Installation Guide for Intel oneAPI Toolkit on Debian

Prerequisites

Before proceeding with the installation of the Intel oneAPI HPC Toolkit, ensure that you have the necessary permissions by having sudo access. Install the prerequisites using the following command:

```
$ apt-get install libgl1-mesa-glx libegl1-mesa libxrandr2 libxrandr2
libxss1 libxcursor1 libxcomposite1 libasound2libxi6 libxtst6
```

Step 1: Installing Intel oneAPI Base Toolkit (Version 2023.2.0)

1. Download the latest version (2023.2.0) of the Intel oneAPI Base Toolkit using the following command in the terminal:

   ```
   $ wget https://registrationcenter-
   download.intel.com/akdlm/IRC_NAS/992857b9-624c-45de-9701-
   f6445d845359/l_BaseKit_p_2023.2.0.49397.sh
   ```

   then install it via:

   ```
   $ sudo sh ./l_BaseKit_p_2023.2.0.49397.sh
   ```

   This will launch a graphical user interface. Click "Continue" and install oneAPI to the default folder.

2. Download a critical update for the DPC++/C++ Compiler using the following command:

   ```
   $ wget https://registrationcenter-
   download.intel.com/akdlm/IRC_NAS/ebf5d9aa-17a7-46a4-b5df-
   ace004227c0e/l_dpcpp-cpp-compiler_p_2023.2.1.8.sh
   ```

   and then install it via:

   ```
   $ sudo sh ./l_dpcpp-cpp-compiler_p_2023.2.1.8.sh
   ```

Step 2: Installing Intel oneAPI HPC Toolkit (Version 2023.2.0)

1. Download and install the latest version (2023.2.0) of the Intel oneAPI HPC Toolkit using the following commands:

   ```
   $ wget https://registrationcenter-
   download.intel.com/akdlm/IRC_NAS/0722521a-34b5-4c41-af3f-
   d5d14e88248d/l_HPCKit_p_2023.2.0.49440.sh

   $ sudo sh ./l_HPCKit_p_2023.2.0.49440.sh
   ```

   This will launch a GUI similar to the previous one. Click "Continue" and install the oneAPI HPC Toolkit to the default folder.

2. Download and install a critical update for the Intel Fortran Compiler version 2023.2.1:

```
$ wget https://registrationcenter-
download.intel.com/akdlm/IRC_NAS/0d65c8d4-f245-4756-80c4-
6712b43cf835/l_fortran-compiler_p_2023.2.1.8.sh

$ sudo sh ./l_fortran-compiler_p_2023.2.1.8.sh
```

After installation, running the installer package again for the previous installations should confirm a normal configuration.

Post-Installation Steps

1. After installation, initialize the environment variables in the terminal using the command:

   ```
   $ . /opt/intel/oneapi/setvars.sh
   ```

   Note that you must do this **every time** you open a new terminal session and wish compile any version of MobCal-MPI's .f source code using mpiifort.

2. To check the version of ifort, use the command:

   ```
   $ mpiifort --version
   ```

   For a one-time setup of setvars.sh following typical Ubuntu syntax, you can explore options in the official documentation.

Step 3: Compiling and Running MobCal-MPI

1. After initializing the environmental variables, navigate to the folder containing the Fortran code.
2. Compile the Fortran code using the following command:

   ```
   $ mpiifort -o MobCal_MPI_201.exe MobCal_MPI_201.f -Ofast
   ```

   The compilation should be error-free and nearly instantaneous.

3. Run a test MobCal-MPI job (.mfj input files can be found in the GUI sample files directory) via the following command (or using one of the submission scripts):

   ```
   $ mpirun -np 8 ./MobCal_MPI_201.exe AMIFOSTINE_3.sub
   ```

Note: The number 8 in the command requests 8 cores. This should be adjusted based on your machine specifications.

If you encounter any issues with this guide, please report them to the Issues section on GitHub. Provide as much detail about your system and workflow to install oneAPI as possible.

Installation Guide for Intel oneAPI HPC Toolkit on Arch Linux

Prerequisites

Before proceeding with the installation of the Intel oneAPI HPC Toolkit on Arch Linux, ensure that you have the necessary permissions by having sudo access. If you do not have the "glibc" library installed or face dependency issues, run the following command:

```
$ sudo pacman -S glibc cpio
```

If "glibc" is already installed or if you encounter dependency problems, use the command:

```
$ pacman -S cpio
```

Installing libstdc++5 from AUR using YAY

1. Install YAY, an AUR helper, by following the instructions on the YAY GitHub page: https://github.com/Jguer/yay.
2. Download and install libstdc++5 from AUR using YAY. Choose the version with the highest endorsement.

   ```
   $ yay -S lib32-libstdc++5
   ```

   Ensure that the package has at least 21 votes (as of 21-11-2023) before proceeding.

Downloading and Installing Intel oneAPI HPC Toolkit

1. Download the Intel oneAPI HPC Toolkit from the official website: https://www.intel.com/content/www/us/en/developer/tools/oneapi/hpc-toolkit-download.html

   If you prefer using the console, download the toolkit with the following command:

   ```
   $ wget https://registrationcenter-
   download.intel.com/akdlm/IRC_NAS/1b2baedd-a757-4a79-8abb-
   a5bf15adae9a/l_HPCKit_p_2024.0.0.49589_offline.sh
   ```

2. Install the toolkit using the console with the following command:

   ```
   $ sudo sh ./l_HPCKit_p_2024.0.0.49589_offline.sh -a -cli
   ```

   Alternatively, you can install it with a graphical interface using:

   ```
   $ sudo sh ./l_HPCKit_p_2024.0.0.49589_offline.sh
   ```

   Ignore warnings about missing packages like g++. Confirm that g++ is not installed by running by typing the command:

   ```
   $ g++
   ```

You should receive an error message that the package cannot be found. If you have received this error, then you can proceed to the next step.

Setting Environmental Variables

1. After installation, initialize the environment variables in the terminal using the command:

   ```
   $ . /opt/intel/oneapi/setvars.sh
   ```

   Note that you must do this **every time** you open a new terminal session and wish compile the MobCal_MPI.f source code using mpiifort.

Compiling MobCal-MPI using the Intel MPI Compiler

1. Navigate to the directory containing the Fortran code (file ending with ".f").
2. Compile the Fortran code (e.g., MobCal_MPI_201.f) using the Intel MPI Compiler with the following command:

   ```
   $ mpiifort -o MobCal_MPI_201.exe MobCal_MPI_201.f -Ofast
   ```

Successful compilation should produce a file called MobCal_MPI_201.exe in the current working directory. Ensure proper performance by testing the several MobCal-MPI jobs provided within the GUI sample files.

If you encounter any issues with this guide, please report them to the Issues section on GitHub. Provide as much detail about your system and workflow to install oneAPI as possible.

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