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Compute Resources

Have questions or need help with compute, including activation or issues? Follow this link.

User Agreement

Docker Usage

The information on this page assumes that you have a knowledge base of using Docker to create images and push them to a repository for use. If you need to review that information, please see the links below.

https://washu.atlassian.net/wiki/spaces/RUD/pages/1705115761/Docker+and+the+RIS+Compute1+Platform?atlOrigin=eyJpIjoiNzc4YTZjNjIxYmQwNGI3OTk4M2Q0MW

https://washu.atlassian.net/wiki/spaces/RUD/pages/1864892726/Docker+Basics+Building+Tagging+Pushing+A+Custom+Docker+Image?atlOrigin=eyJpIjoiMTVjMjNlM

Software Included

Intel® oneAPI HPC Toolkit 2021.1.1 (https://www.intel.com/content/www/us/en/developer/tools/oneapi/hpc-toolkit.html)

Overview

From the Intel® oneAPI HPC Toolkit Docker Hub,

The Intel oneAPI HPC Toolkit delivers what developers need to build, analyze, optimize, and scale high-performance computing (HPC) applications with the latest techniques in vectorization, multithreading, multi-node parallelization, and memory optimization.

For a complete list of libraries included in the Intel® oneAPI HPC Toolkit, please visit the Intel® oneAPI HPC Toolkit Documentation.

Interactive Command-Line Session

To use the Intel® compilers in an interactive command-line session, follow the steps below.

Submit an interactive job.

Set up the Intel® oneAPI environment.

Compile code.

Please refer to the Intel® documentation for more information on how to compile code.

Multi-Stage Docker Image Build

Compile, Keep Only Binaries

A multi-stage build leverages the compilers in the Intel® oneAPI HPC Toolkit Docker image and copies the compiled binaries and runtime dependencies to a new base image. This method results in a smaller Docker image, reducing computing time/resources/cost, and allows withholding source code from public consumption.

For more information on Docker multi-stage builds, please see the Docker multi-stage build documentation.

Sample Multi-Stage Dockerfile

Single-Stage Docker Image Build

Compile, Compile, Keep Source Code and Binaries

A single-stage build leverages the compilers in the Intel® oneAPI HPC Toolkit Docker image and keeps the compiled binaries, runtime dependencies and source code in the resulting image. This method results in a larger Docker image which may cause increased computing time/resources/cost. This method also caches the source code in build layers resulting in public exposure, which may be unwanted.

Sample Single-Stage Dockerfile

Building and Pushing the Docker image

To build and push a Docker image using one of the above methods, please refer to the our existing documentation for guidance.

https://washu.atlassian.net/wiki/spaces/RUD/pages/1705115761/Docker+and+the+RIS+Compute1+Platform?atlOrigin=eyJpIjoiZWMzZTg5ZDg1NTA1NDFkYjk1ZjRkN

https://washu.atlassian.net/wiki/spaces/RUD/pages/1864892726/Docker+Basics+Building+Tagging+Pushing+A+Custom+Docker+Image?atlOrigin=eyJpIjoiM2E1OWY2

https://washu.atlassian.net/wiki/spaces/RUD/pages/1865285780/Docker+Tutorial?atlOrigin=eyJpIjoiM2YyZWQzNDQxNWMxNGFkYmE0YzY3ZDhiNzI4NDJiZTkiLCJwI

Intel® Base Compiler Tutorial

https://washu.atlassian.net/wiki/spaces/RUD/pages/1793949810/Intel+Compiler+Base+Tutorial?atlOrigin=eyJpIjoiMGMwYmVkZGVhNGZhNGZkNDgzZDA1OGYwOTg

Please see our Intel® Base Compiler Tutorial to learn how to leverage the Intel® Base Compiler Docker image on the RIS Scientific Compute Platform.