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

What is new in the Cray Programming Environment

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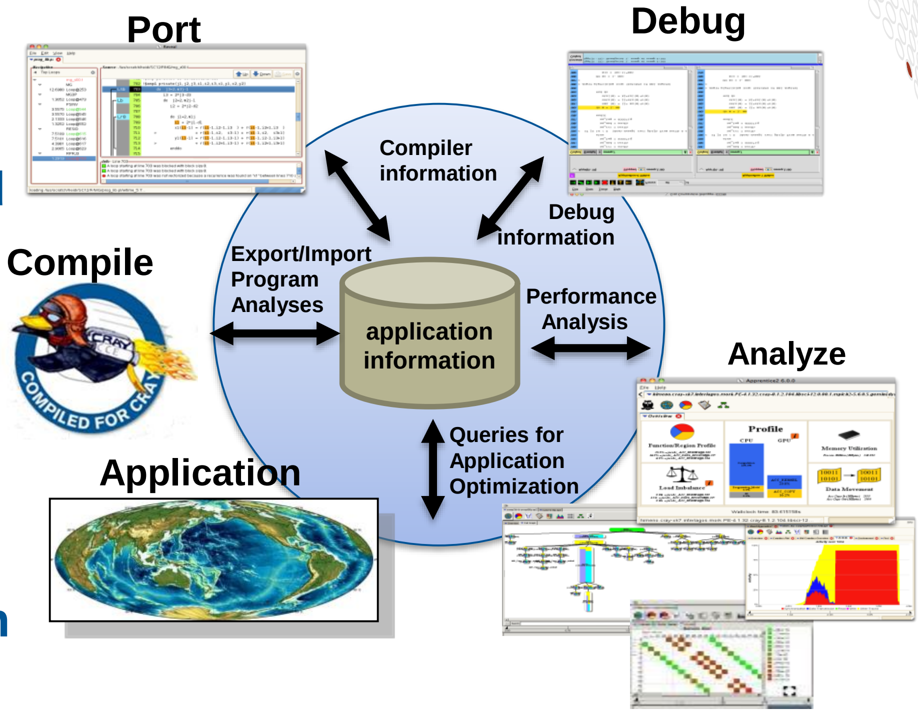
The Cray Programming Environment Mission

- 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**



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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

Cray Performance Tools profile production applications with over 99,000 ranks

Cray MPI runs with 2,001,150 ranks

Programmability Focused Environment

- **GNU Modules simplify build environment**
  - Complexity of compile and link lines (-h –I –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
PrgEnv-
- Cray Compiling Environment
  PrgEnv-cray
- GNU
  PrgEnv-gnu
- 3rd Party compilers
  PrgEnv-xxx

Libraries
Scientific Libraries
- LAPACK
- ScaLAPACK
- BLAS
- Iterative Refinement Toolkit
- FFTW

I/O Libraries
- NetCDF
- HDF5

Development Tools
Environment setup
- Modules

Debuggers
- TotalView
- DDT
- gdb4hpc

Debugging Support
- Abnormal Termination Processing (ATP)
- STAT

Development Tools
Performance Analysis
- CrayPAT
- Cray Apprentice^2

Porting
- Reveal
- CCDB

ML Frameworks
- Cray PE ML Plugin

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

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**

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

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

- **Avoid using –h aggress and –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: -hnodwarf, -hipa0, -hunroll0
    - **-h dev**elop 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

```
%%%    L o o p m a r k   L e g e n d    %%%
     Primary Loop Type         Modifiers
     ------- ---- ----         ---------
     A - Pattern matched       a - atomic memory operation
                               b - blocked
     C - Collapsed             c - conditional and/or computed
     D - Deleted
     E - Cloned
     F - Flat - No calls       f - fused
     G - Accelerated           g - partitioned
     I - Inlined               i - interchanged
     M - Multithreaded         m - partitioned
                               n - non-blocking remote transfer
                               p - partial
     R - Rerolling             r - unrolled
                               s - shortloop
     V - Vectorized            w - unwound
```

Example: Cray loopmark Messages

- –hlist=a ...

```
b-------<  do i3=2,n3-1
b b-----<     do i2=2,n2-1
b b Vr--<        do i1=1,n1
b b Vr            u1(i1) = u(i1,i2-1,i3) + u(i1,i2+1,i3)
b b Vr     *        + u(i1,i2,i3-1) + u(i1,i2,i3+1)
b b Vr            u2(i1) = u(i1,i2-1,i3-1) + u(i1,i2+1,i3-1)
b b Vr     *        + u(i1,i2-1,i3+1) + u(i1,i2+1,i3+1)
b b Vr-->        enddo
b b Vr--<        do i1=2,n1-1
b b Vr            r(i1,i2,i3) = v(i1,i2,i3)
b b Vr     *       - a(0) * u(i1,i2,i3)
b b Vr     *       - a(2) * ( u2(i1) + u1(i1-1) + u1(i1+1) )
b b Vr     *       - a(3) * ( u2(i1-1) + u2(i1+1) )
b b Vr-->        enddo
b b----->     enddo
b------->  enddo
```

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 "<u>var</u>" between lines <u>num</u> and <u>num</u>.

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_ERROUT now supports rank reordering and user-defined labels**
  - The user-defined labels may be set using PMI_LABEL_ERROUT_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

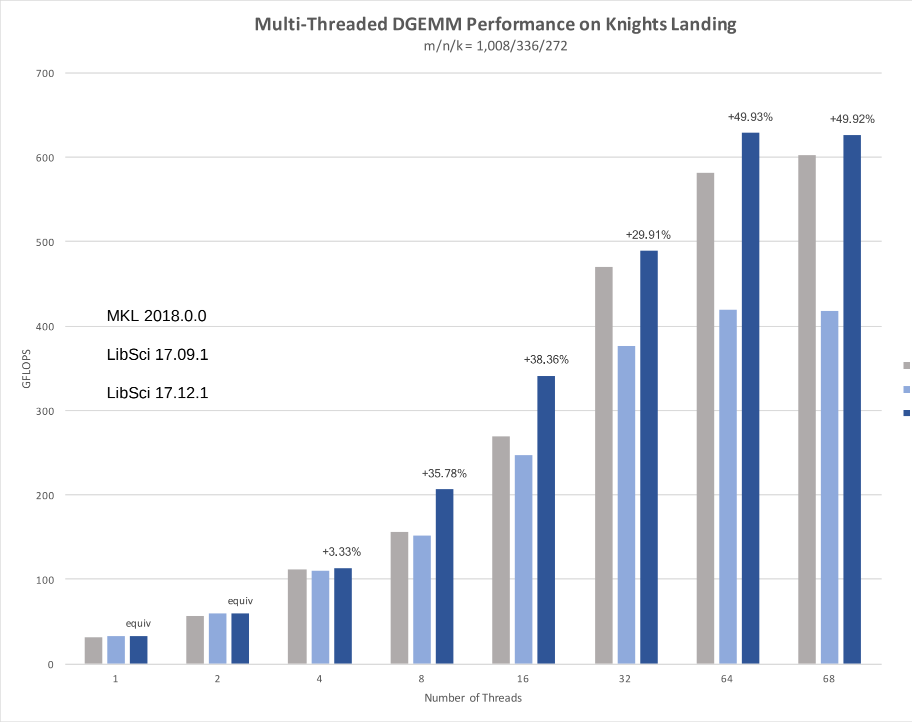
- **Improved support for hugepages in Cray MPICH and Cray SHMEM**
- **Support has been added to improve the default Cray MPI one-sided performance on XC systems**
  - Initial performance improvement over the previous default MPI one-sided version has been observed to be over 4X for both latency and bandwidth
- **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.

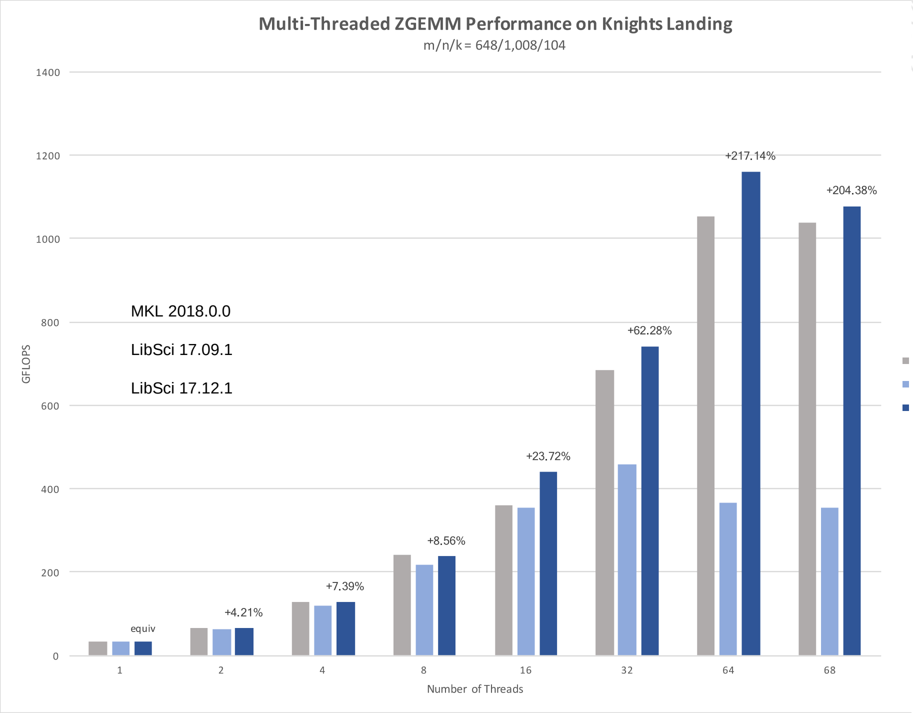
CSML Highlights

- **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

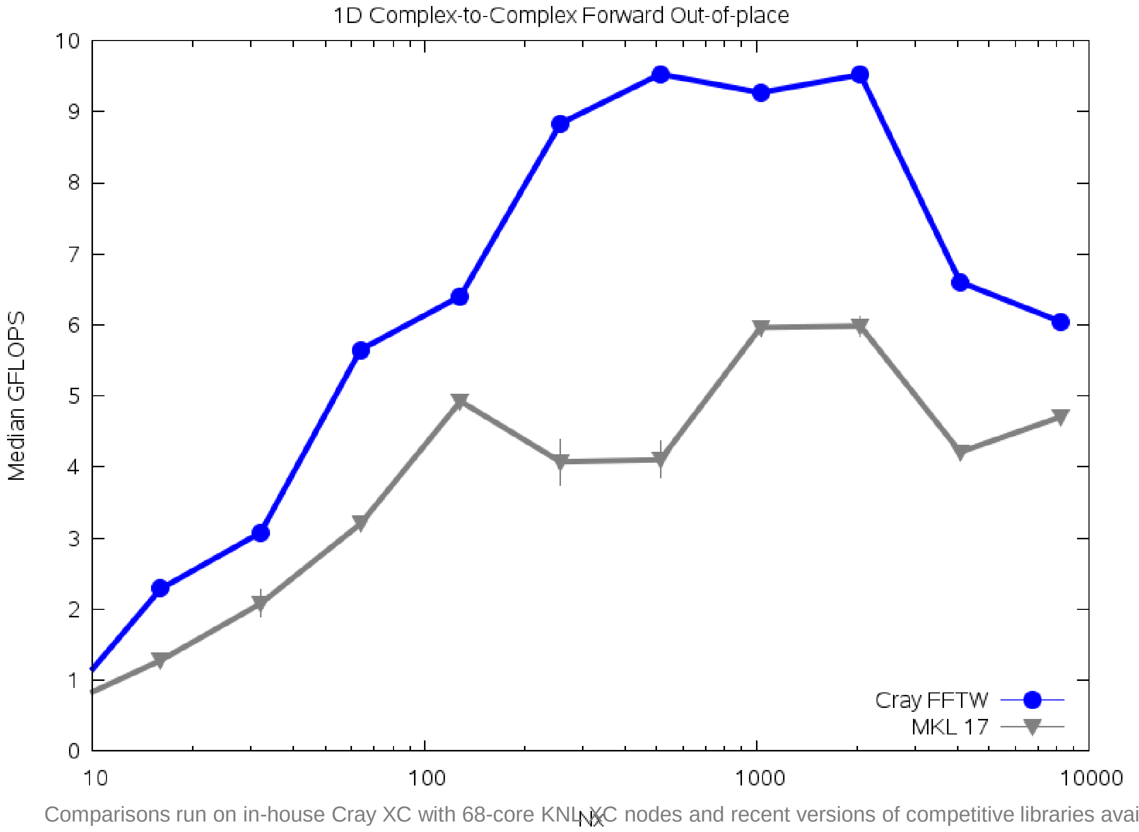
Cray LibSci DGEMM and ZGEMM for KNL





Comparisons run on in-house Cray XC with 68-core Knight's Landing XC nodes and recent versions of competitive libraries available

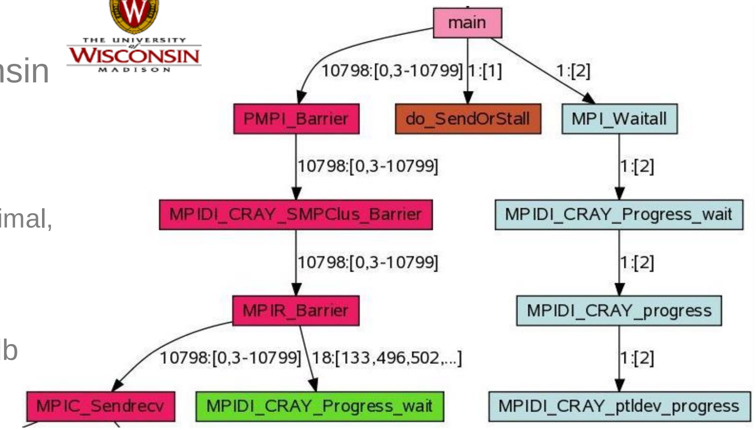
Cray FFTW Performance on KNL



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



gdb4hpc

```
$ lgdb
lgdb 3.0 - Cray Line Mode Parallel Debugger
With Cray Comparative Debugging Technology.
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Reserved.

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-ldr/slurmLMKIoe/slurm_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..3,12..19,28..35,44..51,60..67,76..83,92..99,108..11
5,124..127}: 129
App1{4..11,20..27,36..43,52..59,68..75,84..91,100..107,116.
.123}: 130
dbg all>
```

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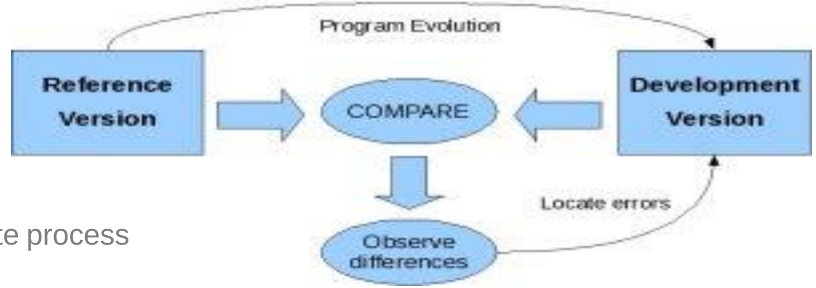
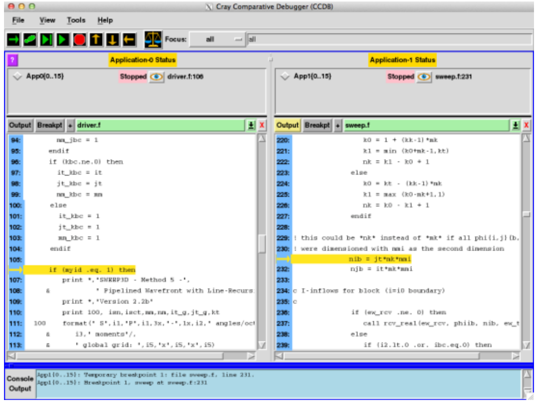
Comparative Debugger

- **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

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

- **Collaboration with University of Queensland**

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Questions?

Thank You!