THE SUPERCOMPUTER COMPANY

Hybrid Multi-core Programming for Exascale Computing

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Key Challenges to Get to an Exascale

Power

- Traditional voltage scaling is over
- Power now a major design constraint
- Cost of ownership
- Driving significant changes in architecture

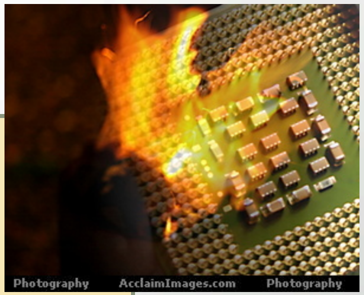
Concurrency

- A billion operations per clock
- Billions of refs in flight at all times
- Will require *huge* problems
- Need to exploit *all* available parallelism

Programming Difficulty

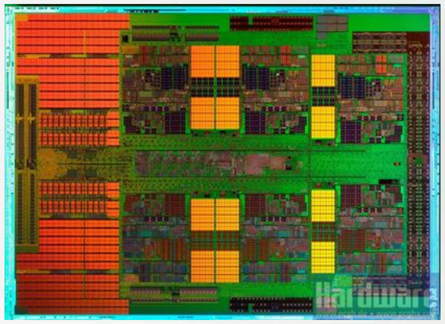
- Concurrency and new micro-architectures will significantly complicate software
- Need to hide this complexity from the users

Resiliency



- Many more components
- Components getting less reliable
- Checkpoint bandwidth not scaling

Improving Processor Efficiency



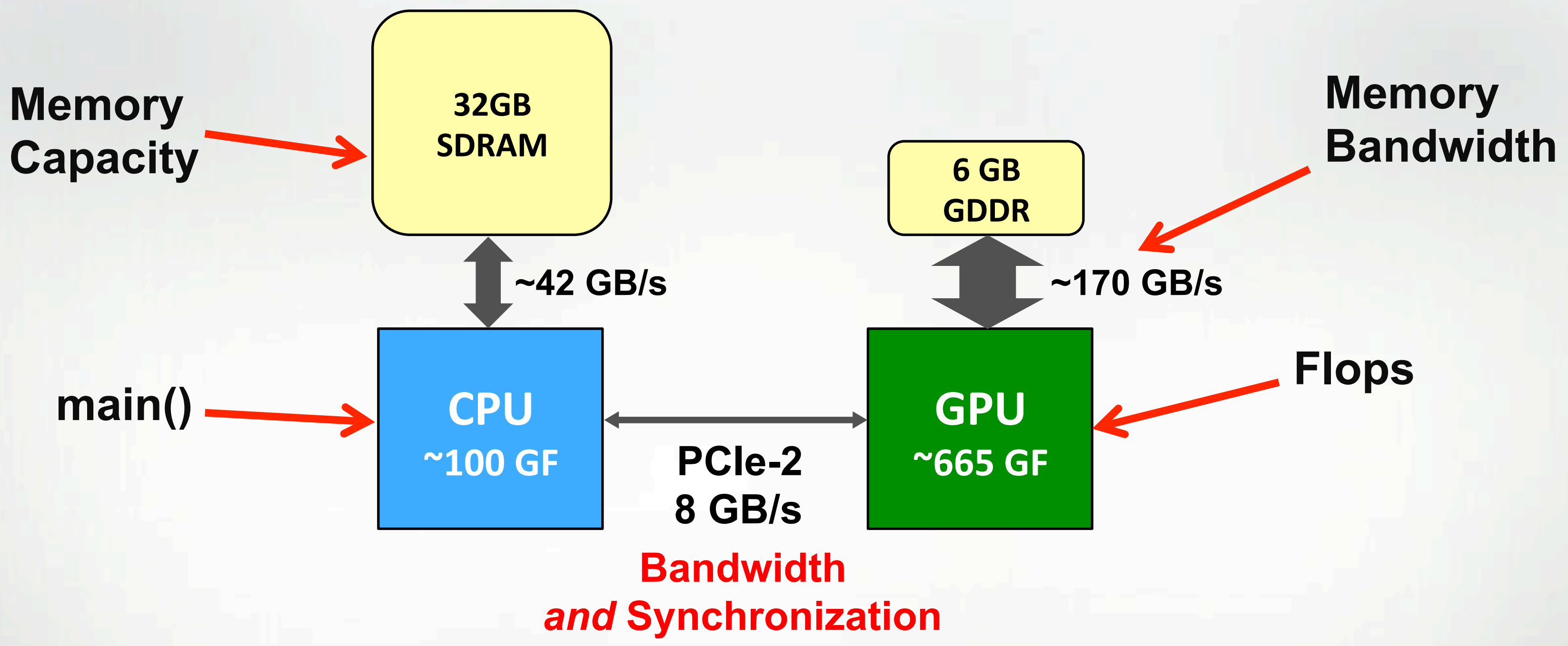
- Multi-core was a good first response to power issues
  - Performance through parallelism
  - Modest clock rate
  - Exploit on-chip locality
- However, conventional processor architectures are optimized for single thread performance rather than energy efficiency
  - Fast clock rate with latency(performance)-optimized memory structures
  - Wide superscalar instruction issue with dynamic conflict detection
  - Heavy use of speculative execution and replay traps
  - Large structures supporting various types of predictions
  - Relatively little energy spent on actual ALU operations
- Could be much more energy efficient with multiple simple processors, exploiting vector/SIMD parallelism and a slower clock rate
- But serial thread performance is really important (Amdahl's Law):
  - If you get great parallel speedup, but hurt serial performance, then you end up with a niche processor (less generally applicable, harder to program)

Conclusion: Heterogeneous Computing

- To achieve scale and sustained performance per {$,watt}, must adopt:
  - …a *heterogeneous* node architecture
    - fast cores for serial code
    - many power-efficient cores for parallel code
  - …a deep, explicitly managed memory hierarchy
    - to better exploit locality, improve predictability, and reduce overhead
  - …a microarchitecture to exploit parallelism at all levels of a code
    - distributed memory, shared memory, vector/SIMD, multithreaded
    - (related to the "concurrency" challenge—leave no parallelism untapped)
- Sounds a lot like GPU accelerators…
- NVIDIA Fermi^{TM} has made GPUs feasible for HPC
  - Robust error protection and strong DP FP, plus programming enhancements
- Expect GPUs to make continued and significant inroads into HPC
  - Compelling technical reasons
  - High volume market
  - It looks like they can credibly support both masters (graphics and compute)

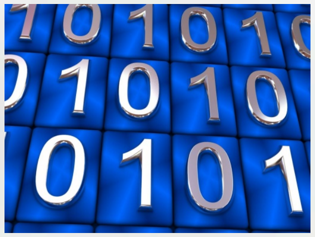
- *Two issues w/ GPU acceleration: STRUCTURAL and PROGRAMMING*

Structual Issues with Accelerated Computing



- This is a short-lived situation
  - NVIDIA Denver and AMD Fusion
- Try to keep kernel data structures resident in GPU memory
  - Avoids copying b/w CPU and GPU; work on GPU-network communication
- May limit breadth of applicability over next 2-3 years

Programming Issues with Accelerated Computing



- Primary issues with programming for GPUs:
  - Learn new language/programming model
  - Maintain two code bases/lack of portability
  - Tuning for complex processor architecture (and split CPU/GPU structure)
- Need a single programming model that is portable across machine types, and also forward scalable in time
  - Portable expression of heterogeneity and multi-level parallelism
  - Programming model and optimization should not be significantly difference for "accelerated" nodes and multi-core x86 processors
  - *Allow users to maintain a single code base*
- Need to shield user from the complexity of dealing with heterogeneity
  - High level language with good complier and runtime support
  - Optimized libraries for heterogeneous multicore processors
- Directive-based approach makes sense (adding to OpenMP 4.0)
- Getting the division of labor right:
  - User should focus on identifying parallelism (we can help with good tools)
  - Compiler and runtime can deal with mapping it onto the hardware

Short Term Petascale Systems – Node Architecture

	Cores on the node	Total threading	Vector Length	Programming Model
Blue Waters	16	32	8	OpenMP/MPI/ Vector
Blue Gene Q	16	32	8	OpenMP/MPI/ Vector
Magna-Cours	24	24	4	OpenMP/MPI/ Vector
Titan	16	32 (768*)	16	Threads/ Cuda/Vector
Intel MIC	32	128	8	OpenMP/MPI/ Vector
Istanbul	32	64	8	OpenMP/MPI/ Vector

* Nvidia allows oversubscription to SIMT units

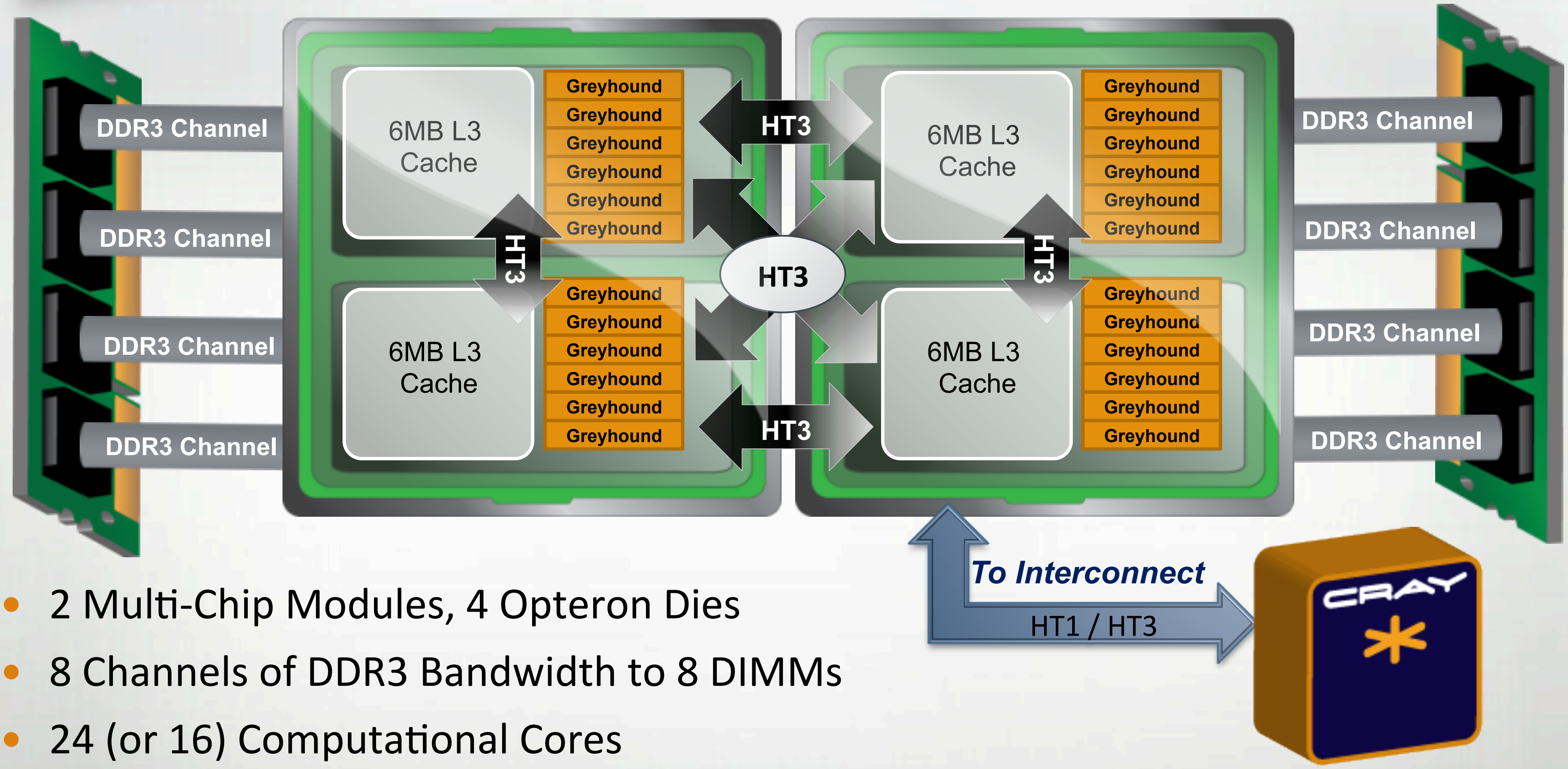
Hybrid Multi-core Architecture

- Massively Parallel System with high powered nodes that exhibit
  - Multiple levels of parallelism
    - Shared Memory parallelism on the node
    - SIMD vector units on each core or thread
  - Potentially disparate processing units
    - Host with conventional X86 architecture
    - Accelerator with highly parallel – SIMD units
  - Potentially disparate memories
    - Host with conventional DDR memory
    - Accelerator with high bandwidth memory

Hybrid Multi-core Architecture

- All MPI may not be best approach
  - Memory per core will decease
  - Injection bandwidth/core will decease
  - Memory bandwidth/core will decrease
- Hybrid MPI + threading on node may be able to
  - Save Memory
  - Reduce amount of off node communication required
  - Reduce amount of memory bandwidth required

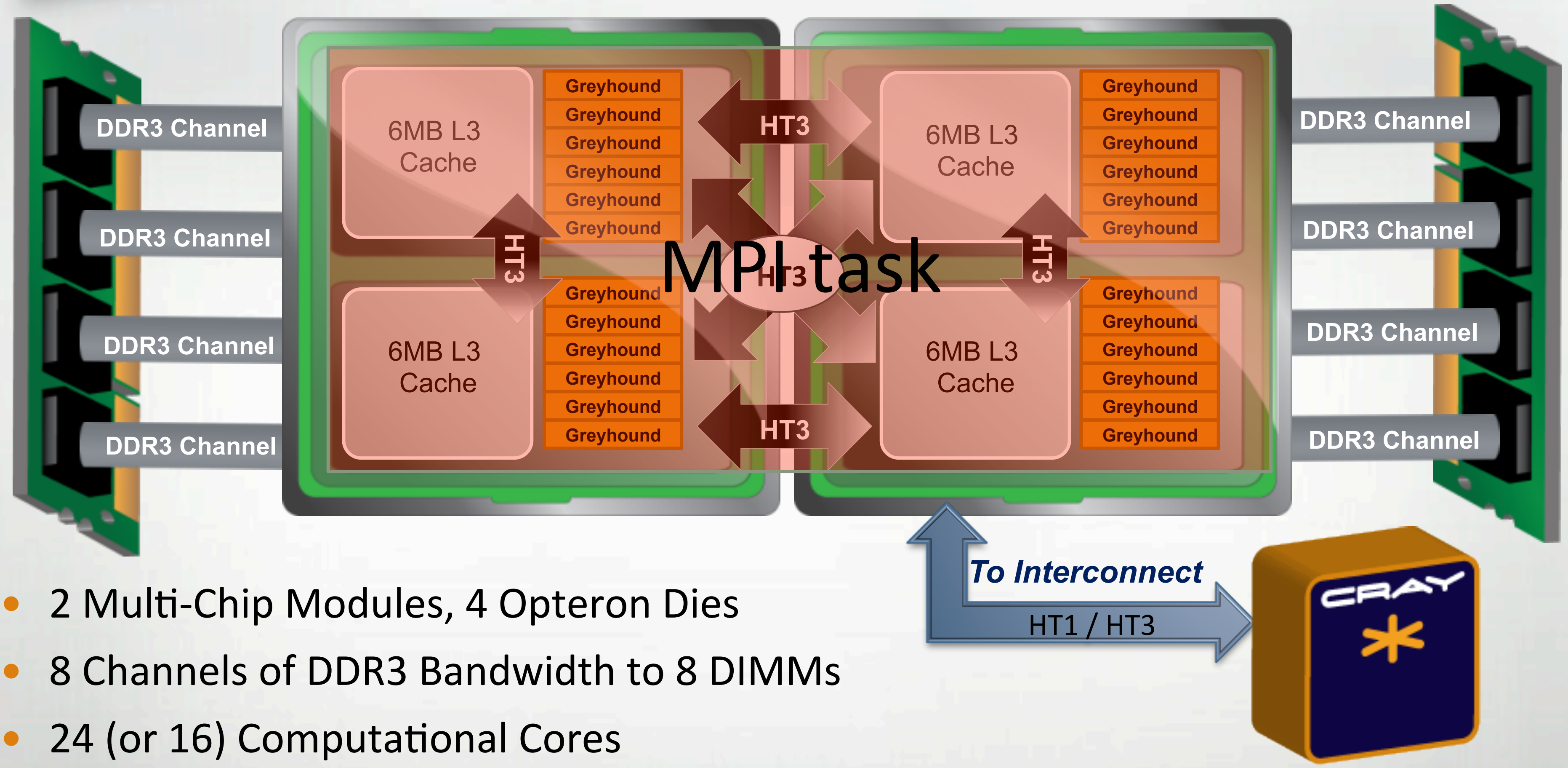
XE6 Node Details: 24-core Magny Cours



- 2 Multi-Chip Modules, 4 Opteron Dies
- 8 Channels of DDR3 Bandwidth to 8 DIMMs
- 24 (or 16) Computational Cores
  - 64 KB L1 and 512 KB L2 caches for each core
  - 6 MB of shared L3 cache on each die
- Dies are fully connected with HT3
- Snoop Filter Feature Allows 4 Die SMP to scale well

XE6 Node Details: 24-core Magny Cours

Run using 1 MPI task on the node



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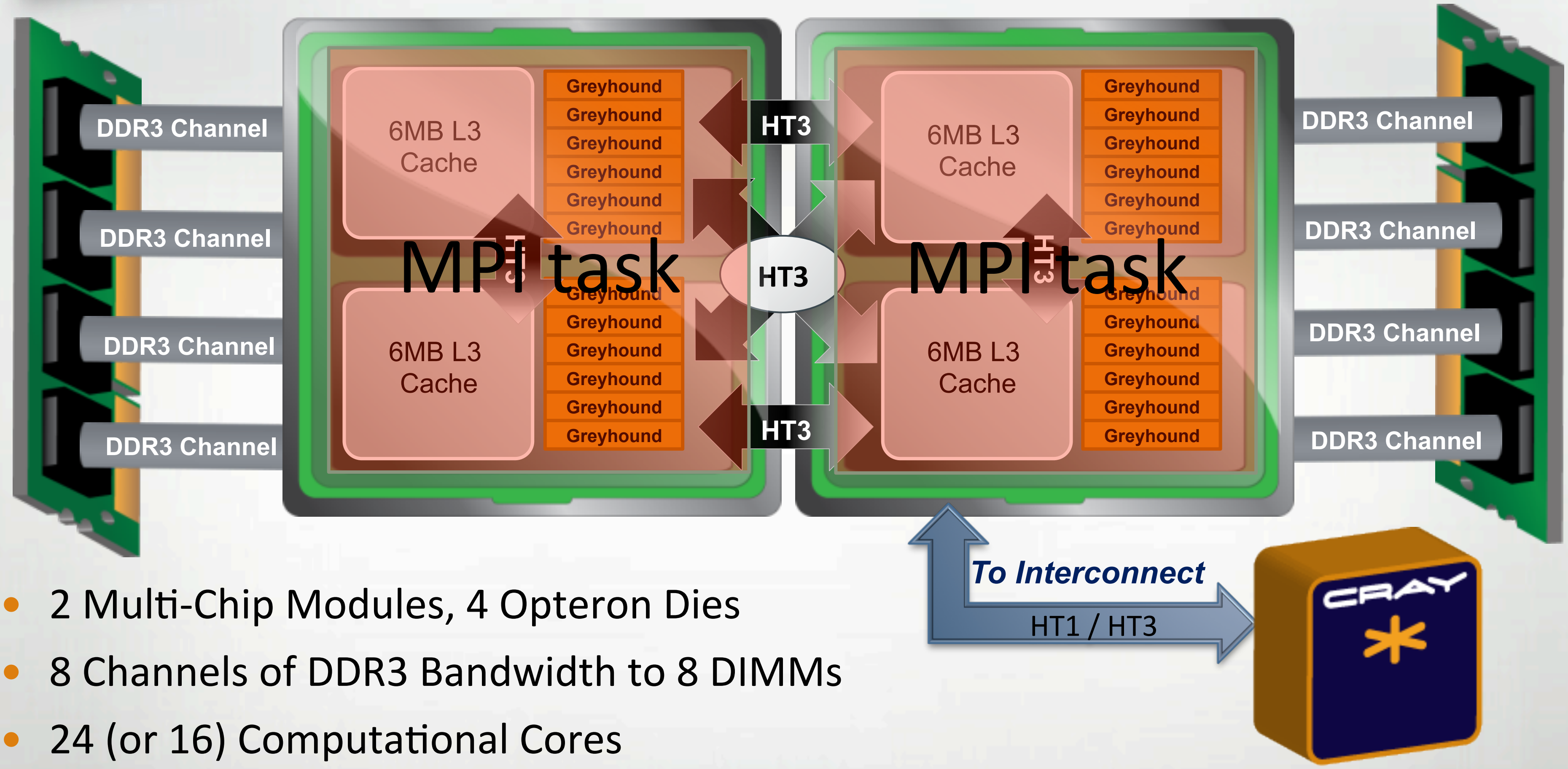
Use OpenMP across all 24 cores

XE6 Node Details: 24-core Magny Cours

Run using 2 MPI tasks on the node
One on Each Die



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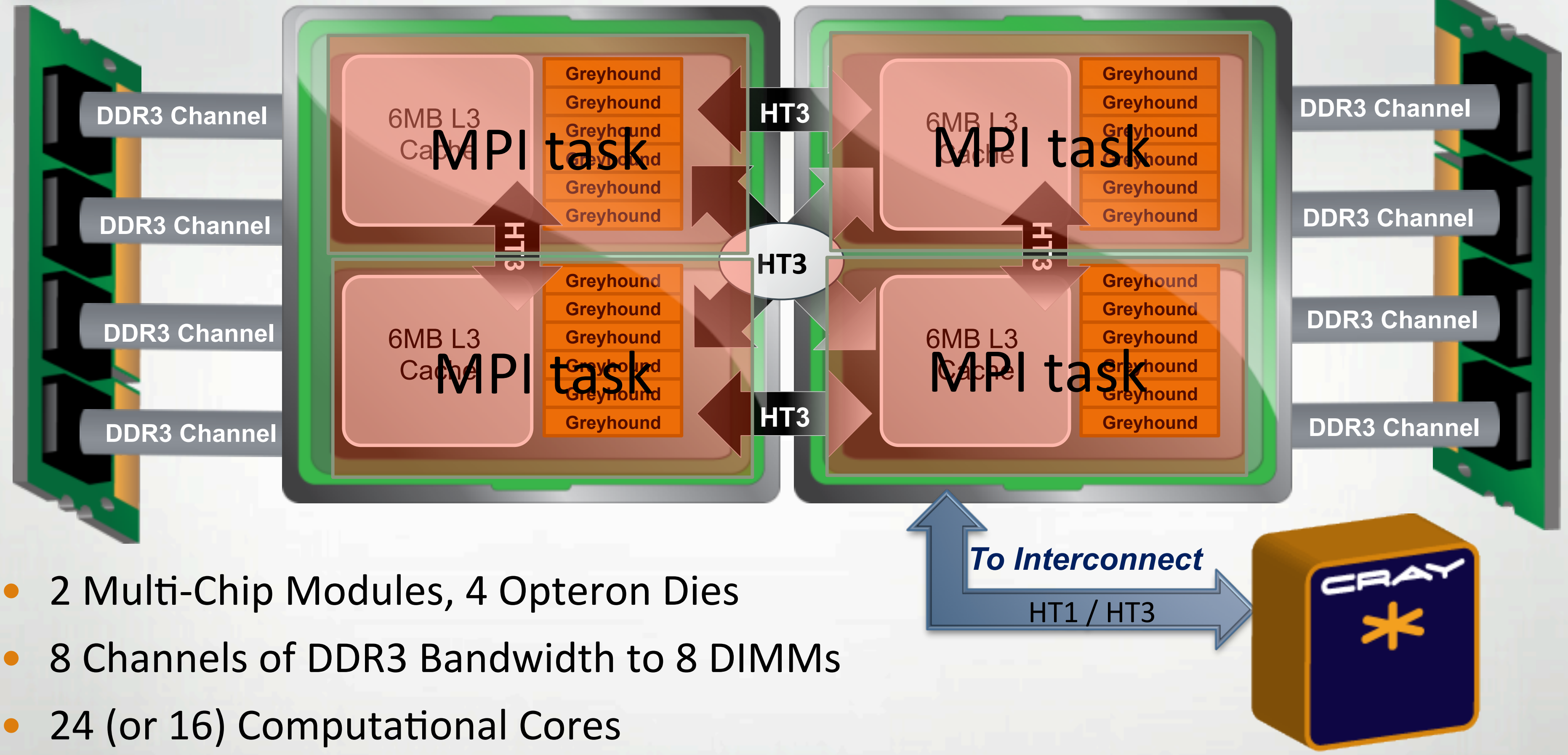
Use OpenMP across all 12 cores in the Die

XE6 Node Details: 24-core Magny Cours

Run using 4 MPI tasks on the node
One on Each Socket



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Use OpenMP across all 6 cores in the Socket

Proposed Programming Paradigm for Hybrid Multi-core

- MPI or PGAS between nodes and/or sockets
- OpenMP, Pthreads or some other shared memory parallelism across a portion of the cores on the node
- Vectorization to utilize the SSE# or SIMD units on the cores

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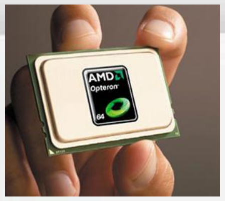
Cray XE6

2011 Cray Upgrade Paths

XT5



Interlagos and Gemini

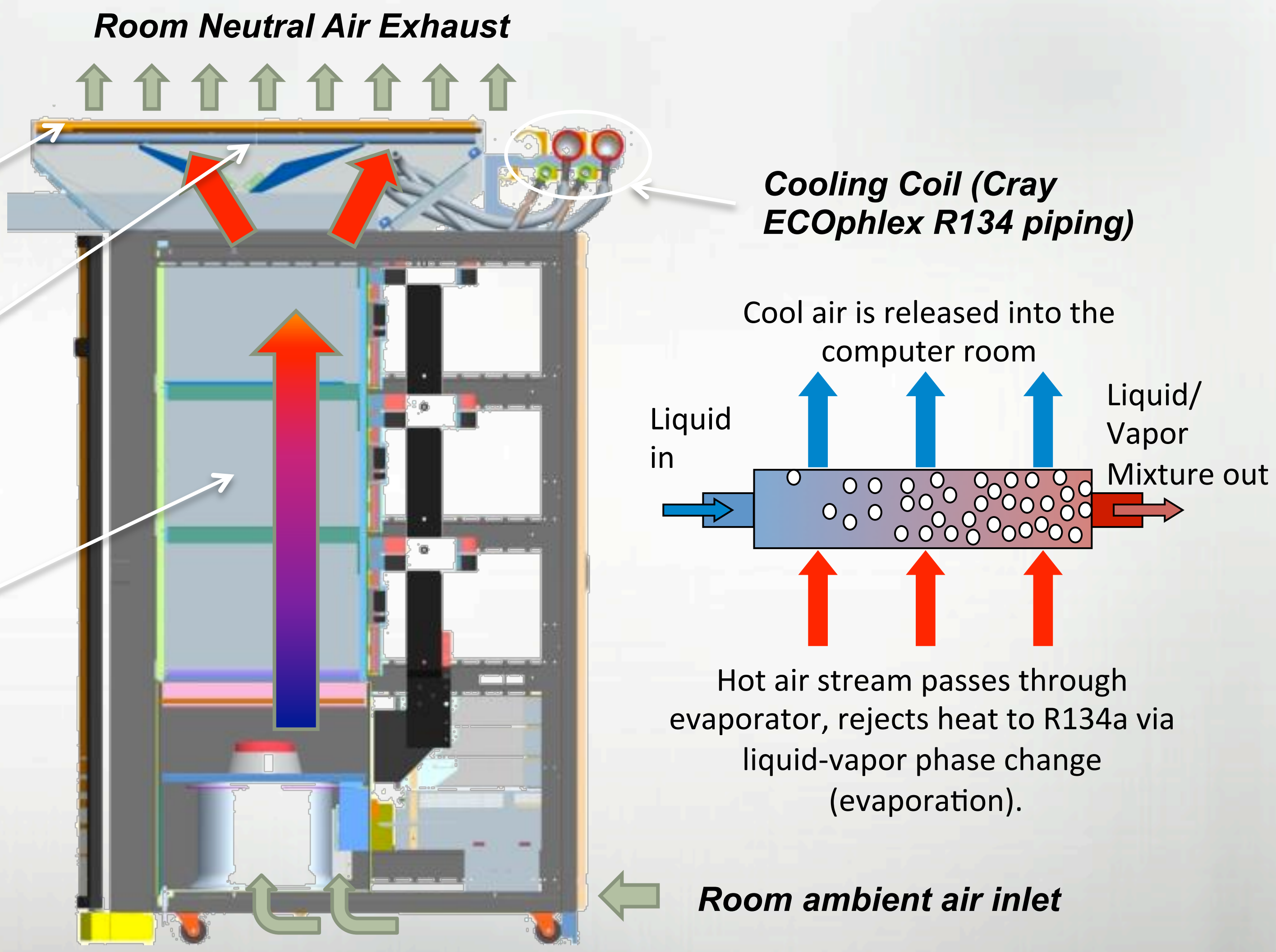
Faster XE6

XE6

GPU Accelerator

“XK6”

Air to Liquid Cooled is also a field upgrade…



Room Neutral Air Exhaust
Exit Evaporators
Cooling Coil (Cray ECOphlex R134 piping)
Hot air is cooled using liquid cooling before being exhausted into the computer room
Air heats as it passes through the compute blades
Cool air is released into the computer room
Liquid in
Liquid/ Vapor Mixture out
Hot air stream passes through evaporator, rejects heat to R134a via liquid-vapor phase change (evaporation).
Room ambient air inlet

Gemini Interconnect

Cray Network Evolution

SeaStar

- Built for scalability to 250K+ cores
- Very effective routing and low contention switch

Gemini

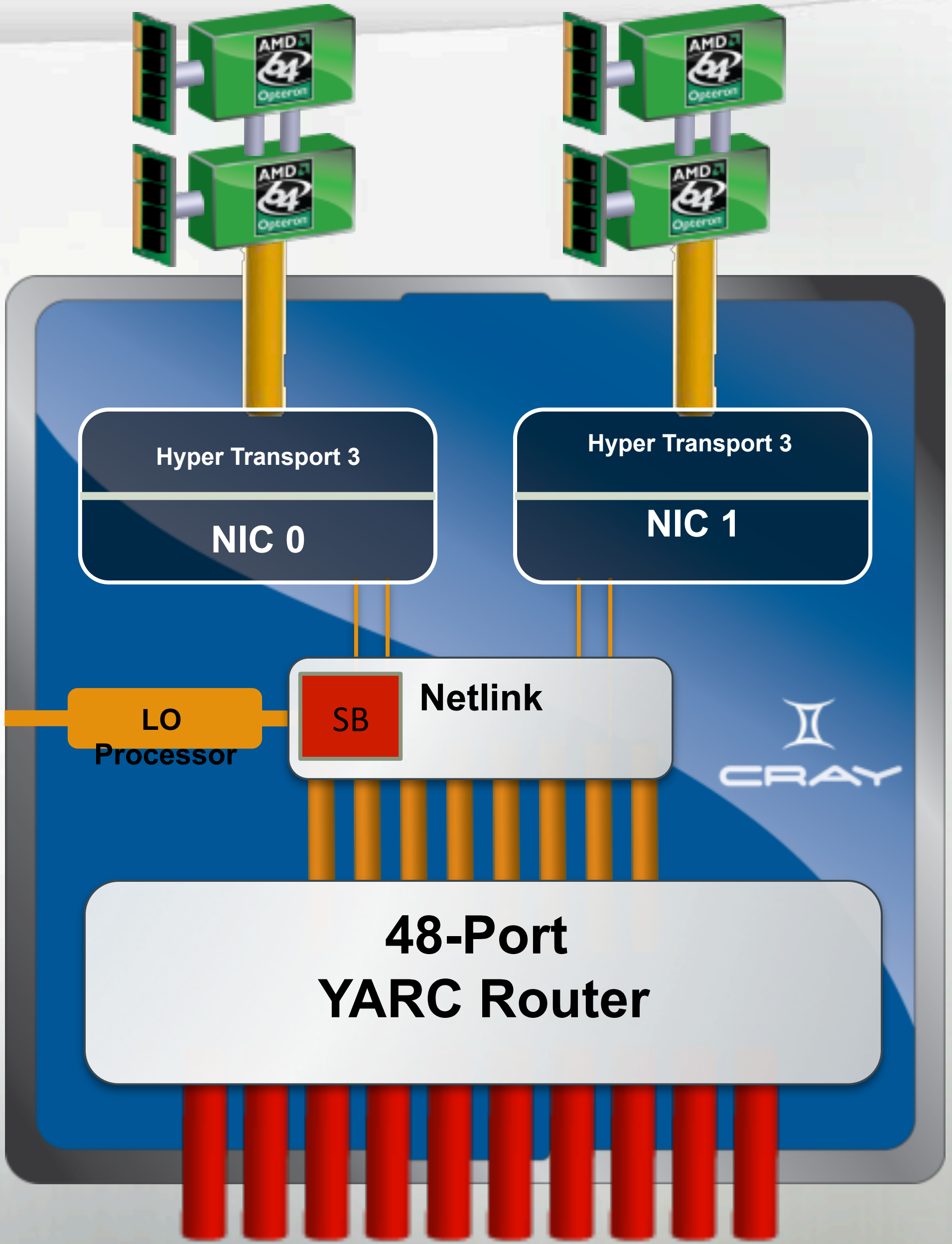
- 100x improvement in message throughput
- 3x improvement in latency
- PGAS Support, Global Address Space
- Scalability to 1M+ cores

Aries

- Ask me about it

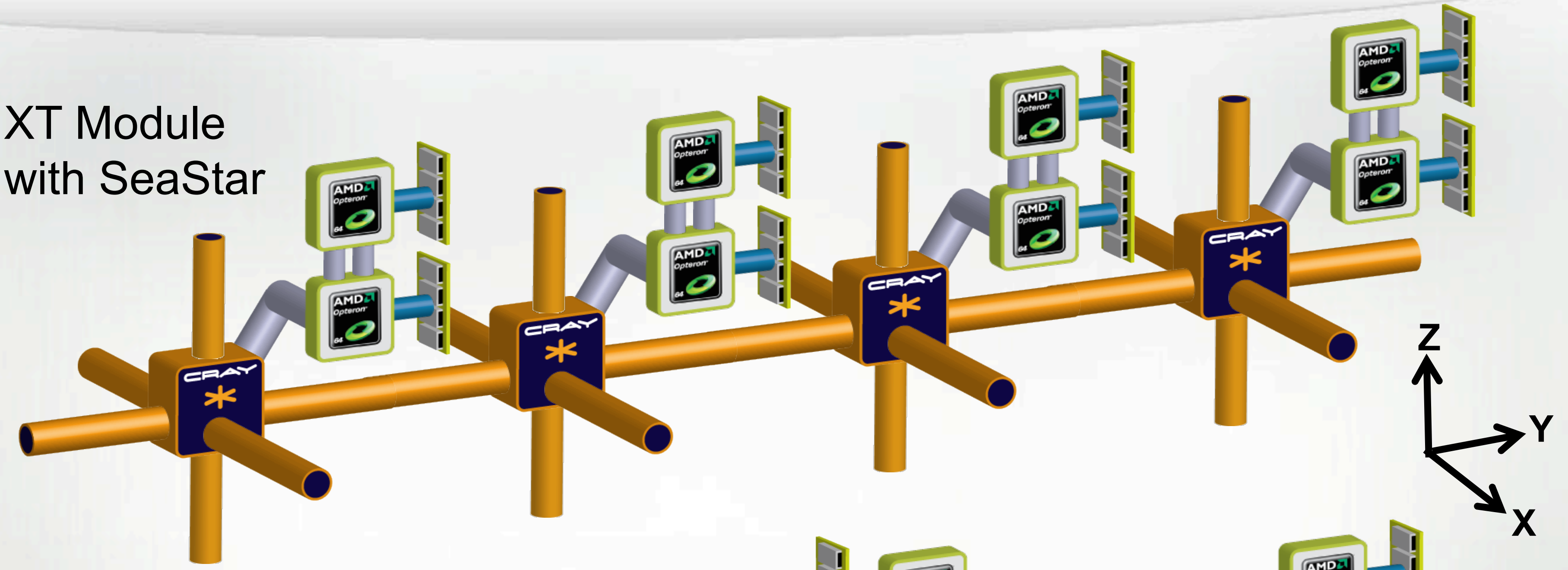
Cray Gemini

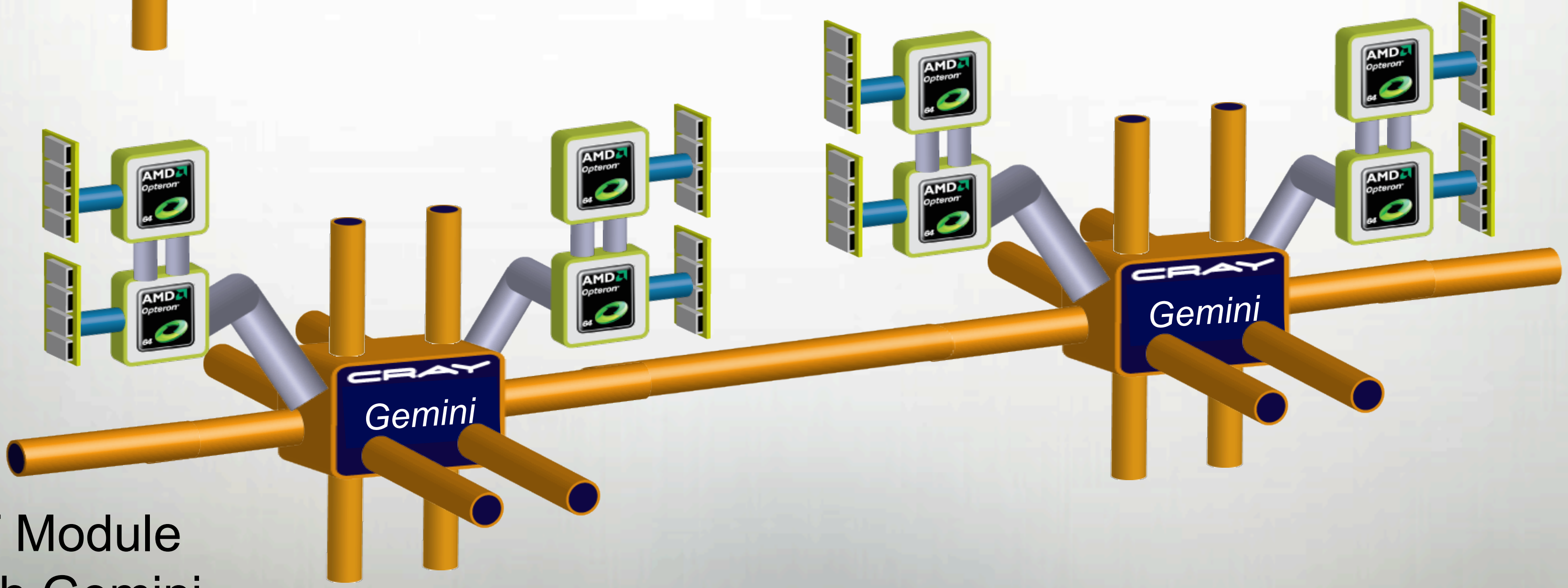
- 3D Torus network
- Supports 2 Nodes per ASIC
- 168 GB/sec routing capacity
- Scales to over 100,000 network endpoints
  - Link Level Reliability and Adaptive Routing
  - Advanced Resiliency Features
- Provides global address space
- Advanced NIC designed to efficiently support
  - MPI
    - Millions of messages/second
  - One-sided MPI
  - UPC, FORTRAN 2008 with coarrays, shmem
  - Global Atomics



Gemini vs SeaStar – Topology

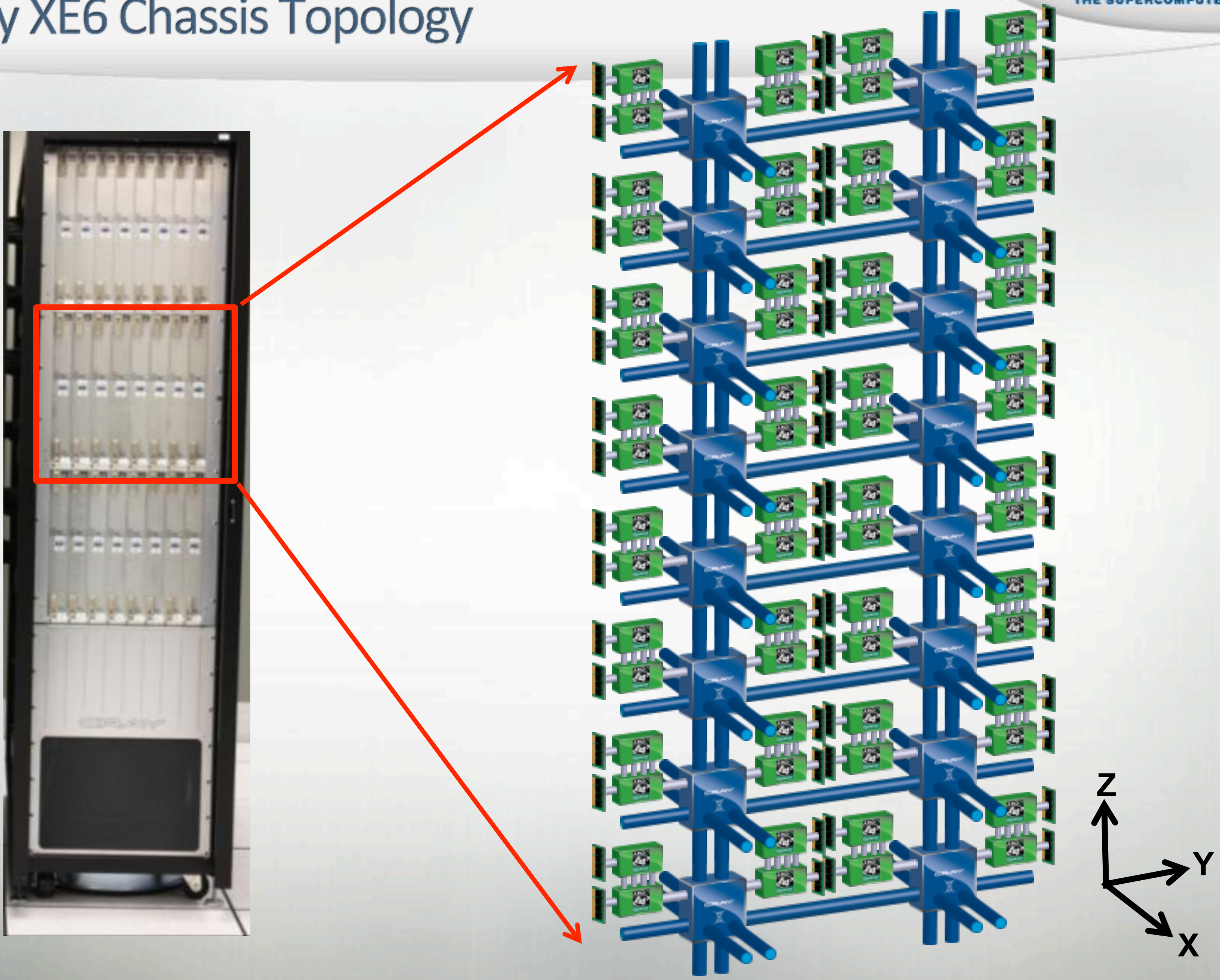
XT Module with SeaStar





XT Module with Gemini

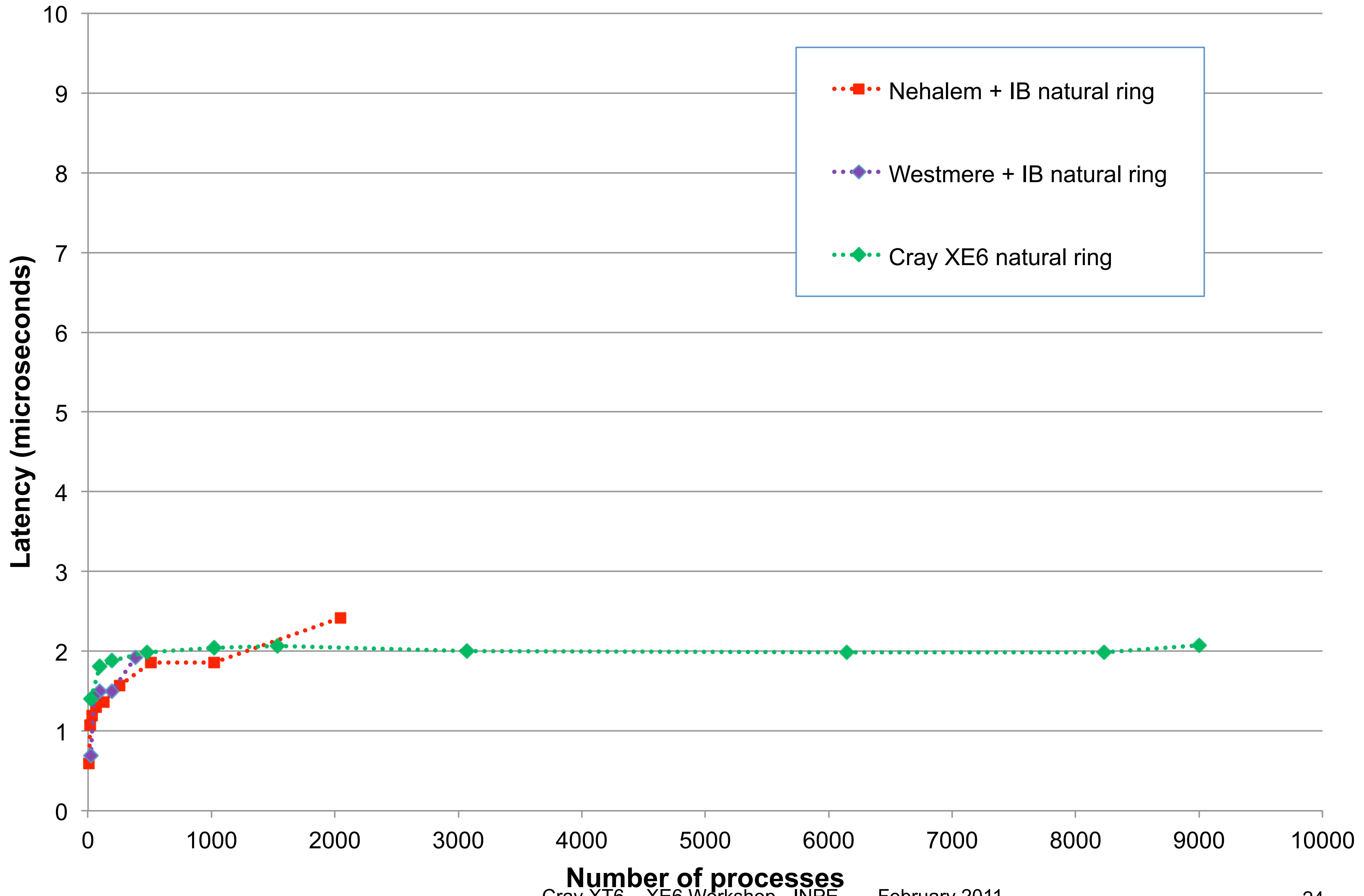
Cray XE6 Chassis Topology



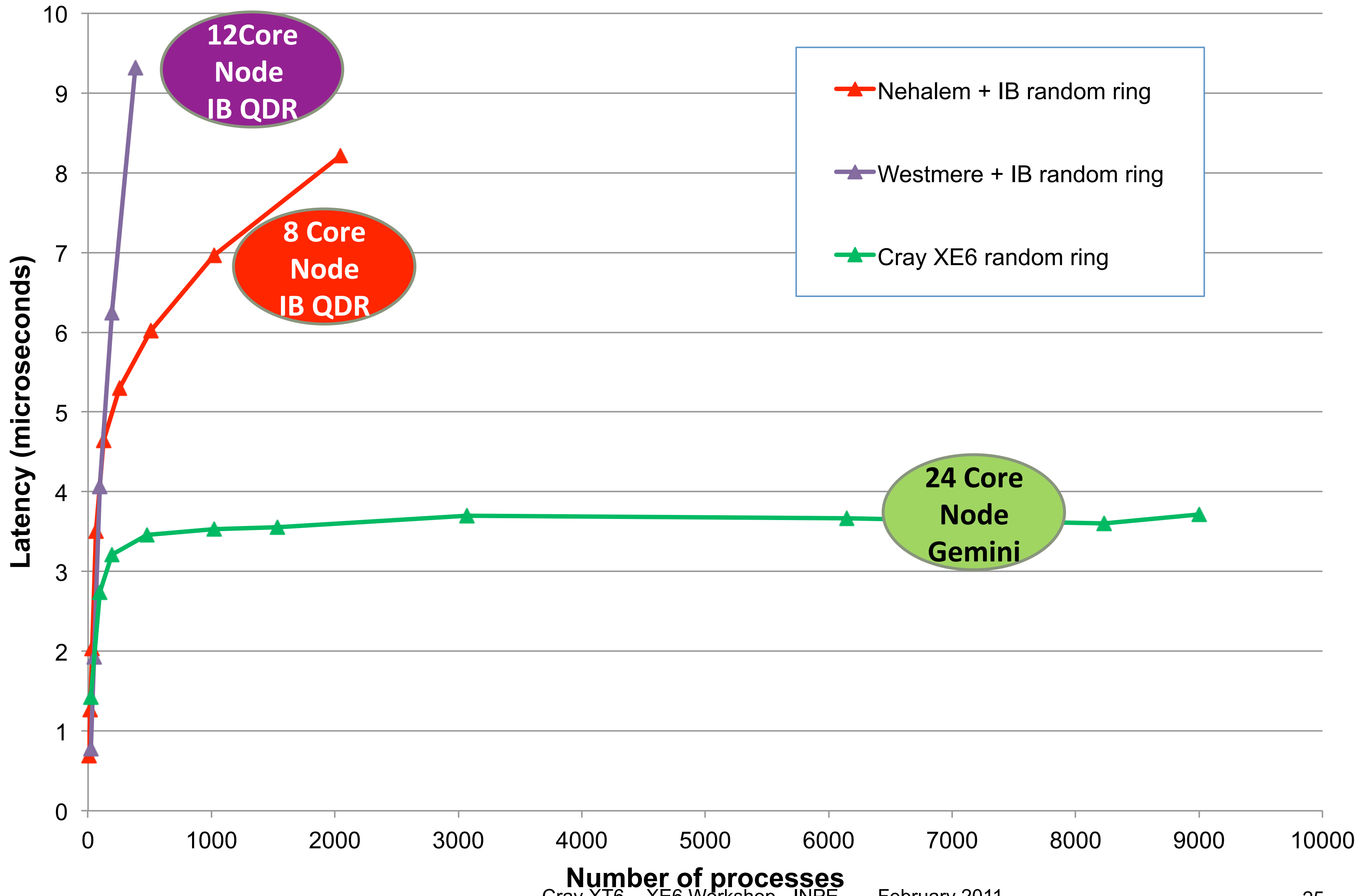
Gemini Advanced Features

- Globally addressable memory provides efficient support for UPC, Co-array FORTRAN, Shmem and Global Arrays
  - Cray Programming Environment will target this capability directly
- Pipelined global loads and stores
  - Allows for fast irregular communication patterns
- Atomic memory operations
  - Provides fast synchronization needed for one-sided communication models

Gemini – QDR Comparison
HPCC Natural Ring Latency Benchmark

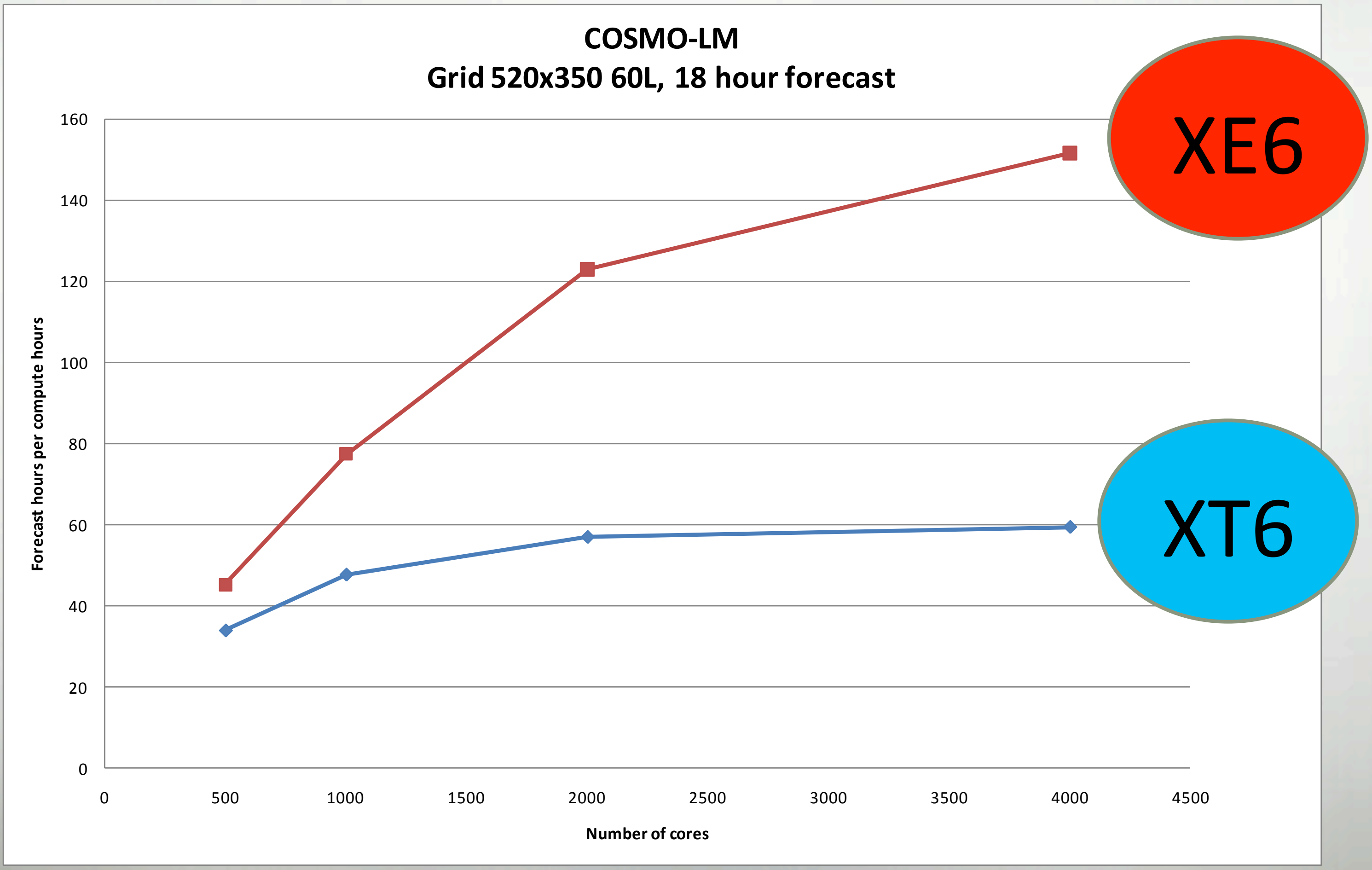


Gemini – QDR Comparison
HPCC Random Ring Latency Benchmark



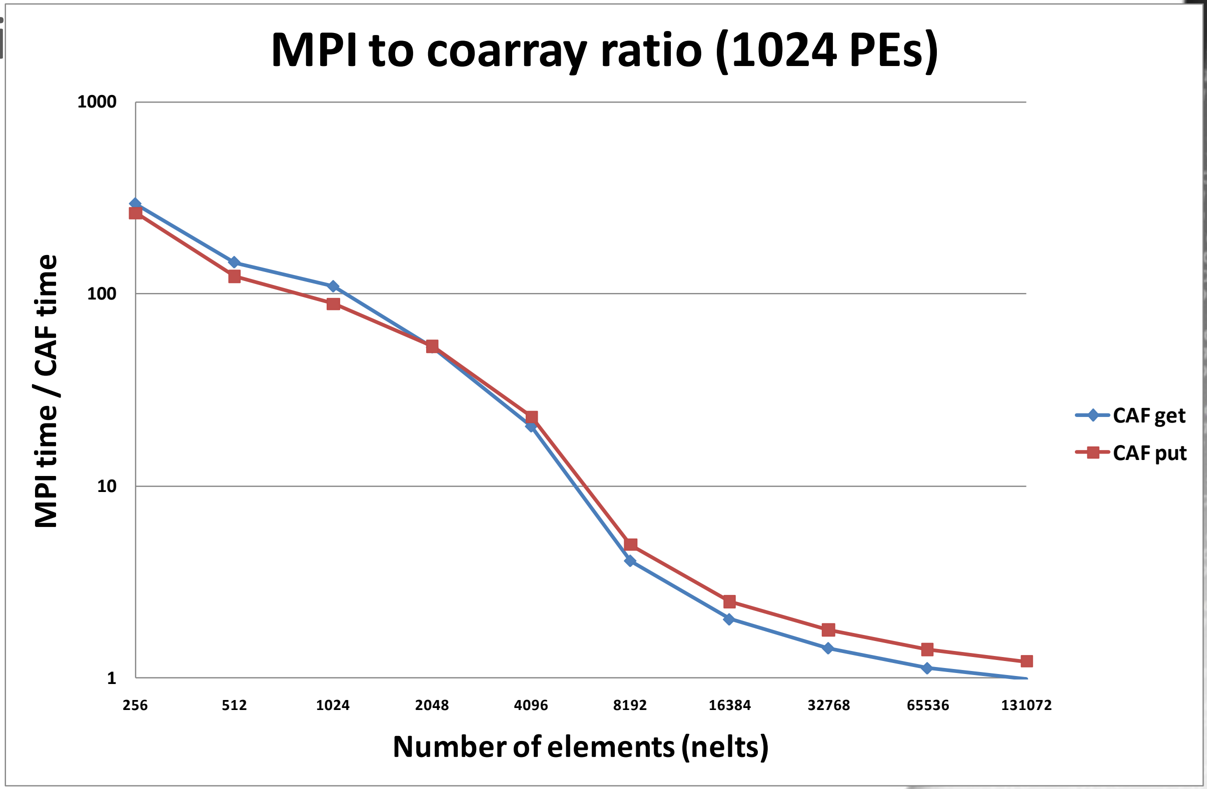
Scalability and simulation rate

- Forecast Hours per compute Hours
- Typical performance improvement



Remote gather: coarray vs MPI

- Coarray implementations are much simpler
- Coarray syntax allows the expression of remote data in a natural way – no need of complex protocols
- Coarray implementation is orders of magnitude faster for small numbers of indi



The Guiding Principle behind Co-Array Fortran

- What is the smallest change required to make Fortran 90 an effective parallel language?
- How can this change be expressed so that it is intuitive and natural for Fortran programmers?
- How can it be expressed so that existing compiler technology can implement it easily and efficiently?

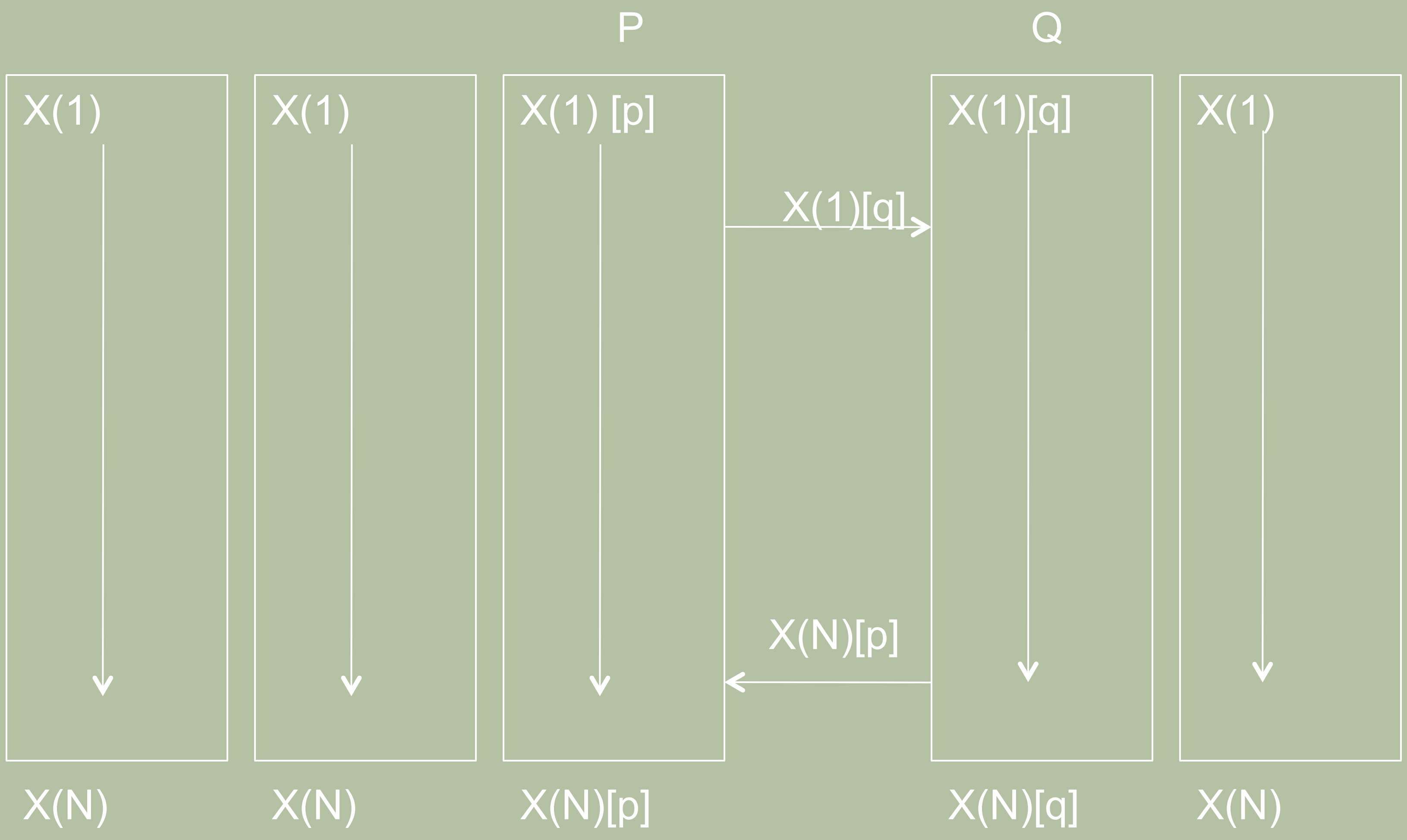
What is Co-Array Syntax?

- Co-Array syntax is a simple extension to normal Fortran syntax.
  - It uses normal rounded brackets ( ) to point to data in local memory.
  - It uses square brackets [ ] to point to data in remote memory.
  - Syntactic and semantic rules apply separately but equally to ( ) and [ ].

Examples of Co-Array Declarations

```
real :: s[*]
real :: a(n)[*]
complex :: z[*]
integer :: index(n)[*]
real :: b(n)[p, *]
real :: c(n,m)[0:p, -7:q,
11:*]
real, allocatable :: w(:)
[:]
type(field) :: maxwell[p,*]
```

CAF Memory Model



What Do Co-Dimensions Mean?

- real :: x(n)[p,q,*]

  - Replicate an array of length n, one on each image.
  - Build a map so each image knows how to find the array on any other image.
  - Organize images in a logical (not physical) three dimensional grid.
  - The last co-dimension acts like an assumed size array: * ➔num_images()/(pxq)
- A specific implementation could choose to represent memory hierarchy through the co-dimensions.

The CAF Execution Model

- The number of images is fixed and each image has its own index, retrievable at run-time:
  - 1 <,= num_images()
  - 1 <,= this_image() <,= num_images()
- Each image executes the same program independently of the others.
- The programmer inserts explicit synchronization and branching as needed.
- An “object” has the same name in each image.
- Each image works on its own local data.
- An image moves remote data to local data through, and only through, explicit CAF syntax.

Co-Array Fortran Extension

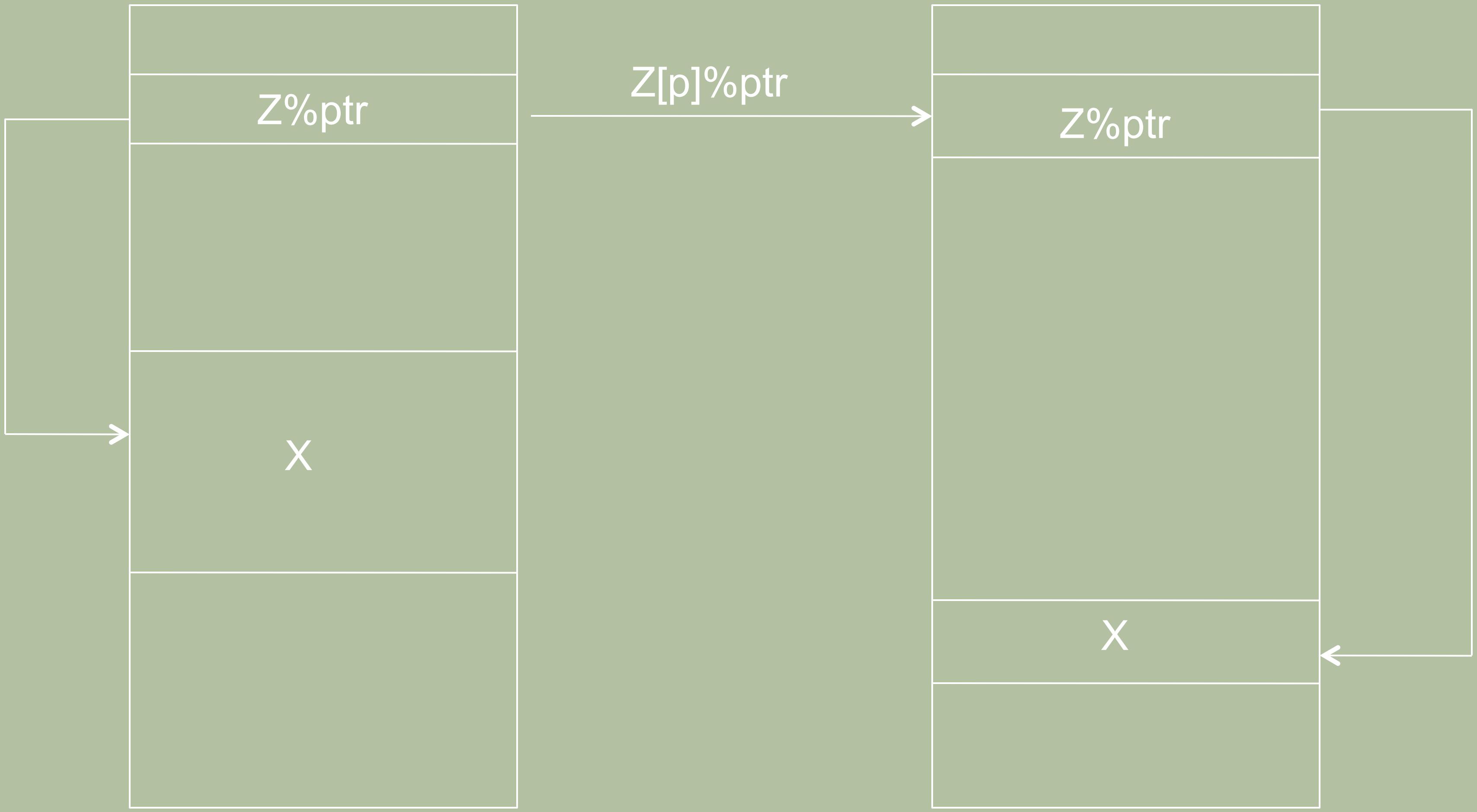
- Incorporate the SPMD Model into Fortran 90
  - Multiple images of the same program
  - Text and data are replicated in each image
- Mark some variables with co-dimensions
  - Co-dimensions behave like normal dimensions
  - Co-dimensions express a logical problem decomposition
  - One-sided data exchange between co-arrays using a Fortran-like syntax
- Require the underlying run-time system to map the logical problem decomposition onto specific hardware.

Communication Using CAF Syntax

- y(:) = x(:)[p]
- myIndex(:) = index(:)
- yourIndex(:) = index(:)[you]
- x(index(:)) = y[index(:)]
- x(:)[q] = x(:) + x(:)[p]

Absent co-dimension defaults to the local object.

Irregular and Changing Data Structures



Co-Array Fortran

- Can be implemented:
  - Directly in the compiler; on those systems where the compiler can issue memory fetches and stores directly to remote processors memory, the statement becomes a simple remote store.
    - Allows co-array reference in a loop to be combined into a vector load or store
    - Allows compiler to use normal prefetch mechanism to move fetches ahead of reference
  - Via a pre-processor; Rice University is currently working on such a translator which generates subroutine calls for transferring data to the remote processor
    - Significantly more difficult to get performance better than MPI

Importance of Vectorizing loop with the CAF reference

```
    7.               iz = this_image(a)
    8.   V----<   do ix = 1, kx
    9.   V r--<     do iy = 1, ky
   10.   V r          a(ix,iy) = b(iy,iz)[ix]
   11.   V r-->     end do
   12.   V---->   end do
ftn-3021 ftn: INLINE File = data_distro.f90, Line = 7
  Routine _THIS_IMAGE3 was not inlined because the compiler was unable to
  locate the routine to expand it inline.
ftn-6204 ftn: VECTOR File = data_distro.f90, Line = 8
  A loop starting at line 8 was vectorized.
ftn-6005 ftn: SCALAR File = data_distro.f90, Line = 9
  A loop starting at line 9 was unrolled 4 times.
ftn-6208 ftn: VECTOR File = data_distro.f90, Line = 9
  A loop starting at line 9 was vectorized as part of the loop starting at line
  8.
```

Another Example

```
 629.  V------------<         do im = 1, 10000
 630.  V                        if(blockid.eq.imon_in(4,im) .and.
 631.  V                  &        ibegin(sx)   .le.imon_in(1,im) .and.
 632.  V                  &        ibegin(sx+1).gt.imon_in(1,im) .and.
 633.  V                  &        jbegin(sy)   .le.imon_in(2,im) .and.
 634.  V                  &        jbegin(sy+1).gt.imon_in(2,im) .and.
 635.  V                  &        kbegin(sz)   .le.imon_in(3,im) .and.
 636.  V                  &        kbegin(sz+1).gt.imon_in(3,im)) then
 637.  V                          num_mon_me = num_mon_me+1
 638.  V                          lmon(im) = .true.
 639.  V                          proc_mon[ioid]%array(im)=procid_global
 640.  V                        endif
 641.  V------------>         end do

ftn-6375 ftn: VECTOR File = main_3d.f, Line = 629
  A loop starting at line 629 would benefit from "!dir$ safe_address".

ftn-6204 ftn: VECTOR File = main_3d.f, Line = 629
  A loop starting at line 629 was vectorized.
```

Special features of Baker relating to CAF/UPC

- On X1, X1E, and ‘BlackWidow’, the custom processor directly emits addresses for any memory location in the machine. Scalar or vector loads/stores can be done to any global address in the system
- On XE6 the Gemini NIC used to ‘extend’ address space of Opteron references to access memory on remote nodes
  - Fortran or C compilers recognize CAF references, x(i)[dest_pe], or UPC ‘shared’ references, x[i][threads], and generates appropriate ncHT messages to Gemini to load from or store to remote memory
  - Users can stride on local offsets or across processor space with any stride, including Gather/Scatter
  - Compiler should generate vector requests as appropriate

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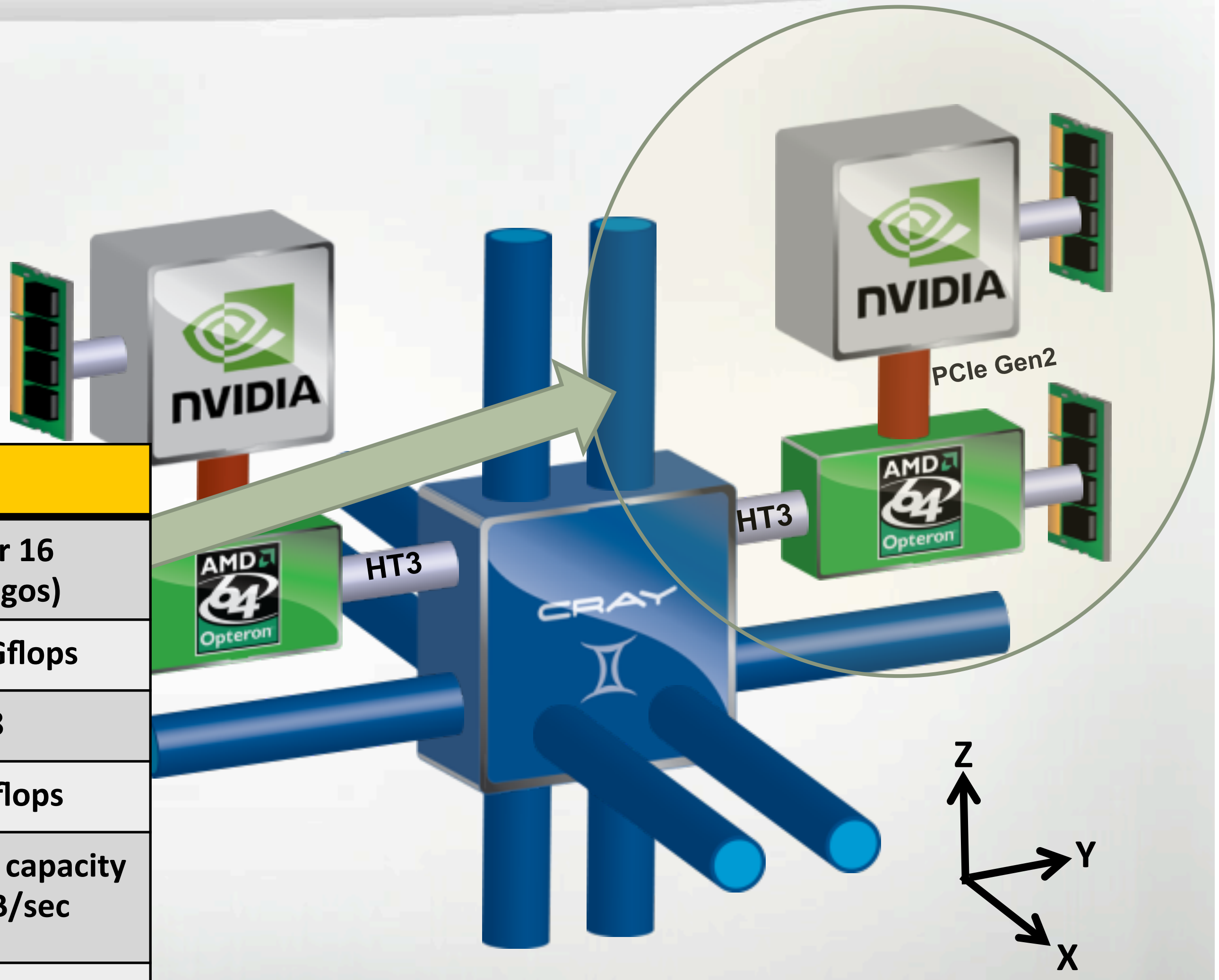
“Glacier” Project

XXX XXX

XK6 Product

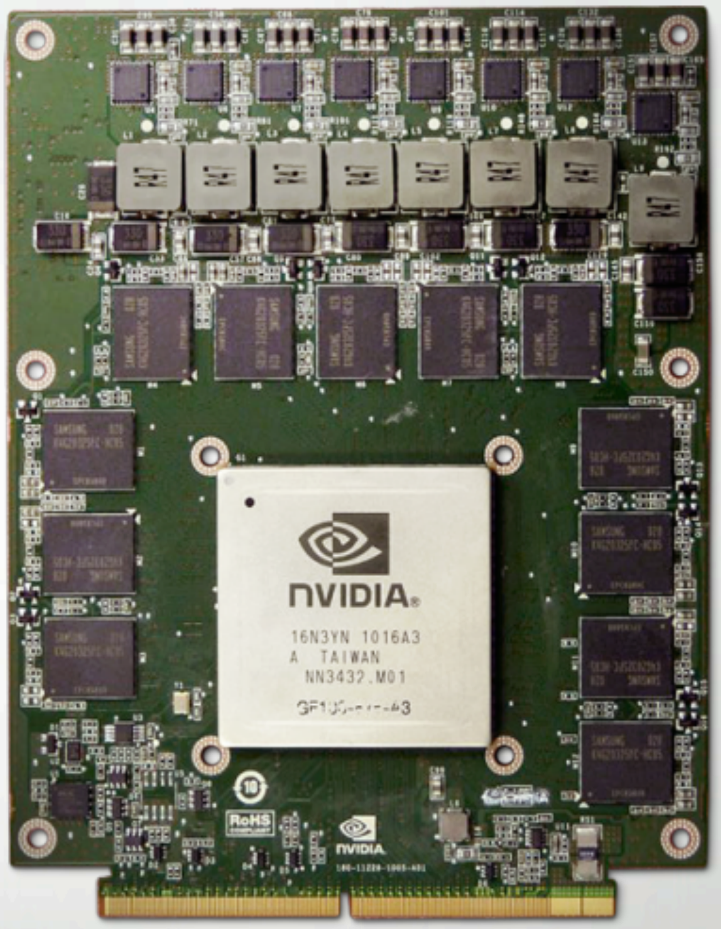
Cray "Glacier" Node



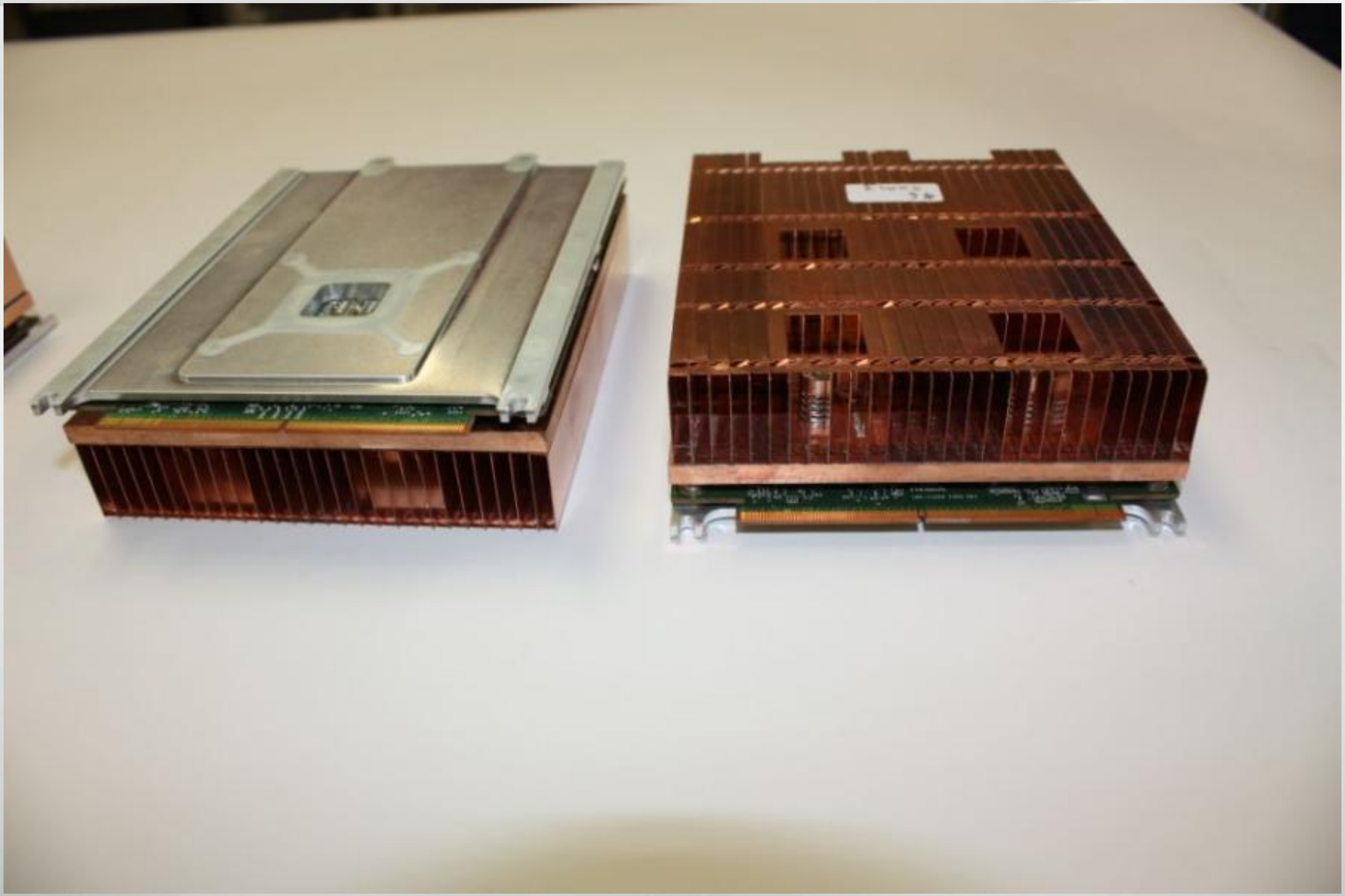
Node Characteristics	
Number of X86 Cores	8, 12 or 16 (Interlagos)
X86 Peak	90-147 Gflops
Accelerator Cores	448
Accelerator Peak	600+ Gflops
X86 Memory	16 or 32GB capacity at 51 GB/sec
Accelerator Memory	6GB capacity at 180 GB/sec

NVIDIA Tesla™ X2070 GPU (today)

- CUDA Core count 448
- GPU Frequency 1.15GHz
- Peak Performance (DP) 515GFlops
- Power consumption 225W
- Memory type and size 6GB of GDDR5 (ECC)
- Memory frequency 1.566GHz
- Memory interface width 384bit
- Custom heat sink for Glacier blade
- Can be upgraded with follow-on GPU



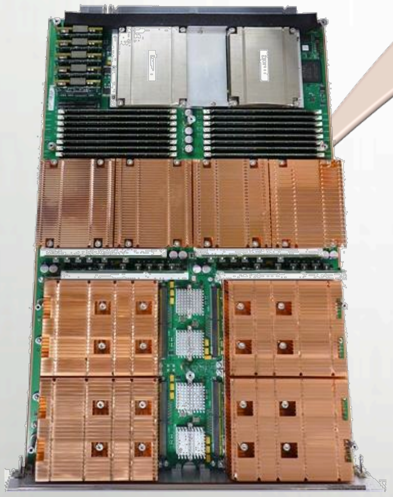
Heat Sinks and Backer Plate



Full Glacier Accelerator Blade

- Four nodes per blade
- Gemini Mezzanine
- Plug compatible with XE6 blade
- Configurable processor, memory and SXM GPU card
- Currently running on system with 175 nodes

Glacier Roadmap

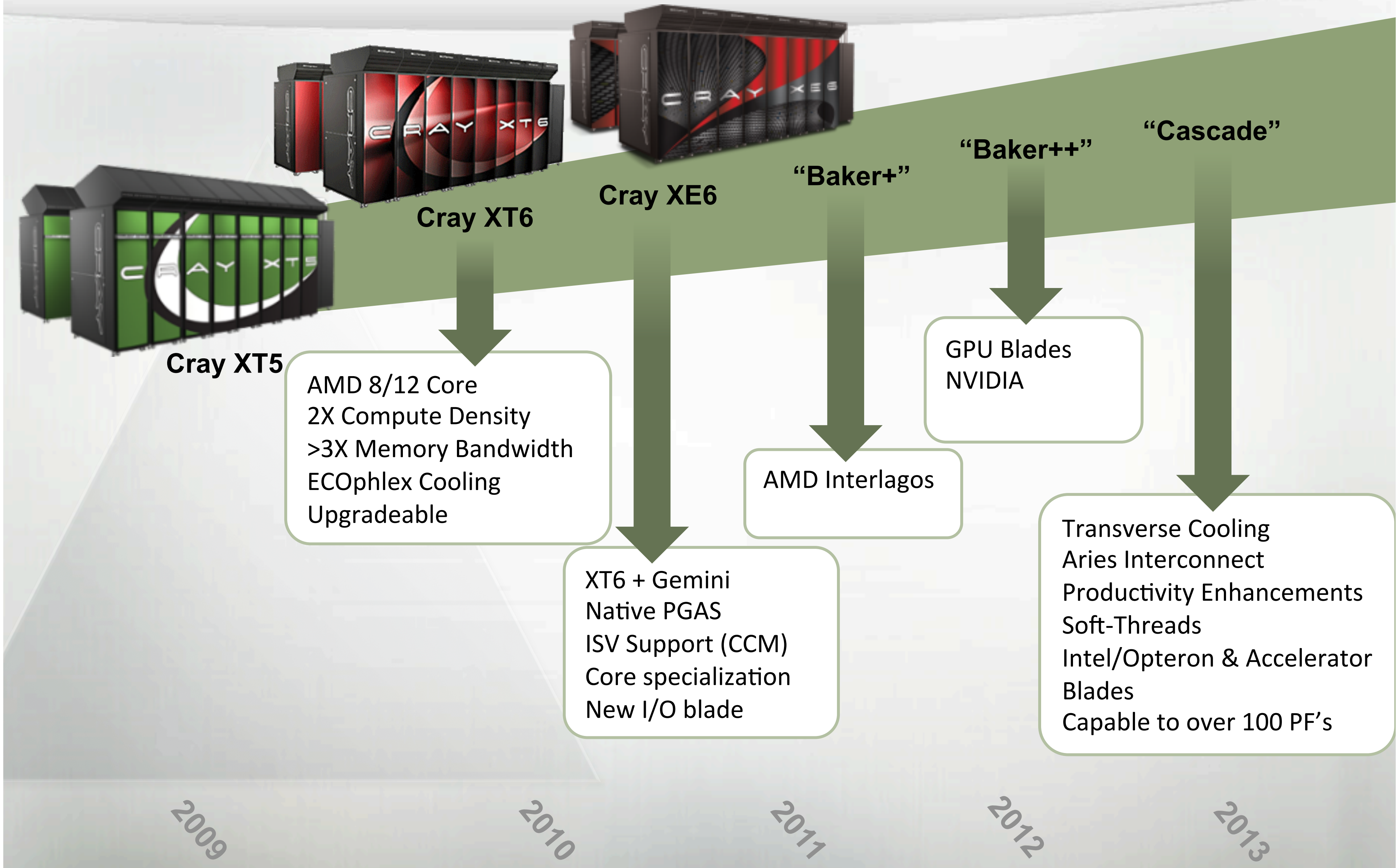


NVIDEA Tesla 640 Gflops Sept - 2011

NVIDEA Kepler Accelerator > 1 Tflop June - 2012

- Glacier will have a series of accelerator modules available
- Peak per cabinet will range from ~75 Tflops to ~130 Tflops
- All Glacier nodes will use the Interlagos processor

Supercomputing Road Map



Cray XT5

Cray XT6

- AMD 8/12 Core
- 2X Compute Density
- >3X Memory Bandwidth
- ECOphlex Cooling
- Upgradeable

Cray XE6

- XT6 + Gemini
- Native PGAS
- ISV Support (CCM)
- Core specialization
- New I/O blade

"Baker+"

- AMD Interlagos

"Baker++"

- GPU Blades
- NVIDIA

"Cascade"

- Transverse Cooling
- Aries Interconnect
- Productivity Enhancements
- Soft-Threads
- Intel/Opteron & Accelerator Blades
- Capable to over 100 PF's

Cray Software Objectives for Accelerators

1. Provide baseline accelerator environment
   - Don't preclude use of tools developers/programmers are used to
2. Integrated Programming Environment
   - Extension of PE Cray has provided on XT/XE systems
   - Provide "bundled" 3rd party commonly used or expected software (compilers, libraries, tools)
3. Cray integrated programming environment include:
   - Greatly enhance the productivity of the programming writing new applications or porting existing applications to accelerators
   - Improve performance of existing applications by exploiting greater levels of parallelism
   - Maintain source compatibility between multi-core and accelerator versions of the code

Programming for Future

Multi-Petaflop and Exaflop Computers

aka

Finding more parallelism in existing applications

Back to the Futures – Combining different levels of parallelism

- Fact
    - For the next decade all HPC system will basically have the same architecture
        - Message passing between nodes
        - Multi-threading within the node – MPI will not do
        - Vectorization at the lower level -

- Fact
    - Current petascale applications are not structured to take advantage of these architectures
        - Current – 80-90% of application use a single level of parallelism, message passing between the cores of the MPP system
        - Looking forward, application developers are faced with a significant task in preparing their applications for the future

Cray's Programming Environment

- Tools for identifying additional parallel structures within the application
  - Investigation of looping structures within a complex application
  - Scoping tools for investigating the parallelizability of high level looping structures

- Tools for maintaining performance portable applications
  - Supply compiler that accepts directives from OpenMP sub-committee formulating extensions to target companion accelerators
    - Application developer able to develop a single code that can run efficiently on multi-core nodes with or without accelerator

Hybridization* of an All MPI Application

* Creation of an application that exhibits three levels of parallelism, MPI between nodes, OpenMP** on the node and vectorized looping structures

** Why OpenMP? To provide performance portability. OpenMP is the only threading construct that a compiler can analyze sufficiently to generate efficient threading on multi-core nodes and to generate efficient code for companion accelerators.

Additional Note about Accelerators

- Many application developers, particularily ISVs have not put in the effort to convert their application to MPI. These applications potentially can utilize accelerators on the node to significantly enhance their performance
  - Most of these do use OpenMP parallelization – by adding OpenMP accelerator extensions, these application should be able to benefit from accelerators

CAUTION!!

- Do not read "Automatic" into this presentation, the Hybridization of an application is difficult and efficient code only comes with a thorough interaction with the compiler to generate the most efficient code and
  - High level OpenMP structures
  - Low level vectorization of major computational areas
- Performance is also dependent upon the location of the data. Best case is that the major computational arrays reside on the accelerator. Otherwise computational intensity of the accelerated kernel must be significant

Cray's Hybrid Programming Environment supplies tools for addressing these issues

Three levels of Parallelism required

- Developers will continue to use MPI between nodes or sockets
- Developers must address using a shared memory programming paradigm on the node
- Developers must vectorize low level looping structures
- While there is a potential acceptance of new languages for addressing all levels directly. Most developers cannot afford this approach until they are assured that the new language will be accepted and the generated code is within a reasonable performance range

Possible Programming Models for the Node

- Cuda
- OpenCL
- Existing Fortran, C and C++ with extensions
    - Pthreads, Thread Building Blocks
    - Comment line directives
        - OpenMP extensions for Accelerators

All of these programming models require the application developer to replace MPI within the node – to develop Hybrid versions of the application

Comparison of Programming Models for the Node

	portability	Performance	Perf/portability	Ease of Use
Cuda	2	5	1	2
OpenCL	2	5	1	1
Existing Language with threading	3	4	2	3
Existing Language with directives	5	4	5	5

Portability

	Nvida GPGPU	AMD GPGPU	IBM Power	IBM BG	X86 multi-core
Cuda	x				
OpenCL	x	x			
Existing Language with threading			x	x	x
Existing Language with directives	x	x	x	x	x

Comparisons between Cuda and OpenMP accelerator extensions

- Cuda
  - Widely used programming model for effectively utilizing the accelerator
  - Flexibility to obtain good performance on the accelerator
- OpenMP accelerator extensions – things to prove
  - Are the directives powerful enough to allow the developer to pass information on to the compiler
  - Can the compiler generate code that get performance close to Cuda.

Consider the following kernel

```
do k = 1,nz
 do j=1,ny
   SPECIES: do n=1,n_spec-1
     do i = 1,nx
       diffFlux(i,j,k,n,1) = - Ds_mixavg(i,j,k,n) * ( grad_Ys(i,j,k,n,1)  &
                             + yspecies(i,j,k,n) * grad_mixMW(i,j,k,1) )
       diffFlux(i,j,k,n,2) = - Ds_mixavg(i,j,k,n) * ( grad_Ys(i,j,k,n,2)  &
                             + yspecies(i,j,k,n) * grad_mixMW(i,j,k,2) )
       diffFlux(i,j,k,n,3) = - Ds_mixavg(i,j,k,n) * ( grad_Ys(i,j,k,n,3)  &
                             + yspecies(i,j,k,n) * grad_mixMW(i,j,k,3) )
     enddo
     do i = 1,nx
      diffFlux(i,j,k,n_spec,1) = diffFlux(i,j,k,n_spec,1) - diffFlux(i,j,k,n,1)
      diffFlux(i,j,k,n_spec,2) = diffFlux(i,j,k,n_spec,2) - diffFlux(i,j,k,n,2)
      diffFlux(i,j,k,n_spec,3) = diffFlux(i,j,k,n_spec,3) - diffFlux(i,j,k,n,3)
     enddo
    enddo SPECIES
    do i = 1,nx
     grad_T(i,j,k,1) = -lambda(i,j,k) * grad_T(i,j,k,1)
     grad_T(i,j,k,2) = -lambda(i,j,k) * grad_T(i,j,k,2)
     grad_T(i,j,k,3) = -lambda(i,j,k) * grad_T(i,j,k,3)
    enddo
    do n=1,n_spec
      do i = 1,nx
       grad_T(i,j,k,1) = grad_T(i,j,k,1) + h_spec(i,j,k,n)*diffFlux(i,j,k,n,1)
       grad_T(i,j,k,2) = grad_T(i,j,k,2) + h_spec(i,j,k,n)*diffFlux(i,j,k,n,2)
       grad_T(i,j,k,3) = grad_T(i,j,k,3) + h_spec(i,j,k,n)*diffFlux(i,j,k,n,3)
      enddo
    enddo
   enddo
  enddo
```

A rewrite for Cuda Fortran
First extract to kernel and call

```
! transfer

 grad_Ys_d = grad_Ys_h
 diffFlux_d = diffFlux_h
 yspecies_d = yspecies_h
 h_spec_d = h_spec_h
 ds_mixavg_d = ds_mixavg_h
 grad_t_d = grad_t_h
 grad_mixMW_d = grad_mixMW_h
 lambda_d = lambda_h

 grid = dim3((nxyz-1)/512+1,1,1)
 threadBlock = dim3(512,1,1)

 call calcDiffFlux<<<grid,threadBlock>>>(lambda_d, grad_T_d, grad_mixMW_d, diffFlux_d, &
      Ds_mixavg_d, yspecies_d, grad_Ys_d, h_spec_d)
 ierr = cudaThreadSynchronize()
```

A rewrite for Cuda Fortran
And now the kernel (1)

```
i = (blockIdx%x-1)*blockDim%x + threadIdx%x
 if (i <= nxyz) then
    ! move first part of grad T here
    lambda_r = lambda(i)
    grad_T_1 = -lambda_r*grad_T(i,1)
    grad_T_2 = -lambda_r*grad_T(i,2)
    grad_T_3 = -lambda_r*grad_T(i,3)
    ! now diffFlux
    diffFlux_n_spec_1 = diffFlux(i,n_spec,1)
    diffFlux_n_spec_2 = diffFlux(i,n_spec,2)
    diffFlux_n_spec_3 = diffFlux(i,n_spec,3)
    grad_mixMW_1 = grad_mixMW(i,1)
    grad_mixMW_2 = grad_mixMW(i,2)
    grad_mixMW_3 = grad_mixMW(i,3)
    do n=1, n_spec-1
       Ds_mixavg_r = Ds_mixavg(i,n)
       yspecies_r = yspecies(i,n)
       diffFlux_1 = - Ds_mixavg_r *(grad_Ys(i,n,1) + yspecies_r*grad_mixMW_1)
       diffFlux_2 = - Ds_mixavg_r *(grad_Ys(i,n,2) + yspecies_r*grad_mixMW_2)
       diffFlux_3 = - Ds_mixavg_r *(grad_Ys(i,n,3) + yspecies_r*grad_mixMW_3)
       diffFlux_n_spec_1 = diffFlux_n_spec_1 - diffFlux_1
       diffFlux_n_spec_2 = diffFlux_n_spec_2 - diffFlux_2
       diffFlux_n_spec_3 = diffFlux_n_spec_3 - diffFlux_3
       h_spec_r = h_spec(i,n)
       grad_T_1 = grad_T_1 + h_spec_r*diffFlux_1
       grad_T_2 = grad_T_2 + h_spec_r*diffFlux_2
       grad_T_3 = grad_T_3 + h_spec_r*diffFlux_3
       diffFlux(i,n,1) = diffFlux_1
       diffFlux(i,n,2) = diffFlux_2
       diffFlux(i,n,3) = diffFlux_3
    enddo
```

1) Unrolled all dir loops
2) Combined two n_spec loops
3) Moved around computation
4) Assigned most arrays to temps

A rewrite for Cuda Fortran
And now the kernel (2)

```
! do n = n_spec iteration and write out final data

    h_spec_r = h_spec(i,n_spec)
    grad_T_1 = grad_T_1 + h_spec_r*diffFlux_n_spec_1
    grad_T_2 = grad_T_2 + h_spec_r*diffFlux_n_spec_2
    grad_T_3 = grad_T_3 + h_spec_r*diffFlux_n_spec_3

    grad_T(i,1) = grad_T_1
    grad_T(i,2) = grad_T_2
    grad_T(i,3) = grad_T_3

    diffFlux(i,n_spec,1) = diffFlux_n_spec_1
    diffFlux(i,n_spec,2) = diffFlux_n_spec_2
    diffFlux(i,n_spec,3) = diffFlux_n_spec_3
 endif
```

Or Add directives

```
!$omp acc_region
!$omp acc_loop collapse(2)
o k = 1,nz
       do j=1,ny
         SPECIES: do n=1,n_spec-1
           do i = 1,nx
             diffFlux(i,j,k,n,1) = - Ds_mixavg(i,j,k,n) * ( grad_Ys(i,j,k,n,1)  &
                                   + yspecies(i,j,k,n) * grad_mixMW(i,j,k,1) )
             diffFlux(i,j,k,n,2) = - Ds_mixavg(i,j,k,n) * ( grad_Ys(i,j,k,n,2)  &
                                   + yspecies(i,j,k,n) * grad_mixMW(i,j,k,2) )
             diffFlux(i,j,k,n,3) = - Ds_mixavg(i,j,k,n) * ( grad_Ys(i,j,k,n,3)  &
                                   + yspecies(i,j,k,n) * grad_mixMW(i,j,k,3) )
           enddo
           do i = 1,nx
            diffFlux(i,j,k,n_spec,1) = diffFlux(i,j,k,n_spec,1) - diffFlux(i,j,k,n,1)
            diffFlux(i,j,k,n_spec,2) = diffFlux(i,j,k,n_spec,2) - diffFlux(i,j,k,n,2)
            diffFlux(i,j,k,n_spec,3) = diffFlux(i,j,k,n_spec,3) - diffFlux(i,j,k,n,3)
           enddo
          enddo SPECIES
          do i = 1,nx
           grad_T(i,j,k,1) = -lambda(i,j,k) * grad_T(i,j,k,1)
           grad_T(i,j,k,2) = -lambda(i,j,k) * grad_T(i,j,k,2)
           grad_T(i,j,k,3) = -lambda(i,j,k) * grad_T(i,j,k,3)
          enddo
          do n=1,n_spec
            do i = 1,nx
             grad_T(i,j,k,1) = grad_T(i,j,k,1) + h_spec(i,j,k,n)*diffFlux(i,j,k,n,1)
             grad_T(i,j,k,2) = grad_T(i,j,k,2) + h_spec(i,j,k,n)*diffFlux(i,j,k,n,2)
             grad_T(i,j,k,3) = grad_T(i,j,k,3) + h_spec(i,j,k,n)*diffFlux(i,j,k,n,3)
            enddo
          enddo
         enddo
        enddo
!$omp end acc_loop
!$omp end acc_region
```

What the Compiler Shows

```
218.  1 G-----------< !$omp acc_region
219.  1 G             !$omp acc_loop collapse(2)
220.  1 G C---------<     do k = 1,nz
221.  1 G C g-------<      do j=1,ny
222.  1 G C g 5-----<          SPECIES: do n=1,n_spec-1
223.  1 G C g 5 gf--<                do i = 1,nx
224.  1 G C g 5 gf                 ! driving force is just the gradient in mole fraction:
225.  1 G C g 5 gf                 diffFlux(i,j,k,n,1) = - Ds_mixavg(i,j,k,n) * ( grad_Ys(i,j,k,n,1)   &
226.  1 G C g 5 gf                                       + yspecies(i,j,k,n) * grad_mixMW(i,j,k,1) )
227.  1 G C g 5 gf                 diffFlux(i,j,k,n,2) = - Ds_mixavg(i,j,k,n) * ( grad_Ys(i,j,k,n,2)   &
228.  1 G C g 5 gf                                       + yspecies(i,j,k,n) * grad_mixMW(i,j,k,2) )
229.  1 G C g 5 gf                 diffFlux(i,j,k,n,3) = - Ds_mixavg(i,j,k,n) * ( grad_Ys(i,j,k,n,3)   &
230.  1 G C g 5 gf                                       + yspecies(i,j,k,n) * grad_mixMW(i,j,k,3) )
231.  1 G C g 5 gf-->            enddo
232.  1 G C g 5 f---<                do i = 1,nx
233.  1 G C g 5 f                 diffFlux(i,j,k,n_spec,1) = diffFlux(i,j,k,n_spec,1) - diffFlux(i,j,k,n,1)
234.  1 G C g 5 f                 diffFlux(i,j,k,n_spec,2) = diffFlux(i,j,k,n_spec,2) - diffFlux(i,j,k,n,2)
235.  1 G C g 5 f                 diffFlux(i,j,k,n_spec,3) = diffFlux(i,j,k,n_spec,3) - diffFlux(i,j,k,n,3)
236.  1 G C g 5 f--->            enddo
237.  1 G C g 5----->          enddo SPECIES
238.  1 G C g g-----<              do i = 1,nx
239.  1 G C g g                  grad_T(i,j,k,1) = -lambda(i,j,k) * grad_T(i,j,k,1)
240.  1 G C g g                  grad_T(i,j,k,2) = -lambda(i,j,k) * grad_T(i,j,k,2)
241.  1 G C g g                  grad_T(i,j,k,3) = -lambda(i,j,k) * grad_T(i,j,k,3)
242.  1 G C g g----->              enddo
243.  1 G C g 5-----<          do n=1,n_spec
244.  1 G C g 5 g---<                    do i = 1,nx
245.  1 G C g 5 g                  grad_T(i,j,k,1) = grad_T(i,j,k,1) + h_spec(i,j,k,n)*diffFlux(i,j,k,n,1)
246.  1 G C g 5 g                  grad_T(i,j,k,2) = grad_T(i,j,k,2) + h_spec(i,j,k,n)*diffFlux(i,j,k,n,2)
247.  1 G C g 5 g                  grad_T(i,j,k,3) = grad_T(i,j,k,3) + h_spec(i,j,k,n)*diffFlux(i,j,k,n,3)
248.  1 G C g 5 g--->                    enddo
249.  1 G C g 5----->          enddo
250.  1 G C g------->         enddo
251.  1 G C--------->         enddo
252.  1 G             !$omp end acc_loop
253.  1 G-----------> !$omp end acc_region
```

Legend to Compiler Notes

```
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 - fused
     G - Accelerated            g - partitioned
     I - Inlined                i - interchanged
     M - Multithreaded          m - partitioned
                                n - non-blocking remote transfer
                                p - partial
                                r - unrolled
                                s - shortloop
     V - Vectorized             w - unwound
```

And a little restructuring

```
!$omp acc_region num_pes(2:512)
!$omp acc_loop collapse(3)
    do k = 1,nz
     do j=1,ny
       do i = 1,nx
           grad_T(i,j,k,1) = -lambda(i,j,k) * grad_T(i,j,k,1)
           grad_T(i,j,k,2) = -lambda(i,j,k) * grad_T(i,j,k,2)
           grad_T(i,j,k,3) = -lambda(i,j,k) * grad_T(i,j,k,3)
           t_1=diffFlux(i,j,k,n_spec,1)
           t_2=diffFlux(i,j,k,n_spec,2)
           t_3=diffFlux(i,j,k,n_spec,3)
         SPECIES: do n=1,n_spec
           if(n < n_spec) then
             diffFlux(i,j,k,n,1) = - Ds_mixavg(i,j,k,n) * ( grad_Ys(i,j,k,n,1)  &
                                   + yspecies(i,j,k,n) * grad_mixMW(i,j,k,1) )
             diffFlux(i,j,k,n,2) = - Ds_mixavg(i,j,k,n) * ( grad_Ys(i,j,k,n,2)  &
                                   + yspecies(i,j,k,n) * grad_mixMW(i,j,k,2) )
             diffFlux(i,j,k,n,3) = - Ds_mixavg(i,j,k,n) * ( grad_Ys(i,j,k,n,3)  &
                                   + yspecies(i,j,k,n) * grad_mixMW(i,j,k,3) )
             t_1 = t_1 - diffFlux(i,j,k,n,1)
             t_2 = t_2 - diffFlux(i,j,k,n,2)
             t_3 = t_3 - diffFlux(i,j,k,n,3)
           end if
           grad_T(i,j,k,1) = grad_T(i,j,k,1) + h_spec(i,j,k,n)*diffFlux(i,j,k,n,1)
           grad_T(i,j,k,2) = grad_T(i,j,k,2) + h_spec(i,j,k,n)*diffFlux(i,j,k,n,2)
           grad_T(i,j,k,3) = grad_T(i,j,k,3) + h_spec(i,j,k,n)*diffFlux(i,j,k,n,3)
         enddo SPECIES
         diffFlux(i,j,k,n_spec,1) = t_1
         diffFlux(i,j,k,n_spec,2) = t_2
         diffFlux(i,j,k,n_spec,3) = t_3
       enddo
     enddo
    enddo
!$omp end acc_loop
!$omp end acc_region
```

What the Compiler Shows

```
219.  1 G----------< !$omp acc_region num_pes(2:512)
220.  1 G            !$omp acc_loop collapse(3)
221.  1 G C--------<     do k = 1,nz
222.  1 G C C------<      do j=1,ny
223.  1 G C C g----<        do i = 1,nx
224.  1 G C C g                 grad_T(i,j,k,1) = -lambda(i,j,k) * grad_T(i,j,k,1)
225.  1 G C C g                 grad_T(i,j,k,2) = -lambda(i,j,k) * grad_T(i,j,k,2)
226.  1 G C C g                 grad_T(i,j,k,3) = -lambda(i,j,k) * grad_T(i,j,k,3)
228.  1 G C C g                 t_1=diffFlux(i,j,k,n_spec,1)
229.  1 G C C g                 t_2=diffFlux(i,j,k,n_spec,2)
230.  1 G C C g                 t_3=diffFlux(i,j,k,n_spec,3)
232.  1 G C C g 6--<          SPECIES: do n=1,n_spec
234.  1 G C C g 6               if(n < n_spec) then
235.  1 G C C g 6                 diffFlux(i,j,k,n,1) = - Ds_mixavg(i,j,k,n) * ( grad_Ys(i,j,k,n,1)  &
236.  1 G C C g 6                                     + yspecies(i,j,k,n) * grad_mixMW(i,j,k,1) )
237.  1 G C C g 6                 diffFlux(i,j,k,n,2) = - Ds_mixavg(i,j,k,n) * ( grad_Ys(i,j,k,n,2)  &
238.  1 G C C g 6                                     + yspecies(i,j,k,n) * grad_mixMW(i,j,k,2) )
239.  1 G C C g 6                 diffFlux(i,j,k,n,3) = - Ds_mixavg(i,j,k,n) * ( grad_Ys(i,j,k,n,3)  &
240.  1 G C C g 6                                     + yspecies(i,j,k,n) * grad_mixMW(i,j,k,3) )
242.  1 G C C g 6                 t_1 = t_1 - diffFlux(i,j,k,n,1)
243.  1 G C C g 6                 t_2 = t_2 - diffFlux(i,j,k,n,2)
244.  1 G C C g 6                 t_3 = t_3 - diffFlux(i,j,k,n,3)
246.  1 G C C g 6               end if
248.  1 G C C g 6               grad_T(i,j,k,1) = grad_T(i,j,k,1) + h_spec(i,j,k,n)*diffFlux(i,j,k,n,1)
249.  1 G C C g 6               grad_T(i,j,k,2) = grad_T(i,j,k,2) + h_spec(i,j,k,n)*diffFlux(i,j,k,n,2)
250.  1 G C C g 6               grad_T(i,j,k,3) = grad_T(i,j,k,3) + h_spec(i,j,k,n)*diffFlux(i,j,k,n,3)
251.  1 G C C g 6
252.  1 G C C g 6-->          enddo SPECIES
254.  1 G C C g               diffFlux(i,j,k,n_spec,1) = t_1
255.  1 G C C g               diffFlux(i,j,k,n_spec,2) = t_2
256.  1 G C C g               diffFlux(i,j,k,n_spec,3) = t_3
258.  1 G C C g---->        enddo
259.  1 G C C------>      enddo
260.  1 G C-------->     enddo
261.  1 G            !$omp end acc_loop
262.  1 G----------> !$omp end acc_region
```

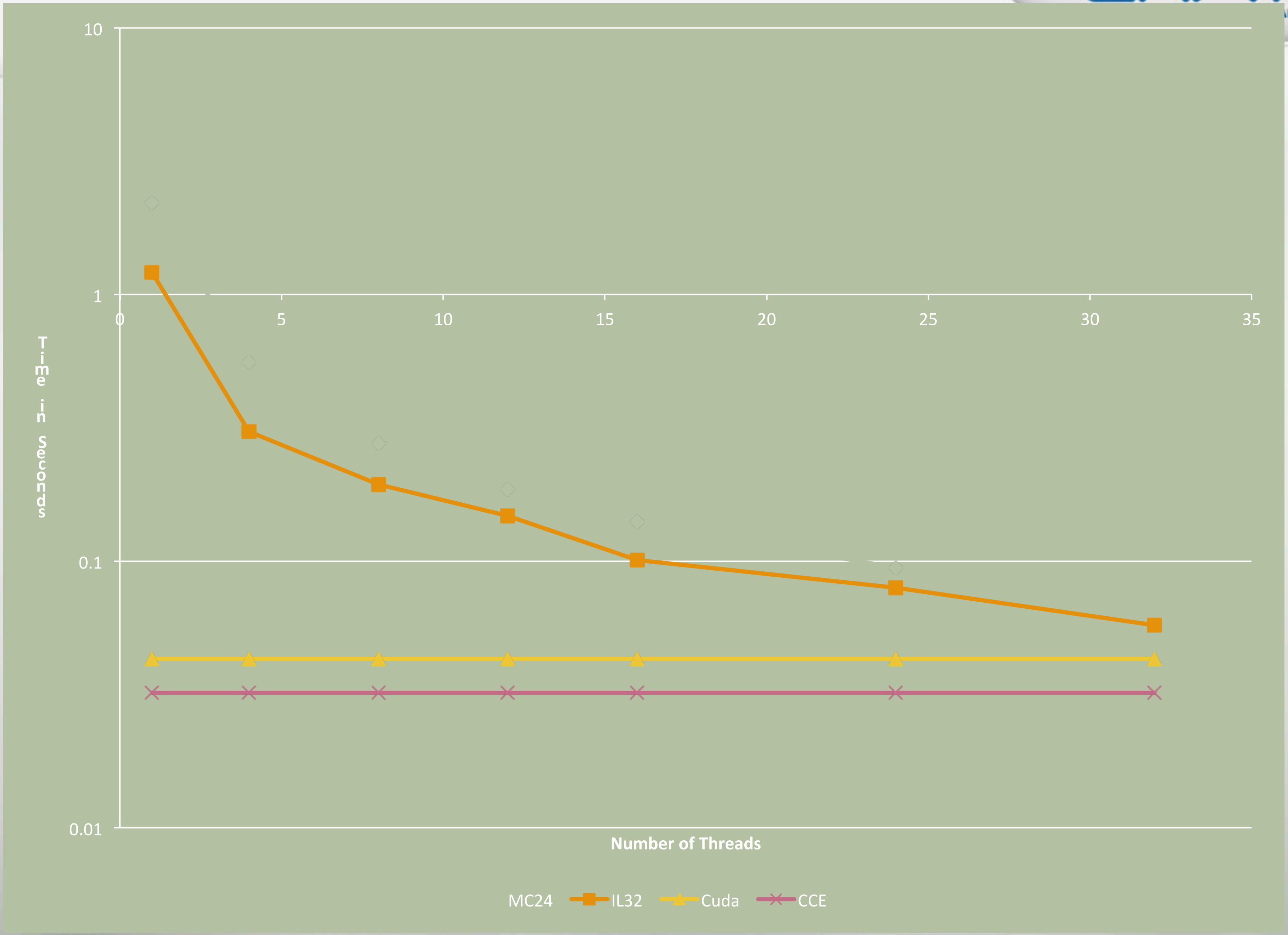
And the timings
Ignoring Data Transfer*

	Original OpenMP Across entire node	Cuda Fortran	Directive Approach	Directive Approach Restructured
Kernel Only	.0417 Seconds	.0061 Seconds	.0113 Seconds	.0067 Seconds

* In S3D all of the arrays used in this computation will reside on the Accelerator prior to the invocation of the kernel.

Ease of Use

Kernel	Lines of Code	Cuda lines of Code Added or changed	Lines of Code added or changed for directives	Directive lines of Code added
Comp_heat	65	45	0	4
Comp_heat (opt)	65	45	9	4
Getrates	5869	6362	0	4
Divergent_sphere	89	44	0	4
Gradient_sphere	45	42	0	4


10
1
0.1
0.01
0
5
10
15
20
25
30
35
Time in Seconds
Number of Threads
MC24
IL32
Cuda
CCE

Converting the MPI application to a Hybrid OpenMP/MPI application

Task 1 – Identification of potential accelerator kernels

- Identify high level computational structures that account for a significant amount of time (95-99%)
  - To do this, one must obtain global runtime statistics of the application
    - High level call tree with subroutines and DO loops showing inclusive/exclusive time, min, max, average iteration counts.
- Tools that will be needed
  - Advanced instrumentation to measure
    - DO loop statistics, iteration counts, inclusive time
    - Routine level sampling and profiling

Gathering High Level looping statistics

```
Table 1:  Profile by Function Group and Function

 Time%   |      Time   |      Imb.  |  Imb.   | Calls   |Group
         |             |      Time  | Time%   |         | Function
         |             |            |         |         |  PE=HIDE
         |             |            |         |         |   Thread=HIDE

 100.0% | 96.774934 |        -- |     -- | 6083.9 |Total
|---------------------------------------------------------------------------------
| 100.0% | 96.766637 |        -- |     -- | 6056.9 |USER
||--------------------------------------------------------------------------------
||  18.7% | 18.125552 | 15.748098 |  49.6% |  200.0 |streaming_.LOOPS
||  16.4% | 15.904828 |  5.941168 |  29.0% |  200.0 |recolor_.LOOP@li.723
||  11.3% | 10.909372 |  0.428680 |   4.0% |    1.0 |initmpi_.LOOP@li.313
||   9.9% |  9.614664 |  0.047006 |   0.5% |    1.0 |read_parallel_.LOOPS
||   8.5% |  8.220680 |  3.385983 |  31.1% |  200.0 |streaming_.LOOP@li.774
||   7.9% |  7.622818 |  1.101631 |  13.5% |  200.0 |streaming_exchange_.LOOPS
||   4.9% |  4.699645 |  1.298570 |  23.1% |  200.0 |collisiona_.LOOP@li.456
||   4.4% |  4.257534 |  1.162477 |  22.9% |  200.0 |collisionb_.LOOP@li.607
||   3.8% |  3.637698 |  0.803541 |  19.3% |  201.0 |cal_velocity_.LOOP@li.874
||   3.5% |  3.421273 |  0.450034 |  12.4% |  200.0 |wall_boundary_.LOOP@li.802
||   2.2% |  2.119447 |  5.224182 |  75.9% |  201.0 |injection_.LOOPS
||   2.1% |  2.031823 |  2.732934 |  61.2% |  200.0 |collisionb_.LOOPS
||   1.3% |  1.252738 |  0.188434 |  13.9% |  201.0 |injection_.LOOP@li.967
```

```
Table 1:  Profile by Function and Callers

 Time%  |      Time  |    Calls  |Group
        |            |           | Function
        |            |           |  Caller
        |            |           |   PE=HIDE

 100.0% | 333.310995 | 120405.1 |Total
|----------------------------------------------------------------------
|  96.0% | 320.005729 |  99841.2 |USER
||---------------------------------------------------------------------
||  90.0% | 299.917011 |   2000.0 |compute_forces_elastic_dev_.LOOPS
3|        |            |          | compute_forces_elastic_dev_
4|        |            |          |  compute_forces_elastic_.LOOPS
5|        |            |          |   compute_forces_elastic_
6|        |            |          |    iterate_time_.LOOPS
7|        |            |          |     iterate_time_
8|        |            |          |      specfem3d_
9|        |            |          |       xspecfem3d_
||   2.2% |   7.348773 |   1000.0 |it_update_displacement_scheme_.LOOPS
3|        |            |          | it_update_displacement_scheme_
4|        |            |          |  iterate_time_.LOOPS
5|        |            |          |   iterate_time_
6|        |            |          |    specfem3d_
7|        |            |          |     xspecfem3d_
||   1.8% |   6.030917 |   1000.0 |compute_forces_elastic_.LOOPS
3|        |            |          | compute_forces_elastic_
4|        |            |          |  iterate_time_.LOOPS
5|        |            |          |   iterate_time_
6|        |            |          |    specfem3d_
7|        |            |          |     xspecfem3d_
||   0.9% |   2.843254 |      1.0 |locate_receivers_.LOOPS
3|        |            |          | locate_receivers_
4|        |            |          |  setup_receivers_.LOOPS
5|        |            |          |   setup_receivers_
6|        |            |          |    setup_sources_receivers_
7|        |            |          |     specfem3d_
8|        |            |          |      xspecfem3d_
||   0.4% |   1.477712 |      1.0 |write_vtk_data_elem_l_.LOOPS
3|        |            |          | write_vtk_data_elem_l_
4|        |            |          |  rmd_setup_inner_outer_elemnts_.LOOPS
5|        |            |          |   rmd_setup_inner_outer_elemnts_
6|        |            |          |    read_mesh_databases_
7|        |            |          |     specfem3d_
8|        |            |          |      xspecfem3d_
```

Gathering High Level looping statistics

```
Table 2:  Loop Stats from -hprofile_generate

   Loop |  Loop Incl |  Loop Incl | Loop Hit |Loop Trips |    Loop |Function=/.LOOP\.
|-----------------------------------------------------------------------------------
|  86.0% | 464.222802 | 464.222802 |        1 |     200.0 |   novec |lbm3d2p_d_.LOOP.4.li.118
|   9.0% |  48.424200 |   0.242121 |      200 |      34.0 |   novec |recolor_.LOOP.0.li.722
|   6.8% |  36.439476 |   0.000455 |    80000 |     101.0 |   novec |recolor_.LOOP.1.li.723
|   6.7% |  36.394050 |   0.000005 |  8080000 |     101.0 |   novec |recolor_.LOOP.2.li.724
|   5.6% |  30.165525 |   0.000001 | 21111225 |      15.0 |   novec |recolor_.LOOP.3.li.744
|   4.6% |  24.770886 |   0.123854 |      200 |      14.0 |   novec |recolor_.LOOP.0.li.773
|   4.5% |  24.500305 |   0.122502 |      200 |      34.0 |   novec |collisionb_.LOOP.5.li.606
|   4.4% |  23.493726 |   0.117469 |      200 |      34.0 |   novec |wall_boundary_.LOOP.0.li.801
|   4.3% |  23.470821 |   0.116770 |      201 |      34.0 |   novec |injection_.LOOP.0.li.966
|   4.3% |  23.415045 |   0.116493 |      201 |      34.0 |   novec |cal_velocity_.LOOP.0.li.873
|   4.3% |  23.307203 |   0.116536 |      200 |      34.0 |   novec |collisiona_.LOOP.0.li.455
|   4.3% |  23.256005 |   0.116280 |      200 |      34.0 |   novec |collisionb_.LOOP.0.li.570
|   3.5% |  18.858521 |  18.858521 |        1 |     400.0 |   novec |read_parallel_.LOOP.0.li.854
|   2.8% |  15.080327 |   0.037701 |      400 | 1014776.0 |   novec |recolor_.LOOP.1.li.774
|   1.5% |   8.200184 |   0.000103 |    80000 |     101.0 |   novec |collisiona_.LOOP.1.li.456
|   1.5% |   8.148148 |   0.000001 |  8080000 |     101.0 |   novec |collisiona_.LOOP.2.li.457
|   1.4% |   7.553060 |   0.000094 |    80000 |     101.0 |   novec |collisionb_.LOOP.6.li.607
|   1.4% |   7.489768 |   0.000001 |  8080000 |     101.0 | sunwind |collisionb_.LOOP.7.li.608
|   1.2% |   6.399606 |   0.000080 |    80400 |     101.0 |   novec |cal_velocity_.LOOP.1.li.874
|   1.2% |   6.344608 |   0.000001 |  8120400 |     101.0 | sunwind |cal_velocity_.LOOP.2.li.875
|   1.2% |   6.229104 |   0.000078 |    80000 |     101.0 |   novec |wall_boundary_.LOOP.1.li.802
|   1.1% |   6.145206 |   0.000001 |  8080000 |     101.0 | sunwind |wall_boundary_.LOOP.2.li.803
```

Current benchmark we are working

```
    do ii=1,ntimes
        if(ip == 0) then
          print *, 'step = ',ii*npasses
        endif

        do jj=1,npasses
          if(ip == 0) then
            write(*,*) '********** step = **********',((ii-1)*npasses)+jj
          endif
          call set_boundary_macro_press2
          call set_boundary_micro_press
          call collisiona
          call collisionb
          call recolor
          call streaming
          call wall_boundary
          call cal_velocity
          call injection
        end do

        etime = mpi_wtime()
        call saturation

      end do
```

Task 2 Parallel Analysis, Scoping and Vectorization

- Investigate parallelizability of high level looping structures
  - Often times one level of loop is not enough, must have several parallel loops
  - User must understand what high level DO loops are in fact independent.
  - Without tools, variable scoping of high level loops is very difficult
    - Loops must be more than independent, their variable usage must adhere to private data local to a thread or global shared across all the threads
- Investigate vectorizability of lower level Do loops
  - Cray compiler has been vectorizing complex codes for over 30 years

Task 2 Parallel Analysis and Scoping

- Tools that will be needed
  - Whole program analysis scoping tool with User interaction
    - The compiler performs an initial parallelization analysis to identify obvious inhibitors to parallelization
    - The User instructs the compiler to ignore various inhibitors if possible
    - The compiler performs an initial scoping analysis and presents the User with concerns with array usage
    - The User works with the environment to trace variables through the high level looping structure, works with the compiler to scope the variables in question.
  - Vectorization Feedback from the Compiler
    - Tremendous experience from years of vector architectures

Lets scope out the potential OpenMP loops

```
-- Loop starting at line 221
auto shared(cell,local_lx,local_ly,lz,rho,uxyz)
-- Loop starting at line 262
auto shared(b,cell,local_lx,local_ly,lz,r,rho,uxyz)
-- Loop starting at line 438
auto shared(b,cell,local_lx,local_ly,lz,r,rho,uxyz)
-- Loop starting at line 558
auto shared(cell,grad,local_lx,local_ly,lz,rho,wet)
-- Loop starting at line 572
auto shared(cell,grad,local_lx,local_ly,lz,wet)
-- Loop starting at line 591
auto shared
(b,cell,ci1,ci10,ci11,ci12,ci13,ci14,ci2,ci3,ci4,ci5,ci6,ci7,ci8,ci9,grad,
        local_lx,local_ly,lz)
-- Loop starting at line 712
auto firstprivate(crit,icrit)
auto shared(b,cell,cix,ciy,ciz,local_lx,local_ly,lz,r,rho,uxyz)

msg-obj: fi FAIL -- Value/Shared Scope Conflict.

-- Loop starting at line 784
auto shared(b,index,index_max,r)
-- Loop starting at line 812
auto shared(b,cell,local_lx,local_ly,lz,r)
-- Loop starting at line 965
auto shared(b,cell,local_lx,local_ly,lz,r,rho,uxyz)
-- Loop starting at line 1125
auto shared(b,bbar,blue,cell,local_lx,local_ly,lz,r,rbar,red,rho,surf)
auto reduction(+:bbar,+:rbar)
```

Vectorization Problem in recolor – call to maxloc

```
723.   1-----------<   do k=0,lz-1
724.   1 2---------<     do j=0,local_ly-1
725.   1 2 3-------<       do i=0,local_lx-1
726.   1 2 3                 if (cell(i,j,k)==0) then
727.   1 2 3                    fi(0) =  r0(i,j,k) +  b0(i,j,k)
728.   1 2 3                    fi(1) =  r1(i,j,k) +  b1(i,j,k)
729.   1 2 3                    fi(2) =  r2(i,j,k) +  b2(i,j,k)
742.   1 2 3
743.   1 2 3 Vw---<>             crit(1:15) = (cix(0:14)*fx(i,j,k)+ciy(0:14)*fy(i,j,k)+&
744.   1 2 3                                  ciz(0:14)*fz(i,j,k))
745.   1 2 3 4-----<             do l=0,14
746.   1 2 3 4 w--<>               max_loc      = maxloc(crit)
747.   1 2 3 4                     mm           = max_loc(1)
748.   1 2 3 4                     crit(mm)     = worst_value
749.   1 2 3 4                     mm           = mm-1
750.   1 2 3 4                     frac_r       = max(0.0d0,min(rho_r(i,j,k),fi(mm)))
751.   1 2 3 4                     rho_r(i,j,k) = rho_r(i,j,k)-frac_r
752.   1 2 3 4
753.   1 2 3 4                     R(i,j,k,mm) = frac_r
754.   1 2 3 4                     B(i,j,k,mm) = fi(mm) - R(i,j,k,mm)
755.   1 2 3 4----->             end do
756.   1 2 3                   end if
757.   1 2 3------->         end do
758.   1 2--------->       end do
759.   1----------->     end do
```

Recolor Routine – now vectorized

```
do k=0,lz-1
   do j=0,local_ly-1
     do i=0,local_lx-1
       crit(i,:)=0.0
       icrit(i,:) = 0
       if (cell(i,j,k)==0) then
          o o o
       do iii = 1,14
        do ii = 1,14
          if(crit(i,ii).gt.crit(i,ii+1))then
          crit_temp = crit(i,ii+1)
          icrit_temp = icrit(i,ii+1)
          crit(i,ii+1)=crit(i,ii)
          icrit(i,ii+1) = icrit(i,ii)
          crit(i,ii)=crit_temp
          icrit(i,ii) = icrit_temp
          endif
        enddo
        enddo

        do ii = 15,1,-1
           mm            = icrit(i,ii)-1
           frac_r        = max(0.0d0,min(rho(2,i,j,k),fi(i,mm)))
           rho(2,i,j,k)  = rho(2,i,j,k)-frac_r
```

Using directives to give the compiler information

- Developing efficient OpenMP regions is not an easy task; however, the performance will definitely be worth the effort
- Compilation of OpenMP regions to accelerator by the compiler is approaching the performance of hand-coded CUDA or OpenCL with the advantage that it results in portable code. And it will only get better.
  - With OpenMP extensions targeting accelerators, data transfers between multi-core socket and the accelerator can be optimized. Utilization of registers and shared memory can also be optimized
  - With OpenMP extensions targeting accelerators, user can control the utilization of the accelerator memory and functional units.
- These directives are currently being discussed by a subgroup of the OpenMP committee which includes Cray, PGI,IBM,Intel

Now we start adding directives -recolor

```
!$omp acc_region_loop private(mm,i,j,k,l,fi,crit,frac_r,ii,crit_max,crit_temp,
!$omp&                          icrit_temp,icrit,iii)
   do k=0,lz-1
    do j=0,local_ly-1
      do i=0,local_lx-1
        crit(i,:)=0.0
        icrit(i,:) = 0
        if (cell(i,j,k)==0) then
           fi(i,0) =  r(i,j,k,0) +  b(i,j,k,0)
           fi(i,1) =  r(i,j,k,1) +  b(i,j,k,1)
           fi(i,2) =  r(i,j,k,2) +  b(i,j,k,2)
           fi(i,3) =  r(i,j,k,3) +  b(i,j,k,3)
           fi(i,4) =  r(i,j,k,4) +  b(i,j,k,4)
           fi(i,5) =  r(i,j,k,5) +  b(i,j,k,5)
           fi(i,6) =  r(i,j,k,6) +  b(i,j,k,6)
           fi(i,7) =  r(i,j,k,7) +  b(i,j,k,7)
           fi(i,8) =  r(i,j,k,8) +  b(i,j,k,8)
           fi(i,9) =  r(i,j,k,9) +  b(i,j,k,9)
           fi(i,10) = r(i,j,k,10) + b(i,j,k,10)
```

Now we start adding directives -collisionb

```
!$omp acc_region_loop private(k,j,i,fx_tmp,fy_tmp,fz_tmp,cif2)
  do k=0,lz-1
    do j=0,local_ly-1
      do i=0,local_lx-1
       fx_tmp = 0.0d0
       fy_tmp = 0.0d0
       fz_tmp = 0.0d0
        if (cell(i,j,k)==0) then
          fx_tmp =grad(i+1,j   ,k   )-grad(i-1,j   ,k   )&
                 +grad(i+1,j+1,k+1)-grad(i-1,j+1,k+1)&
                 +grad(i+1,j-1,k+1)+grad(i+1,j+1,k-1)&
                 -grad(i-1,j-1,k-1)+grad(i+1,j-1,k-1)&
                 -grad(i-1,j+1,k-1)-grad(i-1,j-1,k+1)
          fy_tmp =grad(i   ,j+1,k   )-grad(i   ,j-1,k   )&
                 +grad(i+1,j+1,k+1)+grad(i-1,j+1,k+1)&
                 -grad(i+1,j-1,k+1)+grad(i+1,j+1,k-1)&
                 -grad(i-1,j-1,k-1)-grad(i+1,j-1,k-1)&
                 +grad(i-1,j+1,k-1)-grad(i-1,j-1,k+1)
          fz_tmp =grad(i   ,j   ,k+1)-grad(i   ,j   ,k-1)&
                 +grad(i+1,j+1,k+1)+grad(i-1,j+1,k+1)&
                 +grad(i+1,j-1,k+1)-grad(i+1,j+1,k-1)&
                 -grad(i-1,j-1,k-1)-grad(i+1,j-1,k-1)&
```

Task 3 Correctness Debugging

- Run transformed application on the accelerator and investigate the correctness and performance
  - Run as OpenMP application on multi-core socket
    - Use multi-core socket Debugger - DDT
  - Run as Hybrid multi-core application across multi-core socket and accelerator
- Tools That will be needed
  - Information that was supplied by the directives/user's interaction with the compiler

Task 4 Fine tuning of accelerated program

- Understand current performance bottlenecks
  - Is data transfer between multi-core socket and accelerator a bottleneck?
  - Is shared memory and registers on the accelerator being used effectively?
  - Is the accelerator code utilizing the MIMD parallel units?
    - Is the shared memory parallelization load balanced?
  - Is the low level accelerator code vectorized?
    - Are the memory accesses effectively utilizing the memory bandwidth?

Task 4 Fine tuning of accelerated program

- Tools that will be needed:
  - Compiler feedback on parallelization and vectorization of input application
  - Hardware counter information from the accelerator to identify bottlenecks in the execution of the application.
    - Information on memory utilization
    - Information on performance of SIMT units

Several other vendors are supplying similar performance gathering tools

Useful tools contd.

- Craypat profiling
  - Tracing: "pat_build -u <executable>" (can do APA sampling first)
  - "pat_report -O accelerator <.xf file>"; -T also useful
    - Other pat_report tables (as of perftools/5.2.1.7534)

acc_fu	flat table of accelerator events
acc_time	call tree sorted by accelerator time
acc_time_fu	flat table of accelerator events sorted by accelerator time
acc_show_by_ct	regions and events by calltree sorted alphabetically

Run and gather runtime statistics

```
Table 1:  Profile by Function Group and Function

 Time %  |       Time |Imb. Time |   Imb.  | Calls  |Group
         |            |          | Time %  |        | Function
         |            |          |         |        |  PE='HIDE'
         |            |          |         |        |   Thread='HIDE'

 100.0% | 83.277477 |       -- |     -- | 851.0 |Total
|------------------------------------------------------------------
|  51.3% | 42.762837 |       -- |     -- | 703.0 |ACCELERATOR
||-----------------------------------------------------------------
||  18.8% | 15.672371 | 1.146276 |   7.3% |  20.0 |recolor_.SYNC_COPY@li.790←not good
||  16.3% | 13.585707 | 0.404190 |   3.1% |  20.0 |recolor_.SYNC_COPY@li.793←not good
||   7.5% |  6.216010 | 0.873830 |  13.1% |  20.0 |lbm3d2p_d_.ASYNC_KERNEL@li.116
||   1.6% |  1.337119 | 0.193826 |  13.5% |  20.0 |lbm3d2p_d_.ASYNC_KERNEL@li.119
||   1.6% |  1.322690 | 0.059387 |   4.6% |   1.0 |lbm3d2p_d_.ASYNC_COPY@li.100
||   1.0% |  0.857149 | 0.245369 |  23.7% |  20.0 |collisionb_.ASYNC_KERNEL@li.586
||   1.0% |  0.822911 | 0.172468 |  18.5% |  20.0 |lbm3d2p_d_.ASYNC_KERNEL@li.114
||   0.9% |  0.786618 | 0.386807 |  35.2% |  20.0 |injection_.ASYNC_KERNEL@li.1119
||   0.9% |  0.727451 | 0.221332 |  24.9% |  20.0 |lbm3d2p_d_.ASYNC_KERNEL@li.118
```

Keep data on the accelerator with acc_data region

```
!$omp acc_data acc_copyin(cix,ci1,ci2,ci3,ci4,ci5,ci6,ci7,ci8,ci9,ci10,ci11,&
!$omp& ci12,ci13,ci14,r,b,uxyz,cell,rho,grad,index_max,index,&
!$omp& ciy,ciz,wet,np,streaming_sbuf1, &
!$omp&    streaming_sbuf1,streaming_sbuf2,streaming_sbuf4,streaming_sbuf5,&
!$omp&    streaming_sbuf7s,streaming_sbuf8s,streaming_sbuf9n,streaming_sbuf10s,&
!$omp&    streaming_sbuf11n,streaming_sbuf12n,streaming_sbuf13s,streaming_sbuf14n,&
!$omp&    streaming_sbuf7e,streaming_sbuf8w,streaming_sbuf9e,streaming_sbuf10e,&
!$omp&    streaming_sbuf11w,streaming_sbuf12e,streaming_sbuf13w,streaming_sbuf14w, &
!$omp&    streaming_rbuf1,streaming_rbuf2,streaming_rbuf4,streaming_rbuf5,&
!$omp&    streaming_rbuf7n,streaming_rbuf8n,streaming_rbuf9s,streaming_rbuf10n,&
!$omp&    streaming_rbuf11s,streaming_rbuf12s,streaming_rbuf13n,streaming_rbuf14s,&
!$omp&    streaming_rbuf7w,streaming_rbuf8e,streaming_rbuf9w,streaming_rbuf10w,&
!$omp&    streaming_rbuf11e,streaming_rbuf12w,streaming_rbuf13e,streaming_rbuf14e, &
!$omp&    send_e,send_w,send_n,send_s,recv_e,recv_w,recv_n,recv_s)
  do ii=1,ntimes
         o o o
      call set_boundary_macro_press2
      call set_boundary_micro_press
      call collisiona
      call collisionb
      call recolor
```

Now when we do communication we have to update the host

```
!$omp acc_region_loop private(k,j,i)
  do j=0,local_ly-1
    do i=0,local_lx-1
      if (cell(i,j,0)==1) then
        grad (i,j,-1) = (1.0d0-wet)*db*press
      else
        grad (i,j,-1) = db*press
      end if
      grad (i,j,lz)   = grad(i,j,lz-1)
    end do
  end do
!$omp end acc_region_loop
!$omp acc_update host(grad)
  call mpi_barrier(mpi_comm_world,ierr)
  call grad_exchange
!$omp acc_update acc(grad)
```

But we would rather not send the entire grad array back – how about

Packing the buffers on the accelerator

```
!$omp acc_data present(grad,recv_w,recv_e,send_e,send_w,recv_n,&
!$omp&                recv_s,send_n,send_s)
!$omp acc_region_loop
      do k=-1,lz
        do j=-1,local_ly
          send_e(j,k) = grad(local_lx-1,j        ,k)
          send_w(j,k) = grad(0         ,j        ,k)
        end do
      end do
!$omp end acc_region_loop
!$omp acc_update host(send_e,send_w)
      call mpi_irecv(recv_w, bufsize(2),mpi_double_precision,w_id, &
           tag(25),mpi_comm_world,irequest_in(25),ierr)
          o  o  o
      call mpi_isend(send_w, bufsize(2),mpi_double_precision,w_id, &
           tag(26),& mpi_comm_world,irequest_out(26),ierr)
      call mpi_waitall(2,irequest_in(25),istatus_req,ierr)
      call mpi_waitall(2,irequest_out(25),istatus_req,ierr)
!$omp acc_update acc(recv_e,recv_w)
!$omp acc_region
!$omp acc_loop
      do k=-1,lz
        do j=-1,local_ly
          grad(local_lx  ,j        ,k) = recv_e(j,k)
          grad(-1        ,j        ,k) = recv_w(j,k)
```

Final Profile - bulk of time in kernel execution

```
 |  37.9% | 236.592782 |        -- |     -- | 11403.0 |ACCELERATOR
||-------------------------------------------------------------------
||  15.7% |  98.021619 | 43.078137 |  31.0% |   200.0 |lbm3d2p_d_.ASYNC_KERNEL@li.129
||   3.7% |  23.359080 |  2.072147 |   8.3% |   200.0 |lbm3d2p_d_.ASYNC_KERNEL@li.127
||   3.6% |  22.326085 |  1.469419 |   6.3% |   200.0 |lbm3d2p_d_.ASYNC_KERNEL@li.132
||   3.0% |  19.035232 |  1.464608 |   7.3% |   200.0 |collisionb_.ASYNC_KERNEL@li.599
||   2.6% |  16.216648 |  3.505232 |  18.1% |   200.0 |lbm3d2p_d_.ASYNC_KERNEL@li.131
||   2.5% |  15.401916 |  8.093716 |  35.0% |   200.0 |injection_.ASYNC_KERNEL@li.1116
||   1.9% |  11.734026 |  4.488785 |  28.1% |   200.0 |recolor_.ASYNC_KERNEL@li.786
||   0.9% |   5.530201 |  2.132243 |  28.3% |   200.0 |collisionb_.SYNC_COPY@li.593
||   0.8% |   4.714995 |  0.518495 |  10.1% |   200.0 |collisionb_.SYNC_COPY@li.596
||   0.6% |   3.738615 |  2.986891 |  45.1% |   200.0 |collisionb_.ASYNC_KERNEL@li.568
||   0.4% |   2.656962 |  0.454093 |  14.8% |     1.0 |lbm3d2p_d_.ASYNC_COPY@li.100
||   0.4% |   2.489231 |  2.409892 |  50.0% |   200.0 |streaming_exchange_.ASYNC_COPY@li.810
||   0.4% |   2.487132 |  2.311190 |  48.9% |   200.0 |streaming_exchange_.ASYNC_COPY@li.625
||   0.2% |   1.322791 |  0.510645 |  28.3% |   200.0 |streaming_exchange_.SYNC_COPY@li.622
||   0.2% |   1.273771 |  0.288743 |  18.8% |   200.0 |streaming_exchange_.SYNC_COPY@li.574
||   0.2% |   1.212260 |  0.298053 |  20.0% |   200.0 |streaming_exchange_.SYNC_COPY@li.759
||   0.2% |   1.208250 |  0.422182 |  26.3% |   200.0 |streaming_exchange_.SYNC_COPY@li.806
||   0.1% |   0.696120 |  0.442372 |  39.5% |   200.0 |streaming_exchange_.ASYNC_KERNEL@li.625
||   0.1% |   0.624982 |  0.379697 |  38.4% |   200.0 |streaming_exchange_.ASYNC_KERNEL@li.525
```

Useful tools

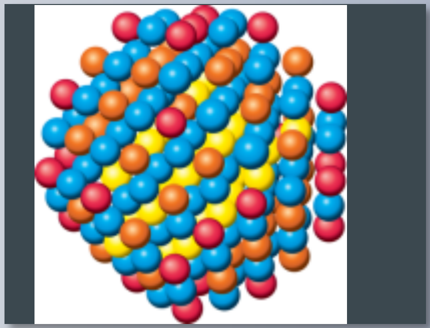
- Compiler feedback:
  - -ra to generate *.lst loopmark files (equivalent for C)
  - -rd to generate *.cg and *.opt files
    - *.cg useful to understand synchronisation points (CAF and ACC)
  - "ptxas -v *.ptx" gives information on register and shared memory usage (no way yet for user to adjust this)
- Runtime feedback (no recompilation needed)
  - "export CRAY_ACC_DEBUG=[1,2,3]" commentary to STDERR
  - NVIDIA compute profiler works with CUDA and directives
    - "export COMPUTE_PROFILE=1"
    - gives information on timings and occupancy in separate file
      - "more /opt/nvidia/cuda/<version>/doc/Compute_Profiler.txt" for documentation
      - Vince Graziano has a great script for summarising the output

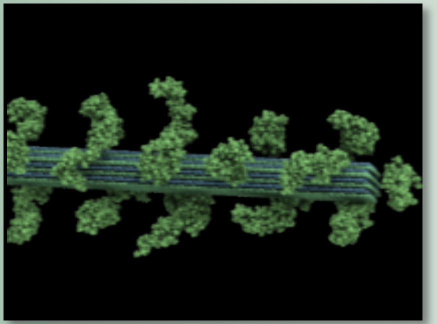
Cray GPU Programming Environment

- Objective: Enhance productivity related to porting applications to hybrid multi-core systems
- Four core components
  - Cray Statistics Gathering Facility on host and GPU
  - Cray Optimization Explorer – Scoping Tools (COE)
  - Cray Compilation Environment (CCE)
  - Cray GPU Libraries

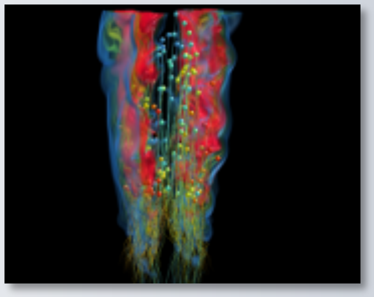
Titan: Early Science Applications

WL-LSMS
Role of material disorder, statistics, and fluctuations in nanoscale materials and systems.



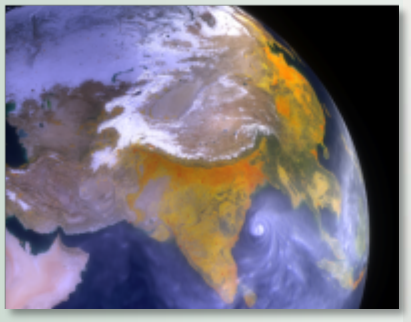


LAMMPS
Biofuels: An atomistic model of cellulose (blue) surrounded by lignin molecules comprising a total of 3.3 million atoms. Water not shown.

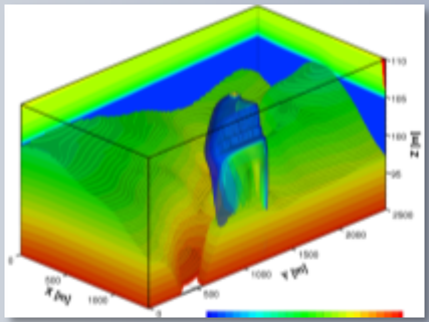


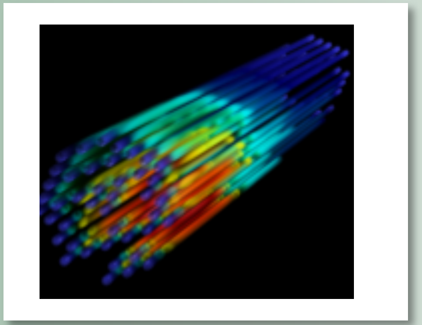
S3D
How are going to efficiently burn next generation diesel/bio fuels?
.

CAM / HOMME
Answer questions about specific climate change adaptation and mitigation scenarios; realistically represent features like precipitation patterns/statistics and tropical storms



PFLOTRAN
Stability and viability of large scale CO_2 sequestration; predictive containment groundwater transport

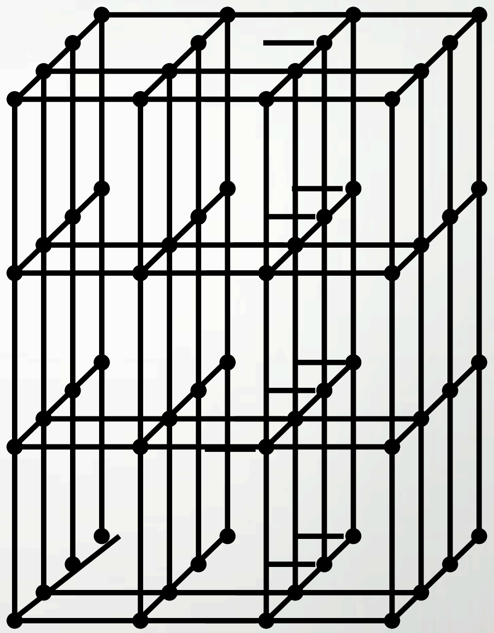




Denovo
Unprecedented high-fidelity radiation transport calculations that can be used in a variety of nuclear energy and technology applications.

S3D – A DNS solver

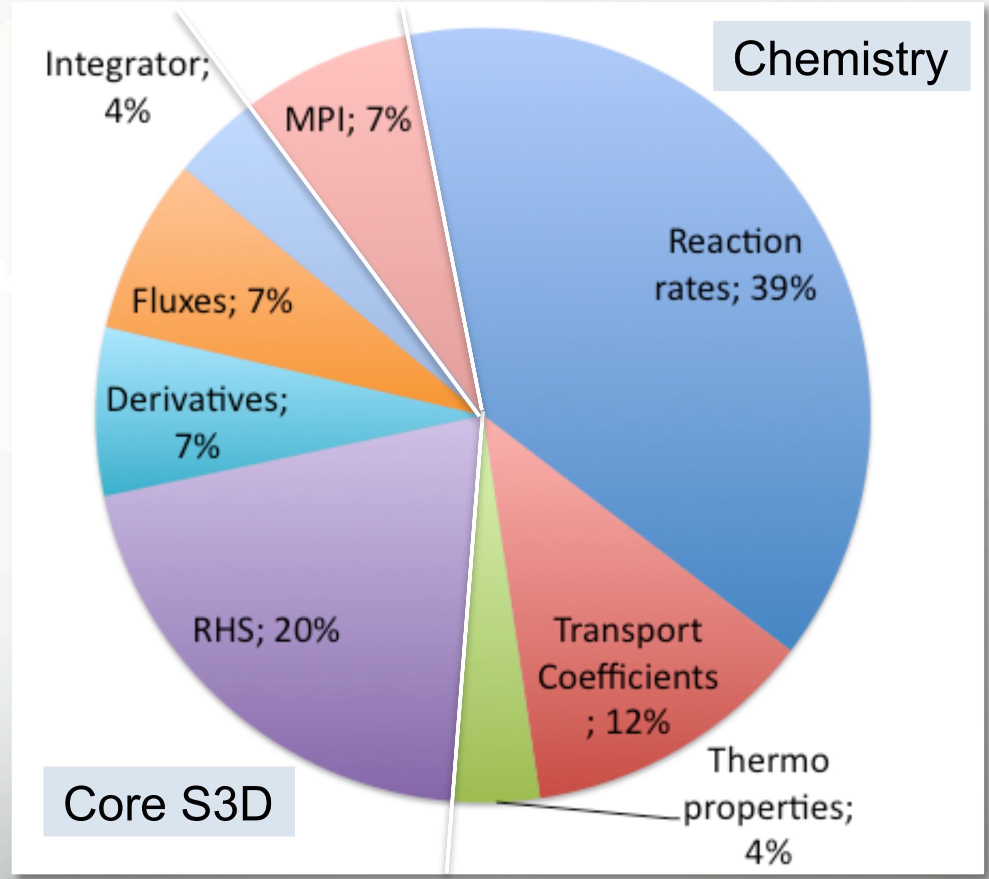
- Structured Cartesian mesh flow solver
- Solves compressible reacting Navier-Stokes, energy and species conservation equations.
  - 8th order explicit finite difference method
  - 4th order Runge-Kutta integrator with error estimator
- Detailed gas-phase thermodynamic, chemistry and molecular transport property evaluations
- Lagrangian particle tracking
- MPI-1 based spatial decomposition and parallelism
- Fortran code. Does not need linear algebra, FFT or solver libraries.



Developed and maintained at CRF, Sandia (Livermore) with BES and ASCR sponsorship. PI – Jacqueline H. Chen (jhchen@sandia.gov)

Benchmark Problem and Profile

- A benchmark problem was defined to closely resemble the target simulation
  - 52 species n-heptane chemistry and 48^3 grid points per node
    - 48^3 * 18,500 nodes = 2 billion grid points
    - Target problem would take two months on today's Jaguar
- Code was benchmarked and profiled on dual-hex core XT5
- Several kernels identified and extracted into stand-alone driver programs



Acceleration Strategy

Team:

Ramanan Sankaran	ORNL
Ray Grout	NREL
John Levesque	Cray

Goals:

- Convert S3D to a hybrid multi-core application suited for a multi-core node with or without an accelerator.
- Be able to perform the computation entirely on the accelerator.
  - Arrays and data able to reside entirely on the accelerator.
  - Data sent from accelerator to host CPU for halo communication, I/O and monitoring only.

Strategy:

- To program using both hand-written and generated code.
  - Hand-written and tuned CUDA*.
  - Automated Fortran and CUDA generation for chemistry kernels
  - Automated code generation through compiler directives
- S3D is now a part of Cray's compiler development test cases

Original S3D

		S3D		
Time Step		Solve_Drive		
Time Step	Runge K	Integrate		
Time Step	Runge K	RHS		
Time Step	Runge K		get mass fraction	I,j,k,n_spec loops
Time Step	Runge K		get_velocity	I,j,k,n_spec loops
Time Step	Runge K		calc_inv_avg	I,j,k,n_spec loops
Time Step	Runge K		calc_temp	I,j,k,n_spec loops
Time Step	Runge K		Compute Grads	I,j,k,n_spec loops
Time Step	Runge K		Diffusive Flux	I,j,k,n_spec loops
Time Step	Runge K		Derivatives	I,j,k,n_spec loops
Time Step	Runge K		reaction rates	I,j,k,n_spec loops

Profile from Original S3D

```
Table 1:  Profile by Function Group and Function

 Time%   |       Time   |     Imb.  |  Imb.   |       Calls   |Group
         |              |     Time  | Time%   |               | Function
         |              |           |         |               |  PE=HIDE
         |              |           |         |               |   Thread=HIDE

 100.0% | 284.732812 |       -- |     -- | 156348682.1 |Total
|------------------------------------------------------------------------------------------------
|  92.1% | 262.380782 |       -- |     -- | 155578796.1 |USER
||-----------------------------------------------------------------------------------------------
||  12.4% |  35.256420 | 0.237873 |   0.7% |    391200.0 |ratt_i_.LOOPS
||   9.6% |  27.354247 | 0.186752 |   0.7% |    391200.0 |ratx_i_.LOOPS
||   7.7% |  21.911069 | 1.037701 |   4.5% |   1562500.0 |mcedif_.LOOPS
||   5.4% |  15.247551 | 2.389440 |  13.6% |  35937500.0 |mceval4_
||   5.2% |  14.908749 | 4.123319 |  21.7% |       600.0 |rhsf_.LOOPS
||   4.7% |  13.495568 | 1.229034 |   8.4% |  35937500.0 |mceval4_.LOOPS
||   4.6% |  12.985353 | 0.620839 |   4.6% |       701.0 |calc_temp$thermchem_m_.LOOPS
||   4.3% |  12.274200 | 0.167054 |   1.3% |   1562500.0 |mcavis_new$transport_m_.LOOPS
||   4.0% |  11.363281 | 0.606625 |   5.1% |       600.0 |computespeciesdiffflux$transport_m_.LOOPS
||   2.9% |   8.257434 | 0.743004 |   8.3% |  21921875.0 |mixcp$thermchem_m_
||   2.9% |   8.150646 | 0.205423 |   2.5% |       100.0 |integrate_.LOOPS
||   2.4% |   6.942384 | 0.078555 |   1.1% |    391200.0 |qssa_i_.LOOPS
||   2.3% |   6.430820 | 0.481475 |   7.0% |  21921875.0 |mixcp$thermchem_m_.LOOPS
||   2.0% |   5.588500 | 0.343099 |   5.8% |       600.0 |computeheatflux$transport_m_.LOOPS
||   1.8% |   5.252285 | 0.062576 |   1.2% |    391200.0 |rdwdot_i_.LOOPS
||   1.7% |   4.801062 | 0.723213 |  13.1% |     31800.0 |derivative_x_calc_.LOOPS
||   1.6% |   4.461274 | 1.310813 |  22.7% |     31800.0 |derivative_y_calc_.LOOPS
||   1.5% |   4.327627 | 1.290121 |  23.0% |     31800.0 |derivative_z_calc_.LOOPS
||   1.4% |   3.963951 | 0.138844 |   3.4% |       701.0 |get_mass_frac$variables_m_.LOOPS
```

Restructured S3D for multi-core systems

		S3D	
Time Step		Solve_Drive	
Time Step	Runge K	Integrate	
Time Step	Runge K	RHS	
Time Step	Runge K	grid loop -OMP	get mass fraction
Time Step	Runge K	grid loop-OMP	get_velocity
Time Step	Runge K	grid loop-OMP	calc_inv_avg
Time Step	Runge K	grid loop-OMP	calc_temp
Time Step	Runge K	grid loop-OMP	Compute Grads
Time Step	Runge K	grid loop-OMP	Diffusive Flux
Time Step	Runge K	grid loop-OMP	Derivatives
Time Step	Runge K	grid loop-OMP	reaction rates

Statistics from running S3D

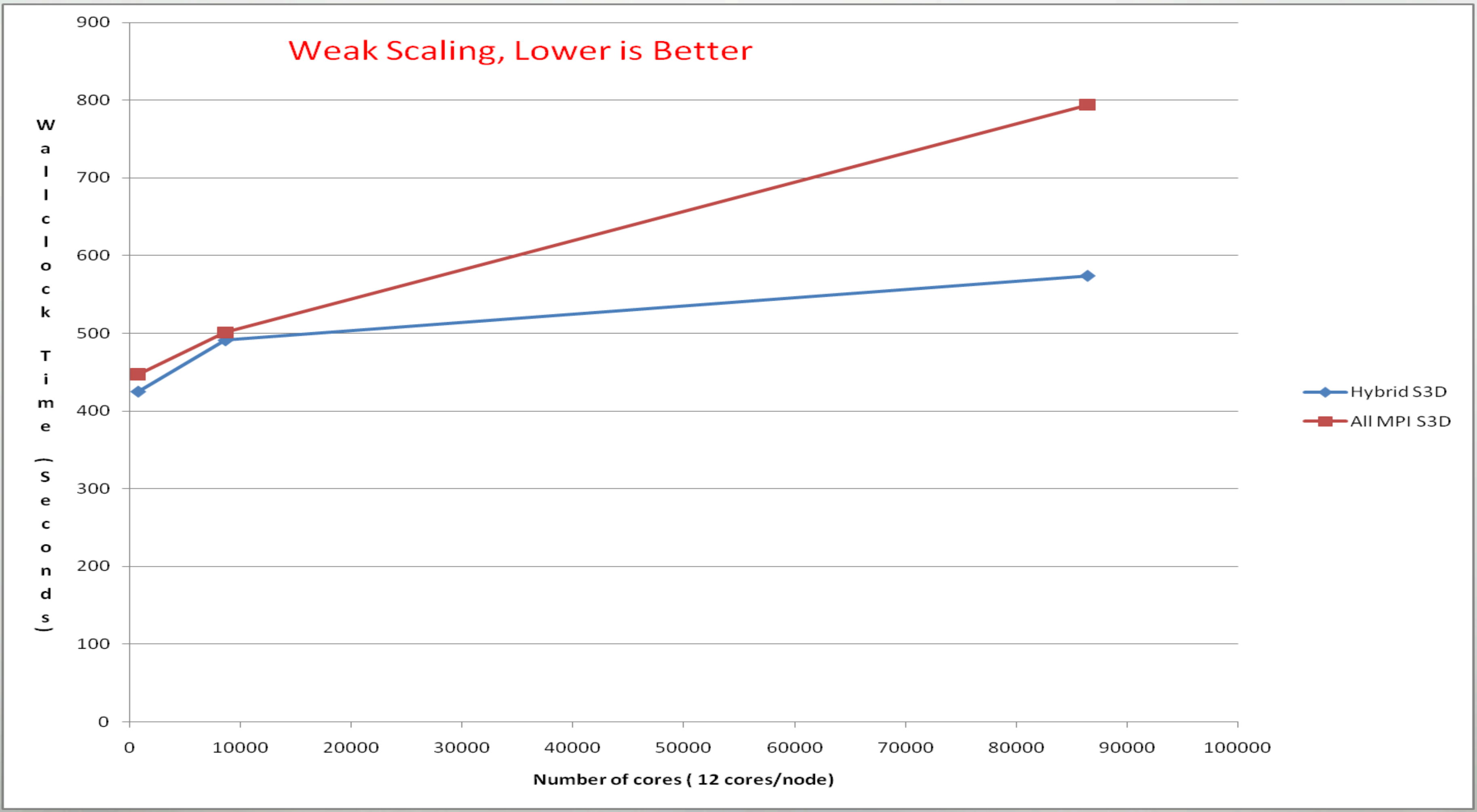
Table 1: Profile by Function Group and Function

```
   Time%  |       Time  |     Imb.  |  Imb.   |    Calls  |Group
          |             |     Time  | Time%   |           | Function|------------------------
    85.3% | 539.077983  |        -- |      -- |  144908.0 |USER
||-----------------------------------------------------------------------------------------------
-------------
||  21.7% | 136.950871 | 0.583731 |   0.5% |     600.0 |rhsf_
||  14.7% |  93.237279 | 0.132829 |   0.2% |     600.0 |rhsf_.LOOP@li.1084
||   8.7% |  55.047054 | 0.309278 |   0.6% |     600.0 |rhsf_.LOOP@li.1098
||   6.3% |  40.129463 | 0.265153 |   0.8% |     100.0 |integrate_
||   5.8% |  36.647080 | 0.237180 |   0.7% |     600.0 |rhsf_.LOOP@li.1211
||   5.6% |  35.264114 | 0.091537 |   0.3% |     600.0 |rhsf_.LOOP@li.194
||   3.7% |  23.624271 | 0.054666 |   0.3% |     600.0 |rhsf_.LOOP@li.320
||   2.7% |  17.211435 | 0.095793 |   0.6% |     600.0 |rhsf_.LOOP@li.540
||   2.4% |  15.471160 | 0.358690 |   2.6% |   14400.0 |derivative_y_calc_buff_r_.LOOP@li.1784
||   2.4% |  15.113374 | 1.020242 |   7.2% |   14400.0 |derivative_z_calc_buff_r_.LOOP@li.1822
||   2.3% |  14.335142 | 0.144579 |   1.1% |   14400.0 |derivative_x_calc_buff_r_.LOOP@li.1794
||   1.9% |  11.794965 | 0.073742 |   0.7% |     600.0 |integrate_.LOOP@li.96
||   1.7% |  10.747430 | 0.063508 |   0.7% |     600.0 |computespeciesdiffflux2$transport_m_.LOOP
||   1.5% |   9.733830 | 0.096476 |   1.1% |     600.0 |rhsf_.LOOP@li.247
||   1.2% |   7.649953 | 0.043920 |   0.7% |     600.0 |rhsf_.LOOP@li.274
||   0.8% |   5.116578 | 0.008031 |   0.2% |     600.0 |rhsf_.LOOP@li.398
||   0.6% |   3.966540 | 0.089513 |   2.5% |       1.0 |s3d_
||   0.3% |   2.027255 | 0.017375 |   1.0% |     100.0 |integrate_.LOOP@li.73
||   0.2% |   1.318550 | 0.001374 |   0.1% |     600.0 |rhsf_.LOOP@li.376
||   0.2% |   0.986124 | 0.017854 |   2.0% |     600.0 |rhsf_.REGION@li.1096
||   0.1% |   0.700156 | 0.027669 |   4.3% |       1.0 |exit
```

Advantage of raising loops

- Create good granularity OpenMP Loop
- Improves cache re-use
- Reduces Memory usage significantly
- Creates a good potential kernel for an accelerator

Resultant Hybrid S3D Performance



Restructured S3D for multi-core systems

		S3D	
Time Step – acc_data		Solve_Drive	
Time Step– acc_data	Runge K	Integrate	
Time Step– acc_data	Runge K	RHS	
Time Step– acc_data	Runge K	grid loop -ACC	get mass fraction
Time Step– acc_data	Runge K	grid loop-ACC	get_velocity
Time Step– acc_data	Runge K	grid loop-ACC	calc_inv_avg
Time Step– acc_data	Runge K	grid loop-ACC	calc_temp
Time Step– acc_data	Runge K	grid loop-ACC	Compute Grads
Time Step– acc_data	Runge K	grid loop-ACC	Diffusive Flux
Time Step– acc_data	Runge K	grid loop-ACC	Derivatives
Time Step– acc_data	Runge K	grid loop-ACC	reaction rates

Sample from S3D – Hybrid-Multi-core Part 1

```
!$omp acc_data acc_copyin(q,volum) acc_shared(yspecies,u,avmolwt,mixMW,temp)
!$omp acc_region_loop private(i,ml,mu)
 do i = 1, nx*ny*nz, ms
  ml = i
  mu =  min(i+ms-1, nx*ny*nz)
  call get_mass_frac_r( q, volum, yspecies, ml, mu)
  call get_velocity_vec_r( u, q, volum, ml, mu)
  call calc_inv_avg_mol_wt_r( yspecies, avmolwt, mixMW, ml, mu)
  voltmp(ml:mu,1,1)=q(ml:mu,1,1,5)*volum(ml:mu,1,1)
  call calc_temp_r(temp, voltmp, u, yspecies, cpmix, avmolwt, ml, mu)
end do
!$omp end acc_region_loop
  ! Start communication - the _prep routines do posts and sends
  ! using buffer identified by itmp
  itmp = 1
!$omp acc_update host(u,temp,yspecies)
  call computeVectorGradient_prep( u, itmp )
  call computeScalarGradient_prep( temp, itmp )
  do n=1,n_spec
      call computeScalarGradient_prep( yspecies(:,:,:,n), itmp  )
  enddo
! Compute remaining properties whilst communication is underway
!$omp acc_region_loop private(i,ml,mu)
 do i = 1, nx*ny*nz, ms
  ml = i
  mu =  min(i+ms-1, nx*ny*nz)
  call calc_gamma_r( gamma, cpmix, avmolwt, ml, mu)
  call calc_press_r( pressure, q(:,:,:,4), temp, avmolwt, ml, mu )
  call calc_specEnth_allpts_r(temp, h_spec, ml, mu)
end do
!$omp end acc_region_loop
```

Sample from S3D – Hybrid-Multi-core Part 2

```
!  Now wait for communication
  call derivative_xyz_wait( itmp )
  calc_buff_internal_wait = .false.
  itmp = 1
!$omp acc_update acc(u,temp,yspecies)
  call computeVectorGradient_calc( u, grad_u, itmp )
  call computeScalarGradient_calc( temp, grad_T, itmp )
!$omp acc_region_loop private(n,itmp)
  do n=1,n_spec
      itmp = n + 4
      call computeScalarGradient5d_calc( yspecies(1,1,1,n), &
      grad_Ys(1,1,1,1,1), n_spec, n, itmp,sscale_1x,sscale_1y,sscale_1z  )
  enddo
!$omp end acc_region_loop
!$omp end acc_data
```

Current Status of putting S3D on XK6

- Internal XK6 with 171 nodes of
  - Magna-Cours
  - Fermi +
- Hybrid S3D running across entire system without accelerators
- Computation sections
  - 4 point-wise calculations of primary variables (running)
  - 2 diffusive flux calculations (not running – compiler bug)
    - Trying to inline a very deep call chain – may need to re-code
  - 2 getrates calculations (running)
  - 3 derivative computations (running)
- Once all computational sections are running, will use acc_data to put all data on accelerator and update halos back and forth to host

Interprocedural Analysis with Inlining

- For the next year, until we can call subroutines and functions on the accelerator, the compiler must inline all subroutines and functions within a acc_region.
  - This is performed automatically by the compiler
    - Can be incrementally controlled by using compile line options
      - -hwp –hpl=<path to program library>

Whole Program Analysis -hwp

- There are several things that inhibit the inlining of the call chain beneath the acc_region
  - Call to subroutines and functions that the compiler does not see
  - I/O, STOP, etc (Not anymore)
  - Array shape changing through argument passing
  - Dummy arguments
    - Real*8 dummy(*), dummy_2d(nx,*)

Successful Inlining

```
248.            !$omp acc_region_loop private(i,ml,mu)
 249.  1---------<  do i = 1, nx*ny*nz, ms
 250.  1             ml = i
 251.  1             mu =  min(i+ms-1, nx*ny*nz)
 252.  1  I          call get_mass_frac_r( q, volum, yspecies, ml, mu)            ! get Ys from rho*Ys, volum from rho
 253.  1  I          call get_velocity_vec_r( u, q, volum, ml, mu)                ! fill the velocity vector
 254.  1  I          call calc_inv_avg_mol_wt_r( yspecies, avmolwt, mixMW, ml, mu)  ! set inverse of mixture MW
 255.  1---------> end do
```

Inliner diagnostics

```
 333.  1---------<   do n=1,n_spec
  334.  1               itmp = n + 4
  335.  1               !call computeScalarGradient_calc( yspecies(:,:,:,n), grad_Ys(:,:,:,n,:), itmp )
  336.  1               call computeScalarGradient5d_calc( yspecies(1,1,1,n), &
                         ^
ftn-3007 ftn: ERROR RHSF, File = rhsf.f90, Line = 336, Column = 12
  Routine "write_date_and_time", referenced in "terminate_run", was not inlined because a scalar actual argument at position 1  is
  being mapped to an array dummy argument.

                         ^
ftn-3007 ftn: ERROR RHSF, File = rhsf.f90, Line = 336, Column = 12
  Routine "write_date_and_time", referenced in "terminate_run", was not inlined because a scalar actual argument at position 1  is
  being mapped to an array dummy argument.

                         ^
ftn-3007 ftn: ERROR RHSF, File = rhsf.f90, Line = 336, Column = 12
  Routine "write_date_and_time", referenced in "terminate_run", was not inlined because a scalar actual argument at position 2  is
  being mapped to an array dummy argument.

                         ^
ftn-3007 ftn: ERROR RHSF, File = rhsf.f90, Line = 336, Column = 12
  Routine "write_date_and_time", referenced in "terminate_run", was not inlined because a scalar actual argument at position 1  is
  being mapped to an array dummy argument.
```

Inliner diagnostics (-rmp)

```
 ^
ftn-3007 ftn: ERROR RHSF, File = rhsf.f90, Line = 336, Column = 12
  Routine "write_date_and_time", referenced in "terminate_run", was not inlined because a scalar actual argument at position 1  is
  being mapped to an array dummy argument.

                    ^
ftn-3007 ftn: ERROR RHSF, File = rhsf.f90, Line = 336, Column = 12
  Routine "write_date_and_time", referenced in "terminate_run", was not inlined because a scalar actual argument at position 1  is
  being mapped to an array dummy argument.

                    ^
ftn-3007 ftn: ERROR RHSF, File = rhsf.f90, Line = 336, Column = 12
  Routine "write_date_and_time", referenced in "terminate_run", was not inlined because a scalar actual argument at position 2  is
  being mapped to an array dummy argument.

                    ^
ftn-3007 ftn: ERROR RHSF, File = rhsf.f90, Line = 336, Column = 12
  Routine "write_date_and_time", referenced in "terminate_run", was not inlined because a scalar actual argument at position 1  is
  being mapped to an array dummy argument.
```

Inliner diagnostics (-rmp)

```
^
ftn-3021 ftn: ERROR RHSF, File = rhsf.f90, Line = 336, Column = 12
  Routine "mpi_finalize", referenced in "terminate_run", was not inlined because the compiler was unable to locate the routine to
  expand it inline.

                  ^
ftn-3021 ftn: ERROR RHSF, File = rhsf.f90, Line = 336, Column = 12
  Routine "mpi_barrier", referenced in "terminate_run", was not inlined because the compiler was unable to locate the routine to
  expand it inline.

                  ^
ftn-3021 ftn: ERROR RHSF, File = rhsf.f90, Line = 336, Column = 12
  Routine "mpi_wait", referenced in "derivative_y_calc_buff_r", was not inlined because the compiler was unable to locate the
  routine to expand it inline.

                  ^
ftn-3021 ftn: ERROR RHSF, File = rhsf.f90, Line = 336, Column = 12
  Routine "mpi_wait", referenced in "derivative_y_calc_buff_r", was not inlined because the compiler was unable to locate the
  routine to expand it inline.
```

All Compiler Internal Errors are not errors

- Currently many compiler internal errors are given when forms are encountered that inhibit acceleration
  - Calls within the acc_region
    - These can be identified by using the inliner
  - Derived Types
    - These are being worked
  - Dummy arguments
  - Etc.

Early Software/Hardware Issues

- Finding lots of bugs in tools and compiler
  - Cannot fix them until they are identified
- Identified bottleneck in MPI messaging between GPUs
  - This is being addressed by Cray/Nvidia
    - Want zero transfer messages – GPU directly to other GPU
- Directives are emerging – changing
  - Usage is identifying new capabilities – pipelining
- Future GPUs will have a higher performance advantage over x86 sockets

Himeno Benchmark on Cray XK6: an OpenMP for Accelerators exercise

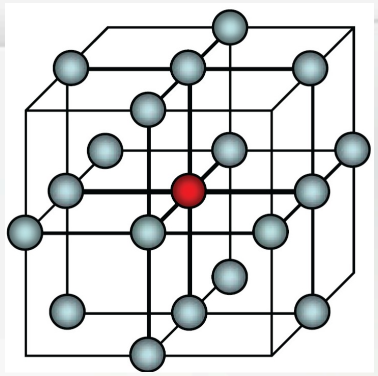
Roberto Ansaloni
Alistair Hart

Cray Performance Symposium, 25.July.11

Contents of talk

- A performance case study
  - The Himeno benchmark
  - Accelerating Himeno using OpenMP directives
    - assume you have met these already
  - Performance and scaling of the Himeno code
- How to accelerate a code using directives
  - A vademecum
- Suitability of codes and examples available
- Useful tools and tricks for accelerator directives

The Himeno Benchmark



- 3D Poisson equation
  - 19-point stencil
  - Highly memory intensive, memory bandwidth bound
- Fortran, C, MPI and OpenMP implementations available from http://accc.riken.jp/HPC_e/himenobmt_e.html
- Several configurations available
  - Tests on XL configuration: 1024 x 512 x 512
- NVIDIA paper on GPU CUDA implementation
  - Phillips, E.H.; Fatica, M.;
    Implementing the Himeno benchmark with CUDA on GPU clusters
    IEEE International Symposium on Parallel & Distributed Processing (IPDPS), 2010 [PDF, or ahart@cray.com]

The Jacobi computational kernel

- The stencil is applied to pressure array p
- Updated pressure values are saved to temporary array wrk2
- Control value wgosa is computed
- In the benchmark this kernel is iterated a fixed number of times (nn)

```
DO K=2,kmax-1
 DO J=2,jmax-1
  DO I=2,imax-1
   S0=a(I,J,K,1)*p(I+1,J, K )
     +a(I,J,K,2)*p(I, J+1,K ) &
     +a(I,J,K,3)*p(I, J, K+1) &
     +b(I,J,K,1)*(p(I+1,J+1,K )-p(I+1,J-1,K ) &
                 -p(I-1,J+1,K )+p(I-1,J-1,K )) &
     +b(I,J,K,2)*(p(I, J+1,K+1)-p(I, J-1,K+1) &
                 -p(I, J+1,K-1)+p(I, J-1,K-1)) &
     +b(I,J,K,3)*(p(I+1,J, K+1)-p(I-1,J, K+1) &
                 -p(I+1,J, K-1)+p(I-1,J, K-1)) &
     +c(I,J,K,1)*p(I-1,J, K ) &
     +c(I,J,K,2)*p(I, J-1,K ) &
     +c(I,J,K,3)*p(I, J, K-1) &
     + wrk1(I,J,K)

   SS=(S0*a(I,J,K,4)-p(I,J,K))*bnd(I,J,K)
   WGOSA=WGOSA+SS*SS
   wrk2(I,J,K)=p(I,J,K)+OMEGA *SS
  ENDDO
 ENDDO
ENDDO
```

fwd n.n.

n.n.n.

bkwd n.n.

Distributed implementation

- The outer loop is performed a fixed number of times
- The Jacobi kernel is executed and new pressure array wrk2 and control value wgosa are computed
- The array is updated with the new pressure values
- The halo region values are exchanged between neighbor PEs
- Send and receive buffers are used
- The maximum control value is computed with an Allreduce operation across all the PEs

```
DO loop = 1, nn
   compute Jacobi kernel → wrk2,wgosa

   copy back wrk2 into p

   pack halo from p into send buffers

   exchange halos with neighbour PEs

   unpack halo into p from recv buffers

   Allreduce to sum wgosa across PEs
ENDDO
```

Porting Himeno to the Cray XK6

- Several versions tested, with communication implemented in MPI or Fortran coarrays
- GPU version using OpenMP Accelerator directives
- Comparing Cray XK6 timings with best Cray XE6 results (hybrid MPI/OpenMP)
- Arrays reside permanently on the GPU memory
- Data transfers between host and GPU are:
  - Communication buffers for the halo exchange
  - Control value

Allocating arrays on the GPU

- Arrays are allocated on the GPU memory in the main program with the *acc_data* directive
- In the subroutines the *acc_data* directive is replicated with the *present* clause, to use the data already present in the GPU memory and avoid extra allocations
- Since present clause is used, no *acc_copy** clauses are used, and data transfers to/from host are implemented by *acc_update* directives

```
PROGRAM himenobmtxp
...
!$omp acc_data acc_shared         &
!$omp&   (p,a,b,c,wrk1,wrk2,bnd,      &
!$omp&   sendbuffx_up,sendbuffx_dn, &
!$omp&   sendbuffy_up,sendbuffy_dn, &
!$omp&   sendbuffz_up,sendbuffz_dn)
...
!$omp end acc_data

SUBROUTINE jacobi(nn,gosa)
!$omp acc_data present          &
!$omp&   (p,a,b,c,wrk1,wrk2,bnd,      &
!$omp&   sendbuffx_up,sendbuffx_dn, &
!$omp&   sendbuffy_up,sendbuffy_dn, &
!$omp&   sendbuffz_up,sendbuffz_dn)
```

Jacobi kernel on the GPU

- The GPU kernel for the main loop is created with the *acc_region_loop* directive
- The scoping of the main variables is specified earlier with the *acc_data* directive - no need to replicated it in here
- wgosa is computed by specifying the *reduction* clause, as in a standard OpenMP parallel loop
- *num_pes* clause is used to indicate the number of threads within a threadblock (compiler default 128)

```
DO loop=1,nn
  gosa = 0
  wgosa = 0
!$omp acc_region_loop                     &
!$omp&  private(s0,ss)                    &
!$omp&  reduction(+:wgosa)                &
!$omp&  num_pes(2:256)
  DO K=2,kmax-1
    DO J=2,jmax-1
      DO I=2,imax-1
        S0=a(I,J,K,1)*p(I+1,J, K )  &
        ...
        wgosa = wgosa + SS*SS
      ENDDO
    ENDDO
  ENDDO
```

Halo region buffers

- Halo values are extracted from the wrk2 array and packed into the send buffers, on the GPU
- A global *acc_region* is specified and buffers in the X, Y, and Z directions are packed within *acc_loop* blocks
- The send buffers are copied to host memory with *acc_update*
- In the same way, after the halo exchange, the recv buffers are transferred to the GPU memory and used to update the array p
- N.B. Currently it's not possible to include array sections in *acc_update* –buffers are necessary

```
!$omp acc_region
!$omp acc_loop
DO j = 2,jmax-1
  DO i = 2,imax-1
    sendbuffz_dn(i,j)= wrk2(i,j,2)
    sendbuffz_up(i,j)= wrk2(i,j,kmax-1)
  ENDDO
ENDDO
!$omp end acc_loop
 ...
!$omp acc_loop
!$omp end acc_loop
!$omp end acc_region

!$omp acc_update &
!$omp&  host(sendbuffz_dn,sendbuffz_up)
```

Coarray implementation

- Coarrays are used to perform the halo exchange
- Non-blocking communication needs *pgas defer_sync* directive
- Programmer now responsible for data synchronization
- By deferring sync point, network comms can be overlapped with CPU or GPU activity
- Updating p from wrk2 (on GPU) overlapped with halo exchange
- N.B. no *sync all*: CAF intrinsic *COSUM* has loose synchronisation (so do need *sync memory* first).

```
!dir$ pgas defer_sync
recvbuffz_up(:,:)[myx,myy,myz-1] = &
   sendbuffz_dn(:,:)
 ...
!$omp acc_region_loop
DO k = 2,kmax-1
  DO j = 2,jmax-1
    DO i = 2,imax-1
      p(i,j,k) = wrk2(i,j,k)
    ENDDO
  ENDDO
ENDDO
!$omp end acc_region_loop
sync memory
gosa = COSUM(wgosa)
!$omp acc_update &
!$omp& acc(recvbuffz_dn,recvbuffz_up)
```

Coarray implementation

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```
!dir$ pgas defer_sync
recvbuffz_up(:,:)[myx,myy,myz-1] = &
    sendbuffz_dn(:,:)
  ...
!$omp acc_region_loop
DO k = 2,kmax-1
  DO j = 2,jmax-1
    DO i = 2,imax-1
      p(i,j,k) = wrk2(i,j,k)
    ENDDO
  ENDDO
ENDDO
!$omp end acc_region_loop
sync memory
gosa = COSUM(wgosa)
!$omp acc_update &
!$omp& acc(recvbuffz_dn,recvbuffz_up)
```

Compiler does not currently support using coarrays in an accelerator region, so this does not work!

You need to make a local copy of the coarray buffers to non-coarray buffers and then transfer them to GPU memory.

This affects the performance, by increasing the host CPU time.

OpenMP for Accelerator GPU version

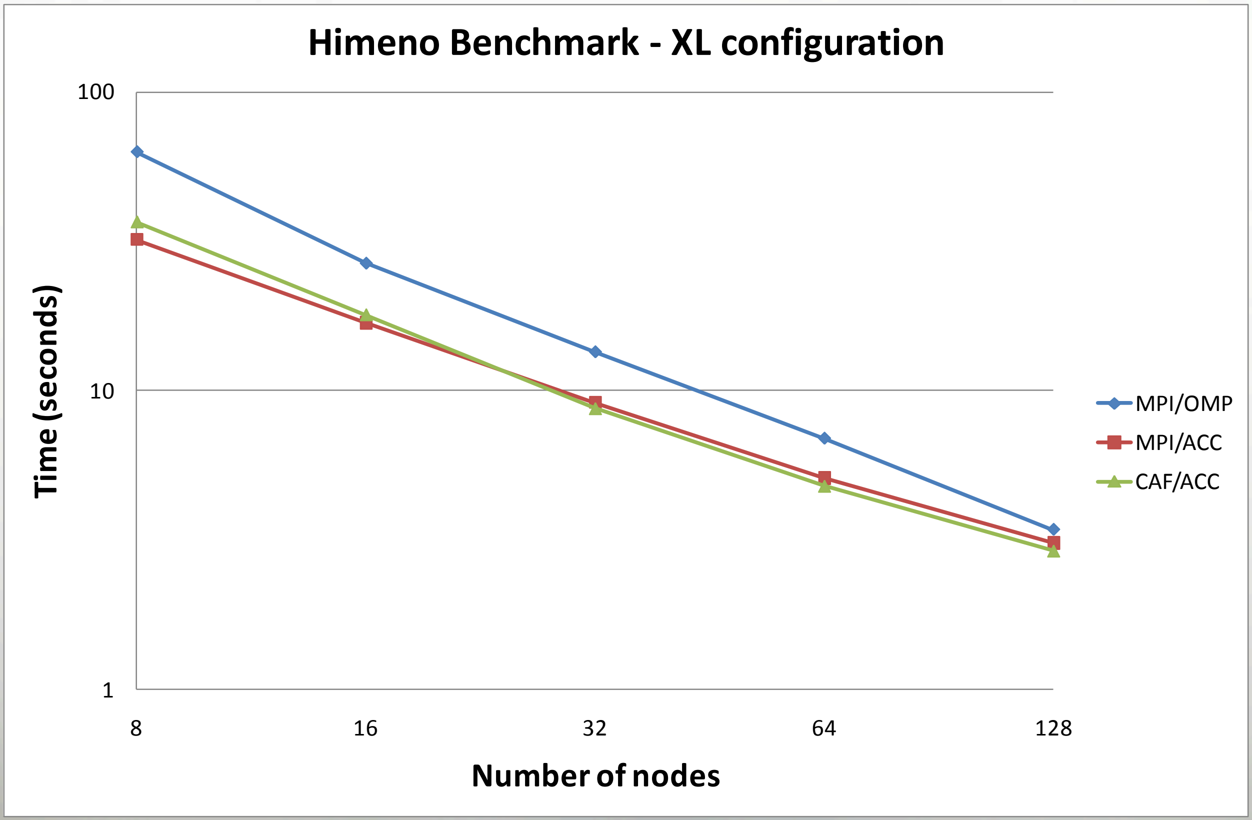
- Total number of lines in the original Himeno MPI-Fortran code: 629
- Total number lines in the modified version with coarrays and accelerator directives: 554
  - don't need MPI_CART_CREATE and the like
- Total number of accelerator directives: 27
  - plus 18 "end" directives

Benchmarking the code

- Cray XK6 configuration (vista)
  - Single AMD MC12 2.1GHz CPU cores, 12 cores per node
  - Nvidia Tesla X2090 GPU, 1 per node
  - Running with 1 PE (GPU) per node
  - Himeno case XL needs at least 8 Cray XK6 nodes
- Cray XE6 configuration (kaibab)
  - Dual AMD MC12 2.1 GHz nodes, 24 cores per node
  - Running on fully packed nodes: all cores used
  - Depending on the number of nodes, 1-6 OpenMP threads per PE are used
- All comparisons are for strong scaling
  - fixed total problem size
  - Nvidia CUDA example is weak scaling

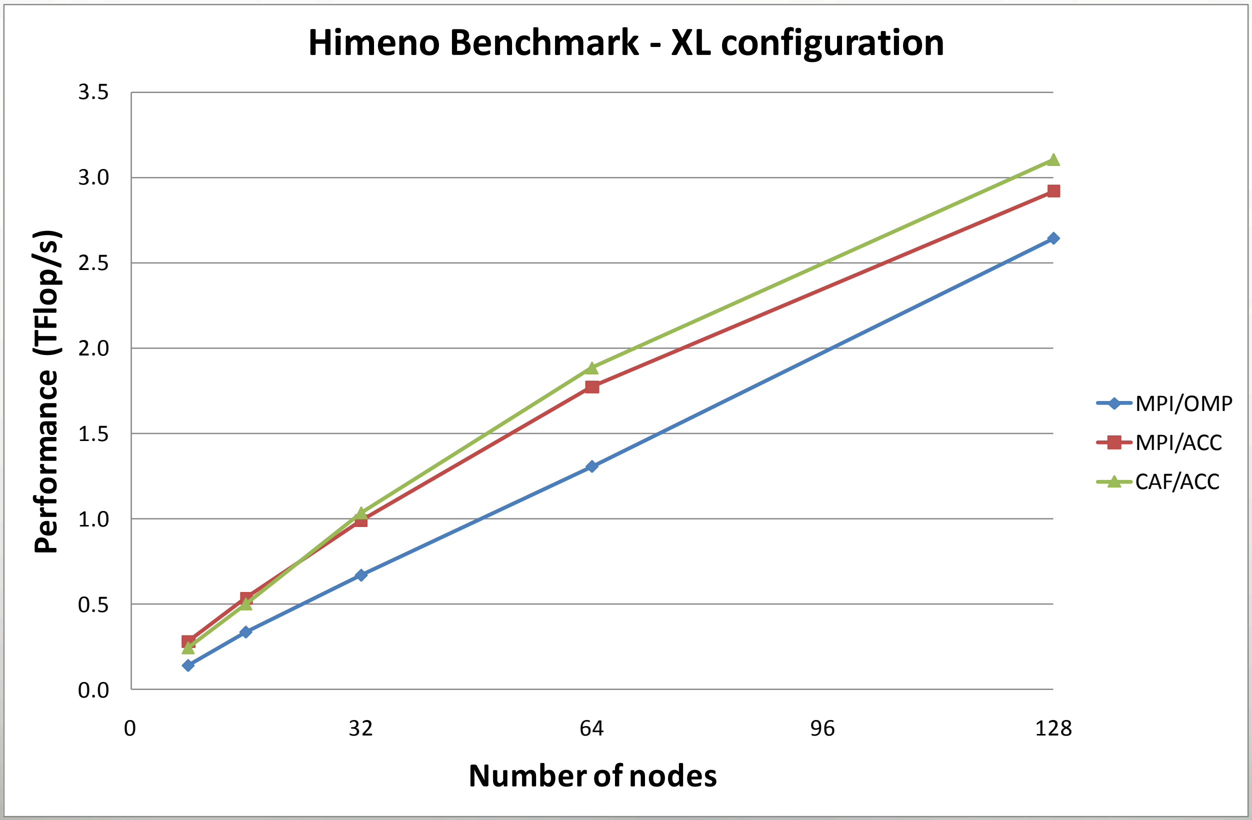
Himeno Timings

- The ACC code on the Cray XK6 outperforms the Cray XE6
- Larger gap on small number of nodes
- CAF communication is more efficient than MPI
  - CAF is worse on small number of nodes – more on this later



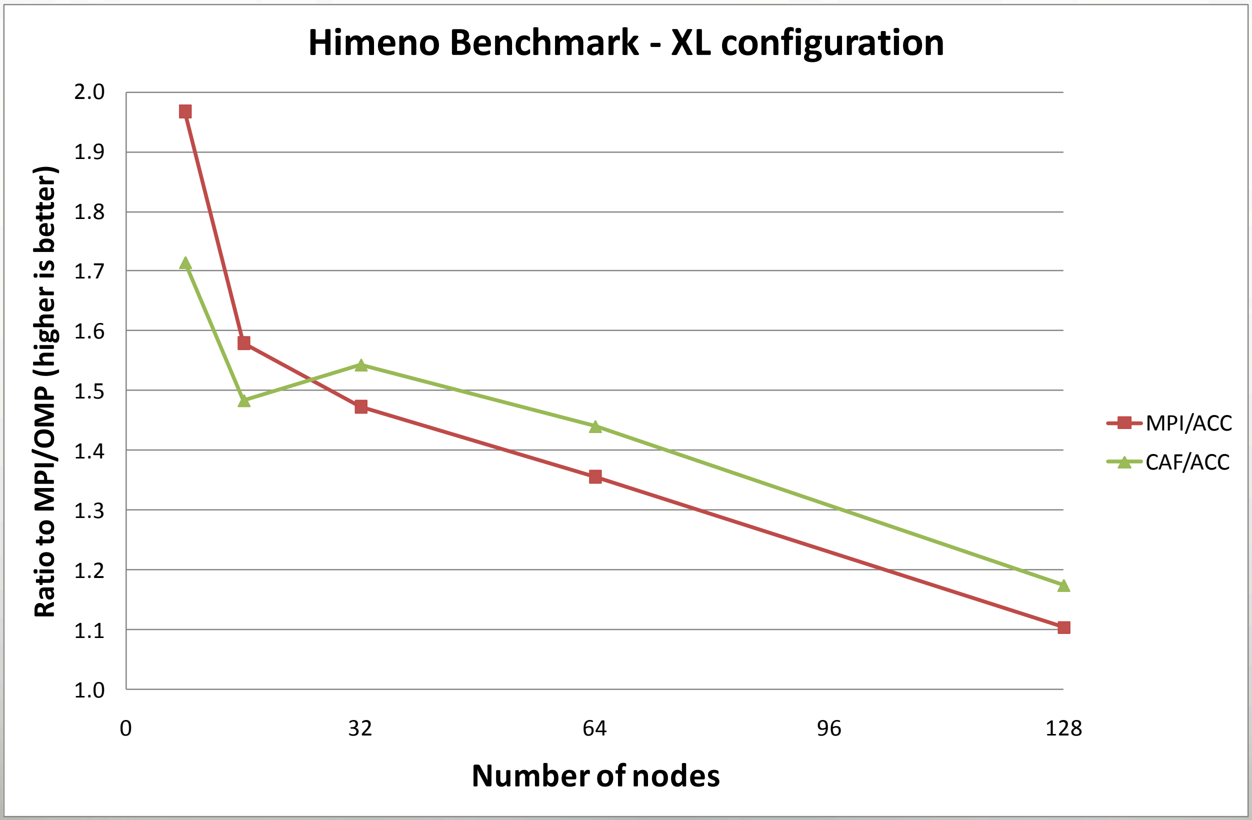
Himeno Performance

- Node-for-node, Cray XK6 (GPU) outperforms Cray XE6 (CPU)
- CAF/ACC is the faster than MPI/ACC on high number of nodes
- ACC code has slightly worse scalability than MPI/OMP
  - more on this later



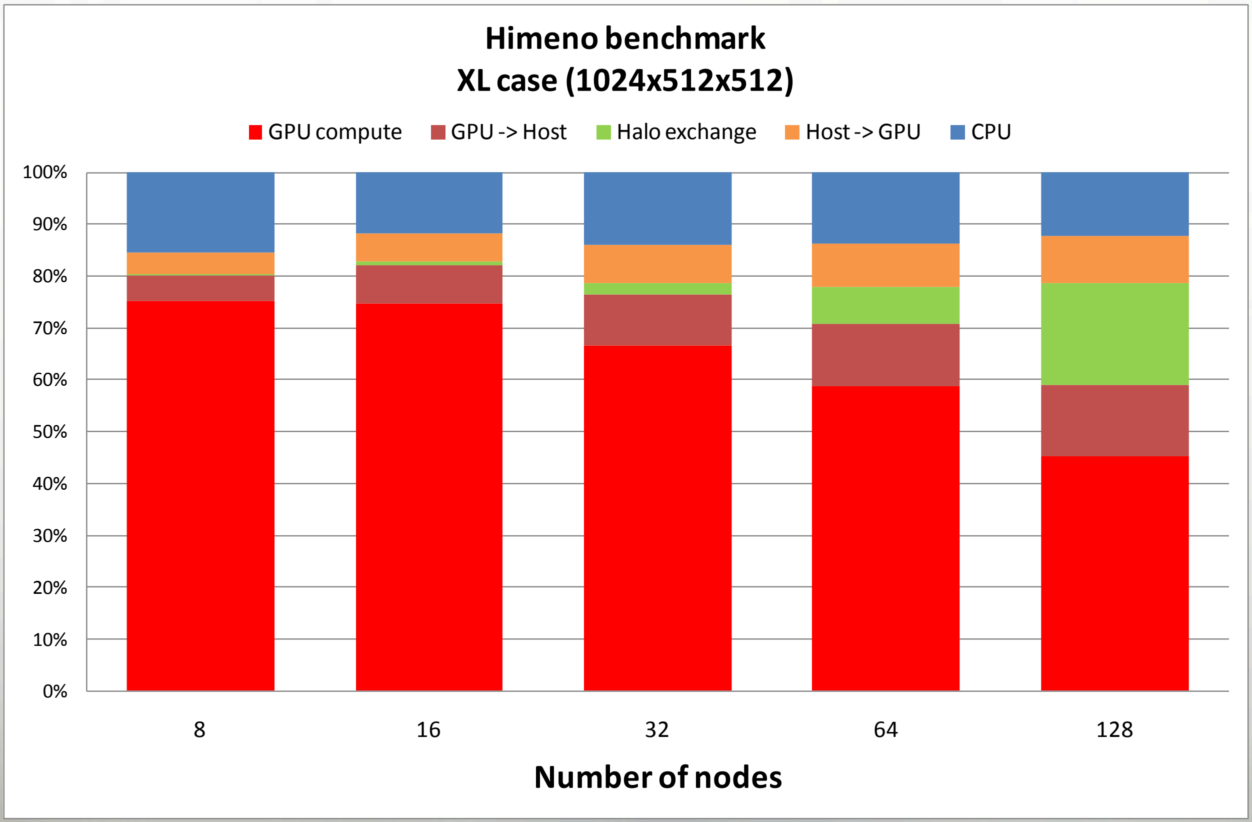
Cray XK6 ratio to Cray XE6

- Cray XK6 is always faster
  - Ratio drops on 16 nodes
  - On 16 nodes the CPU code gets a superlinear boost due to cache effect
- On 128 nodes GPU code is about 20% faster than CPU code



CAF/ACC code breakdown (craypat!)

- Host/GPU transfers always take more time than the halo exchange (network)
  - this code would benefit from an efficient direct GPU-GPU communication
- On 128 nodes less than 50% of the time is spent in the GPU compute kernel
- Extra copy of coarray buffers increases the CPU time (potentially avoidable)
  - This is why CAF code is slower at low node count



Conclusions from the Himeno case study

- It has been very simple to implement the GPU code with OpenMP accelerator directives
- Work has evolved with updates in the (pre-release) compiler
  - Always got the right answers
  - Occasionally needed workarounds before features implemented
  - Compiler team extremely responsive
- Future releases will provide more control of the GPU and allow for better performance
- Codes where data can permanently reside in GPU memory will benefit from an efficient direct GPU-GPU communication
  - N.B. GPUs not on same PCIe bus
  - Many hardware questions need addressing to do this

Future work for Himeno

- Increased overlap of communication and computation
  - async clause for accelerator kernels, data transfers will help this
  - is there enough work in himeno to really hide the comms?
    - we tried precomputing halo regions of temporary array wrk2 for earlier halo exchange
    - allows better overlap with GPU computation (interior of wrk2, copy of wrk2 into p)
    - so far this has not improved code performance
  - measuring overlap is not easy
- Better tuning of GPU kernels
- A distributed CUDA implementation should be implemented to verify the efficiency of the OpenMP for Accelerator directives

Thank you. Questions?

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