Hewlett Packard Enterprise

LUMI Update Webinar Oct 2024

October 02, 2024

Introduction

Agenda

- Introduction
- What has been upgraded (HPE)
- What stacks are available (HPE)
- Changes to the Cray Programming Environment (HPE)
- Updates in the LUMI environment supported by LUST (LUST)
- Changes to the ROCm software environment (AMD)

HPE Cray Supercomputer software updates in general

- The Cray Supercomputing environment includes many components:
  - The Cray System Management software components that manage the service
  - The OS (COS) that runs on the login and compute nodes
  - Cray Programming Environment developer software stack (login and compute nodes)
- All were upgraded in September 2024
- COS updates bring in new Linux kernel (SUSE update), libraries, drivers, and updates to other low-level software (network, Lustre) components
- LUMI was upgraded from a base OS of SLES 15 SP4 to SLES 15 SP5
- The upgrades also introduce new hardware support, new features and optimizations but most are not visible to users
- OS and Programming Environment changes were needed to support the newer ROCm versions
- The most visible changes to users are to the Programming Environment and are identifiable by module changes.

Cray Programming Environment modules

- The default programming environment has changed
  cpe 23.09 $\rightarrow$ cpe 24.03
- Many components of the CPE have been updated
  - CCE 16.0.1 $\rightarrow$ CCE 17.0.1
  - gcc 12.2.0 (system 7.5.0) $\rightarrow$ gcc-native 13.2
  - MPICH 8.1.27 $\rightarrow$ 8.1.29
  - libsci 23.09.1.1 $\rightarrow$ 24.03.0
  - netcdf 4.9.0.7 & HDF5 1.12.2.7 $\rightarrow$ netcdf 4.9.0.11 & HDF5 1.12.2.11
  - perftools 23.09.0 $\rightarrow$ 24.03.0
  - cray-python 3.10.10 $\rightarrow$ 3.11.7
  - cray-R 4.2.1 $\rightarrow$ 4.3.2
  - AOCC cpu compilers updated (see later)

- The AMD ROCm stack is updated
  ROCM 5.2.3 (+ newer LUST versions) $\rightarrow$ ROCM 6.0.3

Status of older software

- Modules do exist for older software versions: cpe 22.08/22.12/23.03/23.09/23.12 etc.
- Lots of older ROCM modules etc.

- You can use the cpe module to change versions of the corresponding modules:

```
> module av cpe
---------------------------- HPE-Cray PE modules ----------------------------
   cpe/22.08    cpe/22.12    cpe/23.03    cpe/23.09    cpe/23.12    cpe/24.03 (D)

   Where:
    D:  Default Module

> module load cpe/23.09

The following have been reloaded with a version change:
  1) PrgEnv-cray/8.5.0 => PrgEnv-cray/8.4.0         5) cray-mpich/8.1.29 => cray-mpich/8.1.27
  2) cce/17.0.1 => cce/16.0.1                       6) cray-python/3.11.7 => cray-python/3.10.10
  3) cray-dsmml/0.3.0 => cray-dsmml/0.2.2           7) craype/2.7.31.11 => craype/2.7.23
  4) cray-libsci/24.03.0 => cray-libsci/23.09.1.1   8) perftools-base/24.03.0 => perftools-base/23.09.0
```

- These are not officially supported? tread carefully!

Python changes

- Cray-python 3.10.10 to 3.11.7 changes

python 3.10.10 $\rightarrow$ 3.11.7
numpy 1.23.5 $\rightarrow$ 1.24.4
pandas 1.4.2 $\rightarrow$ 1.5.3
SciPy 1.10.0 $\rightarrow$ 1.10.1
mpi4py 3.1.4 $\rightarrow$ 3.1.4
dask   2022.7.0 $\rightarrow$ 2023.6.1

CCE 17 (&17.0.1)

- Provides Fortran, C and C++ compilers
- Supports DO CONCURRENT offload to device with unified shared memory
- MI300 support and tuned support for Grace Hopper
- New OpenMP support:
  - 5.1 features
    - 'error' directive
    - 'omp_get_mapped_ptr' routine
    - 'omp_display_env' routine
    - 'thread_limit' clause on 'target' construct (C/C++ only)
    - New initial device number value
    - loop construct
  - Augmented OpenMP 5.X 'declare mapper' to support all Fortran derived types
- CCE 17.0.1
  - ROCM 6.0 support
  - OMPT Device tracing support
  - Tuning for MI300A
- If you have code with objects compiled with older compilers need to relink with CCE 17

CCE 17 New Fortran 2023 Features

- US 01 & 02 Allow much longer statement lines and overall statement length
- US 03 SPLIT and TOKENIZE intrinsics
- US 04 Trig functions that work in degrees
- US 06 selected_logical_kind intrinsic function
- US 07 Additional named constants to specify kinds in ISO_FORTRAN_ENV
- US 10 The at edit descriptor
- US 11 Control over leading zeros in output of real values
- US 15 Simple procedures
- US 20 Reduction specifier for do concurrent
- UK 01 Extend c_f_pointer intrinsic procedure to allow its pointer result to have specified lower bounds

GCC Native

- GCC is now provided by SLES (gcc-native modules), instead of compiled by HPE

```
> module av gcc

----------------------- HPE-Cray PE modules -----------------------
    gcc-mixed/11.2.0                gcc-native-mixed/13.2 (D)    gcc/10.3.0
    gcc-mixed/12.2.0      (D)       gcc-native/12.3                gcc/11.2.0
    gcc-native-mixed/12.3          gcc-native/13.2         (D)    gcc/12.2.0 (D)


    Where:
    D:  Default Module
```

- No functional differences.
  - Check with `-v` flag to see how the compiler was configured

Recent Changes: MPICH

- Supports ROCM 6
- New ongoing implementation using CXI triggered operations for
  MPI_Ibcast
  MPI_Ibgather
  MPI_Iscatter
  MPI_Ireduce
  MPI_Iallreduce

Recent Changes: perftools

- More mature python profiling support:
  - for Sampling:
    $ pat_run python3 app.py
  - for Tracing
    $ pat_run -w python3 app.py
  - an API is available (for example to define regions) (import pat_api)
  - see man pat_python

Other updates

- Singularity module was updated
  - singularity-ce version 4.1.3-150500.10.7
- AMD compilers are updated:
  - Module amd/6.0.3 (GPU): based on LLVM 17
  - Module aocc/4.1.0 (CPU only): based on LLVM 16.0.3

Known Issues

CCE 17

- You may see this error:
  "hidden symbol '<SYMBOL>' in <LIB> is referenced by DSO".
  A workaround is likely to be to add '-lgcc_s' to your link line.
  This is known to affect use of craypat and cray-parallel-netcdf but may happen in other circumstances

Where to get information on new releases

- HPE Cray Programming Environment website:

  https://cpe.ext.hpe.com/docs/latest/index.html

- CPE 24.03 guides:

  https://cpe.ext.hpe.com/docs/24.03/guides/index.html