The Cray Programming Environment: Current Status and Future Directions

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Cray Programming Environments Director
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Agenda

- Cray PE Overview
- Highlights since last CUG and roadmap overview
  - CCE
  - MPT
  - CPMAT
  - CDST
  - CSML
  - CrayPE & Modules
  - Chapel
- Cray Directives
  - Accelerators
  - Memory directives
- Summary
The Cray Programming Environment Mission

- **Focus on Performance and Programmability**
  - It is the role of the Programming Environment to close the gap between observed performance and achievable performance

- **Support the application development life cycle** by providing a tightly coupled environment with compilers, libraries, and tools that will hide the complexity of the system
  - Address issues of scale and complexity of HPC systems
  - Target ease of use with extended functionality and increased automation
  - Close interaction with users
    - For feedback targeting functionality enhancements

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The diagram illustrates the environment's components:

- **Compile**
  - Compiler information
  - Port

- **Application**
  - Debug information
  - Debug
  - Performace Analysis
  - Export/Import

- **Analyze**
  - Queries for Application Optimization
  - Compiler information
  - Application

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CUG 2016

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Cray PE for the CS Series

The Cray Programming Environment Suite for Clusters is a fully integrated programming environment with compilers, tools, and libraries designed to maximize programmer productivity, application scalability, and performance. It consists of:

- **Cray Compiling Environment (CCE)**
  - Fortran, C and C++ compilers supporting OpenMP 4.0 (with OpenMP 4.5 Target) and OpenACC 2.0

- **Cray Performance, Measurement, Analysis, and Porting Tools (CPMAT)**
  - PerfTools (CrayPAT, CrayPAT-light, & Cray Apprentice2)
  - Reveal

- **Cray Scientific Libraries (CSML)**
  - Cray LibSci with Autotuned BLAS library, LAPACK, ScaLAPACK, and Iterative Refinement Toolkit (IRT)
  - Cray LibSci_ACC providing accelerated BLAS and LAPACK routines for GPUs
  - Cray optimized FFTW

- **Cray Comparative Debugger (CCDB / lgdb)**

- **Cray Environment Setup and Compiling support – CENV**

- **MPI libraries supported**
  - Intel MPI
  - MVAPICH
# Cray Programming Environment Roadmap

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<thead>
<tr>
<th>Year</th>
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- Cray Compiling Environment
- CCE
  - ▼8.4
  - ▼8.5b ▼8.5
  - ▼8.5.3 ▼8.5.5
  - ▼8.6b ▼8.6
- Cray Message Passing Toolkit
- MPT
  - ▼7.2
  - ▼7.2.5 ▼7.3
  - ▼7.3.x ▼7.4
  - ▼7.5
  - ▼7.6 ▼7.7
- Cray Performance Measurement & Analysis Tools
- CPMAT
  - ▼6.2.3 ▼6.2.4 ▼6.3
  - ▼6.3.1 ▼6.3.2 ▼6.4
  - ▼6.4.1 ▼6.4.x ▼6.5
- Cray Scientific & Math Libraries
- CSML
  - ▼15.4 ▼15.9 ▼15.12 ▼16.3 ▼16.6 ▼16.9 ▼16.11 ▼17.7
- Cray Debugging Support Tools
- CDST
  - ▼15.4 ▼15.9 ▼15.12 ▼16.3 ▼16.6 ▼16.11 ▼17.7
- Chapel
  - ▼1.11 ▼1.12 ▼1.13 ▼1.14 ▼1.15 ▼1.16

CUG 2016

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# CCE 8.5 Highlights and Roadmap

## 2015
- **Q1:** Hiawatha Up 3
- **Q2:** Itasca
- **Q3:** Itasca Up 1 (Broadwell)
- **Q4:** Jasper LA (CUDA 7.5)

## 2016
- **Q1:** Jasper
- **Q2:** Jasper Up 1 (Athena)
- **Q3:** Jasper Up 2 (CUDA 8.0)
- **Q4:** Kabetogama

## 2017

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### CCE 8.5
- **Intel KNL support**
- **Memory directives**
- **OpenMP 4.5 “target” (accelerator) support**
- **C11 support**
  - Not default with CCE C
    - `-hstd=c99` is the default
    - use `-hstd=c11` to enable
- **Compile time improvements (especially for large codes)**
- **Fortran coarray, UPC, and coarray C++ support on CS**
  - Full Fortran 2008 support
- **Athena support (CCE 8.5.3)**

### CCE 8.6 and beyond
- **NVIDIA Pascal GPU with CUDA 8.0 support**
- **C++14 support**
- **OpenMP 4.5 full support**
- **Fortran 2015 support**
  - Fortran coarray teams
### MPT - Highlights Since Last CUG (MPT 7.2)

<table>
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<th>2016</th>
<th>2017</th>
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- Cray MPI now supports the MPI 3.1 standard (based on MPICH 3.2rc1)
- Added display of high water mark of the memory used by MPI
- GPU-to-GPU support for MPI-3 RMA
- Support to the OpenSHMEM Specification Version 1.3
- Lots of optimizations on MPI and Cray SHMEM
- Reduced MPI memory footprint optimizations
MPT 7.4 Highlights

- Initial KNL support/optimizations
- Cray MPI hugepage support for MCDRAM on KNL
  - (MPI_Alloc_mem and MPI_Win_Allocate)
- Cray SHMEM support for MCDRAM on KNL
- Additional MPI_THREAD_MULTIPLE optimizations (“Thread Hot”)
- Initial MPI-IO optimizations for Cray DataWarp
- MPI-IO Collective Buffering mode allowing multiple aggregators per OST
  - Requires Lustre 2.7 client and server (Lock Ahead feature)

*Krishna Kandalla’s MPT talk at 10:30 on Thursday will cover some of these items in-depth*
### CPMAT - Highlights Since Last CUG (CPMAT 6.2.3)

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<tr>
<td>Kabetogama</td>
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#### Highlights

- Sampling Over Time (6.2.3)
- Power over time display (6.2.3)
- Support to multiple GPUs per node (Cray CS-Storm) (6.2.4)
- Support for Intel MPI on Cray CS Systems (6.3.0)
- New perftools modules (6.3.0)
- SNB / IVB / HSW uncore counter support with privileged access (6.3.0)
- Apprentice2 new sample data over time plots (6.3.0)
- Apprentice2 mosaic in runtime summarization mode (6.3.0)
- Observation for helper threads in reports (6.3.0)
- Apprentice2 compare (6.3.1)
Roadmap Highlights - CPMAT 6.4 and Beyond

- **Reveal**
  - Include time for loops sorted by compiler messages (e.g., find most time consuming loops that didn’t vectorize)
  - auto-parallelization
  - Client for OS X
  - MCDRAM data allocation assistance

- **New trace groups for OpenCL, Lustre API, MemKind, Parallel NetCDF**

- **MPI insight (communication ‘strategy’ thresholds and advice on environment variables)**

- **Memory usage information per NUMA domain**

- **Support for CHARM++**
CSML Highlights Since Last CUG

- Added optimized support for Broadwell target
- Improved BLAS GEMM performance for Haswell and Broadwell CPU targets on XC and CS platforms
- Expanded set of optimizations for ScaLAPACK eigensolver routines
- Improved OpenMP threading support for BLAS and LAPACK routines
- Added FASTPLAN optimizations for Haswell and Broadwell targets
- Added FFT support of arbitrary dimension and size for both real and complex data types
- Added 64-bit integer support for Cray PETSc and Cray TPSL
- Added support for HDF5 in Cray PETSc
- Support for latest Kokkos multithreading libraries
Cray FFTW FASTPLAN Performance

1D Complex-to-Real Haswell (Single thread)

Cray-FFTW (FASTPLAN Enabled)
Cray-FFTW (FASTPLAN Disabled)

Higher GFLOPS Equals Better Performance

Custom 3D-FFT Application (Real-to-Complex 1024^3) Haswell, 16 MPI Ranks

Cray-FFTW (FASTPLAN Disabled)
Cray-FFTW (FASTPLAN Enabled)
Alternate FFT Library

Lower Elapsed Time Equals Better Performance

FFT Portion of Walltime

FASTPLAN enable with environment variable FFTW_CRAY_FASTPLAN=1
CSML Roadmap

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<th>Year</th>
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- Support KNL targets on XC and CS systems
- Small GEMM optimizations for BLAS
- Athena support
- Support for Nvidia Pascal GPU targets on XC and CS systems running CUDA 8.0
## CDST Highlights and Roadmap

### CDST since last CUG
- STAT 2.1 with ALPS DSL tool helper
- ATP, STAT & LGDB SLURM 15 support
- CCDB and LGDB CUDA 7.5 support
- CCDB and LGDB on Cray CS Systems

### CDST Roadmap
- KNL support
- ATP, STAT & LGDB single release to support multiple SLURM versions
- LGDB Pascal GPU and CUDA 8.0 support
- LGDB additional improvements for C++
- LGDB better UPC support
- CCDB better comparisons for large data structures

### CDST Roadmap Timeline

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<tr>
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### CDST Version Numbers
- ▼15.4
- ▼15.9
- ▼15.12
- ▼16.3
- ▼16.6
- ▼16.11
- ▼17.7
CCDB Overview

- **What is comparative debugging?**
  - Data centric approach instead of the traditional control-centric paradigm
  - Two applications, same data
  - Key idea: The data should match
  - Quickly isolate deviating variables

- **Comparative debugging tool**
  - NOT a traditional debugger!
  - Assists with comparative debugging
  - CCDB GUI hides the complexity and helps automate process
    - Creates automatic comparisons
    - Based on symbol name and type
    - Allows user to create own comparisons
    - Error and warning epsilon tolerance
    - Scalable

- **How does this help me?**
  - Algorithm re-writes
  - Language ports
  - Different libraries/compilers
  - New architectures

- **Collaboration with University of Queensland**
● **Module substring feature (PE 16.04)**
  ● Returns results if the argument is a part of any module name, rather than just modules that start with substring argument
    ● Example: “`module --s avail hdf5`” would find all modules with “hdf5” anywhere in the name

● **New CDT module for each XC PE release (PE 16.04)**
  ● Switches currently loaded modules to the version associated with a specific CDT release
  ● Subsequently loaded modules also load the version associated with CDT release
  ● Started with the April 2016 PE release (cdt.16.04)

*Note unloading the cdt module is not sufficient to restore your loaded modules to the system defaults. A script, `restore_system_defaults.sh`, can be sourced to restore your currently loaded modules to the system defaults*
New cdt module for each PE release on XC

```
ldr@cdt-test:~> module list
Currently Loaded Modulefiles:
  1) modules/3.2.10.3
  2) cce/8.4.3
  3) craype-network-aries
  4) craype/2.5.1
  5) cray-libsci/13.3.0
  6) cray-mpich/7.3.1
...
ldr@cdt-test:~> module avail cce
------------------------------ /opt/modulefiles ------------------------
cce/8.4.3(default) cce/8.4.5
...
ldr@cdt-test:~> module avail cray-mpich
------------------------------- /opt/cray/modulefiles -----------------
cray-mpich/7.3.1(default)
cray-mpich/7.3.1(cray-mpich-abi/7.3.1)
cray-mpich/7.3.3(cray-mpich-abi/7.3.3)
```

```
ldr@cdt-test:~> module load cdt/16.04
...
Switching to cce/8.4.5.
Switching to cray-libsci/16.03.1.
Switching to craype/2.5.4.
Switching to modules/3.2.10.4.
Switching to cray-mpich/7.3.3.
...
ldr@cdt-test:~> module avail cce
------------------------------ /opt/modulefiles ------------------------
cce/8.4.3 cce/8.4.5(default)
...
ldr@cdt-test:~> module avail cray-mpich
------------------------------- /opt/cray/modulefiles -----------------
cray-mpich/7.3.1 cray-mpich-abi/7.3.1
```
## Chapel Highlights and Roadmap

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<th>Platform</th>
<th>Notes</th>
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### Chapel Highlights since 1.11
- Improved string and record implementation
  - dramatically improved string performance
  - greatly reduced memory leaks
  - standard string library routines supported
- New module namespace control features
- Improved compiler stability
- Improved library support
- Parallelize large numeric array initialization
  - improved first touch with NUMA domains
- Performance improvement highlights
  - reduction operations
  - convert RMA to local access as permitted
  - significant performance improvements for 'ugni' comm on Crays
  - bulk communication optimization for improved scaling

### Chapel Roadmap
- Continuously improving performance and scalability
- UTF8 string and library support
- Eliminate memory leaks
- Improved Error handling
- Task Teams
- Improved Object Oriented Story
- Additional general purpose libraries
- Additional platform support
  - KNL, ARM, GPUS, etc.
CCE Directives Update (OpenMP / OpenACC / Memory)

<table>
<thead>
<tr>
<th>CCE 8.4</th>
<th>CCE 8.5 (June 2016)</th>
<th>CCE 8.6 (tentative)</th>
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<tr>
<td>OpenMP 4.0</td>
<td>OpenMP 4.5 (target)</td>
<td>OpenMP 4.5 (complete)</td>
</tr>
<tr>
<td>OpenACC 2.0</td>
<td>OpenACC 2.5 (no planned support)</td>
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<td>KNL “memory” directive</td>
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● Cray will continue to support OpenACC 2.0
  ● No plans to support OpenACC 2.5

● Recommendation: migrate to OpenMP “target”
  ● OpenMP 4.0 provides constructs for base functionality
  ● **OpenMP 4.5 provides constructs for competitive performance**
    ● Asynchronous data transfers and kernel execution
    ● Default scoping behavior of scalars as firstprivate
    ● Unstructured data regions, “host data” regions, device pointers
    ● Device memory API
KNL Memory from CCE Perspective

● Node has two different types of memory
  ● DDR: high-capacity, low-bandwidth
  ● MCDRAM: high-bandwidth, low-capacity

● Typical memory footprints exceed MCDRAM
  ● Best performance requires MCDRAM

● Users must allocate specific variables in MCDRAM
  ● Not everything will fit at once
  ● Latency-sensitive variables should probably go in DDR

● CCE solution: provide mechanisms for developers to place specific variables and allocations in MCDRAM
CCE Support for MCDRAM

- Cray Directive (pragma) to support data allocation in MCDRAM
  - Provide a directive-only solution
  - Cover more use cases
- Support for Fortran, C, and C++
  - The directive can be used on **both local and global variables**
    - to place the variables in high bandwidth memory
  - The directive **can also be used on a statement**
    - to change any allocation routines on that statement (allocate, malloc, etc.) to use HBM
- **If Clause** for dynamic control of directive
- **Fallback Clause** to control behavior if allocation fails
- Future direction for memory hierarchy control
  - Ideally will become part of a standard, possibly OpenMP
CCE Proposed API for KNL HBM

- Directive (pragma) to control placement for high bandwidth memory
  - Support for Fortran, C and C++
  - Proposed directive
    - \texttt{!dir$ memory(attributes) [list of variables]}
    - \texttt{#pragma memory(attributes) [list of variables or allocatable members]}
      - \textit{Attributes} – list of desired memory attributes (bandwidth, capacity, nonvolatile, etc.)
      - Initially “bandwidth” is the only allowed attribute
      - Other attributes may be added in the future

- Statements
  - Appears prior to an allocation/deallocation statement
  - Changes explicit allocation routines in the next statement to use HBM
    - \texttt{Fortran: allocate}
    - \texttt{C/C++: malloc, calloc, realloc, posix_memalign, free}
    - \texttt{C++: new, delete, new[], delete[]}
      - Directive on deallocation must match (C/C++ only)
CCE Directive for Variable Declarations

!dir$ memory(attributes) list-of-vars
#pragma memory(attributes) list-of-vars

- **Specified at declaration of variable**
  - For global variables, directive must be visible for every use of global
  - Within type for allocatable members

- **Allowed on:**
  - Local and global variables
  - Scalars, structs and arrays (fixed size and variable length)
  - Fortran allocatables (including members of derived types)
    - Memory allocated will use high bandwidth memory

- **Not allowed on:**
  - Dummy arguments
  - Common blocks or variables within a common block
  - Fortran pointers
  - Variables involved in equivalences
  - Coarray or UPC shared variables
Cray Memory Directive – Current Status

- Initial implementation and basic testing of the Cray memory directive is complete for CCE 8.5
  - Target June 2016 release
    - Support for Intel’s FASTMEM attribute is deferred to a future CCE release

- Internal users are starting to use the feature and providing feedback

- Cray is working with OpenMP to incorporate this feature into the OpenMP 5.0 specification (2017/2018)
  - Cray presented to the OpenMP accelerator subcommittee in April
  - Intent is to initially include the feature in the annual OpenMP TR by SC’2016
Summary

- Application developers need a programming environment that can address and hide the issues of scale and complexity of supercomputers

- Cray’s advanced programming environment continue to focus on Performance and Programmability
  - Cray Compiling Environment (CCE) focused on application performance
    - Fully automatic loop vectorization
    - Directives for accelerators and multiple levels of the memory hierarchy
  - Cray Performance Analysis Tools
    - Focus on automation, scaling, and ease of use
  - Reveal
    - Scoping analysis and parallelization assistant
  - Parallel debugger support
  - Auto-tuned Scientific Libraries support
    - Getting performance from the system … no assembly required
Thank You