#### The Next Generation of High Performance Computing

William Gropp <u>www.cs.illinois.edu/~wgropp</u>



### Extrapolation is Risky

- 1989 T 23 years
  - Intel introduces 486DX
  - Eugene Brooks writes "Attack of the Killer Micros"
  - ♦ 4 years before TOP500
  - Top systems at about 2 GF Peak
- 1999 T 13 years



- NVIDIA introduces its GPU (GeForce 256)
  - Programming GPUs still a challenge 13 years later
- Top system ASCI Red, 9632 cores, 3.2 TF Peak (about 3 GPUs in 2012)
- MPI is 7 years old





# **HPC Today**

- High(est)-End systems
  - 1 PF (10<sup>15</sup> Ops/s) achieved on a few "peak friendly" applications
  - Much worry about scalability, how we're going to get to an ExaFLOPS
  - Systems are all oversubscribed
    - DOE INCITE awarded almost 900M processor hours in 2009; 1600M-1700M hours in 2010-2012; (big jump planned in 2013 – over 5B hours)
    - NSF PRAC awards for Blue Waters similarly competitive
- Widespread use of clusters, many with accelerators; cloud computing services
  - These are transforming the low and midrange
- Laptops (far) more powerful than the supercomputers I used as a graduate student





# HPC in 2012

- <u>Sustained</u> PF systems
  - K Computer (Fujitsu) at RIKEN, Kobe, Japan (2011)
  - "Sequoia" Blue Gene/Q at LLNL
  - NSF Track 1 "Blue Waters" at Illinois
  - Undoubtedly others (China, ... )
- Still programmed with MPI and MPI+other (e.g., MPI+OpenMP or MPI+OpenCL/CUDA)
  - But in many cases using toolkits, libraries, and other approaches
    - And not so bad applications will be able to run when the system is turned on
  - Replacing MPI will require some compromise e.g., domain specific (higher-level but less general)
    - Lots of evidence that fully automatic solutions won't work





# HPC in 2020-2023

- Exascale systems are likely to have
  - Extreme power constraints, leading to
    - Clock Rates similar to today's systems
    - A wide-diversity of simple computing elements (simple for hardware but complex for software)
    - Memory per core and per FLOP will be much smaller
    - Moving data anywhere will be expensive (time and power)
  - Faults that will need to be detected and managed
    - Some detection may be the job of the programmer, as hardware detection takes power
  - Extreme scalability and performance irregularity
    - Performance will require enormous concurrency
    - Performance is likely to be variable
      - Simple, static decompositions will not scale
  - A need for latency tolerant algorithms and programming
    - Memory, processors will be 100s to 10000s of cycles away. Waiting for operations to complete will cripple performance







# What Do Current Systems Tell Us?

- Examples of trends
  - Supercomputers: Blue Waters
  - Exploiting Commodity Computing: GPU Clusters
  - Post GPU: Radical architectures
- Parallelism is about getting *performance* 
  - Productivity is important, but only if performance is achieved
  - All systems already "heterogeneous"
    - "Vector" instructions really a separate unit



Sustained performance is the goal



#### Focus on Sustained Performance

- Blue Water's and NSF are focusing on sustained performance in a way few have been before.
- *Sustained* is the computer's performance on a broad range of applications that scientists and engineers use every day.
  - Time to solution is the metric not Ops/s
  - Tests include time to read data and write the results
- NSF's call emphasized sustained performance, demonstrated on a collection of application benchmarks (application + problem set)
  - Not just simplistic metrics (e.g. HP Linpack)
  - Applications include both Petascale applications (effectively use the full machine, solving scalability problems for both compute and I/O) and applications that use a fraction of the system
- Blue Waters project focus is on delivering sustained PetaFLOPS performance to all applications
  - Develop tools, techniques, samples, that exploit all parts of the system





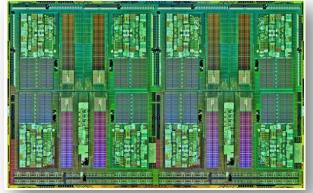


## Blue Waters Science Team Characteristics

Science Area	Number of Teams	Codes	Structured Grids	Unstructured Grids	Dense Matrix	Sparse Matrix	N- Body	Monte Carlo	FFT	Significant I/O
Climate and Weather	3	CESM, GCRM, CM1, HOMME	x	x		х		х		
Plasmas/ Magnetosphere	2	H3D(M), OSIRIS, Magtail/ UPIC	x				X		x	x
Stellar Atmospheres and Supernovae	2	PPM, MAESTRO, CASTRO, SEDONA	x			x		X		x
Cosmology	2	Enzo, pGADGET	X			Х	Х			
Combustion/ Turbulence	1	PSDNS	x						X	
General Relativity	2	Cactus, Harm3D, LazEV	X			X				
Molecular Dynamics	4	AMBER, Gromacs, NAMD, LAMMPS			X		x		X	
Quantum Chemistry	2	SIAL, GAMESS, NWChem			X	X	X	x		x
Material Science	3	NEMOS, OMEN, GW, QMCPACK			X	X	X	x		
Earthquakes/ Seismology	2	AWP-ODC, HERCULES, PLSQR, SPECFEM3D	x	x			X			x
Quantum Chromo Dynamics	1	Chroma, MILC, USQCD	x		X	X	X		X	
Social Networks	1	EPISIMDEMICS								
Evolution	1	Eve								
Computer Science	1			x	x	x			x	x
1867										-67



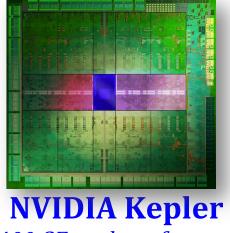
### Heart of Blue Waters: Two New Chips



**AMD Interlagos** 157 GF peak performance

#### **Features:**

2.3-2.6 GHz 8 core modules, 16 threads On-chip Caches L1 (I:8x64KB; D:16x16KB) L2 (8x2MB) Memory Subsystem Four memory channels 51.2 GB/s bandwidth



1,400 GF peak performance

#### **Features:**

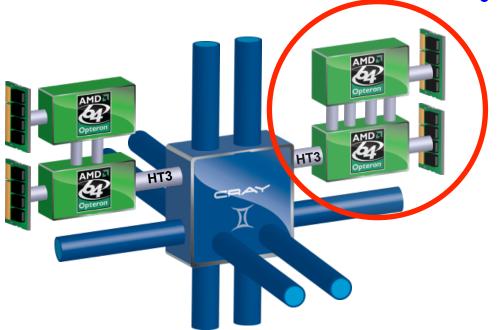
15 Streaming multiprocessors (SMX) SMX: 192 sp CUDA cores, 64 dp
units, 32 special function units L1 caches/shared mem (64KB, 48KB) L2 cache (1536KB)
Memory subsystem Six memory channels 180 GB/s bandwidth





# Cray XE6 Nodes





Blue Waters contains 22,640 Cray XE6 compute nodes.

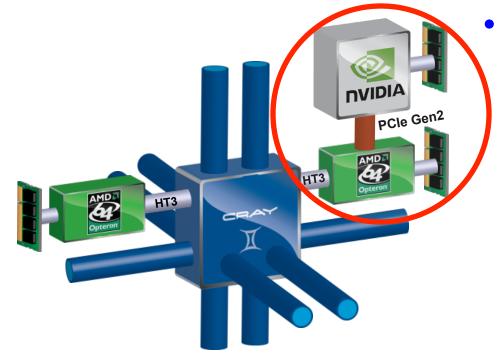
- Dual-socket Node
  - Two AMD Interlagos chips
    - 16 core modules, 64 threads
    - 313 GFs peak performance
    - 64 GBs memory
      - 102 GB/sec memory bandwidth
  - ♦ Gemini Interconnect
    - Router chip & network interface
    - Injection Bandwidth (peak)
      - 9.6 GB/sec per direction





#### Cray XK7 Nodes



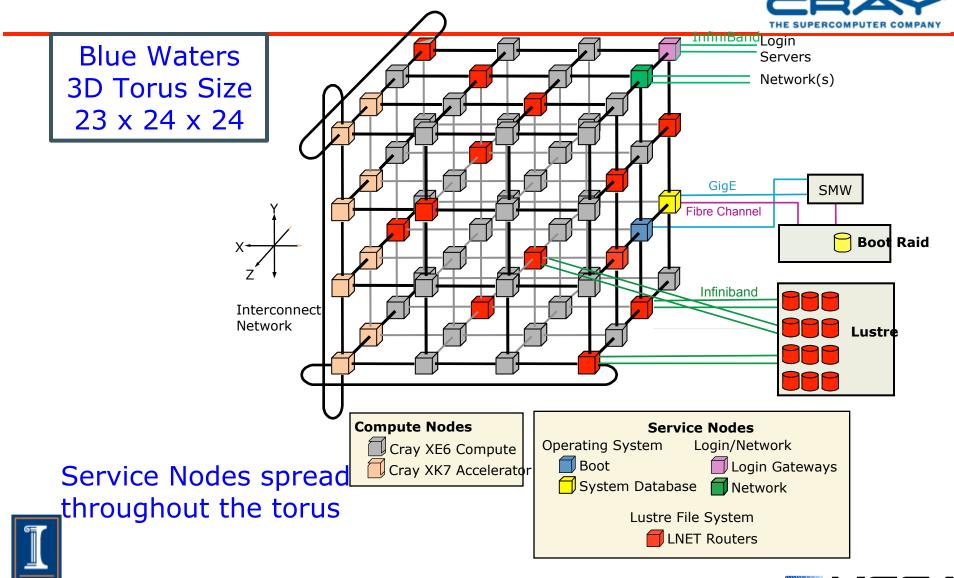


Blue Waters contains 3,072 Cray XK7 compute nodes. Dual-socket Node

- One AMD Interlagos chip
  - 32 GBs memory
    - 51.2 GB/s bandwidth
- One NVIDIA Kepler chip
  - 1.4 TFs peak performance
  - 6 GBs GDDR5 memory
    - 180 GB/sec bandwidth
- Gemini Interconnect
  - Same as XE6 nodes



#### Gemini Interconnect Network





# Blue Waters Disk Subsystem



- Cray Sonexion 1600
  - Lustre file system
  - Reliable, Modular, Scalable
  - Fully integrated
    - Servers
    - Disk drives (Scalable Storage Units)
    - QDR Infiniband switches
  - Hierarchical monitoring
- Blue Waters Disk Subsystem
  - Capacity: 34.6 PBs (raw), 25.9 PBs (usable)
  - Bandwidth: >1 TB/s (sustained)







### Blue Waters Archive System

#### • Spectra Logic T-Finity

- Dual-arm robotic tape libraries
- High availability and reliability, with built-in redundancy

#### • Blue Waters Archive

- Capacity: 380 PBs
   (raw), 300 PBs (usable)
- Bandwidth: 100 GB/sec (sustained)

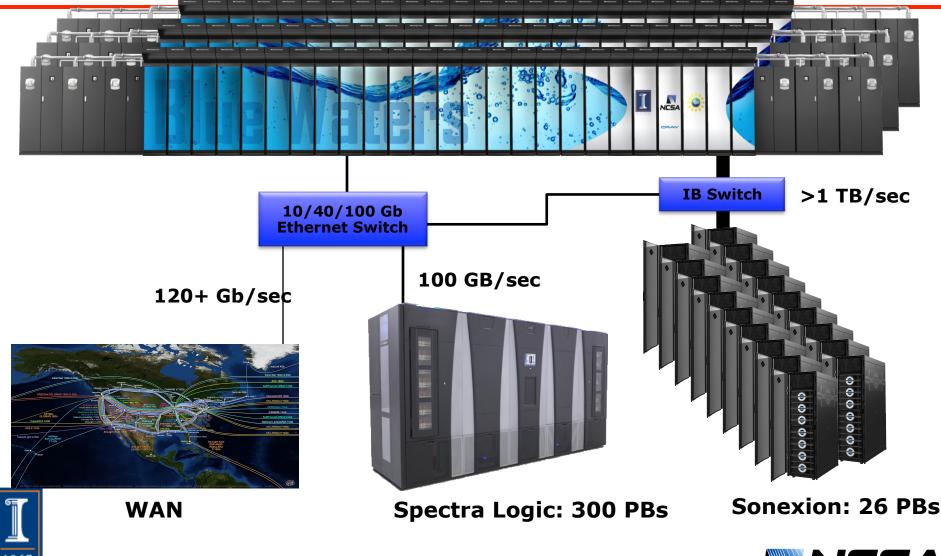


 RAIT for increased reliability





#### **Blue Waters Computing System**





# Blue Waters and Titan Computing Systems

System Attribute	NCSA Blue Waters	ORNL Titan
Vendors Processors	Cray/AMD/NVIDIA Interlagos/Kepler	Cray/AMD/NVIDIA Interlagos/Kepler
Total Peak Performance (PF) Total Peak Performance (C	11.9 CPU/GPU) 7.6/4.3	>20 3/17
Number of CPU Chips Number of GPU Chips	48,576 3,072	18,688 14,592
Amount of CPU Memory (TB)	) 1,510	688
Interconnect	3D Torus	3D Torus
Amount of On-line Disk Stora Sustained Disk Transfer (TB/ Amount of Archival Storage Sustained Tape Transfer (GB)	(sec) >1 300	20(?) 0.4-0.7 15-30 7





# Blue Waters and Kei Computing Systems

System Attribute	NCSA Blue Waters	RIKEN Kei
Vendors Processors	Cray/AMD/NVIDIA Interlagos/Kepler	Fujitsu SPARC64 VIIIfx
Total Peak Performance (PF) Total Peak Performance (		11.3 11.3/0.0
Number of CPU Chips Number of GPU Chips	48,576 3,072	88,128 0
Amount of CPU Memory (TE	3) 1,510	1,410
Interconnect	3D Torus	6D Torus
Amount of On-line Disk Stor Sustained Disk Transfer (TB Amount of Archival Storage	/sec) >1 300	11/30 ? ?
Sustained Tape Transfer (GB	B/sec) 100	?



Blue Waters and Sequoia Computing Systems

System Attribute	NCSA Blue Waters	LLNL Sequoia
Vendor(s) Processors	Cray/AMD/NVIDIA Interlagos/Kepler	IBM PowerPCA2 variant
Total Peak Performance (PF Total Peak Performance (		20.1 20.1/0.0
Number of CPU Chips (8, 1) Number of GPU Chips	6 cores/chip) 48,576 3,072	98,304 0
Amount of CPU Memory (TE	3) 1,510	1,572
Interconnect	3D Torus	5D Torus
Amount of On-line Disk Sto Sustained Disk Transfer (TE		50(?) 0.5-1.0
Amount of Archival Storage Sustained Tape Transfer (G		? ?



# Petascale Computing Facility



Partners EYP MCF/ Gensler

IBM

Yahoo!

- Modern Data Center
  - 90,000+ ft<sup>2</sup> total
  - 30,000 ft<sup>2</sup> raised floor 20,000 ft<sup>2</sup> machine room gallery
- Energy Efficiency
  - LEED certified Gold
  - Power Utilization Efficiency = 1.1–1.2



#### Another Example System

- 128 node GPU Cluster
- #3 on Green500 in 2010
- Each node has
  - One Core i3 530 2.93 GHz dual-core CPU
  - One Tesla C2050 GPU per node
- 33.62 TFLOPS on HPL (10x ASCI Red)
- 934 MFLOPS/Watt
- But how do you program it?







#### An Even More Radical System



- Rack Scale
  - Processing:128 Nodes, 1 (+) PF/s
  - Memory:
    - 128 TB DRAM
    - 0.4 PB/s Aggregate Bandwidth
  - NV Memory



- 1 PB Phase Change Memory (addressable)
- Additional 128 for Redundancy/RAID
- Network
  - 0.13 PB/sec Injection, 0.06 PB/s Bisection

Deployment	Nodes	Topology	Compute	Mem BW	Injection BW	Bisection BW
Module	1	N/A	8 TF/s	3 TB/s	1 TB/s	N/A
Deployable Cage	22	All-to-All	176 TF/s	67.5 TB/s	22.5 TB/s	31 TB/s
Rack	128	Flat. Butterfly	1 PF/s	.4 PB/s	0.13 PB/s	0.066 PB/s
Group Cluster	512	Flat. Butterfly	4.1 PF/s	1.6 PB/s	0.52 PB/s	0.26 PB/s
National Resource	128k	Hier. All-to-All	1 EF/s	0.4 EB/s	0.13 EB/s	16.8 PB/s
Max Configuration	2048k	Hier. All-to-All	16 EF/s	6.4 EB/s	2.1 EB/s	0.26 EB/s





# How Do We Make Effective Use of These Systems?

- Better use of our existing systems
  - Blue Waters will provide a sustained PF, but that typically requires ~10PF peak
- Improve node performance
  - Make the compiler better
  - Give better code to the compiler
  - Get realistic with algorithms/data structures
- Improve parallel performance/scalability
- Improve productivity of applications
  - Better tools and interoperable languages, not a (single) new programming language
- Improve algorithms
  - Optimize for the real issues data movement, power, resilience, ...





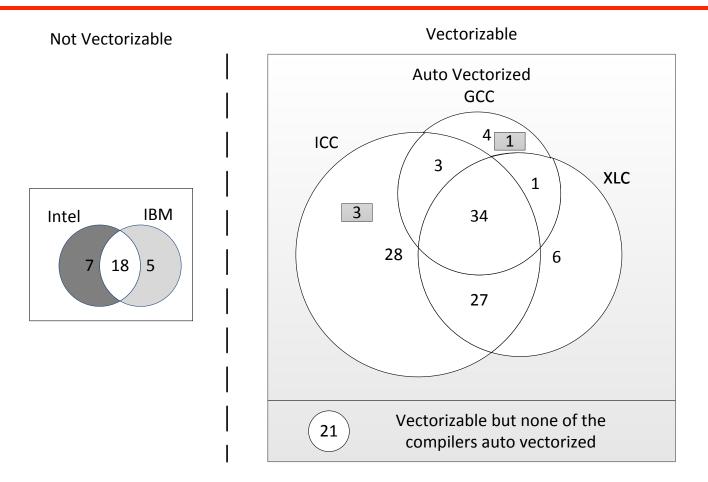
# Make the Compiler Better

- It remains the case that most compilers cannot compete with hand-tuned or autotuned code on simple code
  - Just look at dense matrix-matrix multiplication or matrix transpose
  - Try it yourself!
    - Matrix multiply on my laptop:
    - N=100 (in cache): 1818 MF (1.1ms)
    - N=1000 (not): 335 MF (6s)





#### How Good are Compilers at Vectorizing Codes?



S. Maleki, Y. Gao, T. Wong, M. Garzarán, and D. Padua. *An Evaluation of Vectorizing Compilers*. PACT 2011.



# Media Bench II Applications

Appl	XLC	ICC	GCC	XLC	ICC	GCC
	Automatic		Manual			
JPEG Enc	-	1.33	-	1.39	2.13	1.57
JEPG Dec	-	-	-	-	1.14	1.13
H263 Enc	-	-	-	1.25	2.28	2.06
H263 Dec	-	-	-	1.31	1.45	-
MPEG2 Enc	-	-	-	1.06	1.96	2.43
MPEG2 Dec	-	-	1.15	1.37	1.45	1.55
MPEG4 Enc	-	-	-	1.44	1.81	1.74
MPEG4 Dec	-	-	-	1.12	-	1.18



Table shows whole program speedups measured against unvectorized application S. Maleki, Y. Gao, T. Wong, M. Garzarán, and D. Padua. *An Evaluation of Vectorizing Compilers*. PACT 2011.



# How Do We Change This?

- Test compiler against "equivalent" code (e.g., best hand-tuned or autotuned code that performs the same computation, under some interpretation or "same")
  - In a perfect world, the compiler would provide the same, excellent performance for all equivalent versions
- As part of the Blue Waters project, Padua, Garzaran, Maleki are developing a test suite that evaluates how the compiler does with such equivalent code
  - Working with vendors to improve the compiler
  - Identify necessary transformations
  - Identify opportunities for better interaction with the programmer to facilitate manual intervention.
  - Main focus has been on code generation for vector extensions
  - Result is a compiler whose realized performance is less sensitive to different expression of code and therefore closer to that of the best hand-tuned code.
  - Just by improving automatic vectorization, loop speedups of more than 5 have been observed on the Power 7.
- But this is a long-term project
  - What can we do in the meantime?





Give "Better" Code to the Compiler

- Augmenting current programming models and languages to exploit advanced techniques for performance optimization (i.e., *autotuning*)
- Not a new idea, and some tools already do this.
- But how can these approaches become part of the mainstream development?





How Can Autotuning Tools Fit Into Application Development?

- In the short run, just need effective mechanisms to replace user code with tuned code
  - Manual extraction of code, specification of specific collections of code transformations
- But this produces at least two versions of the code (tuned (for a particular architecture and problem choice) and untuned). And there are other issues.
- What does an application <u>want</u> (what is the Dream)?





# **Application Needs Include**

- Code must be portable
- Code must be persistent
- Code must permit (and encourage) experimentation
- Code must be maintainable
- Code must be correct
- Code must be faster





# Implications of These Requirements

- Portable augment existing language. Either use pragmas/ comments or extremely portable precompiler
  - Best if the tool that performs all of these steps looks like just like the compiler, for integration with build process
- Persistent
  - Keep original and transformed code around: Golden Copy
- Maintainable
  - Let user work with original code and ensure changes automatically update tuned code
- Correct
  - Do whatever the application developer needs to believe that the tuned code is correct
    - In the end, this <u>will</u> require running some comparison tests
- Faster
  - Must be able to interchange tuning tools pick the best tool for each part of the code
  - No captive interfaces
  - Extensibility a clean way to add new tools, transformations, properties, ...





# Application-Relevant Abstractions

- Language for interfacing with autotuning must convey concepts that are meaningful to the application programmer
- Wrong: unroll by 5
  - Though could be ok for performance expert, and some compilers already provide pragmas for specific transformations
- Right (maybe): Performance precious, typical loop count between 100 and 10000, even, not power of 2
- We need work at developing higher-level, performance-oriented languages or language extensions
  - This would be the "good" future





# Better Algorithms and Data Structures

- Autotuning only offers the best performance with the given data structure and algorithm
  - That's a big constraint
- Processors include hardware to address performance challenges
  - "Vector" function units
  - Memory latency hiding/prefetch
  - Atomic update features for shared memory
  - Etc.

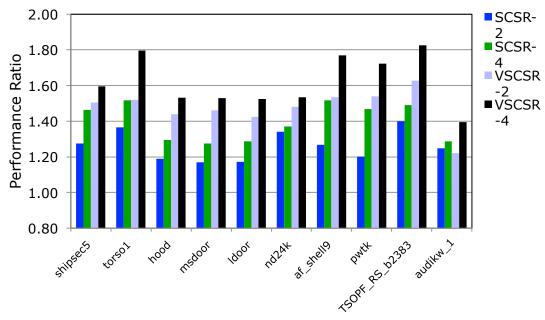




### Sparse Matrix-Vector Multiply

#### **Barriers to faster code**

- "Standard" formats such as CSR do not meet requirements for prefetch or vectorization
- Modest changes to data structure enable both vectorization, prefetch, for 20-80% improvement on P7



Prefetch results in *Optimizing Sparse Data Structures for Matrix Vector Multiply* http:// hpc.sagepub.com/content/25/1/115





# What Does This Mean For You?

- It is time to rethink data structures and algorithms to match the realities of memory architecture
  - We have results for x86 where the benefit is smaller but still significant
  - Better match of algorithms to prefetch hardware is necessary to overcome memory performance barriers
- Similar issues come up with heterogeneous processing elements (someone needs to *design* for memory motion and concurrent and nonblocking data motion)





#### Performance on a Node

- Nodes are SMPs
  - You have this problem on anything (even laptops)
- Tuning issues include the usual
  - Getting good performance out of the compiler (often means adapting to the memory hierarchy)
- New (SMP) issues include
  - Sharing the SMP with other processes
  - Sharing the memory system





# New (?) Wrinkle – Avoiding Jitter

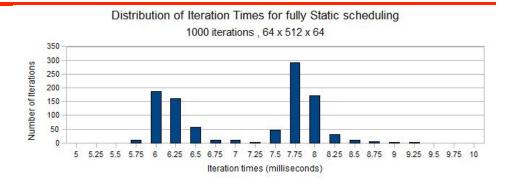
- Jitter here means the variation in time measured when running identical computations
  - Caused by other computations, e.g., an OS interrupt to handle a network event or runtime library servicing a communication or I/O request
- This problem is in some ways less serious on HPC platform, as the OS and runtime services are tuned to minimize impact
  - However, cannot be eliminated entirely

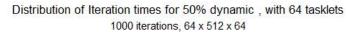


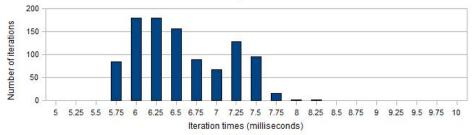


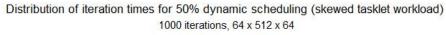
# Sharing an SMP

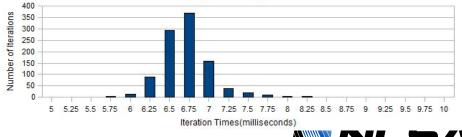
- Having many cores available makes everyone think that they can use them to solve other problems ("no one would use all of them all of the time")
- However, compute-bound scientific calculations are often *written* as if all compute resources are owned by the application
- Such *static* scheduling leads to performance loss
- Pure dynamic scheduling adds overhead, but is better
  - Careful mixed strategies are even better
    - Thanks to Vivek Kale



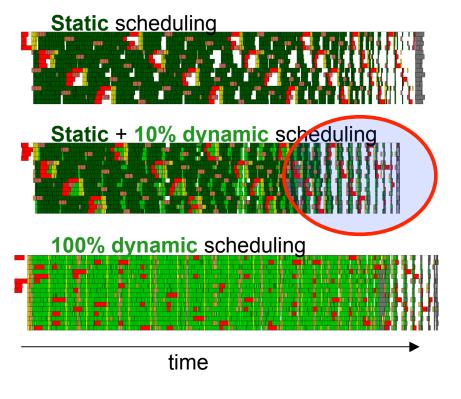






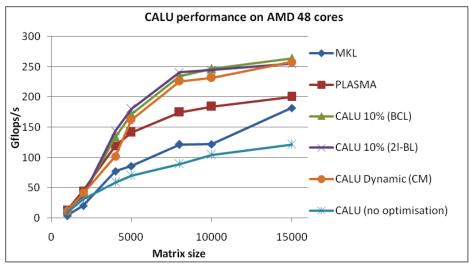


# Happy Medium Scheduling



Communication Avoiding LU factorization (CALU) algorithm

S. Donfack, L .Grigori, V. Kale, WG, IPDPS '12







### Synchronization and OS Noise

 "Characterizing the Influence of System Noise on Large-Scale Applications by Simulation," Torsten Hoefler, Timo Schneider, Andrew Lumsdaine

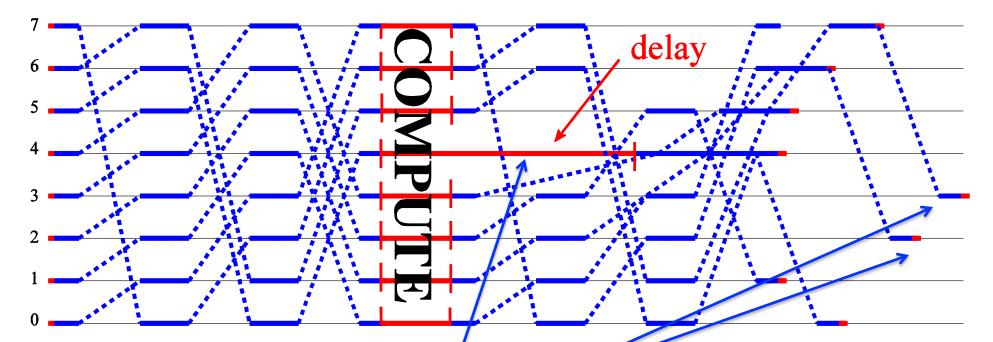
Best Paper, SC10

• Next 3 slides based on this talk...





# A Noisy Example – Dissemination Barrier

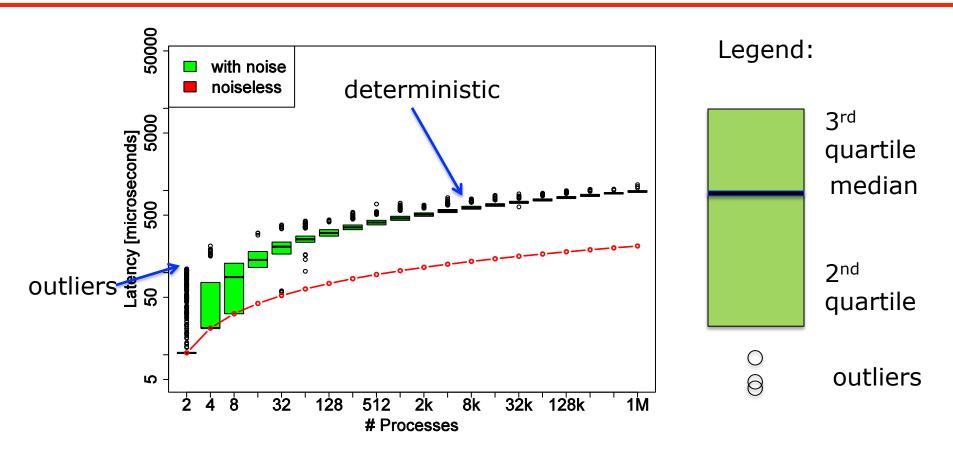


- Process 4 is delayed
  - Noise propagates "wildly" (of course deterministic)





# Single Collective Operations and Noise





1 Byte, Dissemination, regular noise, 1000 Hz, 100 µs



The problem is blocking operations

- Simple, data-parallel algorithms easy to reason about but inefficient
  - True for decades, but ignored (memory)
- One solution: fully asynchronous methods
  - Very attractive, yet efficiency is low and there are good reasons for that
  - Blocking can be due to fully collective (e.g., Allreduce) or neighbor communications (halo exchange)



 Can we save methods that involve global, synchronizing operations?



# Saving Allreduce

- One common suggestion is to avoid using Allreduce
  - But algorithms with dot products are among the best known
  - Can sometimes aggregate the data to reduce the number of separate Allreduce operations
  - But better is to reduce the impact of the synchronization by hiding the Allreduce behind other operations (in MPI, using MPI\_Iallreduce)
- We can adapt CG to nonblocking Allreduce with some added floating point (but perhaps little time cost)





# The Conjugate Gradient Algorithm

• While (not converged) niters +=1;s = A \* p; t = p' \*s; alpha = gmma / t; x = x + alpha \* p; r = r - alpha \* s; if rnorm2 < tol2 ; break ; end z = M \* r; gmmaNew = r' \* z;beta = gmmaNew / gmma; gmma = gmmaNew;  $\bar{p} = z + beta * p;$ end





# The Conjugate Gradient Algorithm

• While (not converged) niters +=1; $S \longrightarrow = A *_A p;$ <u>n'7s;</u> alpha = gmma / t; x = x + alpha \* p; r = r - alpha \* s; if rnorm2 < tol2 ; break ; end gmmaNew = r' \* z; beta = gmmaNew / gmma; gmma = gmmaNew; p = z + beta \* p; end





### CG Reconsidered

- By reordering operations, nonblocking dot products (MPI\_Iallreduce in MPI-3) can be overlapped with other operations
- Trades extra local work for overlapped communication
  - On a pure floating point basis, the nonblocking version requires 2 more DAXPY operations
  - A closer analysis shows that some operations can be merged



More work does not imply more time



### What's Different at Peta/Exascale

- Performance Focus
  - Only a little basically, the resource is expensive, so a premium placed on making good use of resource
  - Quite a bit node is more complex, has more features that must be exploited
- Scalability
  - Solutions that work at 100-1000 way often inefficient at 100,000-way
  - Some algorithms scale well
    - Explicit time marching in 3D
  - Some don't
    - Direct implicit methods
  - Some scale well for a while
    - FFTs (communication volume in Alltoall)
  - Load balance, latency are critical issues
- Fault Tolerance becoming important
  - Now: Reduce time spent in checkpoints
  - Soon: Lightweight recovery from transient errors





Preparing for the Next Generation of HPC Systems

- Better use of existing resources
  - Performance-oriented programming
  - Dynamic management of resources at all levels
  - Embrace hybrid programming models (you have already if you use SSE/VSX/OpenMP/...)
- Focus on results
  - Adapt to available network bandwidth and latency
  - Exploit I/O capability (available space crew faster than processor performance!)
- Prepare for the future
  - Fault tolerance
  - Hybrid processor architectures
  - Latency tolerant algorithms
  - Data-driven systems 48





# **Recommended Reading**

- Bit reversal on uniprocessors (Alan Karp, SIAM Review, 1996)
- Achieving high sustained performance in an unstructured mesh CFD application (W. K. Anderson, W. D. Gropp, D. K. Kaushik, D. E. Keyes, B. F. Smith, Proceedings of Supercomputing, 1999)
- Experimental Analysis of Algorithms (Catherine McGeoch, Notices of the American Mathematical Society, March 2001)
- Reflections on the Memory Wall (Sally McKee, ACM Conference on Computing Frontiers, 2004)





#### Thanks

- Torsten Hoefler
  - Performance modeling lead, Blue Waters; MPI datatype
- David Padua, Maria Garzaran, Saeed Maleki
  - Compiler vectorization
- Dahai Guo
  - Streamed format exploiting prefetch, vectorization, GPU
- Vivek Kale
  - SMP work partitioning
- Hormozd Gahvari
  - AMG application modeling
- Marc Snir and William Kramer



- Abhinav Bhatele
  - Process/node mapping
- Elena Caraba
  - Nonblocking Allreduce in CG
- Van Bui
  - Performance model-based evaluation of programming models
- Funding provided by:
  - Blue Waters project (State of Illinois and the University of Illinois)
  - Department of Energy, Office of Science
  - National Science Foundation



