HPE CRAY PROGRAMMING ENVIRONMENT

John Levesque     CTO-Office
Technical Adviser for Cray Programming Environment
Performance Evangelist for Coral-2 CoE

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**HPE Cray Programming Environment**

Comprehensive set of tools for developing, porting, debugging, and tuning of HPC applications on HPE & HPE Cray systems

### Programming Models
- HPE Cray MPI
- SHMEM
- OpenMP | OpenACC 2.0
- AMD ROCm | NVIDIA CUDA
- UPC | Fortran co-arrays

### Global Arrays
- Programming Environments
  - Compiling Environment
    - GNU
    - Intel Programming Environment
    - AMD Programming Environment
    - NVIDIA HPC SDK

### Programming Languages
- C
- C++
- R
- Python
- Fortran

### Optimized Libraries
- LibSci (BLAS)
- LAPACK & ScALAPACK
- LibSci, ACC
- IRT
- FFTW

### I/O Libraries
- NetCDF
- Adios 2
- HDFS
- DL / AI Tools
- Deep Learning Plug-in

### Comparative Debugger
- GDB for HPC
- Parallelized gdb for HPC

### Performance Analysis Tool (PAT)
- Whole program performance analysis, exposing wide set of indicators, identifying bottlenecks and automatically generating suggestions to improve performance.

### Visualization Tool
- Quick assessment of severity of issues

### Code Parallelization Assistant
- Reveal hidden potential of an application via code restructuring

### Supported systems:
- HPE Cray supercomputers
- HPE Apollo 2000 & Apollo 80 systems
- HPE ProLiant DL
- Legacy Cray systems
HPE CRAY PROGRAMMING ENVIRONMENT COMPONENTS

• Cray Compiling Environment (CCE)
  • Cray Fortran Compiler
  • Cray Enhanced Clang/LLVM C/C++ Compiler
• Cray Scientific and Math Libraries (CSML)
  • BLAS, LAPACK, ScaLAPACK, and FFTW
• Cray Message Passing Toolkit (CMPT)
  • Cray MPI (mpich), Cray OpenSHMEMX
• Cray Environment Setup and Compiling Support (CENV)
  • Modules, compiler drivers
• Cray Performance Measurement & Analysis Tools (CPMAT)
  • Cray Perftools and the Performance API (PAPI)
• Cray Debugging Support Tools (CDST)
  • STAT, ATP, gdb4hpc, valgrind4hpc, and CCDB
COMPONENT VERSIONS FOR EX SYSTEMS WITH HPCM – BY RELEASE


<table>
<thead>
<tr>
<th>HPE Cray Programming Environment Component</th>
<th>21.05</th>
<th>21.04</th>
</tr>
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<tbody>
<tr>
<td>Cray Compiling Environment (CCE)</td>
<td>11.0.4</td>
<td>11.0.4</td>
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<tr>
<td>GNU Compiler Collection (GCC)</td>
<td>10.3.0</td>
<td>10.2.0</td>
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<tr>
<td>Cray Message Passing Toolkit - MPICH</td>
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<td>8.1.4</td>
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<tr>
<td>Cray Message Passing Toolkit - OpenSHMEMX</td>
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<td>11.2.0</td>
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<tr>
<td>Cray Scientific and Math Libraries – LibSci</td>
<td>21.04.1</td>
<td>21.04.1</td>
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<tr>
<td>Cray Scientific and Math Libraries - FFTW</td>
<td>3.3.8.10</td>
<td>3.3.8.9</td>
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<tr>
<td>Perftools (CPMAT)</td>
<td>21.05.1</td>
<td>21.02.0</td>
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<tr>
<td>Performance API (PAPI)</td>
<td>6.0.0.7</td>
<td>6.0.0.6</td>
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<tr>
<td>Cray Debugging Support Tools – gdb4hpc</td>
<td>4.13.1</td>
<td>4.12.4</td>
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<tr>
<td>Cray Debugging Support Tools – STAT</td>
<td>4.11.1</td>
<td>4.10.1</td>
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</table>
# CPE 2021 Roadmap for Cray EX, Apollo

|----------------------|----------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------|
| **Hardware**         | • Grizzly Peak A100  
• Apollo/DL with Slingshot-10 fabric*  
• Apollo/DL MI-100*  
|                       | • Apollo/DL Gen10+ Milan  
• Apollo/DL MI-100 (Tech Preview) |                                                                                       | • Cray EX with Slingshot-11 fabric  
• Next Gen AMD  
• Apollo/DL Gen10+ Icelake | • Next Gen Intel  
• Next Gen AMD |
| **CSM (OS support)** | • SHASTA V1.3, V1.4                                                                                         | • COS 2.1 (SLES15 SP2)                                                                | • COS 2.2 (SLES15 SP3)  
• COS 2.2 (SLES15 SP3) | |
| **HPCM (OS support)** | • SLES15 SP2 (EX)  
• RHEL 8 (Apollo/DL)                                                                                     | • COS 2.1 (EX)  
• RHEL 8 (Apollo/DL) | • COS 2.2 (EX)  
• RHEL 8 (Apollo/DL) | • COS 2.2 (EX)  
• RHEL 8 (Apollo/DL) |
| **CPE Features**     | • MPI GPU-to-GPU support for NVIDIA A100 and AMD MI-100  
• gdb for HPC support for PBSpro with HPCM  
• Support for ‘cpe’ module on EX  
• Support LMOD on Apollo | • CCE 12.0 with additional OpenMP 5.0 features  
• SPACK environment enablement  
• OpenSHMEX 1.5 compliance  
• ROCm 4.1 support  
• Perftools support for OpenMP target offload for AMD MI-100  
• LibSci OpenMP threaded kernel updates for AMD CPU targets on EX and Apollo  
• Transition from module collections to metamodules  
• Module support for 3 combinations of Intel OneAPI compilers | • MPI support for HPE NIC traffic classes, scalable startup, Rosetta hardware collectives  
• Perftools support for next Gen AMD  
• Code parallelization assistant tool scoping and OpenMP device directive generation | • CCE 13.0 with full OpenMP 5.0 support |
| **3rd Party compilers** | • NVIDIA HPC SDK (PrgEnv-nvidia)  
|                       | • Intel OneAPI (PrgEnv-intel)  
• ROCm compilers (PrgEnv-amd)                                                                              |                                                                                       |                                                                                       |                                                                                       |

*Limited availability
HPE CRAY PROGRAMMING ENVIRONMENT

- A cross-compiler environment
  - Compiler runs on a User Access Node (UAN)
  - Executable runs on the compute nodes

- Cray written compiler driver scripts
  - HPE Cray OS compiler options
  - HPE Cray OS system libraries and header files
  - Compiler specific programming environment libraries

- Modules utility
  - Consists of the `module` command and module files
  - Initializes the environment for a specific compiler
  - Allows easy swapping of compilers and compiler versions
  - Spock and Frontier will use Lmod modules based on Lua
## PROCESSOR, ACCELERATOR, AND NETWORK MODULES

<table>
<thead>
<tr>
<th>Module</th>
<th>Contents</th>
</tr>
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<tbody>
<tr>
<td>craype-x86-rome</td>
<td>Specifies CPU Target of AMD EPYC 2\textsuperscript{nd} Generation CPU - Rome</td>
</tr>
<tr>
<td>craype-x86-milan</td>
<td>Specifies CPU Target of AMD EPYC 3\textsuperscript{nd} Generation CPU - Milan</td>
</tr>
<tr>
<td>craype-accel-amd-gfx908</td>
<td>Sets options and paths to build for the AMD MI100 GPU</td>
</tr>
<tr>
<td>craype-network-ofi</td>
<td>Sets options and paths for network to use libfabric from OpenFabrics Interfaces (OFI)</td>
</tr>
<tr>
<td>craype-network-ucx</td>
<td>Sets options and paths for network to use Nvidia (Mellanox) HPC-X toolkit using Unified Communication X (UCX)</td>
</tr>
</tbody>
</table>
COMPILER DRIVER SCRIPTS

• Do not call compilers directly; use Cray compile drivers
  • ftn
  • cc
  • CC

• Driver actions:
  • Select compiler version
  • Add system libraries and header files
  • Add compiler-specific programming environment libraries
  • Execute the actual compiler command with added options

• Use vendor man pages for details of compiler options
  • HPE Cray man pages: crayftn, craycc, crayc++
  • GCC man pages: gfortran, gcc, g++