# The Cray Programming Environment: Current Status and Future Directions


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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**


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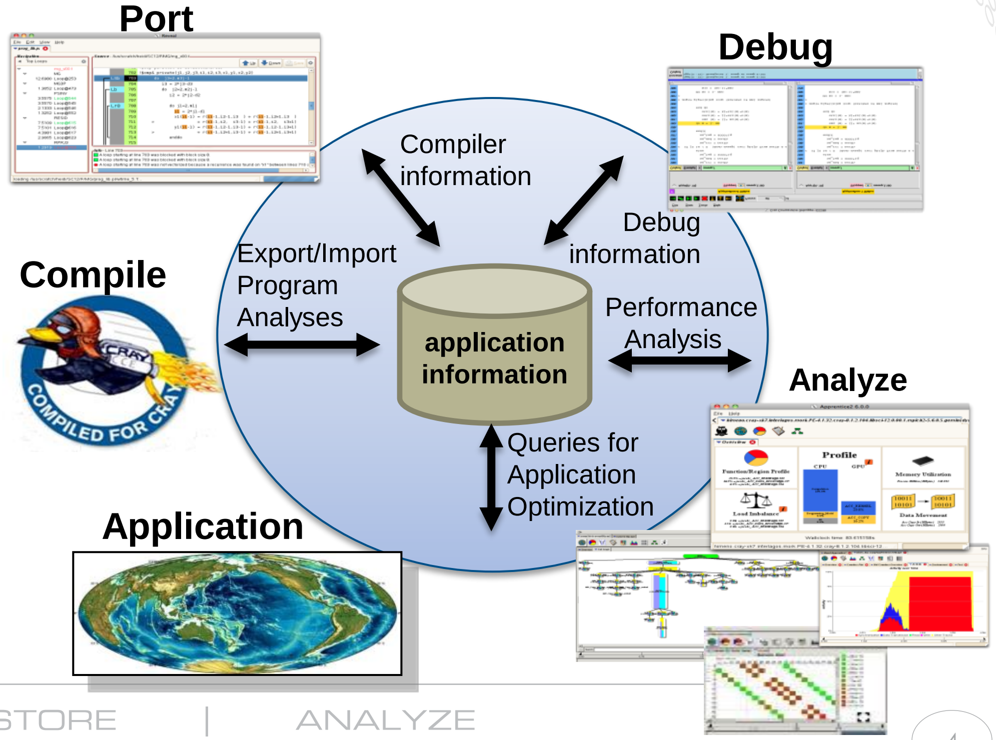
# The Cray Programming Environment Mission

- 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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# 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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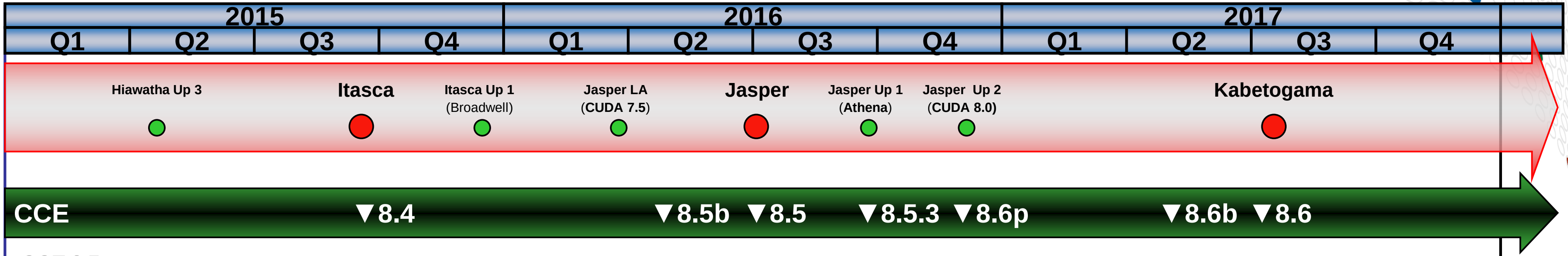
# CCE 8.5 Highlights and Roadmap




**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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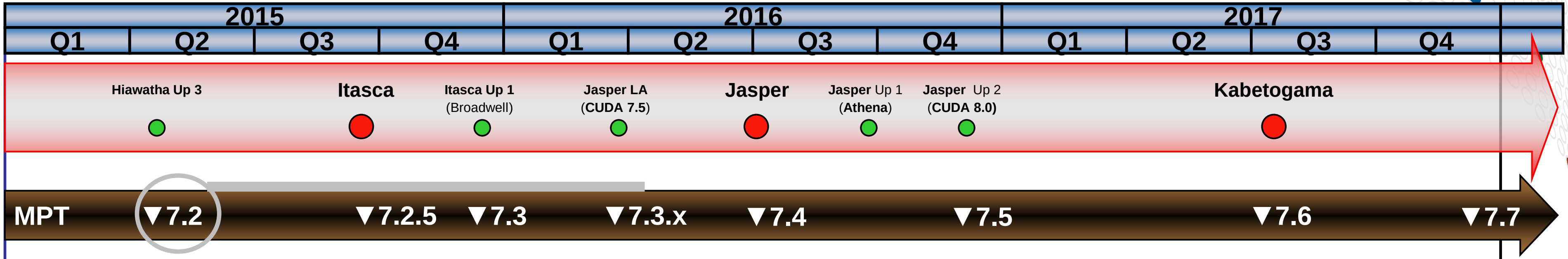
# MPT - Highlights Since Last CUG (MPT 7.2)




- 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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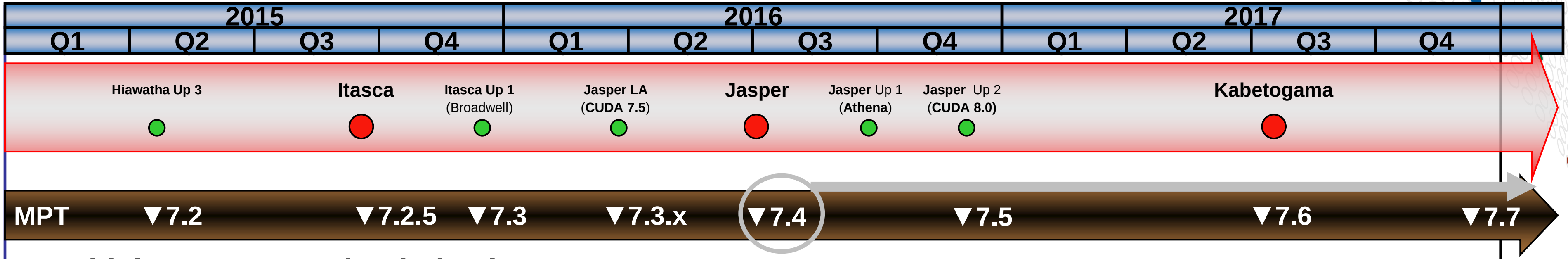
# MPT 7.4 Highlights




- **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**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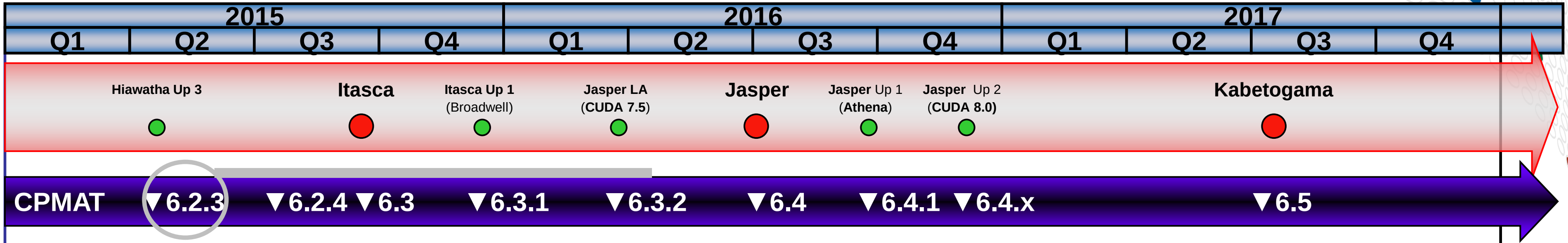
# CPMAT - Highlights Since Last CUG (CPMAT 6.2.3)




- 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)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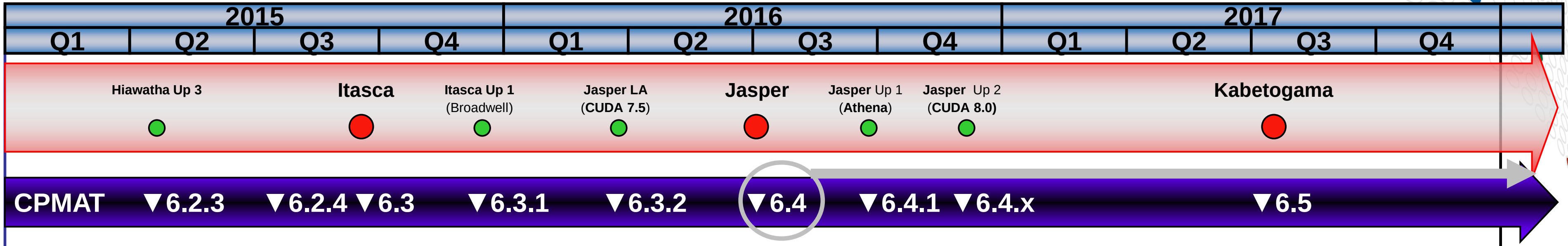
# Roadmap Highlights - CPMAT 6.4 and Beyond




- **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++**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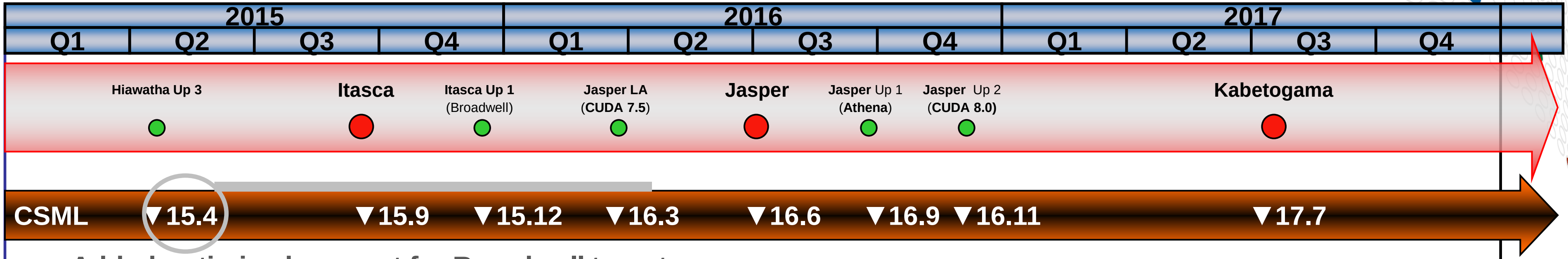
# CSML Highlights Since Last CUG




- 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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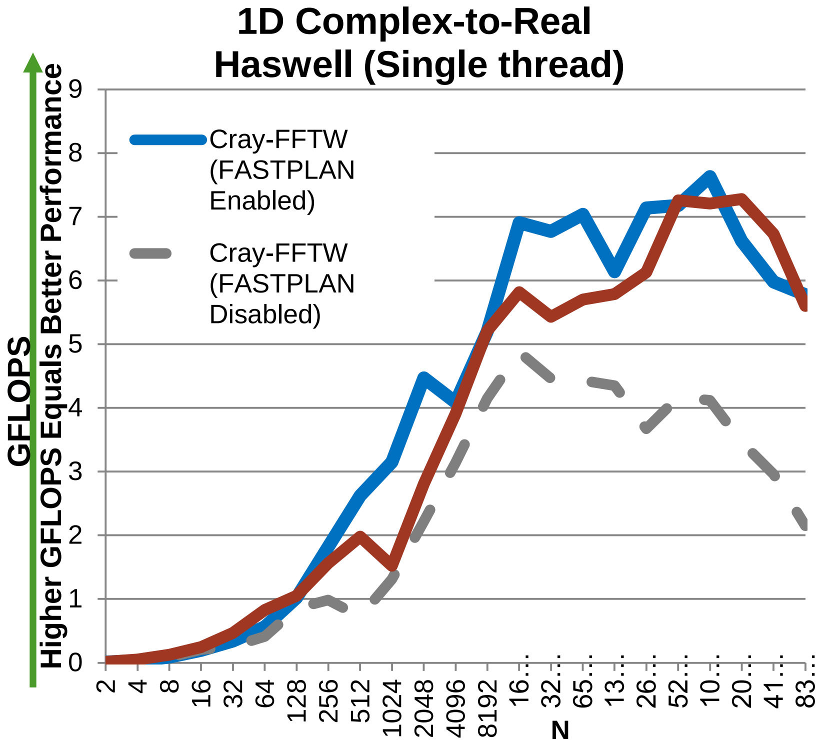
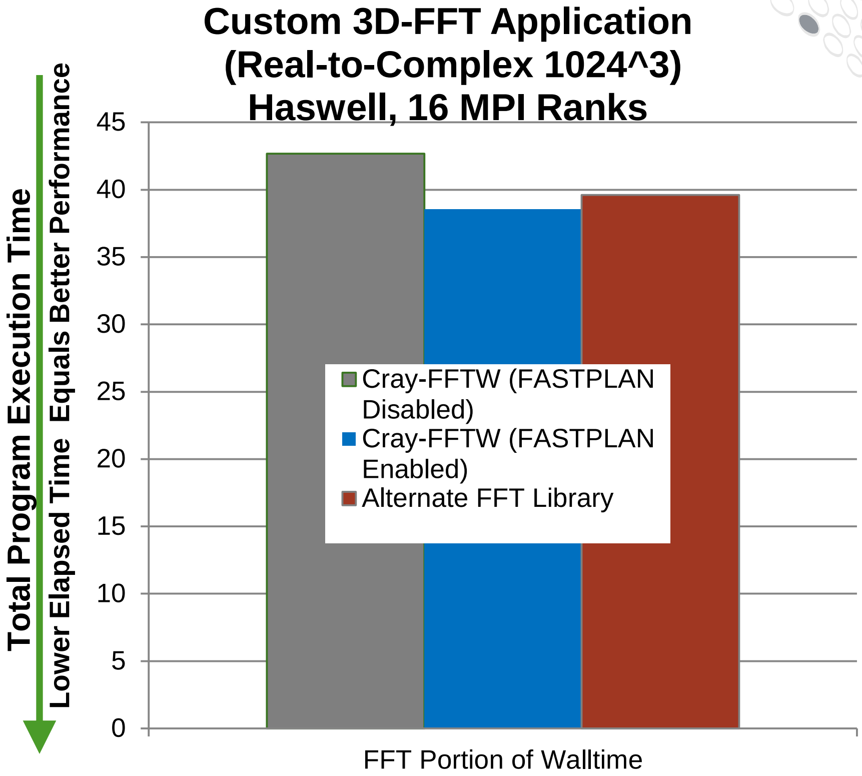
# Cray FFTW FASTPLAN Performance




**FASTPLAN enable with environment variable FFTW_CRAY_FASTPLAN=1**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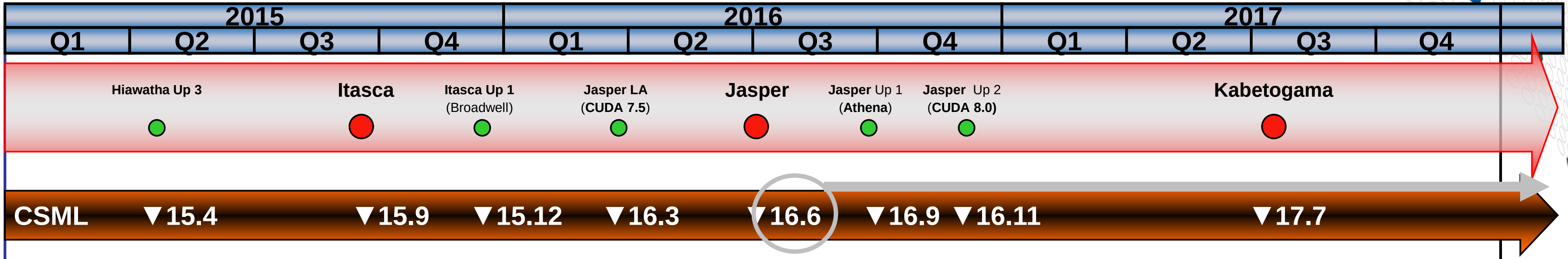
# CSML Roadmap




- 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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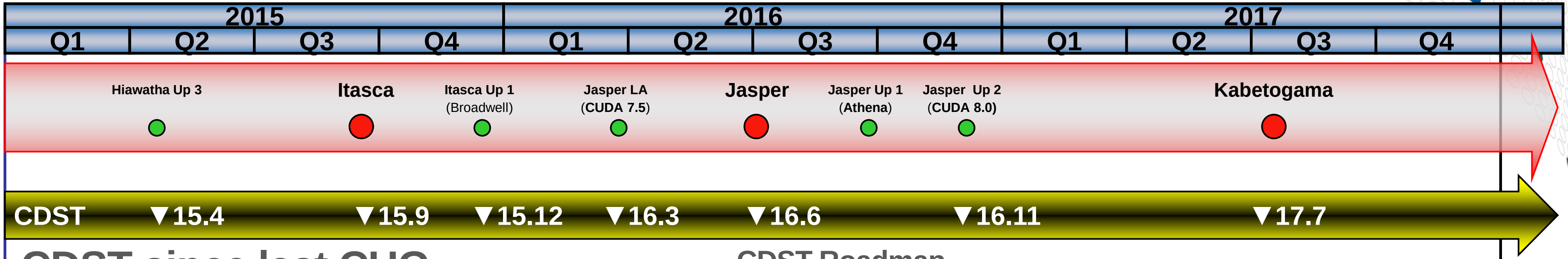
# CDST Highlights and Roadmap




## 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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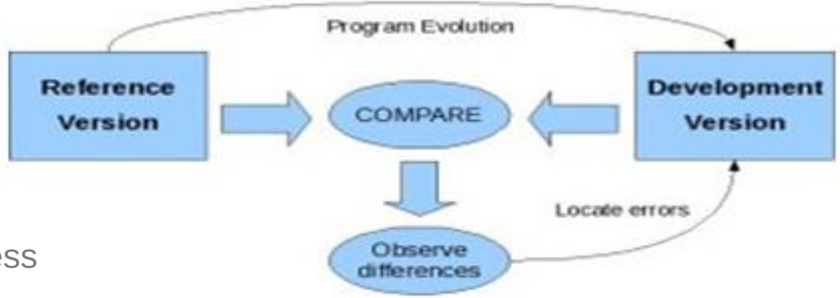
# CCDB Overview

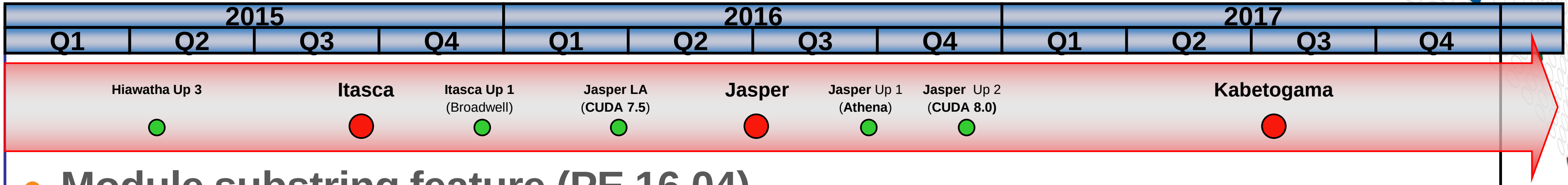
- **What is comparative debugging?**
  - Data centric approach instead of the traditional control-centric paradigm
  - Two applications, same data
  - Key idea: The data should match
  - Quickly isolate deviating variables
- **Comparative debugging tool**
  - NOT a traditional debugger!
  - Assists with 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**





The University Of Queensland
AUSTRALIA

# Craype/modules Highlights




- **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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# 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-abi/7.3.1(default)
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
cray-mpich/7.3.3(default)   cray-mpich-abi/7.3.3(default)
```


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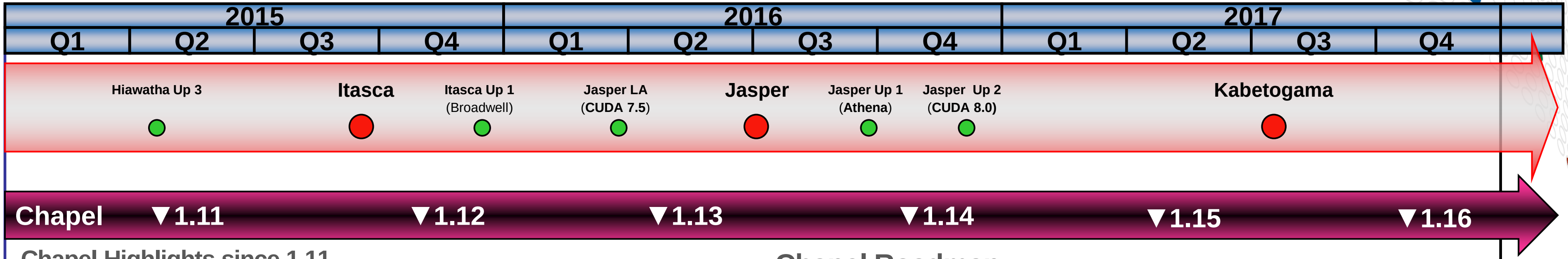
# Chapel Highlights and Roadmap




### 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.



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# CCE Directives Update (OpenMP / OpenACC / Memory)

| CCE 8.4 | CCE 8.5 (June 2016) | CCE 8.6 (tentative) |
|---|---|---|
| OpenMP 4.0 | OpenMP 4.5 (target) | OpenMP 4.5 (complete) |
| OpenACC 2.0 | ~~OpenACC 2.5~~ (no planned support) | |
| | KNL “memory” directive | |

- **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


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# 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**


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# 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


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# CCE Proposed API for KNL HBM

- **Directive (pragma) to control placement for high bandwidth memory**
  - Support for Fortran, C and C++
  - Proposed directive
    - **!dir$ memory(*attributes*) *[list of variables]***
    - **#pragma memory(*attributes*) *[list of variables or allocatable members]***
      - *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
    - **Fortran: allocate**
    - **C/C++: malloc, calloc, realloc, posix_memalign, free**
    - **C++: new, delete, new[], delete[]**
      - Directive on deallocation must match (C/C++ only)


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# 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


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# 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


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# 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**



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CRAY

COMPUTE | STORE | ANALYZE

# Thank You