An Introduction to the Cray X1E

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Outline

Phoenix is the world's largest X1E system (well, almost)

- 1024 multi-streaming processors
- 2 TB aggregate memory

This talk will introduce Phoenix and briefly discuss:

1. X1E hardware platform
2. Some practicalities:
   - Compiling and linking code
   - Running jobs
   - Debugging
3. Performance analysis and tuning

Part I: X1E hardware platform

- NUMA system consisting of up to 2048 nodes (1024 modules)
- Nodes are logical entities of 4 multi-streaming processors (MSPs)

- Memory shared SMP-style within a node
- Jobs that span nodes behave as on MPP distributed memory system
  - Each node has local memory…
  - …but memory is globally addressable between nodes

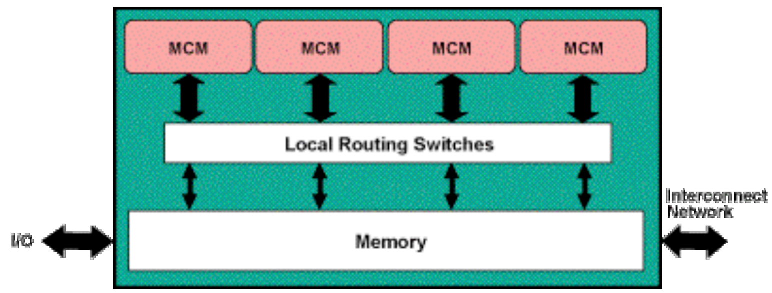
Models of parallelism

The X1E architecture supports several models of parallelism:

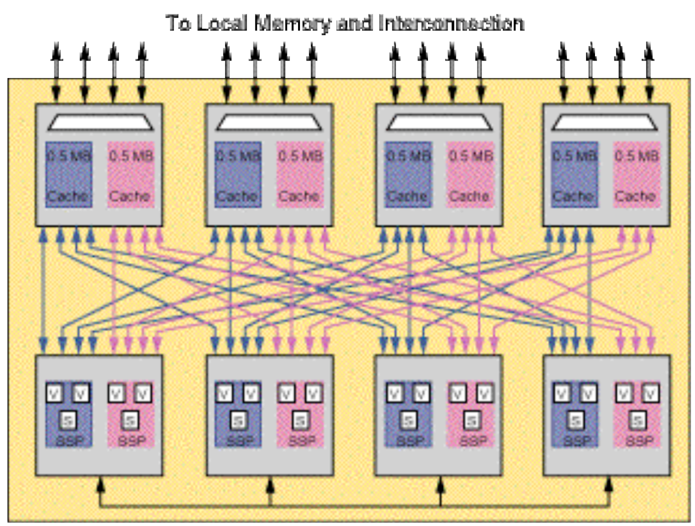
- Two levels of SIMD, loop-level parallelism:
  - Vectorization within SSP
  - Multistreaming within MSP
- OpenMP within node
- Between nodes (or processors)
  - MPI-1 two-sided message passing
  - MPI-2 one-sided communication
  - SHMEM one-sided communication
  - Co-Array Fortran remote memory
  - Direct load/store using pointers

Cray X1E compute module

- Compute module contains 4 multichip modules (MCMs):

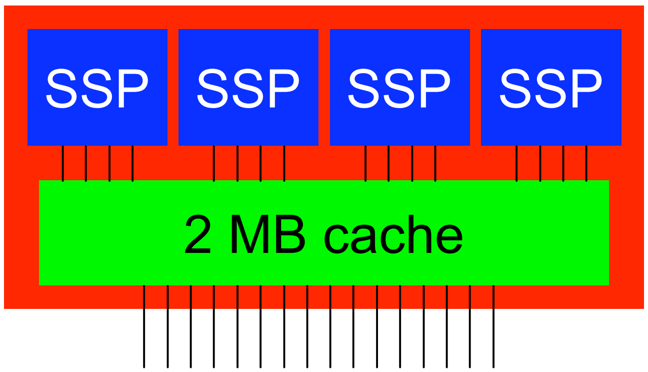


- Each MCM consists of 2 multistreaming processors (MSPs):



Cray X1E multistreaming processor (MSP)

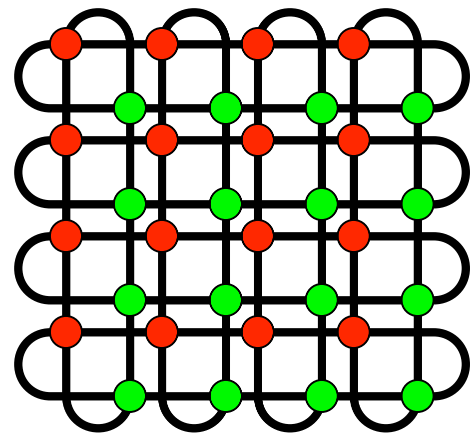
- MSP consists of 4 tightly-coupled single-streaming processors (SSPs)
- Each SSP consists of:
  - One 2-way superscalar processing unit (565 MHz)
  - Two-pipe vector processing unit (1.13 GHz)



Is an MSP one or four processors?

- One!
  - Fast synchronization, shared cache
  - Can be treated as one 8-pipe processor
- Four!
  - Each SSP can operate independently
  - Treat as MPI processor or use OpenMP-like directives

X1E Interconnect



- "Enhanced" 3D torus
  - Modules connected in a 3D torus.
  - One torus dimension is fully connected.
- 12 GB/s measured MPI bandwidth

- Globally addressable memory:
  - Load/store memory on any node
  - Remote memory refs routed through interconnect
  - W/ contiguous nodes, remote address translation possible (System scales w/ number of nodes w/o additional TLB misses)
  - Low latency

Phoenix strengths and weaknesses

- Strengths:
  - Very powerful processors (18 Gflop/sec peak)
  - Low effective latency
    - Vector processors hide local latency
    - Globally addressable memory hides/minimizes global latency
  - Very high memory bandwidth (global and local)
    - Good for stride-1, strided, and random access
- Weaknesses:
  - Scalar processing slow
  - "Some tuning required"
  - Limited memory per MSP

Part II: Practicalities

- Logging into a front end
- Using the Programming Environment
  - Choosing compiler versions
  - Special features of Cray compilers
  - Libraries provided by Cray
- Code-porting issues
- Running jobs
- Debugging

Phoenix front-ends

- Users can ssh into two different front-ends for Phoenix:
  - phoenix.ccs.ornl.gov
    - Compile, load, performance tool commands transparently offloaded to Cray Programming Environment Server (CPES)
    - Some standard tools (e.g., emacs, complete Python) unavailable
  - robin.ccs.ornl.gov
    - Linux cross-compiler box
    - Cross-mounts Phoenix scratch space
    - Can submit and manage Phoenix jobs
    - Much faster than CPES! (5x or more!)

Phoenix front-ends

We recommend working on robin whenever possible.

It is much faster and friendlier!

There are a few cases where you need to use phoenix:

- Using ‘psview’ to display Psched (system scheduler) information
- Using ‘nm’ command to view symbols in binary objects
- autoconf that does not support cross-compilation
  (Note: Python-based configuration needs to be done on robin!)

Cray Programming Environment

Cray Programming Environment provides:

- Fortran compiler 'ftn'
- C compiler 'cc'
- C++ compiler 'CC'
- MPI include files and libraries available by default

- Compiler, MPT versions determined by PrgEnv module version
- `pe-version` tells version of PrgEnv and components
- To load another PE version, do
  `module swap PrgEnv PrgEnv.newversion`
- Best to swap entire PrgEnv, not individual components
  - Possible exception: MPT version

Special Cray compiler flags

Compiler flags are documented completely in man pages.
We outline some Cray-specific ones here.

`-G` options to specify debug level:

- `-g`: Full debugging w/ breakpoints on every executable line.
  - Very slow; all optimizations turned off.
  - Bugs often dissapear!
- `-G1` (ftn) or `-Gp` (CC/cc): block-by-block debugging
  - Multistreaming disabled
- `-G2` (ftn) or `-Gf`: Debugging w/ full optimization
  - In Fortran, only postmortem debugging
  - In C/C++, can set breakpoints at function entry/exit

Special Cray compiler flags

- Executables can be built for three different modes on Phoenix
  - MSP mode (the default)
    - May also want to use `-h gen_private_callee` so that subroutines can be called from multistreamed regions
  - SSP mode (compiler flag: `-h ssp`)
  - "command" mode (compiler flag: `-h command`)
    - Executable can run on service node w/o help from aprun
    - Probably no real need for this now that Robin is available

- Which to use?
  - Lots of loop-level parallelism suggests MSP
  - Very scalable code suggests SSP
- Best to start w/ MSP but try both

Cray LibSci routines

Cray provides a collection of several highly-optimized kernels in LibSci:

Single processor support for:

- Fast Fourier Transform (FFT), convolution, filtering
- BLAS, LAPACK
- Basic Linear Algebra Communication Subprograms (BLACS)
- Sparse direct solvers

- Multiprocessor distributed memory support for
  - FFT routines
  - Scalable LAPACK (ScaLAPACK) routines
  - Basic Linear Algebra Communication Subprograms (BLACS)
- OpenMP versions of all level 3 BLAS and some level 2 BLAS

- Link with `-lsci` normally
  - `-lsci64` of `-sdefault64` routines
  - `-lompsci` for OpenMP support

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Common code porting problems

- Beware of old `#ifdef CRAY` directives!
- X1E is very different from old Cray machines:
  - Some library calls may be unsupported, or work differently.
  - Default Fortran data sizes: 32 bit integers, 32 bit reals
  - Use `-sdefault64` to default to 64 bit integers and reals (and to link w/ MPI, BLAS, etc., that assume this)
  - Can also use `-sreal64` to get 32 bit integers, 64 bit reals
- Need to manually check each #ifdef CRAY to see if it makes sense.

- Auto-configuration problems
  - Configure scripts that cannot cross-compile must be run on Phoenix
  - Build systems relying on Python may need to run on Robin

Running jobs

- Phoenix uses PBS for job submission (see http://info.nccs.gov/resources/phoenix/batch)
- Use `aprun` within job script to launch parallel jobs

- Specify number of MSPs in resource list with `mppe=N`. (This also works for SSP jobs -- ask for `mppe=N/4`, `N` the # SSPs)
- Multi-node jobs (>4 MSPs) must request a multiple of 8 MSPs! (Scheduler places jobs on hardware module boundaries)
- Run out of `/tmp/work/$USER` if doing even moderate IO
- Memory limits:
  - Default memory limit is 2 GB per MSP (512 MB per SSP)
  - Request more with `-m` option to `aprun`
  - If requesting more, ask PBS for more MPPE's than aprun will use
  - May also need to increase env variables; see `man 7 memory`

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Debugging: Postmortem

- Set `TRACEBK` to 30 to get automatic traceback when code crashes
- `aprun` needs '`-c core=unlimited`' to generate core files
  DO NOT do this unless running in "`/tmp/work/$USER`"!

- Can view corefiles with gdb or Totalview
  - `phoenix> gdb a.out core`
  - `phoenix> totalview a.out core`

- Traceback gives hints as to what corefiles to look at:

```
Traceback for process 64311(ssp mode) apid 64184.229 on node 7
```

Suggests starting with core file 229.

Debugging: Interactive

- To use Totalview interactively to debug an N process job:
  - `totalview -app "-n N" a.out` [totalview options] [`-a` <program options>]
  - Use `totalviewcli` for command-line
- This can be very useful, but may be slow

- Can also use gdb
  - Fast and responsive
  - Debugging parallel programs difficult (impossible?)
  - Unsupported by Cray

Part III: Performance analysis and tuning

- Always generate performance profile BEFORE code tuning!
  - Routines that are negligible on other systems may be bottlenecks on X1E!

- Basic code tuning steps:
  1. Generate performance profile and identify hotspots.
  2. Examine loopmark listings for hotspots.
  3. Then do some combination of:
     1. Insert compiler directives
     2. Manually unroll loops, switch loop indices, etc.
     3. Rearrange data structures
  4. Return to step 1 and iterate until performance is “good enough”.

Introduction to CrayPAT

Basic steps in using Cray Performance Analysis Toolkit:

1. Generate executable for Phoenix
2. run 'pat_build' to generate instrumented executables
   - `robin> pat_build [options] a.out a.out.inst`
   - Note that object files must be present!
3. submit batch jobs using 'qsub'
   - Run with 'aprun' to generate '.xf' file,
     then run 'pat_report' to generate performance report
   - OR, run with 'pat_run' to run and generate report
     (Provides somewhat simpler interface)
4. Optionally, use Cray Apprentice ('app2') to visualize performance

Types of performance experiments

- Three basic types of performance experiments
  - "Profiling"
    - Simplest experiment; lowest overhead
    - Samples program counter by user and system time
  - Sampling
    - Sample program counter, call stack, HW counters at specified intervals or specific events
  - Tracing
    - At function entry/exit, record performance data, function arguments, return values
    - pat_build must be instructed to instrument specific functions

- Many options for pat_run, pat_report. Too many to list here! See
  - http://info.nccs.gov/resources/phoenix/pat
  - Chapter 2 of Optimizing Applications on Cray X1 Series Systems (available at docs.cray.com)

Performance reports

- I like PAT_RT_EXPERIMENT='samp_cs_time' to profile and sample callstack (Very useful: See where time is spent in calltree)

```
100.0% |    100.0% | 154438 |Total
|-----------------------------------------------
|  25.0% |     25.0% |  38644 |pe.3
||----------------------------------------------
||   7.9% |      7.9% |  12160 |MatSetValuesLocal
|||---------------------------------------------
|||   7.9% |      7.9% |  12159 |matsetvalueslocal_
|||        |           |        | thcjacobian@thc_module_
|||        |           |        |  oursnesjacobian
|||        |           |        |   SNESComputeJacobian
|||        |           |        |    SNESSolve_LS
|||        |           |        |     SNESSolve
|||        |           |        |      snessolve_
|||        |           |        |       pflowgrid_step@pflow_grid_module_
|||        |           |        |        main
|||   0.0% |      7.9% |      1 |DAGetMatrix3d_MPIAIJ
|||        |           |        | DAGetMatrix
|||        |           |        |  dagetmatrix_
|||        |           |        |   pflowgrid_setup@pflow_grid_module_
|||        |           |        |    main
```

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Optimization priorities

- Profile should always guide where optimization is done
- In hotspots routines, optimization priorities:
  1. Vectorization (10x or more speedup)
  2. Multistreaming (4x)
  3. Low-latency communication (2x)
  4. Register blocking (< 2x)
  5. Cache blocking (< 2x)

Vectorization

Exploiting fine-grain parallelism with vectorization is #1 priority on X1E!

- One vector instruction == many loop iterations
- Need a large enough number of loop iterations
  - SSP vector register holds 64 doubles
  - More than 64 iterations is ideal (for pipelining, multistreaming)
  - Fewer iterations means lower efficiency
- No procedure calls inside loop
- No loop-carried data dependencies
  - Some exceptions, e.g., reduction operations

Multistreaming

- Multistreaming takes additional advantage of loop-level parallelism.
- Loop iterations divided among 4 SSPs within an MSP
- Usually 2nd most important priority: Up to 4x speedup

- Many of the same considerations as w/ vectorization
- Additional wrinkle: When to stream vs. vectorize?
  - For streamed and vectorized loop nests,
    want to vectorize loop with trip count that results in long vectors
  - May need to help the compiler by telling it
    - what to stream (!dir$ preferstream)
    - what to vectorize (!dir$ prefervector)

What compilers can/can't do

The compiler can do a lot for us:

- Re-arrange loop nests
- Reductions, (un)pack, scatter/gather
- Fuse loops and array statements
- Inline procedures (one level down)
- if statements within loops (Vector masks, some loss of efficiency)

But it cannot do things like:

- Make short vector loops efficient
- Make stride-1 (or -0) scatter/gather efficient
- Know that index arrays don't repeat
- do j = 1, n
  x(i(j)) = x(i(j)) + …
- Effectively inline many levels down

Loopmark listings

- With profile in hand, examine loopmark listings for hotspot routines, to see what the compiler could and couldn't do.

- Loopmark listings show the compiler optimizations applied:
  - What vectorized?
  - What multistreamed?
  - What was unrolled?
  - Why was X not vectorized?

- To obtain:
  - `robin> ftn -rm myprog.f`
  - `robin> cc -hlist=m myprog.c`

Example loopmark listing: Vectorized/streamed

```
 1.           subroutine vectorize1(nx,a,b,c,d)
 2.           real a(nx),b(nx),c(nx),d
 3.
 4.   MVr--< do i = 1, nx
 5.   MVr       c(i) = a(i) * b(i) + d
 6.   MVr--> end do
 7.
 8.           end subroutine

ftn-6005 ftn: SCALAR File = vectorize1.ftn, Line = 4
  A loop starting at line 4 was unrolled 2 times.

ftn-6204 ftn: VECTOR File = vectorize1.ftn, Line = 4
  A loop starting at line 4 was vectorized.

ftn-6601 ftn: STREAM File = vectorize1.ftn, Line = 4
  A loop starting at line 4 was multi-streamed.
```

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What if code doesn't vectorize/multistream?

- Last slide showed perfectly vectorized/multistreamed loop
- When this doesn't happen, try (in order of difficulty):
  1. Using compiler option flags:
     - `-h aggress` to attempt more aggressive loop optimizations
  2. Using compiler directives to give compiler hints:
     - !dir$ in Fortran, #pragma _CRI in C/C++
     - e.g. !dir$ concurrent to assert loop is free of dependencies
  3. Rewriting code
     - Simple stuff: switching loop indices, fusing loops, etc.
     - Complicated stuff: Rewriting data structures,
       choosing more vectorizable algorithms (extreme case)

Example loopmark: partial vectorization

Here, indirect addressing prevents compiler from knowing if index collisions occur:

```
 6.   Vp----<                    DO i = 1,n
 7.   VP r-<>                          e(ix1(i)) = e(ix1(i)) - a(i)
 8.   VP---->                    END DO
 9.
10.                                          end
```

```
f90-6371 f90: VECTOR File = gs-2.f, Line = 6
  A vectorized loop contains potential conflicts due to indirect
  addressing at line 7, causing less efficient code to be generated.

f90-6204 f90: VECTOR File = gs-2.f, Line = 6
  A loop starting at line 6 was vectorized.
```

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Example loopmark: Using 'concurrent' directive

Fix by using `!dir$ concurrent` to assert that loop has no vector dependencies:

```
  6.          !dir$ concurrent
  7.   MV--<        DO i = 1, n
  8.   MV             e(ix1(i)) = e(ix1(i)) - a(i)
  9.   MV-->        END DO
 10.
 11.               end
```

```
f90-6203 f90: VECTOR File = gs-2.f, Line = 7
  A loop starting at line 7 was vectorized because an IVDEP
  or CONCURRENT compiler directive was specified.

f90-6203 f90: STREAM File = gs-2.f, Line = 7
  A loop starting at line 7 was streamed because an IVDEP
  or CONCURRENT compiler directive was specified.
```

Example loopmark: IO within loop

Here, IO needs to be moved outside of a loop by the programmer:

```
 1.          subroutine io1(nx,a,b,c)
 2.          real a(nx),b(nx),c(nx)
 3.
 4.          open(8,file='c_array',access='direct', &
 5.               form='formatted',status='replace')
 6.    1--<  do i = 1, nx
 7.    1       c(i) = a(i) * b(i)
 8.    1       write(8,'(1x,f12.4)',rec=i) c(i)
 9.    1-->  end do
10.
11.          end subroutine

ftn-6286 ftn: VECTOR File = io1.ftn, Line = 6
  A loop starting at line 6 was not vectorized because it contains
  input/output operations at line 8.

ftn-6709 ftn: STREAM File = io1.ftn, Line = 6
  A loop starting at line 6 was not multi-streamed because it contains
  input/output operations.
```

Example loopmark: IO moved outside

The problem is fixed by manually segmenting the loop:

```
 1.           subroutine io2(nx,a,b,c)
 2.           real a(nx),b(nx),c(nx)
 3.
 4.           open(8,file='c_array',access='direct', &
 5.                form='formatted',status='replace')
 6.
 7.   MVr--< do i = 1, nx
 8.   MVr       c(i) = a(i) * b(i)
 9.   MVr--> end do
10.
11.           write(8,'(1x,f12.4)',rec=i) (c(i),i=1,nx)
12.
13.           end subroutine

ftn-6005 ftn: SCALAR File = io2.ftn, Line = 7
  A loop starting at line 7 was unrolled 2 times.

ftn-6204 ftn: VECTOR File = io2.ftn, Line = 7
  A loop starting at line 7 was vectorized.

ftn-6601 ftn: STREAM File = io2.ftn, Line = 7
  A loop starting at line 7 was multi-streamed.
```

Other optimization priorities

Haven't discussed other priorities:

- Communication latency can be reduced by
  - Strategic use of Co-Array Fortran
  - Use of SHMEM, UPC, or MPI-2
  - Remote load-store using pointers
  - See docs.cray.com. Or see the Cray folks at this meeting!

- Register blocking, cache blocking
  - Standard techniques covered in many sources
  - E.g., O'Reilly *High Performance Computing* by Severance and Dowd

Where to go for more help

- Much of the information discussed here can be found at
  http://info.nccs.gov/resources/phoenix

- Many more documents available at http://docs.cray.com
  - Cray X1 Series System Overview
  - Migrating Applications to the Cray X1 Series Systems
  - Optimizing Applications on Cray Series Systems
    (Some of my examples came from here)
  - Cray Fortran, C/C++ reference manuals

- Attend the Cray tutorial/workshop this Wednesday.

- Email help@nccs.gov