Cray Programming Environment Workshop

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Cray PE Workshop - Agenda

09:00 – 09:15  introduction

09:15 – 10:45  Applying a “Whack-a-mole” Method using Cray’s perftools to identify the Moles

10:45 – 11:00  Break

11:00 – 12:00  Continue with Applying a “Whack-a-mole” Method using Cray’s perftools to identify the Moles

12:00 – 13:00  Lunch

13:00 – 13:30  What is new in PE

13:30 – 14:30  Perftools tips and tricks, data interpretation

14:30 – 14:45  Break

14:45 – 15:15  Tips when using Cray MPI

15:15 – 15:45  Cray PE DL Scalability Plugin

15:45 – 16:00  Wrap-up & Questions
The Cray Programming Environment Mission

- Provide **scalable performance, portability, and programmability** on homogeneous and heterogeneous Cray systems
- Provide the best environment to develop, debug, analyze, and optimize applications for **production supercomputing** with tightly coupled compilers, libraries, and tools
  - Address issues of scale and complexity of HPC systems
  - Intuitive behavior and best performance with the least amount of effort
  - Target **ease of use** with extended functionality and increased automation
  - Close interaction with users
Performance at Scale

- Drive maximum computing performance while focusing on programmability and portability

- **Close the gap** between observed performance and achievable performance

- Maximize the cycles to the application

- **Address issues of scale** and complexity of HPC systems

- A **performance portable programming environment**
  - Same look and feel, independently of processor architecture
Programmability Focused Environment

- **GNU Modules** simplify build environment
  - Complexity of compile and link lines (-h -l -l -L) reduced

- **Multiple product versions, compilers, and compiler versions** available on system at the same time offers more flexibility and convenience

- **Product agnostic drivers** (cc, CC, ftn) are used to compile for supported Programming Environments
  - Customer-integrated and Cray libraries share the same driver interface

- Support available to plug 3rd party software into Cray software environment (craypkg-gen)
# Cray Developer Environment on XC Systems

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

## Programming Models
- Distributed Memory
  - Cray MPI
  - SHMEM
- Shared Memory / GPU
  - OpenMP
  - OpenACC
- Global Arrays
- PGAS & Global View
  - UPC
  - Fortran coarrays
  - Coarray C++
  - Chapel

## Programming Environments
- Cray Compiling Environment
  - PrgEnv-cr
- GNU
  - PrgEnv-gnu
- 3rd Party compilers
  - PrgEnv-xxx

## Libraries
- Scientific Libraries
  - LAPACK
  - ScaLAPACK
  - BLAS
  - Iterative Refinement Toolkit
  - FFTW
  - NetCDF
  - HDF5

## Development Tools
- Environment setup
  - Modules
- Debuggers
  - TotalView
  - DDT
  - gdb4hpc
- Debugging Support
  - Abnormal Termination Processing (ATP)
  - STAT
- I/O Libraries
  - NetCDF
  - HDF5

## Development Tools
- Performance Analysis
  - CrayPAT
  - Cray Apprentice²
- Porting
  - Reveal
  - CCDB
- ML Frameworks
  - Cray PE ML Plugin

## Notes
- Cray Developed
- Cray added value to 3rd party
- 3rd party packaging
- Licensed ISV SW

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Using the Compiler

- Cray Systems come with compiler wrappers to simplify building parallel applications
  - Fortran Compiler: ftn
  - C Compiler: cc
  - C++ Compiler: CC

- Using these wrappers ensures that your code is built for the compute nodes and linked against important libraries
  - Cray MPT (MPI, Shmem, etc.)
  - Cray LibSci (BLAS, LAPACK, etc.)
  - ...

- Do not call the Cray compilers directly

- Cray Compiler wrappers try to hide the complexities of using the proper header files and libraries
Compiler man Pages

- The cc(1), CC(1), and ftn(1) man pages contain information about the compiler driver commands

- The craycc(1), crayCC(1), and crayftn(1) man pages contain descriptions of the Cray compiler command options

- To verify that you are using the correct version of a compiler, use:
  - -V option on a cc, CC, or ftn command with CCE
The Cray Compiling Environment (CCE)

- Cray technology designed for real scientific applications, not just for benchmarks

- Fully integrated heterogeneous optimization capability

- Focus on standards compliance for application portability and investment protection

Languages:
- C++ 14
- Fortran 2008
- OpenMP 4.5
- C11
- UPC 1.3
Some Cray Compiling Optimization Basics

● **Start with default options**, then add options as desired/needed for performance tuning or optional features
  ● Optimization: `-O2` is the default and you should usually use this
  ● It’s the equivalent of most other compilers –`O3` or –`fast`
  ● It is also our most thoroughly tested configuration

● Use the **restrict keyword** on all of a function's pointer parameters, provided that they do not alias

● **Limit functions to a reasonable size**
  ● **Thousands of lines of code in a single function will drive up compile time and memory usage**
Recommended CCE Compilation Options

- Using \texttt{-O3,fp3} (or \texttt{-O3 -hfp3}, or some variation)
  - \texttt{-O3} only gives you slightly more than \texttt{-O2} \textit{(but more compilation time)}
  - We also test this thoroughly
    - Notice that higher numbers are not always correlated with better performance
  - \texttt{-hfp3} gives you a lot more floating point optimization, esp. 32-bit

- With C++:
  - Use \texttt{-hipa4}
    - This is now the default in CCE 8.7
  - \texttt{Use the predefined complex type} rather than the standard template implementation

- Avoid using \texttt{-h aggress} and \texttt{-h ipa5}
  - Few codes actually see a performance benefit (these options are available for rare cases)

- Optimizing for compile time rather than execution time
  - Compile time can sometimes be improved by disabling certain optimizations
    - Some common things to try: \texttt{-hnodwarf, -hipa0, -hunroll0}
    - \texttt{-h develop} reduces compile time at the expense of optimization, by omitting optimizations that are known to increase compile time. This option is intended to be used when a program is under development and being recompiled frequently
Helpful Directives

● See ‘man intro_directives’ for a summary
  ● Many directives also have their own man page

● Use the “optimize” directive to apply an optimization to a function
  ● Overrides the command line for that function
    ● See ‘man optimize’.

● Use the “safe_address” directive when possible for loops to improve performance
  ● See 'man safe_address'
Tips and Hints on using CCE - Vectorization

- **Compiler options:**
  - -h cpu={x86-skylake,mic-knl,...}
  - -h preferred_vector_width={64,128,256,512}
    - For Xeon Skylake, using AVX512VL at 256 bits can sometimes be faster than the full 512 bit vector width
  - -h nofp_trap (the default) allows the compiler to optimize more aggressively

- **Directives:**
  - OpenMP SIMD is a portable way to identify a loop nest for vectorization
  - #pragma concurrent. See ‘man concurrent’.
  - #pragma ivdep. See ‘man ivdep’.

- **Other tips:**
  - **CCE is not limited to vectorizing innermost loops**
    - Entire loop nests are candidates for vectorization
  - Based on target hardware characteristics, CCE may decide to leave a loop as scalar if that is expected to be faster than the vectorized counterpart
    - This can be overridden by #pragma prefervector or #pragma omp simd
OpenMP

● On CCE OpenMP is **ON** by default
  ● Optimizations controlled by `-hthread`#

● **Autothreading is NOT** on by default;
  ● `-hautothread` to turn on
  ● Modernized version of Cray X1 streaming capability
  ● **Interacts with OpenMP directives**

● **If you do not want to use OpenMP and have OMP directives in the code, make sure to shut off OpenMP at compile time**
  ● To shut off use `-hthread0` or `-xomp` or `-hnoomp`
Communications From CCE

- “Positive” and “negative” optimization messages
  - “Positive” messages report
    - Key optimizations that were performed
    - Various optimization concerns (like overuse of registers)
    - Possible functional issues
      - like potential numeric differences and use-before-definition problems
    - … and a few other situations
  - “Negative” messages report
    - Most important reason why a key optimization was not performed
    - Compiler tries very hard to report only the most critical optimization inhibitors – otherwise basically looking at a lot of “noise”
  - “explain” utility to obtain detailed information on each message

- Loopmark
  - Annotated listing
  - Generally easier to use than raw message output

- Assembly language output
Loopmark: Compiler Feedback

- Compiler can generate an filename.lst file
  - Contains annotated listing of your source code with letter indicating important optimizations

<table>
<thead>
<tr>
<th>Primary Loop Type</th>
<th>Modifiers</th>
</tr>
</thead>
<tbody>
<tr>
<td>A - Pattern matched</td>
<td>a - atomic memory operation</td>
</tr>
<tr>
<td></td>
<td>b - blocked</td>
</tr>
<tr>
<td>C - Collapsed</td>
<td>c - conditional and/or computed</td>
</tr>
<tr>
<td>D - Deleted</td>
<td></td>
</tr>
<tr>
<td>E - Cloned</td>
<td></td>
</tr>
<tr>
<td>F - Flat - No calls</td>
<td>f - fused</td>
</tr>
<tr>
<td>G - Accelerated</td>
<td>g - partitioned</td>
</tr>
<tr>
<td>I - Inlined</td>
<td>i - interchanged</td>
</tr>
<tr>
<td>M - Multithreaded</td>
<td>m - partitioned</td>
</tr>
<tr>
<td></td>
<td>n - non-blocking remote transfer</td>
</tr>
<tr>
<td>R - Rerolling</td>
<td>r - unrolled</td>
</tr>
<tr>
<td>V - Vectorized</td>
<td>s - shortloop</td>
</tr>
<tr>
<td></td>
<td>w - unwound</td>
</tr>
</tbody>
</table>

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29. b-------< do i3=2,n3-1
30. b b------< do i2=2,n2-1
31. b b Vr--< do i1=1,n1
32. b b Vr u1(i1) = u(i1,i2-1,i3) + u(i1,i2+1,i3)
33. b b Vr * + u(i1,i2,i3-1) + u(i1,i2,i3+1)
34. b b Vr u2(i1) = u(i1,i2-1,i3-1) + u(i1,i2+1,i3-1)
35. b b Vr * + u(i1,i2-1,i3+1) + u(i1,i2+1,i3+1)
36. b b Vr--> enddo
37. b b Vr--< do i1=2,n1-1
38. b b Vr r(i1,i2,i3) = v(i1,i2,i3)
39. b b Vr * - a(0) * u(i1,i2,i3)
40. b b Vr * - a(2) * ( u1(i1) + u1(i1-1) + u1(i1+1) )
41. b b Vr * - a(3) * ( u2(i1-1) + u2(i1+1) )
42. b b Vr--> enddo
43. b b------> enddo
44. b--------> enddo

Example: Cray loopmark Messages

● –hlist=a ...

Outer loops were blocked

Inner-loops wa vectorized and unrolled
Example: Cray loopmark messages (cont)

ftn-6289 ftn: VECTOR File = resid.f, Line = 29
A loop starting at line 29 was not vectorized because a recurrence was found on "U1" between lines 32 and 38.

ftn-6049 ftn: SCALAR File = resid.f, Line = 29
A loop starting at line 29 was blocked with block size 4.

ftn-6289 ftn: VECTOR File = resid.f, Line = 30
A loop starting at line 30 was not vectorized because a recurrence was found on "U1" between lines 32 and 38.

ftn-6049 ftn: SCALAR File = resid.f, Line = 30
A loop starting at line 30 was blocked with block size 4.

ftn-6005 ftn: SCALAR File = resid.f, Line = 31
A loop starting at line 31 was unrolled 4 times.

ftn-6204 ftn: VECTOR File = resid.f, Line = 31
A loop starting at line 31 was vectorized.

ftn-6005 ftn: SCALAR File = resid.f, Line = 37
A loop starting at line 37 was unrolled 4 times.

ftn-6204 ftn: VECTOR File = resid.f, Line = 37
A loop starting at line 37 was vectorized.
Example of Explain Utility

users/ldr> explain ftn-6289

VECTOR: A loop starting at line %s was not vectorized because a recurrence was found on "var" between lines num and num.

Scalar code was generated for the loop because it contains a linear recurrence. The following loop would cause this message to be issued:

```
DO I = 2,100
    B(I) = A(I-1)
    A(I) = B(I)
ENDDO
```
CCE 8.7 Key New Features

- More aggressive C++ inlining at default
  - Default inlining level for C++ is now -hipa4
    - The Fortran and C default inlining level remains -hipa3 (unchanged)

- The -hfp3 option is now enabled when -O3 is specified
  - Previously, -O3 did not modify the -hfp level

- New -hnofma option disables the use of fused-multiply-add instructions
  - Applications sensitive to rounding differences may benefit from disabling fused multiply add (FMA) instructions.
    - This switch is intended for application debugging purposes

- Fortran 2018 features: SELECT RANK, COSHAPE, GENERIC

- Enhancements for better automatic OpenMP affinity and wait policy settings
  - The cray-specific extension, AUTO, is our new default value for OMP_PROC_BIND and OMP_WAIT_POLICY
    - our default used to be FALSE and ACTIVE respectively
  - See the intro_openmp(7) manpage for details

- C11 atomics
  - Atomic operations were an optional part of the C11 standard

- PGAS support for large memory nodes
  - Automatic node partitioning to accommodate address space limitations
  - Transparent to users
Cray MPT Highlights – Cray PMI

- New topology and placement-aware rank reordering option
  - This option determines an optimized rank placement based on the hardware resources available to the job at the time of job launching
    - This option has no effect on the resources selected by the workload manager
  - Initial results have shown some applications have improved by as much as 35% using this option

- PMI_LABEL_ERRROUT now supports rank reordering and user-defined labels
  - The user-defined labels may be set using PMI_LABEL_ERRROUT_FORMAT environment variable
Cray MPT Highlights - Dynamic Process Management

- **Cray MPI now supports a subset of Dynamic Process Management (DPM) from the MPI-2 and MPI-3 standards**
  - This support is available as a separate version of the Cray MPICH library, invoked using the new “-craympich-dpm” compiler driver option
  - Full DPM support is targeted for June 2018

- **Cray MPI now supports a larger MPI_TAG_UB value**
  - This feature is linked to the DPM support

- **Cray MPI now supports optimized message matching**
  - Since this feature was needed for the feature to increase the max tag size it is also only available when using the new “-craympich-dpm” option
  - Initial results have shown improvements of as much as 16% in some micro-benchmarks
Additional Cray MPT Highlights

- Improved support for hugepages in Cray MPICH and Cray SHMEM

- Support has been added to improve the default Cray MPI one-sided performance on XC systems
  - Initial performance improvement over the previous default MPI one-sided version has been observed to be over 4X for both latency and bandwidth

- Improvements have been made to the Cray MPI async-progress algorithms

- MPI_Reduce_scatter and MPI_Reduce_scatter_block has been modified to scale better on high process counts by using much less memory

- Cray MPI has been enhanced so that MPI-IO will recognize the new DataWarp Cache FileSystem feature

- Cray MPI has been optimized to improve network communication bandwidth performance for Intel Skylake
  - Performance improvements of up to 22% have been seen when running with more than 8 ranks per node.
CSML Highlights

● **Cray LibSci**
  ● New QDWH, KSVD, and ELPA backends for Scalapack eigensolvers
  ● Backend integration with recent releases of cray-R
  ● NumPy and SciPy integration with cray-python

● **Cray FFTW3**
  ● FASTPLAN optimizations for Intel Skylake CPU targets
  ● Default threading model is now OpenMP for all targets
  ● Continued support for arbitrary dimension and size for real/complex
Comparisons run on in-house Cray XC with 68-core Knight’s Landing XC nodes and recent versions of competitive libraries available.
Cray FFTW Performance on KNL

Comparisons run on in-house Cray XC with 68-core KNL XC nodes and recent versions of competitive libraries available.
Debugging on Cray Systems

- Systems with thousands of threads of execution need a new debugging paradigm
- Support for traditional debugging mechanism
  - RogueWave TotalView and Allinea DDT
- Cray’s focus is to build tools around traditional debuggers with innovative techniques for productivity and scalability

- **Scalable** Solutions based on MRNet from University of Wisconsin
  - STAT - Stack Trace Analysis Tool
    - Scalable generation of a single, merged, stack backtrace tree
  - ATP - Abnormal Termination Processing
    - Scalable analysis of a sick application, delivering a STAT tree and a minimal, comprehensive, core file set.

- **gdb4hpc / CCDB**
  - Ability to see data from multiple processors in the same instance of gdb
    - without the need for multiple windows
  - Comparative debugging
    - A *data-centric paradigm* instead of the traditional control-centric paradigm
    - Collaboration with University of Queensland
$ gdb
lgdb 3.0 - Cray Line Mode Parallel Debugger
With Cray Comparative Debugging Technology.
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Type "help" for a list of commands.
Type "help <cmd>" for detailed help about a command.

dbg all> launch --launcher-args="--N 4 --tasks-per-node=32 --cpus-per-task=1 --exclusive --partition=hsw16" $App1{128} himeno
Starting application, please wait...
Creating MRNet communication network...
184871928.475738: UNKNOWN_THREAD(0x7f34b9fe0840): Network.C[840] init FrontEnd - WARNING: Topology Root (falcon) is not local host-(falcon.cray.com)
SLURM PID FILE: /tmp/cray_cti-lkr/slurmLMKloeslurm_pid
Waiting for debug servers to attach to MRNet communications network...
Timeout in 400 seconds. Please wait for the attach to complete.
Number of dbgsrvs connected: [1]; Timeout Counter: [0]
Number of dbgsrvs connected: [34]; Timeout Counter: [0]
Number of dbgsrvs connected: [44]; Timeout Counter: [0]
Number of dbgsrvs connected: [92]; Timeout Counter: [0]
Number of dbgsrvs connected: [128]; Timeout Counter: [0]
Finalizing setup...
Launch complete.
App1{0..127}: Initial breakpoint, initcomm at himeno.f:381
dbg all> break jacobi
App1{0..127}: Breakpoint 1: file himeno.f, line 209.
dbg all> c
App1{0..127}: Breakpoint 1, jacobi at himeno.f:209

dbg all> l
App1{0..127}: 209 subroutine jacobi(nn,gosa)
App1{0..127}: 210
C******************************************************************************
App1{0..127}: 211 IMPLICIT NONE
App1{0..127}: 212 C
App1{0..127}: 213 include 'mpif.h'
App1{0..127}: 214 include 'param.h'
App1{0..127}: 215 C
App1{0..127}: 216 integer :: nn,i,j,k,loop,ierr
App1{0..127}: 217 real (kind=4) ::
gosa,wgosa,s0,ss
App1{0..127}: 218
dbg all> backtrace
App1{0..127}: #0 0x0000000000402020 in jacobi at
himeno.f:209
App1{0..127}: #1 0x00000000004012de in himenobmtxp at
himeno.f:91
dbg all> print npe
App1{0..127}: 128
dbg all> p jmax
App1{0..127}: 128
App1{0..127}: 3,11,20,27,36,43,52,59,68,75,84,91,100,107,116,123: 130
dbg all>
Comparative Debugger

- 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

assert P1::T1[0..99]@"file.c":240 = P2::Y2(1,100)@"prog.f":300
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