Cray’s Programming Environment for Portable Performance and Programmability on Systems with High-Bandwidth Memory

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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
Cray Programming Environment for KNL

### Programming Languages
- Fortran
- C
- C++
- Chapel

### Programming models
- Distributed Memory (Cray MPT)
  - MPI
  - SHMEM
  - GA
- Shared Memory
  - OpenMP 4.0
  - OpenACC 2.0
- PGAS
  - UPC
  - CAF
  - CoArray C++

### Compilers
- Cray Compiling Environment (CCE)
- GNU
- Intel Compilers

### Tools
- Debuggers
  - DDT
  - TotalView
  - Igdb
- Debugging Tools
  - ATP
  - STAT
- Performance Analysis
  - CrayPat & Cray Apprentice2
  - Porting Tools
  - Reveal
  - CCDB

### Optimized Scientific Libraries
- Dense
- BLAS
- LAPACK
- ScaLAPACK
- Iterative Refinement Toolkit
- Sparse
- Cray PETSc (with CASK)
- Cray Trilinos (with CASK)
- FFT
- FFTW

### I/O Libraries
- NetCDF
- HDF5

Cray developed
Licensed ISV SW
3rd party packaging
Cray added value to 3rd party

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CCE Support for High Bandwidth Memory

- Cray Directive (pragma) to support data allocation in HBM
  - 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
    - `!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)
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
If Clause

!dir$ memory(attributes) if(expression)
#pragma memory(attributes) if(expression)

● Dynamic control of directive

● For declarations
  ● Expression is evaluated when variable goes into scope

● For heap allocations
  ● Expression is evaluated when directive is encountered
  ● The expression must match on the deallocation (C/C++ only)
Fallback Clause

!dir$ memory(attributes) fallback
#pragma memory(attributes) fallback

● Controls behavior if allocation fails

● Default behavior: allocation fails

● Fallback behavior: allocation returns normal memory
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 will present the directive to the OpenMP accelerator subcommittee
  ● Intent is to initially include the feature in the annual OpenMP TR by SC’2016