

Hopper Phase-2 Migration

Harvey Wasserman
User Services Group

Nick Wright
Advanced Technologies Group

NUG Training

October 2010



U.S. DEPARTMENT OF
ENERGY

Office of
Science



www.nersc.gov



The NERSC Hopper System

- Cray XT6, 6,392 nodes, 153,408 cores, 2.1-GHz AMD Magny-Cours Opteron processor
- Cray Gemini Interconnect
- 1.25 Petaflops peak performance
- 2-PB disk Lustre filesystem

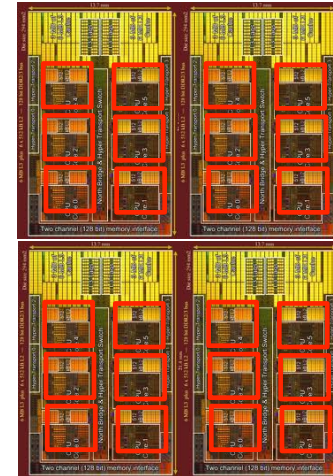


Part 1

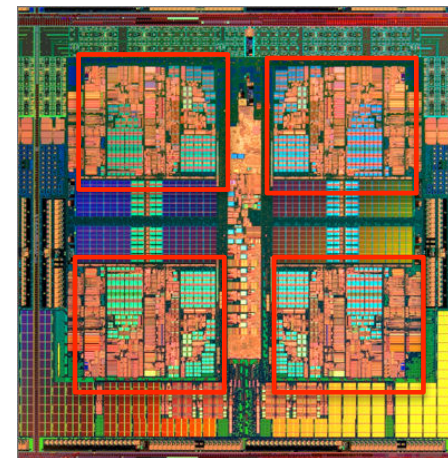
PROGRAMMING

What is Different About Hopper?

- The new Hopper Phase-2 system will have 24 cores per node.
- Franklin has only four.
- The way that you use the new Hopper system may have to change as a result.



AMD Magny-Cours Die



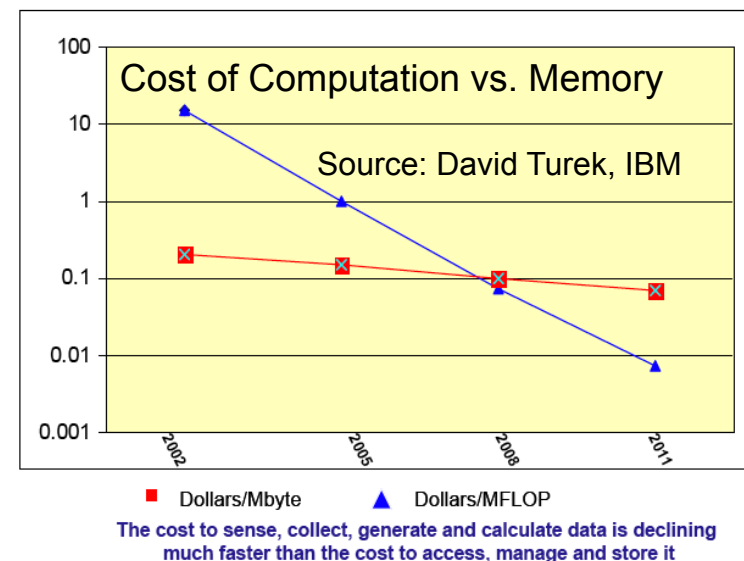
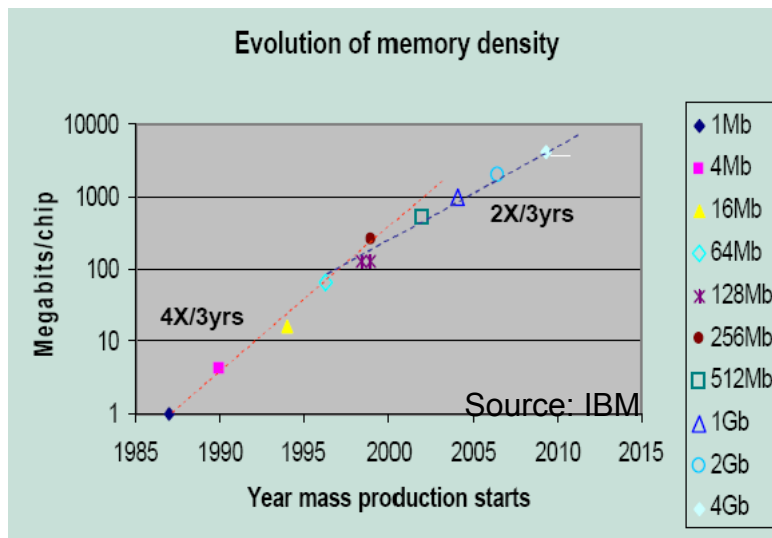
AMD Barcelona Die

What Else is Different ?

- **Less memory per core: 1.33 GB vs. 2.0 GB**
 - 8 GB per node (Franklin);
 - 32 GB per node (Hopper, 6,008 nodes)
- **“OOM killer terminated this process” error**
OOM = Out of Memory
- (Hopper will have 384 larger-memory nodes
64 GB.)

Why Less Memory Per Core?

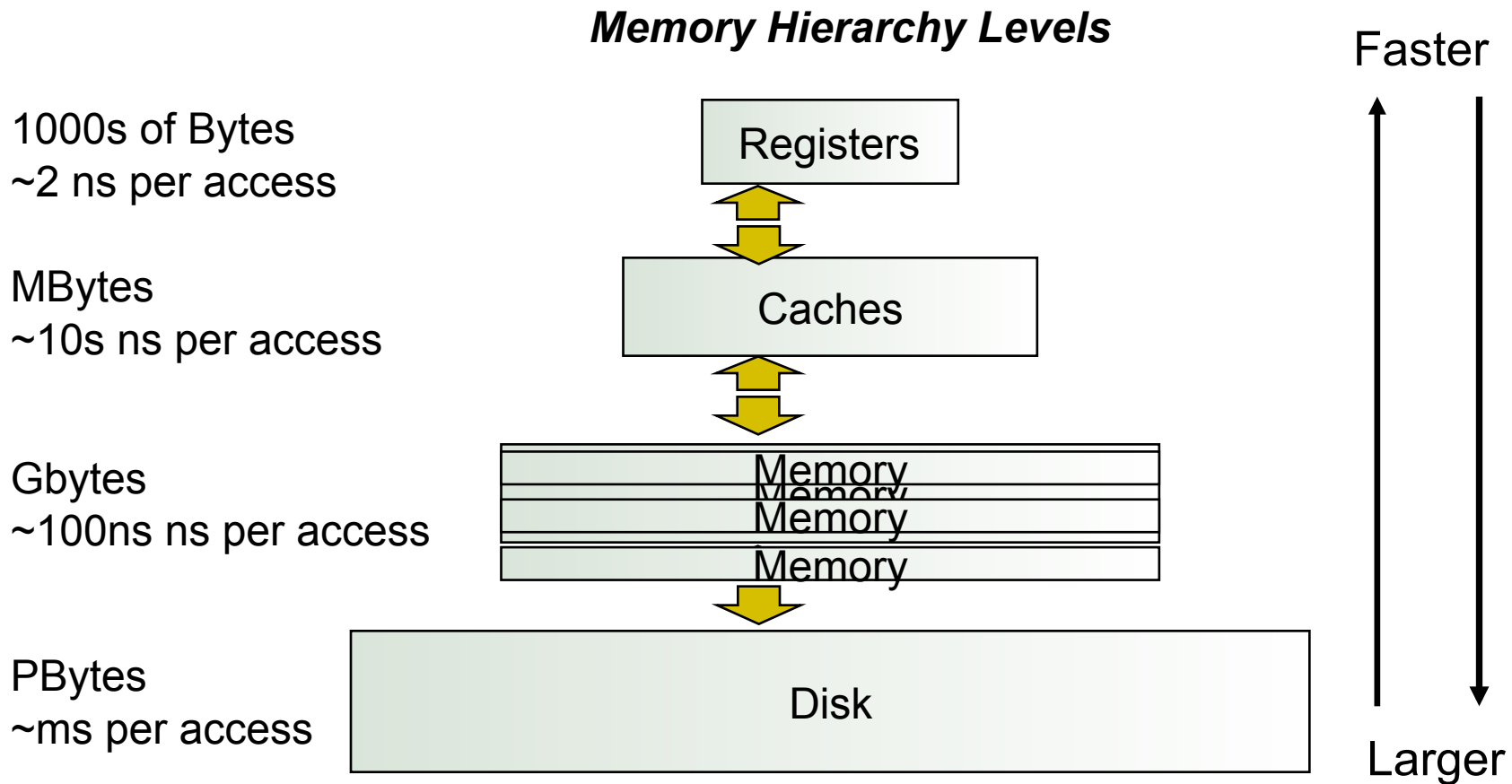
- **Technology trends:**
 - Memory density 2X every 3 yrs; processor logic every 2
 - Storage costs (\$/MB) drops more gradually than logic costs



- **NERSC optimized the Hopper system for a diverse workload**
 - fixed budget; memory cost is already a significant portion.

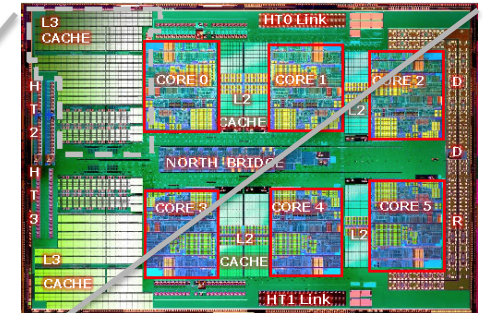
What Else is Different ?

- “Deeper” Memory Hierarchy in Hopper



What Else is Different ?

- “Deeper” Memory Hierarchy
 - NUMA: Non-Uniform Memory Architecture
 - All memory is transparently accessible but...
 - Longer memory access time to “remote” memory
 - A process running on NUMA node 0 accessing NUMA node 1 memory can adversely affect performance.



2xDDR1333 channel

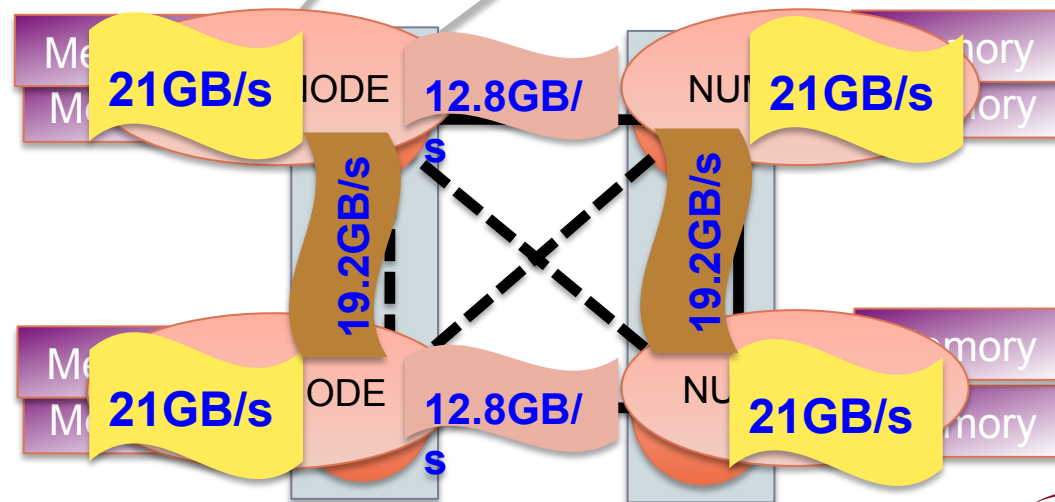
21.3 GB/s

3.2GHz x16 lane HT

12.8 GB/s bidirectional

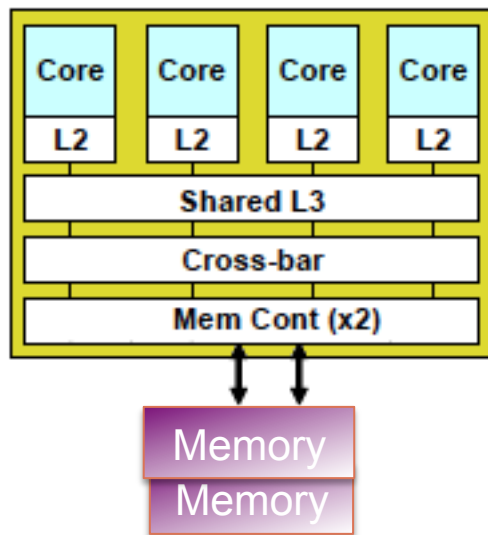
3.2GHz x8 lane HT

6.4 GB/s bidirectional

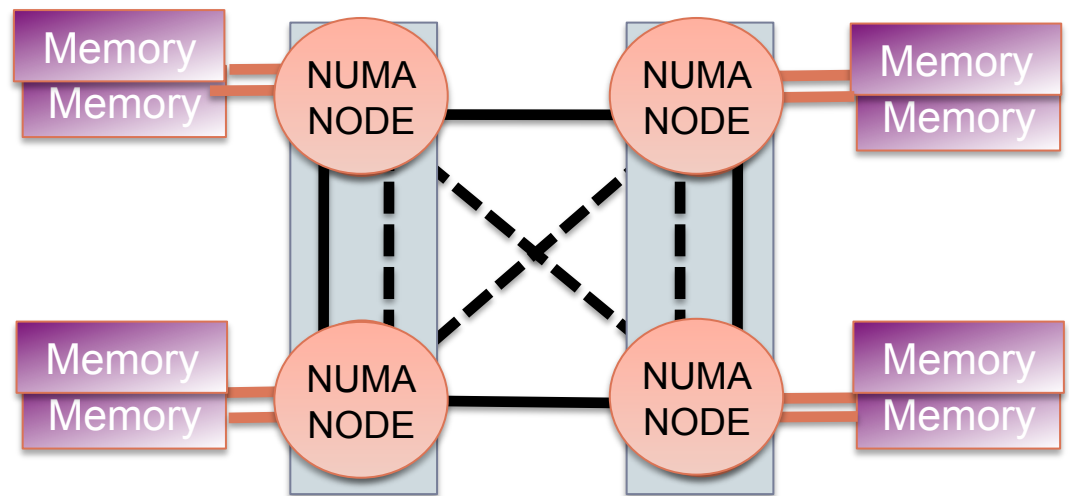


Hopper Node

Hopper vs. Franklin



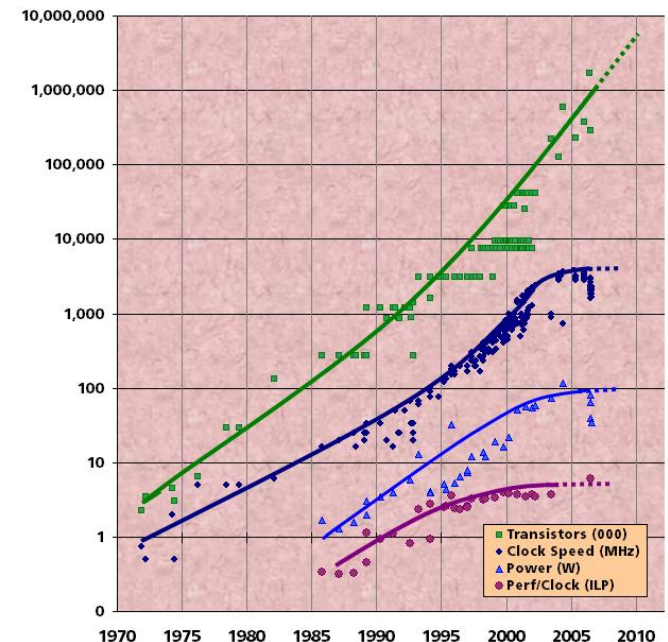
Franklin: Uniform Memory Architecture





Hopper: Non-Uniform Memory Architecture

What About the Future?

- The technology trends point to
 - Little or no gain in clock speed or performance per core;
 - Rapidly increasing numbers of cores per node;
 - Decreased memory *capacity* per core (possible slight increase per node)
 - Decreased memory *bandwidth* per core
 - Decreased interconnect bandwidth per core
 - Deeper memory hierarchy
- Hopper is the first example at NERSC but surely not the last



Will My Existing Code Run?

- **Probably, yes, your MPI code will run.** 
- **But the decrease in memory available per core may cause problems ...**
 - **May not be able to run the same problems.**
 - **May be difficult to continue “weak” scaling (problem size grows in proportion to machine size).** 
- **(and your MPI code might not use the machine most effectively.)**
- **Time to consider alternative programming models?**

What is NERSC Doing About All This?

- NERSC-Cray
“Programming Models Center of Excellence”
- Close ties to UCB and LBNL Computing Research Division
- Investigation of Advanced Programming Models
- Study of application software that NERSC provides
 - OpenMP ready?
 - OpenMP capable?

Stencil Computation Optimization and Auto-tuning on State-of-the-Art Multicore Architectures

Kaushik Datta^{*†}, Mark Murphy[†], Vasily Volkov[†], Samuel Williams^{*†}, Jonathan Carter^{*}, Leonid Oliker^{*†}, David Patterson^{*†}, John Shalf^{*}, and Katherine Yelick^{*†}

^{*}CRD/NERSC, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA
[†]Computer Science Division, University of California at Berkeley, Berkeley, CA 94720, USA

Abstract

Understanding the most efficient design and utilization of emerging multicore systems is one of the most challenging questions faced by the mainstream and scientific computing industries in several decades. Our work explores multicore stencil (nearest-neighbor) computations — a class of algorithms at the heart of many structured grid codes, including PDE solvers. We develop a number of effective optimization strategies, and build an auto-tuning environment that searches over our optimizations and their parameters to minimize runtime, while maximizing performance portability. To evaluate the effectiveness of these strategies we explore the broadest set of multicore architectures in the current HPC literature, including the Intel Clovertown, AMD Barcelona, Sun Victoria Falls, IBM QS22 PowerPC Cell 8i, and NVIDIA GTX280. Overall, our auto-tuning optimization methodology results in the fastest multicore stencil performance to date. Finally, we present several key insights into the architectural trade-offs of emerging multicore designs and their implications on scientific algorithm development.

1. Introduction

The computing industry has recently moved away from exponential scaling of clock frequency toward chip multiprocessors (CMPs) in order to better manage trade-offs among performance, energy efficiency, and reliability [1]. Because this design approach is relatively immature, there is a vast diversity of available CMP architectures. System designers and programmers are confronted with a confusing variety of architectural features, such as multicore, SIMD, simultaneous multithreading, core heterogeneity, and unconventional memory hierarchies, often combined in novel arrangements. Given the current flux in CMP design, it is unclear which architectural philosophy is best suited for a given class of algorithms. Likewise, this architectural diversity leads to uncertainty on how to refactor existing algorithms and tune them to take the maximum advantage of existing and emerging platforms. Understanding the most efficient design and utilization of these increasingly parallel multicore systems is one of the most challenging

questions faced by the computing industry since it began. This work presents a comprehensive set of multicore optimizations for stencil (nearest-neighbor) computations — a class of algorithms at the heart of most calculations involving structured (rectangular) grids, including both implicit and explicit partial differential equation (PDE) solvers. Our work explores the relatively simple 3D heat equation, which can be used as a proxy for more complex scientific calculations. In addition to their importance in stencil calculations, stencils are interesting as an architectural evaluation benchmark because they have abundant parallelism and low computational intensity, offering a mixture of opportunities for on-chip parallelism and challenges for associated memory systems.

Our optimizations include NUMA affinity, array padding, core/register blocking, prefetching, and SIMDization — as well as novel stencil algorithmic transformations that leverage multicore resources: thread blocking and circular queues. Since there are complex and unpredictable interactions between our optimizations and the underlying architectures, we develop an *auto-tuning* environment for stencil codes that searches over a set of optimizations and their parameters to minimize runtime and provide performance portability across the breadth of existing and future architectures. We believe such application-specific auto-tuners are the most practical near-term approach for obtaining high performance on multicore systems.

To evaluate the effectiveness of our optimization strategies we explore the broadest set of multicore architectures in the current HPC literature, including the dual-socket quad-core AMD Barcelona and the dual-socket quad-core Intel Clovertown, the heterogeneous core fast double precision STI Cell QS22 PowerPC Cell 8i Blade, as well as one of the first scientific core eight-thread Sun Victoria Falls machine. Additionally, we present results on the single-socket dual-socket eight-threaded streaming NVIDIA GeForce GTX280 general purpose graphics processing unit (GPGPU).

This suite of architectures allows us to compare the mainstream multicore approach of replicating conventional cores that emphasize serial performance (Barcelona and

SC2008 November 2008, Austin, Texas, USA 978-1-4244-2835-9/08 \$25.00 ©2008 IEEE

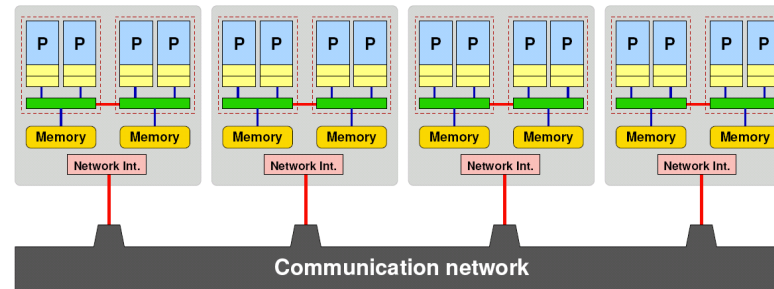


What Does NERSC Recommend?

- **NERSC recognizes the huge investment in MPI.**
- **But given the technology trends...**
- **We suggest a move towards programming models other than pure MPI**
- **A good place to start: MPI + OpenMP (“Hybrid”)**
 - **MPI for domain decomposition and OpenMP threads within a domain**
 - **Suggested primarily to help with memory capacity**

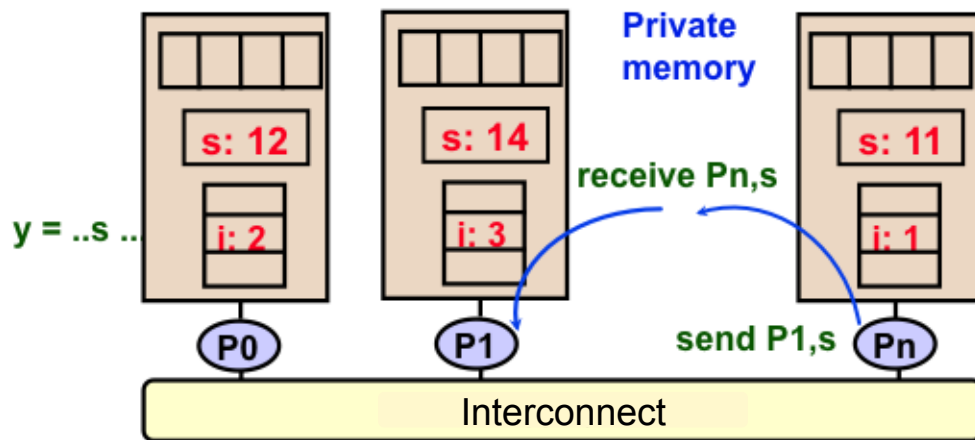
Isn't This the Same as Clusters of SMPs (.ca 2002)?

- **SMP: Symmetric Multiprocessor**
 - aka clusters, Networks of Workstations, CLUMPS, ...
 - SGI Origin, ASCI Q/Blue Mountain, Berkeley NOW, IBM SP, ...



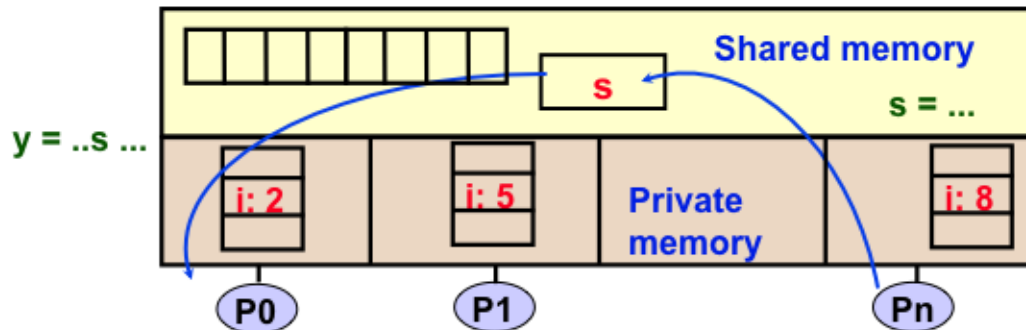
- **In some ways the issues are the same:**
 - Memory architecture is the key
- **But chip multiprocessors have vastly improved inter-core latencies and bandwidth.**
- **With today's trends we have no choice.**

What are the Basic Differences Between MPI and OpenMP?



Message Passing Model

Shared Address Space Model

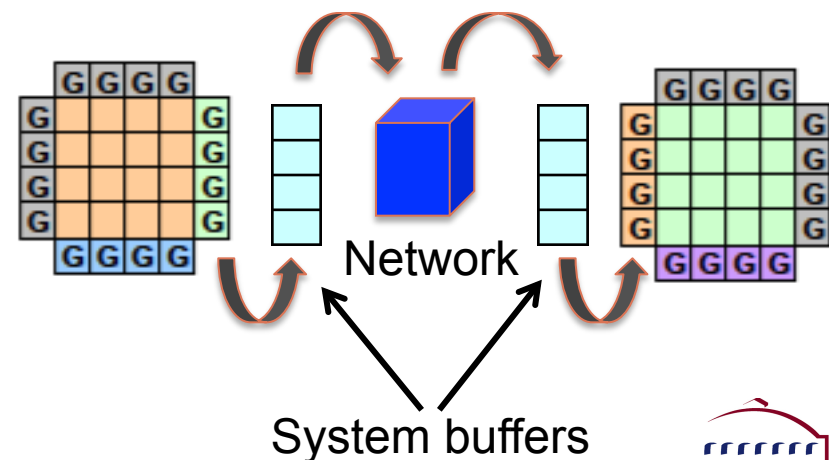
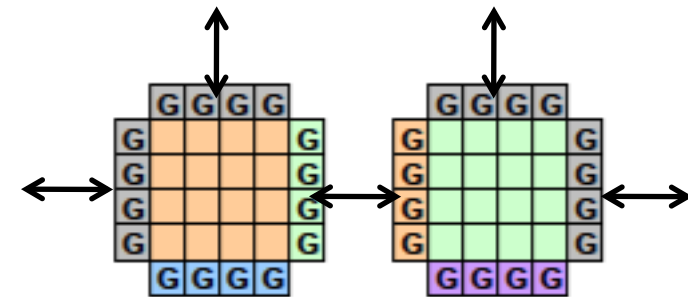


- Program is a collection of processes.
 - Usually fixed at startup time
- Single thread of control plus private address space -- NO shared data.
- Processes communicate by explicit send/receive pairs
 - Coordination is implicit in every communication event.
- MPI is most important example.

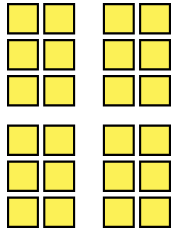
- Program is a collection of threads.
 - Can be created dynamically.
- Threads have private variables and shared variables
- Threads communicate implicitly by writing and reading shared variables.
 - Threads coordinate by synchronizing on shared variables
- OpenMP is an example

Why are MPI-only Applications Memory Inefficient?

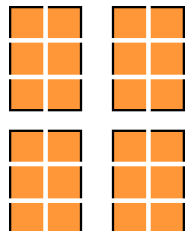
- MPI codes consist of n copies of the program
- MPI codes require *application-level* memory for messages
 - Often called “ghost” cells
- MPI codes require *system-level* memory for messages
 - Assuming the very common synchronous/blocking style



Why Does Hybrid/OpenMP Help?



"Pure" MPI

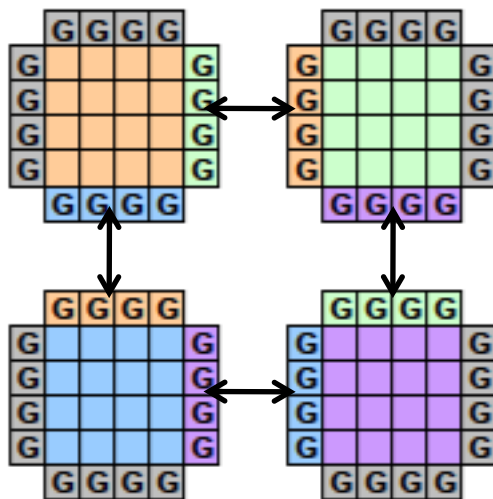


"Pure" OpenMP

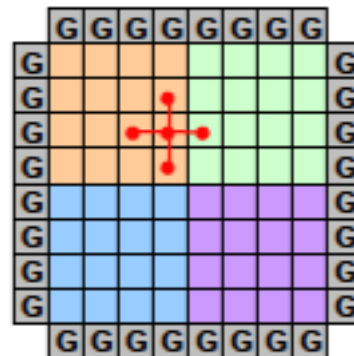


Hybrid: 4 MPI tasks,
6 threads per MPI

- **Reduced Memory Usage:**
 - Fewer instances of your program on the node
 - Eliminate some ghost cell memory



Distributed memory
subgrid distribution



Shared memory
subgrid distribution

Figures from Kaushik Datta, Ph.D. Dissertation, UC Berkeley, 2009

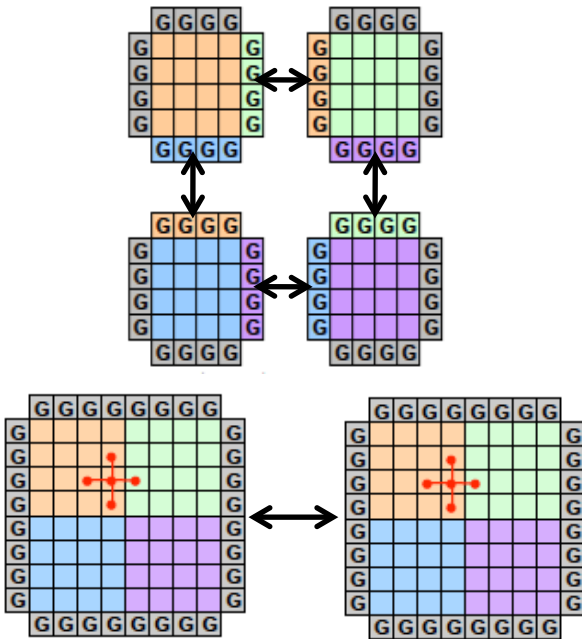


U.S. DEPARTMENT OF
ENERGY

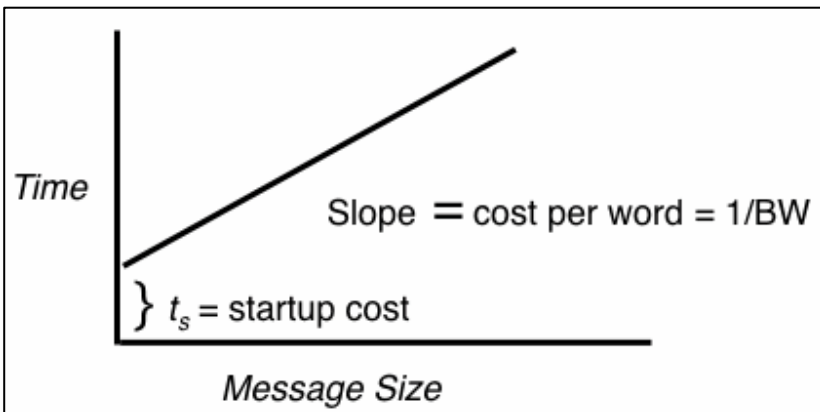
Office of
Science



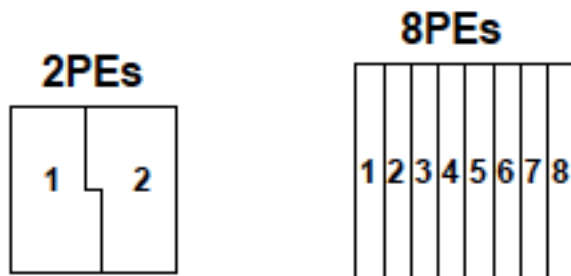
Why Does Hybrid/OpenMP Help?



- Send larger MPI messages
 - small messages are expensive
- No intra-node messages



Why Does Hybrid/OpenMP Help?



- There may be scalability limits to domain decomposition
- OpenMP adds fine granularity (larger message sizes) and allows flexibility of dynamic load balancing.
- Some problems have two levels of parallelism

What are the Benefits of OpenMP?

- **Uses less memory per node**
- **At least equal performance**
- **Additional parallelization may fit algorithm well**
 - especially for applications with limited domain parallelism
- **Possible improved MPI performance and load balancing**
 - Avoid MPI within node
- **OpenMP is a standard so code is portable**
- **Some OpenMP code can be added incrementally**
 - Can focus on performance-critical portions of code
- **Better mapping to multicore architecture**

What are the Disadvantages of OpenMP?

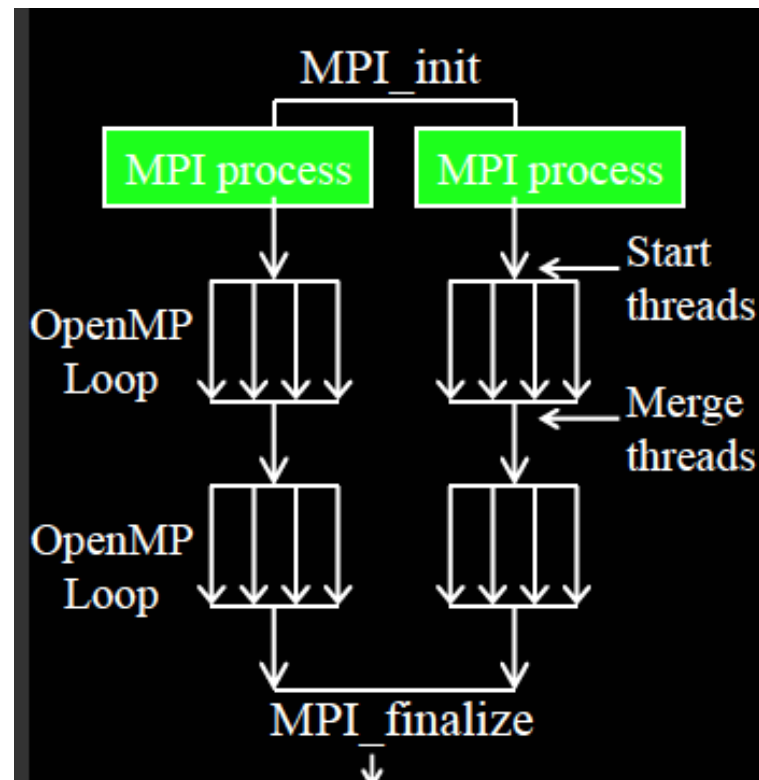
- **Additional programming complexity**
- **Can be difficult to debug race conditions**
- **Requires explicit synchronization**
- **Additional scalability bottlenecks:**
 - **thread creation overhead, critical sections, serial sections for MPI**
- **Cache coherence problems (false sharing) and data placement issues**
 - **Memory locality is key...**
 - **but OpenMP offers no direct control**

Are There Additional Solutions?

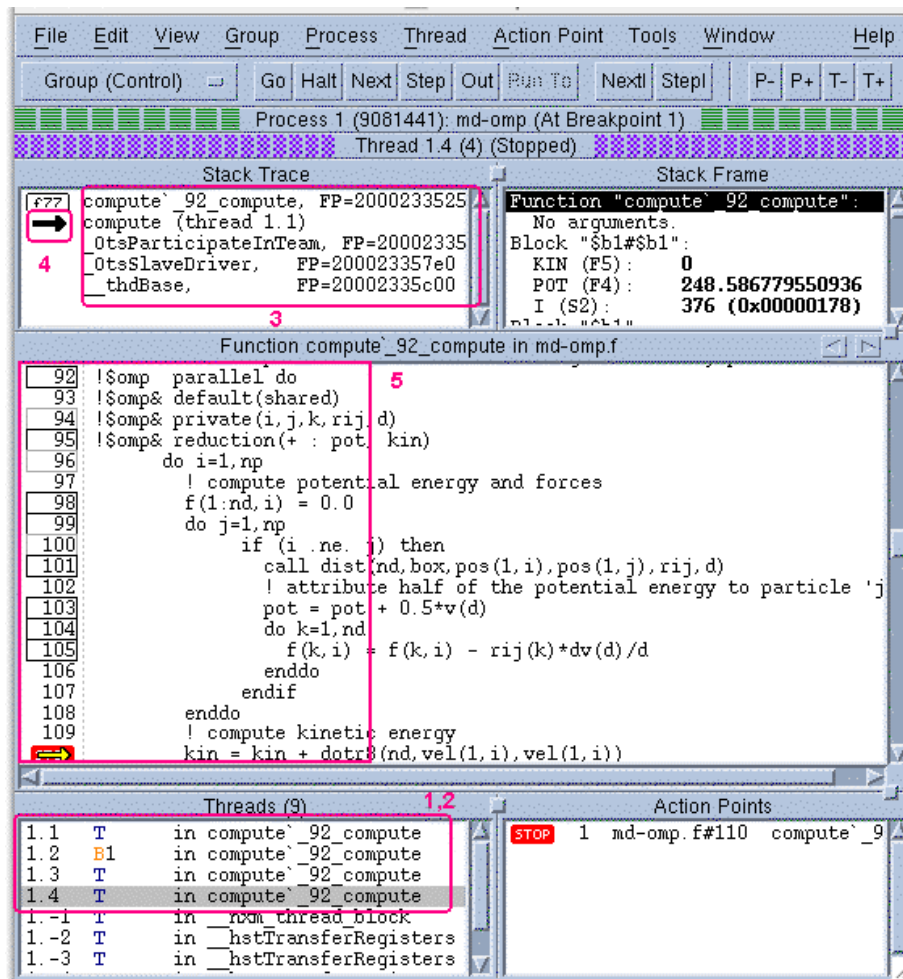
- **Sometimes it may be better to leave cores idle**
 - Improves memory capacity and bandwidth
 - Improves network bandwidth
- **However, you are charged for all cores**

Typical OpenMP Program

- **Execution begins with a single “Master Thread”**
- **Threads “fork” at each parallel region, join at end**

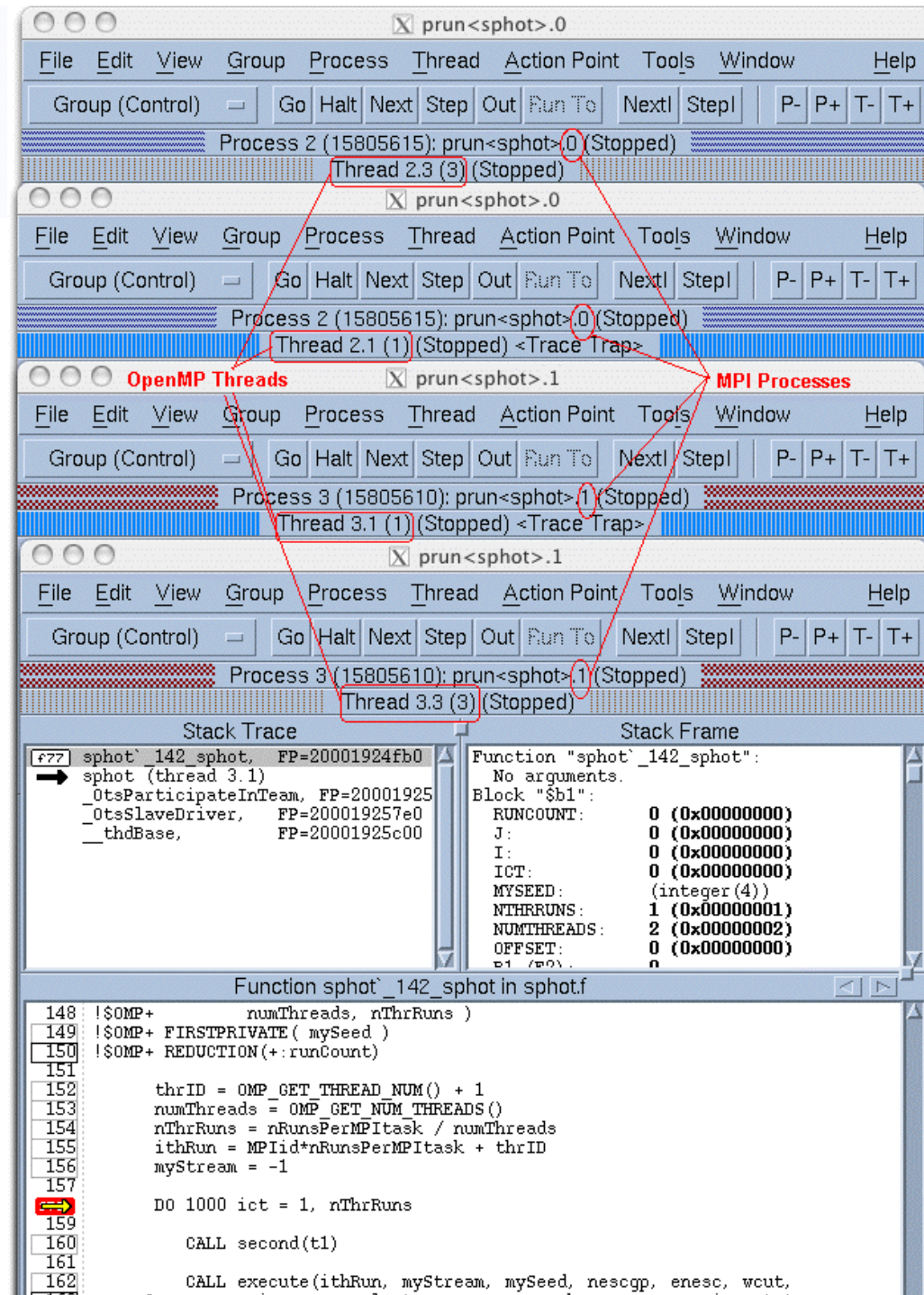


Can I Debug OpenMP and Hybrid Codes?



- Difficult because of *race conditions* – imprecise and non-reproducible ordering of memory read/store operations
- Common bugs:
 - incomplete or misplaced synchronization
 - improper scoping
 - occur often as a result of converting serial code

Screenshot of a Totalview debugging session with a hybrid MPI / OpenMP code.



The screenshot displays a Totalview debugging session for a hybrid MPI/OpenMP application. It shows three stacked windows for different processes, all titled 'prun<sphot>.0' or '.1'. The top window shows Process 2 (15805615) with Thread 2.3 (3) (Stopped). The middle window shows Process 3 (15805610) with Thread 3.1 (1) (Stopped) and Thread 3.3 (3) (Stopped). The bottom window shows Process 3 (15805610) with Thread 3.3 (3) (Stopped). Red circles and arrows highlight the thread IDs across the windows. The 'Stack Trace' pane shows the call stack for thread 3.1, with the top frame being 'sphot' (thread 3.1) at address f77. The 'Stack Frame' pane shows the function 'sphot' _142_sphot' with various variables like RUNCOUNT, J, I, ICT, MYSEED, NTHRRUNS, NUMTHREADS, and OFFSET. The 'Function sphot' _142_sphot in sphot.f' pane shows the source code for the function, including OpenMP directives and a loop.

Process 2 (15805615): prun<sphot>.0 (Stopped)
Thread 2.3 (3) (Stopped)

Process 3 (15805610): prun<sphot>.1 (Stopped)
Thread 3.1 (1) (Stopped) <Trace Trap>
Thread 3.3 (3) (Stopped)

Stack Trace

Address	Function	FP
f77	sphot' _142_sphot,	FP=20001924fb0
→	sphot (thread 3.1)	
	_otsParticipateInTeam,	FP=20001925
	_otsSlaveDriver,	FP=200019257e0
	_thdBase,	FP=20001925c00

Stack Frame

Variable	Value
Function "sphot" _142_sphot:	No arguments.
Block "\$b1":	
RUNCOUNT:	0 (0x00000000)
J:	0 (0x00000000)
I:	0 (0x00000000)
ICT:	0 (0x00000000)
MYSEED:	(integer(4))
NTHRRUNS:	1 (0x00000001)
NUMTHREADS:	2 (0x00000002)
OFFSET:	0 (0x00000000)
p1 / p2:	0

Function sphot' _142_sphot in sphot.f

```

148 |$OMP+      numThreads, nThrRuns )
149 |$OMP+ FIRSTPRIVATE( mySeed )
150 |$OMP+ REDUCTION(+:runCount)
151
152 |      thrID = OMP_GET_THREAD_NUM() + 1
153 |      numThreads = OMP_GET_NUM_THREADS()
154 |      nThrRuns = nRunsPerMPITask / numThreads
155 |      ithRun = MPIId*nRunsPerMPITask + thrID
156 |      myStream = -1
157
158 |      DO 1000 ict = 1, nThrRuns
159
160 |          CALL second(t1)
161
162 |          CALL execute(ithRun, myStream, mySeed, nescgp, enesc, wcut,

```

Can I Analyze OpenMP Performance?

Yes: Use CrayPat Tool

```
module load xt-craypat
```

```
cd $SCRATCH/...
```

```
make (e.g., ftn -o my.exe mycode.f)
```

```
pat_build -g omp
```

```
qsub ...
```

```
aprun -n $_cores my.exe+pat
```

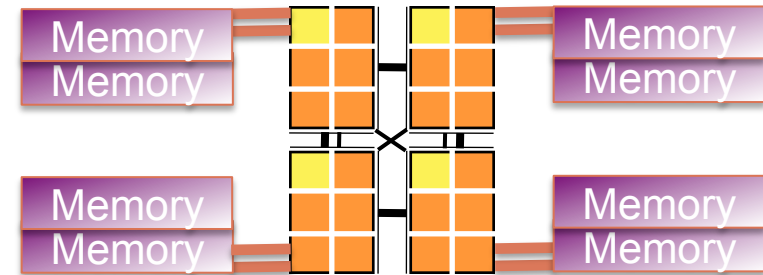
```
pat_report datafile.xf > out
```

What are the Disadvantages of OpenMP?

- Additional programming complexity
- Can be difficult to debug race conditions
- Requires explicit synchronization
- Additional scalability bottlenecks:
 - thread creation overhead, critical sections, serial sections for MPI
- Cache coherence problems (false sharing) and **data placement issues**
 - **Memory locality is key...**
 - **but OpenMP offers no direct control**

What's All This About Locality?

- **Remember: All memory accesses on the node happen transparently**
 - but remote access takes longer
- **Need NUMA control - memory and process affinity**
 - Improve performance
 - Eliminate performance variability
 - Avoid resource contention

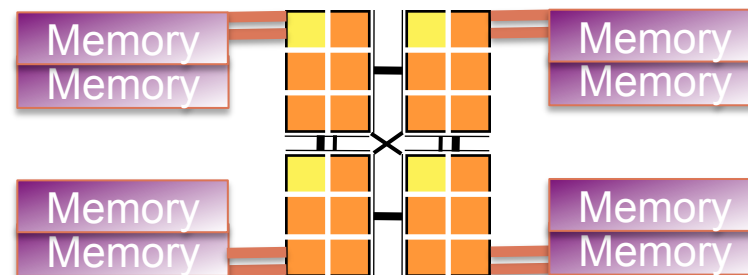


Where do processes, threads, and their memory go on the Hopper node?

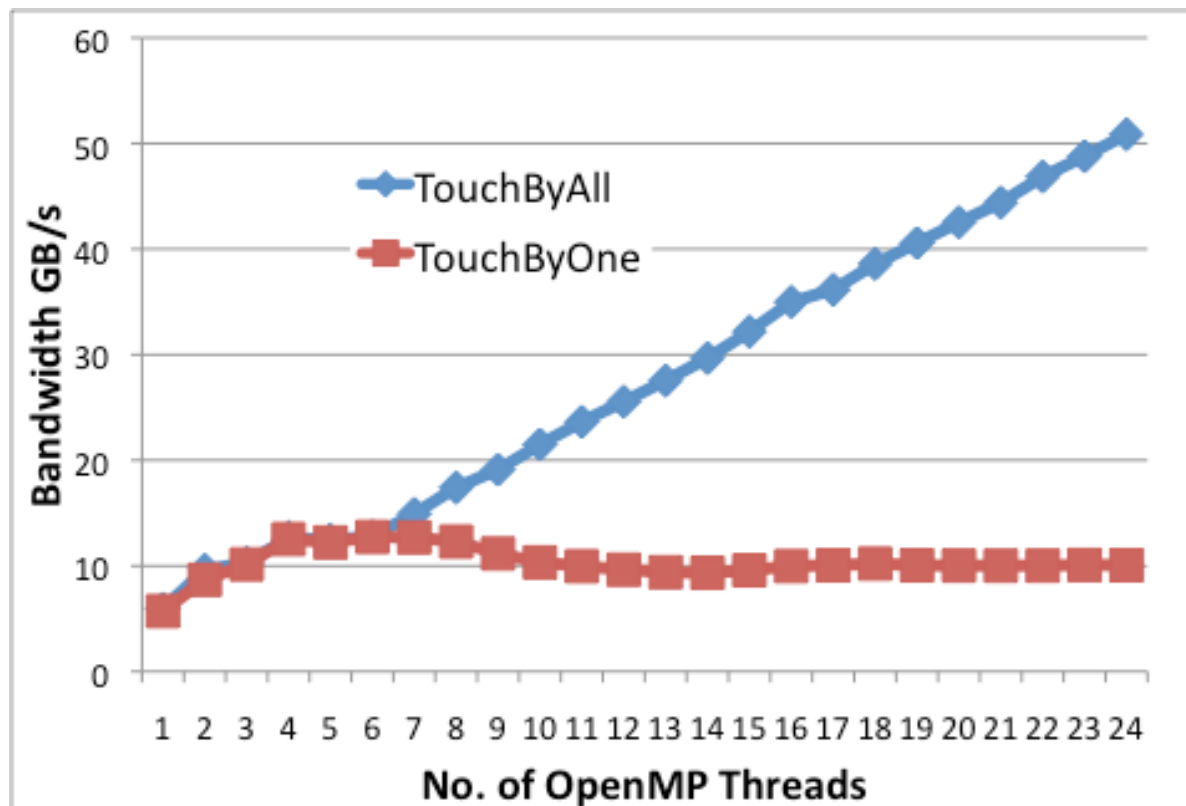
Memory Affinity via “First Touch”

- Memory is mapped to the NUMA node containing the core that first touches that memory.
- “Touch” means write (not allocate)
- Solution (Golden Rule): have each thread initialize the points that it will later be processing
 - Initialize memory immediately after allocating it
 - Initialize memory in parallel regions, not in serial code

Recommended: Tutorial M16 at SC10



$S_i = AX_i + Y_i$ Performance



Measurements by
Hongzhang Shan
(CRD)

More on Locality & Other Factors

Wednesday, Oct. 20th

Training	Time (PDT)	Topic	Presenter
	8:00-8:30am	Arrive at NERSC	
	8:30am-noon	<ul style="list-style-type: none"> • Single processor optimizations for Magny Cours. • Tips and tricks for running on the Hopper XE6 system 	Cray
	20 minute break from 10:30-10:50am		
	noon-1pm	Lunch + hands on sessions. Ask questions to Cray and NERSC staff	
	1-2pm	Best Practices for Hybrid OpenMP/MPI Programming on Hopper	Nick Wright

Part 2

RUNNING ON HOPPER

Running on Hopper

- **Submit a job to the batch system requesting resources**
 - Interactive
 - Batch
 - #PBS -l mppwidth = *Total_Number_of_cores_needed*
- **Launch executable with aprun**
 - Need to ensure that aprun command is consistent with batch resources requested

Running on Hopper

- **You must recompile**
 - **Franklin and Hopper Phase 1 binaries include SeaStar**
 - **Hopper Phase 2 binaries need Gemini**
- => you must recompile**

aprun: Example 1

- **Pure MPI application, using all cores in a node: 32 MPI tasks on 32 cores**

```
#PBS -l mppwidth=32  
aprun -n 32 a.out
```

Franklin

8 nodes, fully-populated,
(32 cores charged against allocation)

Hopper

2 nodes, not fully-populated
NOTE: you are charged for all the cores allocated
(48 cores charged against allocation)
(8 cores on one node, 24 on other node is default)

On Hopper, you can request actual number needed; batch system will allocate required number of nodes.
NOT RECOMMENDED!!!
Request full nodes
(#PBS -l mppwidth=48)

Important Note About Defaults

- Non-local Hopper NUMA node memory is not available unless your combination of #PBS directives and aprun command request it.
- Example: If you use 1/2 the cores in the node, and all are on two NUMA nodes only 1/2 the Hopper node memory is available.
- If you don't fully populate the node be sure to spread your cores over all NUMA nodes

aprun: Example 2

- Underpopulate nodes by 1/2 to save memory, 48 MPI tasks

Franklin

Requires 48 tasks ÷ 2 tasks per node X 4 cores per node
= 96 cores (24 nodes * 4 cores per charged against allocation)

```
#PBS -l mppwidth=96  
aprun -n 48 -N 2 a.out
```

Hopper

Requires 48 tasks ÷ 12 tasks per node X 24 cores per node
= 96 cores (4 nodes * 24 cores per charged against allocation)

```
#PBS -l mppwidth=96  
aprun -n 48 -N 12 -S 3 a.out
```

aprun NUMA options

- Important to ensure that MPI tasks are assigned separate NUMA nodes when underpopulating the node

Cores per NUMA node; 1-6, default 6;

```
aprun -S cores
```

NUMA nodes per Hopper node; 1-4, no default:

```
aprun -sn nodes
```

NUMA node list; 0,1,2,3 comma or hyphen delimited:

```
aprun -sl node-list
```

Hopper

aprun: Example 2

- Underpopulate nodes by 1/2 to save memory, 48 MPI tasks

Requires 48 tasks ÷ 12 tasks per node X 24 cores per node
= 96 cores (4 nodes * 24 cores per charged against allocation)

Hopper

```
#PBS -l mppwidth=96
aprun -n 48 -N 12 -S 3 a.out
```



optimal

```
#PBS -l mppwidth=96
aprun -n 48 -N 12 -S 4 a.out
```



avoid

aprun NUMA options

Hopper

CPU affinity: Bind processes / threads

- to each core within a NUMA node, or
 - to any core within a NUMA nodes or
 - don't bind at all;
- cc is the default for MPI codes

```
aprun -cc [ cpu | numa_node | none ]
```

Allocate memory only local to the NUMA node; do not use if underpopulating

```
aprun -ss
```

MPI, OpenMP and aprun

- Use both the OMP_NUM_THREADS environment variable + `aprun -n -d` options
- `aprun -n #` option specifies # of MPI processes
- `aprun -d #` option specifies number of threads per MPI task.
 - each of the “-n” MPI processes creates “-d” threads

aprun: Example 3

- Hybrid OpenMP / MPI

Franklin

92 MPI tasks, 4 OpenMP threads each:
Total cores = 92 tasks \div 1 MPI task per node X 4 cores per node = 368 (92 nodes)

```
#PBS mppwidth=368  
export OMP_NUM_THREADS=4  
aprun -n 92 -N 1 -d 4 a.out
```

Hopper

92 MPI tasks, 6 OpenMP threads each:
Total cores = 92 tasks \div 4 MPI tasks per node X 24 cores per node = 552 (23 nodes)

```
#PBS mppwidth=552  
setenv OMP_NUM_THREADS 6  
aprun -n 92 -N 4 -S 1 -d 6 a.out
```

Some Error Messages

- **Claim exceeds reservation's node-count**
 - On Franklin usually caused by requesting fewer cores (`#PBS -l mppwidth=#`) than aprun needs
 - On Hopper may result from improperly spreading processes and threads over NUMA nodes
- **Claim exceeds reservation's memory**
 - On Hopper; happens because having a compute node reserved for your job does not guarantee that you can use all NUMA nodes.

“Prediction is difficult - especially for the future.”

- Y. Berra

“The future will be just like the present - only more so.”

- Groucho Marx

Part 3

PERFORMANCE OF HOPPER

What Performance Should I Expect on Hopper Phase-2?

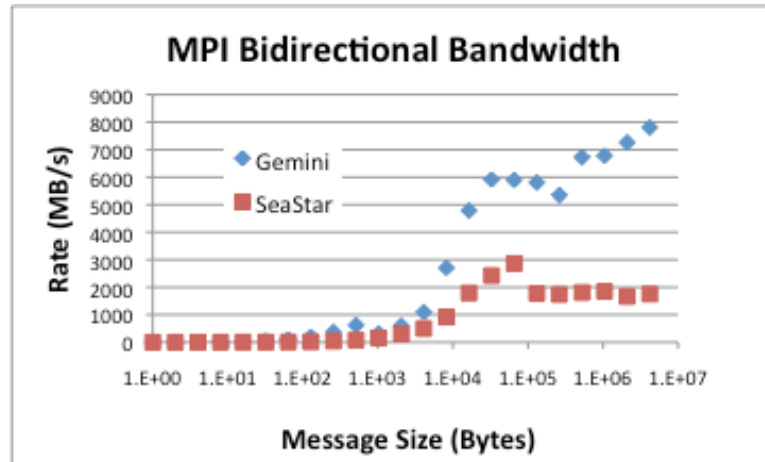
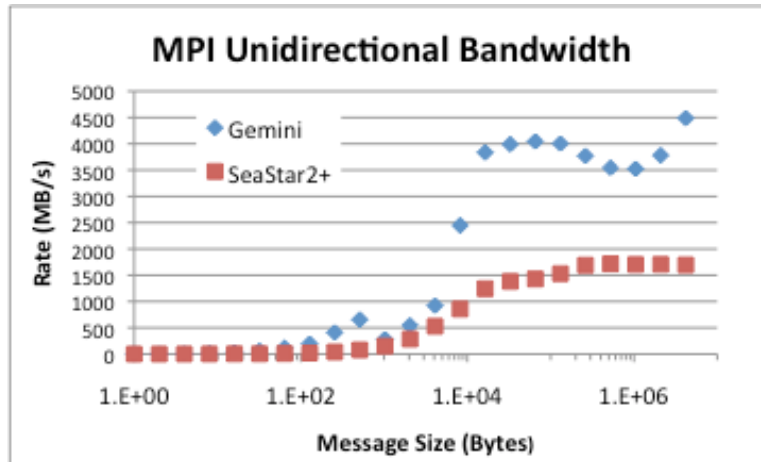
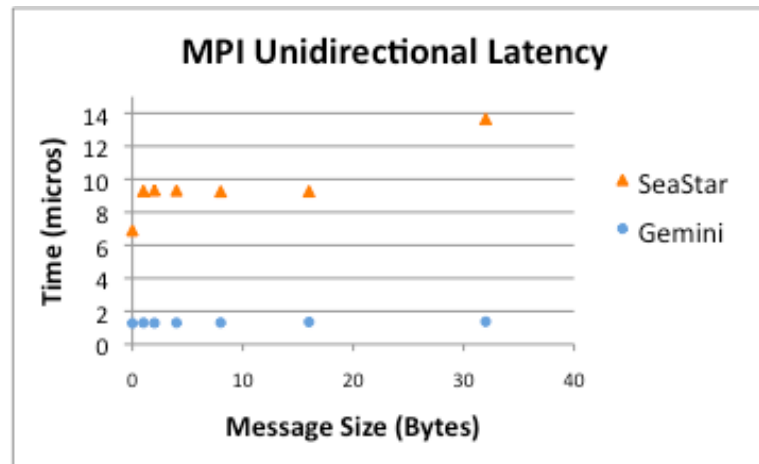
Processor	Cores	Frequency (GHz)	Peak (GFLOPS) per Core	Peak (GFLOPS) per Processor	Bandwidth (GB/s)	Balance (Bytes/Flop)	Hyper-Transport Technology	Memory Technology
Barcelona (Cray XT4)	4	2.3	9.2	36.8	12.8	0.34	3x 2GT/s	2x DDR2 667 per 4 cores
Magny Cours (Cray XT6)	12	2.1	8.4	100.8	42.6	0.42	4x 6.4 GT/s	2x DDR3 1333 per 6 cores

What Performance Should I Expect on Hopper Phase-2?

*PERFORMANCE DATA ARE PROPRIETARY –
NOT TO BE PUBLISHED IN ANY FORM*

*Cray XT6 PERFORMANCE DATA ARE FROM
AN EARLY VERSION OF THE SYSTEM*

What Performance Should I Expect on Hopper Phase-2?



**PRELIMINARY PERFORMANCE DATA:
PROPRIETARY – NOT TO BE PUBLISHED IN
ANY FORM**

NERSC Application Benchmarks

Code	Language	Description
CAM	F77	Community Atmosphere Model, “D” grid
GAMESS	F77	Quantum Chemistry RHF gradient MP2
GTC	F90	Particle in Cell – Fusion turbulence
IMPACT-T	F90 + FFTW	Particle in Cell – Accelerator design
MAESTRO	F90 (C)	Low Mach number flow astrophysical
MILC	C	Lattice QCD
PARATEC	Fortran + FFTW + BLAS	Plane Wave Density Functional Theory
PMEMD	F90	Particle Mesh Ewald Molecular Dynamics

Application Benchmark Times

(run times in seconds)

Code	Cores	Franklin	Hopper	Notes
CAM	240	378	335	
GAMESS	1024	3798	1386	Code rewrite to take advantage of Gemini one-sided communication; some code optimization; add'l parallelization
GTC	2048	1515*	1254**	loop source directives, some source changes; compiler
IMPACT-T	1024	661	600**	Compiler?
MAESTRO	2048	2532*	2036*	
MILC	8192	1285§	902§	
PARATEC	1024	591	381	
PMEMD	256	588	492	

* Pathscale

** Cray CCE / no OpenMP

§ gcc

**PRELIMINARY PERFORMANCE DATA:
PROPRIETARY – NOT TO BE PUBLISHED IN
ANY FORM**



Application Benchmark Times

(run times in seconds)

(This slide intentionally left blank in published version of the slides)



Summary

- **Hopper is performing well.**
- **Even for codes performing well you would be well advised to consider an alternative to MPI-only programming.**
- **The key to success is likely to be careful consideration of locality.**
- **NERSC can help.**

FILESYSTEMS

Home directories are global, meaning common across all NERSC systems. Accessible from login and compute nodes. Quota is 40 GB. Refer to your home space in scripts as `$HOME`.

Scratch directories are configured for parallel I/O, accessible from login and compute nodes, in `/scratch1/scratchdirs/userID` and `/scratch2/scratchdirs/userID`. Refer to these in scripts as `$SCRATCH1` and `$SCRATCH2`. Quota is 2 TB but purging will occur. Use the NERSC web form if more space is temporarily needed.

Project directories are available via the NERSC Global Filesystem (NGF); use these to share data across NERSC platforms or amongst users in a project. Use a NERSC web form to request (under Global File System).

HIGH PERFORMANCE STORAGE SYSTEM (HPSS)

Use HPSS to back up all your code and data. Access is via `ftp`, `pftp`, `htar`, or `hsi` to `archive.nersc.gov`. Use NIM password or generate a token (stored in `~/.netrc`) then no password required. The `hsi` utility uses syntax similar to Unix for most commands; additional commands include `add`, `cdls`, `cput`, `dump`, `get`, `lmdir`, `mdelete`, `mget`, `mput`, `put`, `replace`, `rename`, `save`, `send`, `store`.

Several ways of using `hsi`:

- From a command line: Just type `hsi`, wait for HPSS prompt, type commands, & exit to end.
- Multiple commands at once: `hsi "mkdir foo; cd foo; put data_file"`
- From input file: `hsi "in input_file"`
- From or to standard input or output:
`tar cvf - | hsi put - : d.tar`
`hsi get - : d.tar | tar xvf -`

Hopper QuickReference v1.0 October 2010

NERSC CONSULTING



Left to right, top: Katie Antypas (User Services Group Leader), Richard Gerber, Helen He, Woo-Sun Yang, Harvey Wasserman; bottom: Zhengji Zhao, Viraj Paropkari, Mike Stewart, David Turner, Eric Hjort

consult @ nersc.gov

510 - 486 - 8611 or

800-66-NERSC, menu option 3

<http://www.nersc.gov>

NERSC ACCOUNT MANAGEMENT (Passwords, New Users)



Clayton Bagwell, Mark Heer

510 - 486 - 8612 or

800-66-NERSC, menu option 2

Online Account Management for all users: <http://nim.nersc.gov>



QUICK REFERENCE CARD

NERSC Hopper

Complete documentation available on <http://www.nersc.gov>

Hopper OVERVIEW



The NERSC Hopper system, in full service early 2011, will have 1.25 Petaflops peak performance; 6,392 nodes, each with two 2.1-GHz Opteron 12-core processors, 153,408 total cores, 24 cores per node, 1.33 GB/core; Gemini interconnect in 3-D torus topology; operating system is the Cray Linux Environment, with full Linux on the eight login nodes and Compute Node Linux micro-kernel on the compute nodes.

HOW TO LOG IN

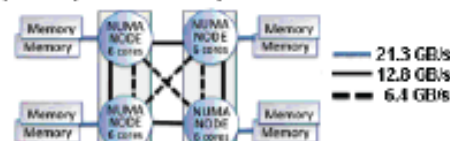
Log in to hopper with:

`ssh [-l user] hopper.nersc.gov`

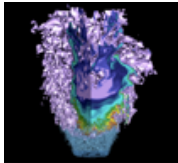
Use `-l user` only if user ID on your local system is different from your user ID on Hopper. Note: use `hopp2.nersc.gov` prior to January 2011. Passwords must not be shared. Login privileges are disabled with three login failures; call Account Management to clear login failures.

Hopper NODE ARCHITECTURE

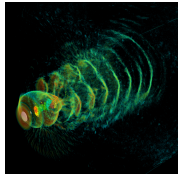
Note the Non-Uniform Memory Architecture (NUMA) with six cores per NUMA node:



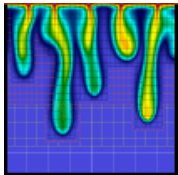
About the Cover



Low swirl burner combustion simulation. Image shows flame radical, OH (purple surface and cutaway) and volume rendering (gray) of vortical structures. Red indicates vigorous burning of lean hydrogen fuel; shows cellular burning characteristic of thermodynamically unstable fuel. Simulated using an adaptive projection code. Image courtesy of John Bell, LBNL.



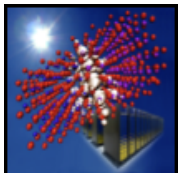
Hydrogen plasma density wake produced by an intense, right-to-left laser pulse. Volume rendering of current density and particles (colored by momentum orange - high, cyan - low) trapped in the plasma wake driven by laser pulse (marked by the white disk) radiation pressure. 3-D, 3,500 Franklin-core, 36-hour LOASIS experiment simulation using VORPAL by Cameron Geddes, LBNL. Visualization: Gunther Weber, NERSC Analytics.



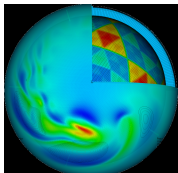
Numerical study of density driven flow for CO₂ storage in saline aquifers. Snapshot of CO₂ concentration after convection starts. Density-driven velocity field dynamics induces convective fingers that enhance the rate by which CO₂ is converted into negatively buoyant aqueous phase, thereby improving the security of CO₂ storage. Image courtesy of George Pau, LBNL



False-color image of the Andromeda Galaxy created by layering 400 individual images captured by the Palomar Transient Factory (PTF) camera in February 2009. NERSC systems analyzing the PTF data are capable of discovering cosmic transients in real time. Image courtesy of Peter Nugent, LBNL.



The exciton wave function (the white isosurface) at the interface of a ZnS/ZnO nanorod. Simulations performed on a Cray XT4 at NERSC, also shown. Image courtesy of Lin-Wang Wang, LBNL.



Simulation of a global cloud resolving model (GCRM). This image is a composite plot showing several variables: wind velocity (surface pseudocolor plot), pressure (b/w contour lines), and a cut-away view of the geodesic grid. Image courtesy of Professor David Randall, Colorado State University.