document.

In these notes we will use:

- 1. the module command to load the common basic Intel software
- 2. the **spack load** command to load a suitable Python installation
- 3. the pip command, in a python environment, to install PyTorch, Tensoflow and some ad-hoc Intel software

Important remark: in the rest of this document we assume that you are interactively logged on one of the five Ponte Vecchio nodes (gpqd0001-gpqd0005) and you are using the BASH shell.

2 Preliminary check

Before to begin, we recommend to preliminary check if all the GPUs are recognized by the operating system. You can accomplish this task with:

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¹Actually, RHEL 9.4 is not officially supported by Intel, but for most applications the GPUs should still work fine.

Code 1: Preliminary check xpu-smi discovery

which should return:

```
Device ID | Device Information
_____+__+___
         | Device Name: Intel(R) Data Center GPU Max 1550
0
         | Vendor Name: Intel(R) Corporation
         | SOC UUID: 00000000-0000-003a-0000-002f0bd58086
         | PCI BDF Address: 0000:3a:00.0
         | DRM Device: /dev/dri/card0
         | Function Type: physical
         | Device Name: Intel(R) Data Center GPU Max 1550
1
         | Vendor Name: Intel(R) Corporation
         | SOC UUID: 00000000-0000-004b-0000-002f0bd58086
         | PCI BDF Address: 0000:4b:00.0
          DRM Device: /dev/dri/card1
         | Function Type: physical
         | Device Name: Intel(R) Data Center GPU Max 1550
2
         | Vendor Name: Intel(R) Corporation
         | SOC UUID: 00000000-0000-00ca-0000-002f0bd58086
         | PCI BDF Address: 0000:ca:00.0
         | DRM Device: /dev/dri/card2
         | Function Type: physical
3
         | Device Name: Intel(R) Data Center GPU Max 1550
         | Vendor Name: Intel(R) Corporation
         | SOC UUID: 00000000-0000-00da-0000-002f0bd58086
         | PCI BDF Address: 0000:da:00.0
         | DRM Device: /dev/dri/card3
         | Function Type: physical
```

If no devices are shown, then the compute node has indeed a problem and you should inform us via the ticketing system, albeit in most cases we should be already aware of the problem and working to fix it.

3 Intel modules

Intel provides a software suite, called <u>Intel One API</u>, whose later version currently installed in the Lichtenberg II cluster can be loaded with:

Code 2: Load required oneAPI packages module load intel/2025.0 module load intelmpi

To better understand the software's possibilities and limitations, it is recommended to look at the <u>oneAPI Samples GitHub</u>. This is especially true for direct programming or code migration, such as SYCL instructions.

4 Spack

Spack is a package management tool that helps in providing a wide variety of software with different versions for multiple environments.

You can decide to use one the Spack installations already available in the system, create <u>your own independent environment</u> within this installation² or resort to a completely independent personal setup. For more information about how to proceed, we refer to the

²Since the /shared filesystem is read-only, it is not possible to create managed environments.

official documentation and tutorial.

The Ponte Vecchio nodes have their own Spack installation, separated from the global installation adopted for the rest of the system. To set up a proper Spack environment for the Ponte Vecchio nodes, please use the following commands³:

Code 3: Spack Ponte Vecchio environment setup

```
export SPACK_DISABLE_LOCAL_CONFIG=true;
export SPACK_ROOT="/shared/gpspack";
source ${SPACK_ROOT}/share/spack/setup-env.sh ;
spack env activate gpqd;
```

To get a list of the available software, type: "spack find -l".

To get a list of the available versions of a specific software, for example <code>intel-oneapi-mkl</code>, type: "spack find -L intel-oneapi-mkl". To load a package, type: "spack load <name-of-the-package>". When multiple versions of the same package are available, it is necessary to specify the desired one and possibly also the compiler which was use to build the software, for example: "spack load openmpi@5.0.3%gcc@11.4.1" (please, note that this is just an example and this specific package might not exist when you try the command). However, sometimes there might still be a residual ambiguity, due to different options or dependencies which were activated at compile time, that can solved by indicating the hash of the package: "spack load \abcdef" (assuming that <code>abcdef</code> is the hash of the package).

Due to the lack of support or work-in-progress issues, a lot of software still lacks the capability to utilize the hardware. As such, the software stack is currently minimal, but we would be much obliged if you could provide us with requests or information for further applications to be included in this environment, thus helping us in saving time to individual users and in making the hardware more usable.

5 Python

5.1 Load Python 3.11

When using different pieces of software, very often not all versions work fine together. Although other combinations are possible, in this tutorial we will use Python 3.11^4 .

After having set up Spack⁵, we type:

```
Code 4: Load pip with python 3.11 spack load py-pip@23.1.2
```

This version of pip was built with Spack imposing a Python 3.11 installation as dependence, therefore, when it is loaded, this installation is automatically activated, too. The command "python –version" should now return the answer "3.11.9".

5.2 Temporary directories

When installing a new package, both Spack and pip need to store an amount of temporary data that often exceeds the space available in the default temporary directory. Therefore, it is very important to define the variable **TMPDIR**, containing the path of a directory mounted on a device with sufficient space.

Although it is not guaranteed that, in a shared node, there will be enough room for the needs of all users, the first choice should be a RAM disk, that is automatically created for every user in \\dev\shm\$. If the space is not enough and at some point you get the error "No space left on device", then you should create a temporary directory in \\work\scratch\$. Assuming that you have created the directory "tmp \$USER" under \\dev\shm\$, the command to let the system know that you have chosen this folder as a temporary directory is:

Code 5: Export the path of a temporary directory and create it

```
export TMPDIR=/dev/shm/tmp_${USER}
mkdir -p ${TMPDIR}
```

³The first line forbids to use a customized setup in the home directory. This precaution reduces the risk of unwanted local side effects, but it is not strictly necessary and often not even desired.

⁴With Python 3.9, the RHEL 9.4 system default, some basic tests with Tensorflow crashed, while with Python 3.12, that can be loaded after the module intel/2025.0, we did not find Tensorflow versions that could be installed with pip which were also officially supported by the Intel Tensorflow extensions. However, it is possible that now the situation has changed. We will check the status every now and then.

⁵See Code 3

5.3 Python modules

Intel provides extensions for popular Python-based frameworks such as PyTorch and TensorFlow. It is strongly recommended to create a virtual environment for your Python modules. In Code 6 you can find the syntax for an environment called "your environment".

Code 6: Create virtual enviroment for your python package.

```
python -m venv <your_environment>
source <your_environment>/bin/activate
```

The environment resides in a directory having the same name and containing all its files, including the python packages installed with pip when it is active. Please, note that you need to create the environment only once (first line of Code 6), but you need to activate it every time before you use it (second line).

To deactivate a python virtual environment, simply type "deactivate". In the next subsections, we will create two virtual environments, one for PyTorch and the other for Tensorflow

5.4 PyTorch

For PyTorch, we follow the procedure described in https://pytorch.org/docs/main/notes/get_start_xpu.html.

With the commands:

```
Code 7: Install Py-Torch
```

```
python -m venv pytorch_env
source pytorch_env/bin/activate
pip install torch torchvision torchaudio --index-url https://download.pytorch.org/whl/test/xpu
```

we:

- 1. create a python virtual environment named pytorch env
- 2. activate the python virtual environment that we just created
- 3. install the version of Py-Torch (and its most common packages) for Intel XPUs

For a quick check that the installation went fine, you can launch python and execute:

```
Code 8: Py-Torch installation quick check
```

```
import torch
torch.xpu.is_available()
```

which should return "True".

It is recommended to try also the examples listed on https://pytorch.org/docs/main/notes/get_start_xpu.html# examples.

At the time of writing these notes, they all worked fine.

5.5 TensorFlow

To install the Tensorflow framework on the Intel GPU Max system, first we set up a python virtual environment, then we install the standard Tensorflow and, finally, the Intel extension for this software:

Code 9: Install Tensorflow

```
python -m venv TF_env
source TF_env/bin/activate
pip install tensorflow==2.15.0
pip install --upgrade intel-extension-for-tensorflow[xpu]
```

Although more recent versions of Tensorflow exist, at the time of writing version 15.0 is explicitly required by the Intel extension.

In order to briefly check that the installation went fine, you can launch python and execute:

Code 10: Py-Tensorflow installation quick check

```
import intel_extension_for_tensorflow as itex
print(itex.__version__)
```

Among the many messages that are printed when importing the module (first command in Code 10), there should be the line: "Intel Extension for Tensorflow* GPU backend is loaded." and, of course, the second command should return the actual version of the Intel Extension for Tensorflow.

Additionally, you can execute the short sample python script in the Tensorflow homepage:

Code 11: Py-Tensorflow basic example script

```
import tensorflow as tf
mnist = tf.keras.datasets.mnist

(x_train, y_train),(x_test, y_test) = mnist.load_data()
x_train, x_test = x_train / 255.0, x_test / 255.0

model = tf.keras.models.Sequential([
tf.keras.layers.Flatten(input_shape=(28, 28)),
tf.keras.layers.Dense(128, activation='relu'),
tf.keras.layers.Dropout(0.2),
tf.keras.layers.Dense(10, activation='softmax')
])

model.compile(optimizer='adam',
loss='sparse_categorical_crossentropy',
metrics=['accuracy'])

model.fit(x_train, y_train, epochs=5)
model.evaluate(x_test, y_test)
```

6 oneAPI SYCL C++ samples using GPUs

In the website https://github.com/oneapi-src/oneAPI-samples Intel provides many examples of code based on the oneAPI framework, including some relatively simple programs that can run also on GPUs. The page https://oneapi-src.github.io/oneAPI-samples/ provides a basic summary of all the available examples. We tested a small subset of them, but unfortunately non always successfully. We suppose that in most cases the failures might depend on small mismatches between Red Hat 9.4, the linux distribution powering the Lichtenberg II cluster, and Ubuntu 22.04, the linux distribution used by Intel to validate the code, but we cannot rule out that, in some cases, they are due to other problems. Therefore we encourage the users to contact us by opening a ticket whenever they encounter unexpected compilation or execution problems.

Here we report a trivial typical usage example, just to give an idea of how to proceed, referring to the Intel documentation for the other samples.

First of all we load the modules delivering oneAPI and CMake:

```
Code 12: Load the necessary modules

module load intel/2025.0

module load intelmpi

module load cmake
```

Then, of course, we need to download the oneAPI git repository and move into the directory of the code sample that we want to compile and run. The chosen example is a simplified version of a typical scientific problem, with some parameters that can be easily changed.

```
Code 13: Get the oneAPI repository
```

```
git clone https://github.com/oneapi-src/oneAPI-samples.git
cd oneAPI-samples/DirectProgramming/C++SYCL/StructuredGrids/particle-diffusion
```

Now we build the executable and, with the last command, we run it:

```
Code 14: Build the code sample
     mkdir build
     cd build
     cmake ..
     make
     make run
The initial part of the output (we omit the rest of it) should be:
**Running with default parameters**
Running on: Intel(R) Data Center GPU Max 1550
Device Max Work Group Size: 1024
Device Max EUCount: 512
Number of iterations: 10000
Number of particles: 256
Size of the grid: 22
Random number seed: 777
Device Offload time: 0.0340798 s
(of course, the device offload time slightly changes from run to run).
```

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