BLUE WATERS SUSTAINED PETASCALE COMPUTING

Blue Waters and the Future of @Scale Computing and Analysis

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PETASCALE COMPUTATION











Outline

- Blue Waters Update
 - System
 - Applications and Usage
- Observations and Challenges for @Scale Computing
- System Wide Performance Assessment SSP/ SPP
- Comments on the Top500 List and its future







Blue Waters Computing System







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CORE, CPUS, SOCKETS, PROCESSORS, ETC. DO NOT HAVE CLEAR DEFINITIONS

What unit is the smallest schedulable unit?

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- There are two independent integer units and a *shared*, 256-bit FP resource
- This architecture is very flexible, and can be applied effectively to a variety of workloads and problems
- No one uses the AMD definitions

	MPI Task 0	Share Comp	ed ponents		MPI Task	1			
	Fetch								
	Int Scheduler	FP Scheduler		Int Scheduler					
5	Int Core 0 eujedia eujedia L1 DCache	128-bit FMAC	128-bit FMAC	L Pipeline	Int Core 1				
	Dedicated Components	Shar	red at the lule level	Shared at the chip level					

Fetch

FP Scheduler

128-bit FMA0

Int Scheduler

Int Unit 0

L1 DCache

Int Scheduler

Int Unit 1

L1 DCache



Single Core Mode, only one integer scheduler unit is used

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- Most common mode for S&E applications
 Implications
 - This core has exclusive access to the 256-bit FP unit and is capable of 8 FP results per clock cycle
 - The core has twice the memory capacity
 - The core has twice the memory bandwidth
 - The L2 cache is effectively twice as large
 - The peak performance of the chip is not reduced
- AMD refers to this as a "Core Module"

Shared L2 Cache

128-bit FN



Interlagos Processor vs Processor Modules

- Each processor die is composed of 4 core modules
- The 4 core modules share a memory controller and 8 MB L3 data cache on one die
- Two die are packaged on a multi-chip module to form a G34-socket Interlagos processor
- Package contains
 - 8 core modules
 - 16 MB L3 Cache
 - 4 DDR3 1600 memory channels



1 Socket









Blue Waters XE6 Node

Blue Waters contains 22,640 XE6 compute nodes

Node Characteristics						
Number of Core Modules*	16					
Peak Performance	313 Gflops/sec	10 22				
Memory Size	64 GB per node	eron				
Memory Bandwidth (Peak)	102 GB/sec					
Interconnect Injection Bandwidth (Peak)	9.6 GB/sec per direction					

*Each core module (aka Bulldozer) includes 1 256-bit wide FP unit and 2 integer units. This is often advertised as 2 "integer" cores, leading to a 32 core node.

HT3

HT3







Cray XK7 and a Path to the Future

Blue Waters contains 4,224 NVIDIA Kepler (GK110 K20X) GPUs

XK7 Compute Node Characteristics

Host Processor	AMD Series 6200 (Interlagos)
Host Processor Performance	156.8 Gflops
Kepler Peak (DP floating point)	1.311 Tflops (DP)
Host Memory	32GB 51 GB/sec
Kepler Memory	6GB GDDR5 capacity 205 GB/sec





CONCLUSION – WE SCHEDULE NODES SO WE USE NODES FOR COMPARISON

Node = Symetric or NUMA Coherent Unit

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On-line Storage Subsystem

- 36 Sonnexion racks about 1 PB raw per rack
- 25+ usable PB
- 3 file systems, 3 metadata servers
 - /home 2.1 usable PB persistent, backup
 - /project 2.1 usable PB persistent, backup
 - /scratch 21 usable PB temporary, 30 day residency by file access
- ~ 4,000 Sandybridge cores
- 528 Lnet routers in Cray system
- Tested at 1.1+ TB sustained
 - Re-tested periodically sustains > 1TB even with 75% full





- World's Largest HPSS storage system
 - Bandwidth, capacity, file creates, ...
 - RAIT implementation

Near-Line Sotrage Subsystem	Phase 1 (test)	Phase 2	Phase 3	Potential
Numbers of HPSS Movers		28	28	
Globus On-line end points	4	50	50	
Number of TS1140 (IBM JAG 4) tape drives	24	244	366	416
Aggregate Bandwidth Performance (GB/s)	5.7	58.5	87.8	100
Number of dual arm SprectraLogic libraries	1	4	6	7
Active Slot count	1,500	63,720	95,580	125,104
Total media capacity	6PB	255PB	382PB	500+PB
HPSS cache		1.3 PB	1.3 PB	







Near-Line Storage



- Have the right data at the right place at the right time
- Eliminate Partner Data Pain
- Cost Efficient
 - RAIT
 - Managing data (limits, transparent movement, consolidation, etc.)
- Import/Export server management and support
- Community Leadership

- Most balanced and intense storage implementation in open science
 - Scale and Performance
- Advanced Technologies
 - RAIT, Lustre-HPSS Interface, ILM, etc.
- Maintain storage related software packages
- Maintain and improve BW developed SW
- Performance testing and tuning
- Import/export facility maintenance and service request management







Interim Full Service Starts April 2, 2013 Full Production Service started September 1, 2013

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NESA



Petascale Usage



Category	Number of Teams
NSF - PRAC	28 active
	+6 exploratory
	5 have completed
University of Illinois	30
	15 General, 15
	Exploratory
GLCPC	10
Education	4
Industry	1
Innovation and Exploration	8









B	Science Area	Number of Teams	Codes	Struct Grids	Unstruct Grids	Dense Matrix	Sparse Matrix	N- Body	Monte Carlo	FFT	PIC	Significant I/O	ł
sus [.]	Climate and Weather	3	CESM, GCRM, CM1/ WRF, HOMME	Х	x		x		Х			x	
	Plasmas/Magnetosphere	2	H3D(M),VPIC, OSIRIS, Magtail/ UPIC	x				x		х		x	
	Stellar Atmospheres and Supernovae	5	PPM, MAESTRO, CASTRO, SEDONA, ChaNGa, MS-FLUKSS	X			Х	x	Х		X	x	
	Cosmology	2	Enzo, pGADGET	Х			Х	Х					
	Combustion/Turbulence	2	PSDNS, DISTUF	Х						Х			
	General Relativity	2	Cactus, Harm3D, LazEV	Х			х						
	Molecular Dynamics	4	AMBER, Gromacs, NAMD, LAMMPS			х		X		х			
	Quantum Chemistry	2	SIAL, GAMESS, NWChem			х	Х	X	х			Х	
	Material Science	3	NEMOS, OMEN, GW, QMCPACK			х	Х	X	х				
	Earthquakes/Seismology	2	AWP-ODC, HERCULES, PLSQR, SPECFEM3D	х	x			х				x	
	Quantum Chromo Dynamics	1	Chroma, MILC, USQCD	х		х	х	Х		х			
	Social Networks	1	EPISIMDEMICS										
	Evolution	1	Eve										
	Engineering/System of Systems	1	GRIPS,Revisit						х				
	Computer Science	1			X	х	Х			х		X	









- Klaus Schulten (PI) and the NAMD group - Code NAMD/ Charm++
- Completed the highest resolution study of the mechanism of HIV cellular infection.
- May 30, 2013 Cover of Nature
- Orders of magnitude increase in number of atoms – resolution at about 1 angstrom





- Paul Woodward PI Code PPM
 - 1.5 Pflop/s sustained on Blue Waters
 - 10,5603 grid
 - A Trillion Cell, Multifluid CFD Simulation
 - 21,962 XE nodes; 702,784 interger cores; 1331 I/Os; 11 MW
 - All message passing and all I/O overlapped w. comput.
 - 12% theoretical peak performance sustained 41 hrs
 - 1.02 PB data written and archived; 16.5 TB per dump.
 - Ran over 12 days in 6-hour increments







Enabling Breakthrough Kinetic Simulations of the Magnetosphere via Petascale Computing

- Homa Karimabadi PI Code PPM
 - Possible extreme solar storms could significantly disrupt many modern infrastructure systems
 - This project studies the initiation and transmission of the solar wind
 - Produced much higher resolution data sets being shared with 1,000's of other scientists







http://bluewaters.ncsa.illinois.edu







http://bluewaters.ncsa.illinois.edu



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24 HOURS	JOBS STARTED 313	JOBS QUEUED	JOBS COMPLETED
About Blue Waters The Blue Waters project provides systems and support science and engineering. The Blue Waters supercomput most powerful systems in the world - achieves sustained of 1 petaflop on a range of science and engineering co more than 25PB of usable storage. View complete syste Blue Waters is supported by the National Science Foun Scientists, engineers, educators and companies can app Waters. For more information, visit the Allocations page The Blue Waters project also includes education and the and engagement with industry. Find out more about the science and engineering impa Waters project at https://bluewaters.ncsa.illinois.edu/im Questions? Contact implements and engineering impa	for petascale er - one of the ed performance des and offers ms specs dation. Jy to use Blue e. alining activities 20% et of the Blue spect-overview.	16.9%	 The Computa Microscope Other Hierarchical n dynamics san assessing para and free ener RNA catalysis binding, and conformationa Latice QCD Waters Petascale Sin Turbulent Ste Hydrodynamic

The Computational

Hierarchical molecular

dynamics sampling for

assessing pathways and free energies of

RNA catalysis, ligand

binding, and conformational change

Lattice QCD on Blue Waters

> Turbulent Stellar Hydrodynamics

Petascale Simulation of





Gross Utilization on Blue Waters



provided during that period. It does not include non-BlueWaters jobs.

It is worth noting that this value is a rough estimate in certain cases where the resource providers don't provide accurate records of their system specifications, over time.







Petascale Usage

- Petascale Definitions of Scale
 - Not Large ≤ 1,284 nodes
 - ≤ 20,544 FP cores
 - ≤ 41,088 integer cores
 - Large \geq 1,285 nodes
 - ≥ 20,560 FP cores
 - ≥ 41,120 integer cores
 - Very Large ≥ 4,584 nodes
 - ≥ 123,344 FP cores
 - ≥ 146,688 integer cores

- Year to Date Computational Usage
 - Not Large 60%

Large - 25%

No longer can define core, processor...

- ~380,000 AMD x86 Floating-point Bulldozer cores,
- ~760,000 AMD x86 integer cores,
- 4,224 NVIDIA Kepler K20x GPUs or
- >12 million "cudacores"
- Very Large 15%
 - Does not include any GPU usage













XK jobs as of end of September



XK aprun nodecnt historgram

Slide Courtesy Greg Bauer







Frontlog/Backlog

Switch to XK Previous Next Zoom Out Zoom In Start: Nov 28,2013 10:26 pm End: Dec 2,2013 9:39 pm Overall Utilization Average: 89.98% Node-Hours lost from Undersubmitted Workload: 589.542 nodehours (0.03% avg) Node-Hours lost by Down nodes: 1180.411 nodehours (0.05% avg) Node-Hours spent Draining: 214284.062 nodehours (9.94% avg) Current Chart Resolution: 30 Minutes

2 people currently viewing this chart







Full Service Job Characteristics

- July-Sept. 2013 Interval
- Large job expansion factor well under target of 10.
 - 1+(time in queue/time requested)



XK nodes	1 -	16 nodes	17 - 256 nodes	25	257 – 4,224 nodes		
Expansion fa	ctor	Very Large job	s Large jobs		Not Large jobs		
XK nodes		1.56	2.85		2.79		
XE nodes		4.75	1.27		1.04		





Community Engagement

- Community Outreach and Education activities to enable the general computational science and engineering community to make effective use of petascale systems. This component includes activities to help train the next generation of petascale computational experts through a coordinated set of courses, workshops, and fellowships.
- Key Activities include
 - Hands-on workshops
 - **Virtual School**: semester-long courses on the web to allow participation by students at multiple institutions across the country. The courses will be offered as a traditional college course, including a syllabus with learning outcomes,
 - Prototype course taught by Wen-Mei Hwu in Spring 2013.
- Graduate Fellowships

Fellowships announced November 11, 2013 http://www.ncsa.illinois.edu/news/story/applications now being accepted for blue waters graduate fellowships

- Candidates must already be enrolled in a PhD program at an accredited US non-profit academic institution at the time of application.
- They must have completed no more than two years of graduate studies. The fellowship support is for one year, renewable based on performance for up to two additional years.
- The level of support is up to \$50,000 per year encompassing a stipend of \$38,000 plus \$12K in support of tuition and fees as well as support for travel to augment their learning and present papers in their field.
- Must be US Citizen or Permanent Resident
- Internships
 - Continuing effort from deployment phase
 - Available to undergraduate and graduate students \$5K, 1 week hands-on workshop at NCSA
 - Interns are paired with researcher(s)
 - · Emphasis on engaging women, minorities and people with disabilities
- Blue Waters Symposium
 - Showcases results from the Blue Waters system, and provides a forum for dealing with community issues and solutions for efficient parallel and heterogeneous petascale computing.
 - Planning for this event is underway, but date and location are still under consideration









What Science Teams Did to Improve

- Another observed social experiment
- NEIS-P² Direct Support
 - Blue Waters directly funded science teams to make improvements in their codes to enable them to "realize the full potential of the Cray XE6/XK7 system."
 - 20 PRAC teams participated
 - Component was completed in Summer 2013
 - Summary of activities and results for each team can be found on the Blue Waters website: <u>https://bluewaters.ncsa.illinois.edu/neis-p2-final-reports</u>
- Reporting by full Science Teams indicated more applications
 - Single node optimization
 - GPU Implementations prefer a single code base
 - Heterogeneous use of x86 and K20x processors
 - Reduce Communication Pressure
 - Topology Awareness
 - Load Balancing
 - I/O and storage Improvements





Goals

- facilitate the creation of new methods and approaches that will dramatically improve the ability to achieve sustained science on petascale systems
- assist the general computational science community in making effective use of systems at all scales.
- Major Areas from Component 1 and Production Experiences
 - Enable application-based topology awareness to more effectively and efficiently use limited bandwidth resources, and to fully exploit the new system functionality for topology aware scheduling that will be available on Blue Waters in 2014.
 - Increasing scalability of full applications, including much work with improving the load balancing within the applications.
 - Improve single node performance for applications, particularly to assist applications in layout, affinity, etc.
 - Increase the number of science applications that can use accelerators and many core technology by lowering the effort to re-engineer applications for these technologies and enabling the teams to maintain a single code base that can be applied to multiple architectures.
 - Enable integrated, at scale applications use of heterogeneous systems that have both general-purpose CPUs and acceleration units.
 - Improve the use of advanced storage and data movement methods to increase the efficiency and time to solution of applications.
 - Assessment and dissemination of science and society impacts resulting from petascale Science





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Much of the Benchmark tuning was topology based

1 poorly placed node out of 4116 (0.02%) can slow an application by >30% (on dedicated system)

Just 1 of 3057 gemini down out in the wrong place of 6114 can slow an application by >20% (P3DNS – 6114 Nodes)

Later Slides for Positive Impacts



Appears in all system and many applications, but scale makes it clear





- Applies to all systems and topologies
- Need a system and application partnership to do the best
- Cray developed new management and tuning functions
 - Bandwidth Injection and Congestion Protection features helps all systems
- BW works with science teams and technology providers to
 - Understand and develop better process-to-node mapping analysis to determine behavior and usage patterns.
 - Better instrumentation of what the network is really doing
 - Topology aware resource and systems management that enable and reward topology aware applications
 - Malleability for applications and systems



- Understanding topology given and maximizing effectiveness
- Being able to express desired topology based on algorithms
- Mid ware support
- Even if applications scale, consistency becomes an increasing issue for systems applications
- This will only get worse in future systems









- Job Job interaction
 - Analysis of key application communication intensity and sensitivity
 - 20% slowdown typical, 100% or more possible.



Communication	MILC	NAMD	NWCHEM	PSDNS	WRF
Intensive	2	2	3	2	1
Sensitive	2	3	1	2	1

1 – low 3 – high as viewed by convex app.

Slide Courtesy Greg Bauer

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Shape Targeting

- Slabs/sheets and cubes of popular node counts pre-defined
- Defined in XZ plane to maximize global bandwidth
- Defined to edges to maximize torus wrap-around benefit
 - Also reduces chance of interfering application
- Designated shapes can dodge dateline boundaries
- Use existing scheduler features to target "one of" qualified targets
- Threatens utilization and turnaround time
 - more than 3d topology awareness would
- Improves consistency
- Improves performance







Alternative ALPS Node ID ordering

- 4x2x8 "bricks" laid out in Z
- Fills XZ plane first
- Return path folding
 - Z-bar returns
 - Plane level
- Ignore XK region remnants



Sheet/slab 2 high in Y

Slide Courtesy Jeremy Enos





Alternative ALPS Node ID ordering

- 4x2x8 "bricks" laid out in Z
- Fills XZ plane first
- Return path folding
 - Z-bar returns
 - Plane level
- 4 high in Y (crude, not Hilbert)
- Not optimized, but compare worthy against 4 wide YZ bias
- Ignore XK region remnants

Slide Courtesy Jeremy Enos



Sheet/slab 4 high in Y





Alternative Node ID ordering

- Surprise even crude 4y high did as well or better in most tests
- 10-17% improvement average over baseline for all applications tested
- 2y high probably choice average skewed by apps that will select for cubic

Application	node count	baseline timing	test 1	test 2
cesm	600	sec	sec	sec
changa	1024	168.9s	169s	177.7s
dns_distuf	512	0.039 sec/step	0.037 sec/step	0.04 sec/step
milc	1372	11.76 sec/step	10.26 sec/step	12.90 sec/step
milc	2744	8.81 sec/step	6.16 sec/step	6.74 sec/step
namd	1368	10.5 ms/step	11.5 ms/step	8.65 ms/step
nwchem	3000	616.0 sec	467.6 sec	442.7 sec
psdns	1024	49.47sec/step	40.68sec/step	28.42sec/step
wrf	1386	0.781025	0.771038	0.771045





Alternative Node ID ordering

- Limit XK plane order to half dimension
- Begin XE allocation in full plane area
- Increases the metric for other topology awareness effort
- Fragmentation still a issue but Moab contiguous allocation may be an option to minimize

System wide rank reordering mechanisms in development

Slide Courtesy Jeremy Enos







Congestion Protection

- To avoid data loss, traffic injection is throttled for a period of time, when reaching a point where forward progress is stalling. Throttling is applied and removed until congestion is cleared.
- System monitors percentage of time that traffic trying to enter the network from the nodes and percentage of time network tiles are stalled.
- Fortunately not a common occurrence. It does happen, typically in bursts.
- Can happen with node-node (MPI, PGAS) or node-LNET (IO) traffic.
- Many-to-one and long-path patterns.
- Libraries and user can control node injection as a precaution.
- In CP reports, flit rates represent data arriving at the node from the interconnection network.

Slide Courtesy Greg Bauer

APID	Name			Nod	les	Flits/s	UID	Start	End	
2220460	Castro3	d.Linux.		20	48	31698	46466	16:00:45	19:41:40	
2220462	Castro3	d.Linux.		20	48	81115	46466	16:01:05	19:37:03	
2218386	namd2			20	0.0		43448	01:58:31	18:02:09	
2220803	psolve			20	0.0	45732	47252	17:12:34	17:30:30	
2218759	su3_rhmo	d_hisq_q		15	36		12940	07:29:16		
2219859	nwchem			10	00		32745	13:58:50	18:02:07	
2220668	nwchem			10	0.0	4128749	32745	17:00:22	18:15:32	
2219678	ks_spect	trum_his		7	68		12940	11:30:04		
2219512	namd2			7	0.0		42864	10:35:55		
							==			
Top Band	dwidth Ap	pplicatio	ons							
							==			
0: apid 3075	2218386	userid	43448	numnids	2000	apname		namd2	Kflits/sec:	Total
1: apid 2743	2219859	userid	32745	numnids	1000	apname		nwchem	Kflits/sec:	Total
2: apid 2715	2220462	userid	46466	numnids	2048	apname	Cast	ro3d.Linux.	Kflits/sec:	Total
3: apid	2220460	userid	46466	numnids	2048	apname	Cast	ro3d.Linux.	Kflits/sec:	Total
2691 4: apid	2219517	userid	42864	numnids	700	apname		namd2	Kflits/sec:	Total
2271								10		
5: apid 2073	2219519	userid	42864	numnids	700	apname		namd2	Kflits/sec:	Total
6: apid 2071	2218759	userid	12940	numnids	1536	apname	su3_	_rhmd_hisq_q	Kflits/sec:	Total
7: apid 1762	2219514	userid	42864	numnids	700	apname		namd2	Kflits/sec:	Total
8: apid	2220646	userid	12940	numnids	512	apname	ks_s	pectrum_his	Kflits/sec:	Total
9: apid 1389	2217219	userid	47296	numnids	500	apname		python	Kflits/sec:	Total

Congestion Candidate COMPUTE Nodes

congestion cumulate contoin nodes

8: c14-1c0s3n0 (19784 flits/sec) (nid 8120; apid 2219756 userid 14394 numnids 32 apname

l: c17-ocls0n1 (64051 flits/sec) (nid 18401; apid 2220473 userid 14394 numnids 32 apname numa_script.sh)

^{2:} c9-Oc0s1n0 (61950 flits/sec) (nid 23036; apid 2219894 userid 14394 numnids 32 apname numa_script.sh)

^{3:} c10-lc0s3n2 (24438 flits/sec) (nid 5798; apid 2219756 userid 14394 numnids 32 apname numa_script.sh)

^{4:} c3-10c0s5n1 (24238 flits/sec) (nid 25867; apid 2219672 userid 35077 numnids 64 apname enzo.exe)

^{5:} c12-1C0s2n2 (22544 flits/sec) (nid 8026; apid 2219756 userid 14394 numnids 32 apname numa_script.sh)

^{6:} c5-10c0s6n3 (20193 flits/sec) (nid 24813; apid 2219672 userid 35077 numnids 64 apname enzo.exe)

^{7:} cl2-lc0s2n0 (20161 flits/sec) (nid 8004; apid 2219756 userid 14394 numnids 32 apname numa_script.sh)





IO and Storage

- LNETs scattered across the torus (orange colored geminis).
- Specific OSTs served by specific LNETs (not a full fat tree for the IB between OSTs and LNETs).
- IO is "topology sensitive".



Slide Courtesy Greg Bauer





Routing of IO write



- 15 compute geminis

 (•) (30 nodes) writing
 to files served by a
 LNET pair (•).
- Color scale is the number of convergent routes on the link.

Slide Courtesy Greg Bauer







I/O Is Complex

- Many Challenges
 - Scale timings
 - Filesystem failure over works just not fast enough all the time
- Data and I/O server placement make this a complicated topology based optimization
- Reads slower than writes at scale

 one to many rather than many to
 one





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Resiliency Needs New Approaches

- Current State on Blue Waters
 - 2-2.5 node failures a day getting less (lower 2's now)
 - Any cause to fail with application running
 - Any cause to fail proactive node health check
 - SWOs average 5 days system wide MTBF over several months and improving
- Hardware is better than expected
 - E.g. just 7 full HDD failures in 6 months
 - Software error rates not measurable yet
- Software causes the majority of the failures
 - Almost all storage failures
 - More than ½ the node failures
 - More than ½ the system wide outages
 - Possible the cause of congestion events
- Most research is about the hardware not software
 - Most resiliency concerns are about hardware not software
- Defensive I/O (checkpoint) is increasingly intrusive.
 - System-assisted application based flexible resiliency as a path to the future
 - Need multi-vendor implementations or applications will continue to do things they can control











- Becoming Intolerable
 - Topology helps sometimes but not enough
 - Same code same nodes different time
- Most is not OS Jitter related
- Congestion Events Intrusive see Blue Waters' presentations later for more details
 - Prediction should be possible but not currently available
- Causes overestimation of run time and less efficient system scheduling
- Impacts resource requirements estimation
- Not just at the largest scales see slide courtesy of Tom Pugh – Australian Met Office







SOURCE	Average MBs/Day	Max MBs/Day
apstat	0.05	0.06
bwbackup	0.06	0.74
esms	229.79	622.71
hpss	345.29	1391.80
hpss_core	0.08	0.22
ibswitch	0.80	1.59
јсс	0.17	0.93
moab	2539.40	5678.32
sched	0.07	0.08
SEL	0.23	0.42
sonexion	326.67	870.15
syslog	12563.31	102626.18
torque	31.66	103.78
volkseti	11.42	27.38

Average

- 15 GBs/day
- >88M events/day
- > 10,500 defined events
 Does not include OVIS CPU,
 Gemini and Darshan data
 collection
- Will be significant increases at 1 minute resolution for all nodes





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Time to Solution is <u>THE</u> Metric

- The consensus of many papers/experts is the only real, meaningful metric that can compare systems or implementations is the time it takes to solve a defined, real problem on systems.
 - Work is a task to carry out or a problem to solve
 - Just like in the real world, work is not a rate, it is not a speed, it is a quantity
- The work is meaningful effort, not overhead work or useless work
- Hence a good evaluation compares how much time it takes to do an amount of meaningful (productive) work
 - Referred to as the System's Potential to do the work
 - Cost effectiveness = system's potential/system's cost
 - Cost can have many components as well





- Time to Solution comparisons have their own challenges
 - Defining what the work is in an discrete manner (i.e. data input set)
 - Defining the work process(es) (application/algorithm/ code path...)
 - Picking a unit to represent the work
 - Defining work across disciplines for multi use systems
 - Defining useful work vs overhead work (to parallelize, to move data, to set up, key steps)
 - Balancing practical issues
 - Complexity, testable system size, tractable length the test runs, number of tests, quality of implementation, optimizations







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What is a Benchmark?

- Benchmark tests are approximations of real, practical work a computer system accomplishes
- Benchmark tests estimate the potential of computer systems to solve a set of problems
- Benchmark tests are made up of computer programs and the input data sets that state a problem for the program to solve
 - Today's real applications are complex and generally solve multiple problems and have different ways to define the methods used
 - Each input data set causes a different code path to execute with possibly different characteristics and performance
 - Many applications have markedly different code paths and characteristics based on input
 - PME steps for chemistry, converging criteria, time step resolution, memory use...
 - E.g MILC for NSF Track1 same code two very different problems and characteristics, MADCAP for NERSC-3/4 same code – multiple different problems and characteristics
 - Hence, one cannot evaluate a benchmark result without defining its input and therefore its code path and execution characteristics
- Sophistication of the approximation represented by the benchmarks depends on the fidelity needed to represent the true workload relative to the goals of getting good measurements













- 1. Evaluation and/or selection of a system from among its competitors.
- 2. Validating a selected system actually works the way it is expected to operate once a system is built and/or arrives at a site.
 - This purpose may be more important than the first and is particularly key when systems are specified and selected based on performance projections rather than actual runs on the actual hardware.
- 3. Assuring the system performance stays as expected throughout the system's lifetime (e.g. after upgrades, changes, and regular use)
- 4. Helping guide future system designs.

Most reports/papers discuss only the first of these four purposes benchmarks play in the life of a system.

The majority of tests claim to do well on the first goal and possibly one other of the goals, but few are effective in all purposes.





From Method To Implementation

- Sustained Petascale Performance Metric is the Blue Waters/NSF implementation of the SSP Method
- To move from the Method to Metric
 - 1. Select number and instances of applications and problem sets
 - 2. Select Input sets that determine the code paths
 - 3. Establish Reference Counts
 - 4. Optimize (or not)
 - 5. Run Tests
 - 6. Composite
 - 7. Evaluate
 - 8. Repeat 4 thru 7 or 2 thru 7 or until complete



BW Sustained Performance Measures

- Original NSF Benchmarks
 - Full Size QCD (MILC), Turbulence (PNSDNS), Molecular Dynamics (NAMD)
 - Modest Size MILC, Paratec, WRF
- Sustained Petascale Performance (SPP) expands the original requirements as it is a time to solution metric that is using the planned applications on representative parts of the science team problems
 - Represents end to end problem run including I/O, pre and post phases, etc.
 - Coverage for science areas, algorithmic methods, scale
- SPP Application full applications (details and method available)
 - NAMD Molecular Dynamics; MILC, Chroma Lattice Quantum Chromodynamics; VPIC, SPECFEM3D – Geophysical Science; WRF – Atmospheric Science; PPM – Astrophysics; NWCHEM, GAMESS – Computational Chemistry; QMCPACK – Materials
- The input, problem sizes, included physics, and I/O performed by each benchmark is comparable to the simulations proposed by the corresponding science team for scientific discovery.
- Well defined reference operation counts used to represent work across disciplines
- Each benchmark sized to use one-fifth to one-half of the number of nodes in the full system.
 - At least three SPP applications run at full system size





Determining Reference Operation Counts

- Determining the total number of reference work operations (e.g. FLOPs) required for each SPP science problem requires specifying the code version and the input problem data set.
- The GigaFLOP value used to calculate $P_{\alpha,i}$ is based on reference FLOP counts obtained using *best practices*. In order of preference, these best practices are:
 - hand-counting the floating-point operations within the code (where feasible),
 - using developer-implemented measures of the number of FLOPs executed, or
 - collecting hardware counter data collected by running the problem on Interlagos processors. When hardware performance counters are collected, the hardware counter data was compared to hand counts or developer-implemented measures (where available) for validation.
 - In order to avoid including extra FLOPs that may result from the extra operations used for scaling such as redundant computations, etc., scaling assessments were collected and compared hardware counter data obtained from multiple runs at different node counts for the same total problem size.
 - Enabled determination of whether the FLOP count for a fixed total problem size increases with the number of nodes, as well as how to eliminate any superfluous FLOPs from FLOP counts obtained at the desired scale.





NCSA



SPP Method Coverage

Science Area	Struct Grids	Unstruct Grids	Dense Matrix	Sparse Matrix	N- Body/ Agent	Monte Carlo	FFT	PIC	Significant I/O
Climate and Weather	Х	X		Х		X			Х
Plasmas/Magnetosphere	Х				Х		Х		x
Stellar Atmospheres and Supernovae	х			х	х	х		X	x
Cosmology	х			х	х				
Combustion/Turbulence	х						Х		
General Relativity	х			х					
Molecular Dynamics			Х		Х		Х		
Quantum Chemistry			Х	х	х	х			Х
Material Science			Х	х	Х	Х			
Earthquakes/Seismology	х	X			х				х
Quantum Chromo Dynamics	х		Х	Х	Х		Х		
Contagion (Social) Networks					х				
Evolution									
Engineering/System of Systems						х			
Computer Science		X	Х	X			Х		X 59





BW SPP Test Components

- SPP is a time to solution metric that is using the planned applications on representative parts of the Science team problems
 - Represents end to end problem run including I/O, pre and post phases, etc.
 - Coverage for science areas, algorithmic methods, scale
- SPP Application Mix (details and method available)
 - NAMD molecular dynamics
 - MILC, Chroma Lattice Quantum Chromodynamics
 - VPIC, SPECFEM3D Geophysical Science
 - WRF Atmospheric Science
 - PPM Astrophysics
 - NWCHEM, GAMESS Computational Chemistry
 - QMCPACK Materials Science
- Minimum SPP for x86 processors plus
- Kepler processors have to add at least 13% more above the x86 SPP
- At least three SPP benchmarks run at full scale







BW SPP Test Components XE XK

Area	Code - version	Run Scale (XE Nodes) (Multiply by 16 or 32 to get cores)	Features
Molecular Dynamics	NAMD v2.0	5,000	C++, Charm++
Quantum Monte-Carlo	QMCPACK v52	4,800	C++/Fortran, MPI+OpenMP
Quantum Chromodynamic s	MILC 7.6.3	4,116	C/C++, MPI/ pthreads
Quantum Chemistry	NWChem 6.1	5,000	C/Fortran, GA
Climate/ Weather	WRF 3.3.1	4,560	C/Fortran, MPI +OpenMP
Earthquakes/ Seismology	SpecFEM3D 5.13	5,419	F90/C++, MPI
Stellar Atmospheres and Supernovae	VPIC	4,608	Fortran/C, MPI +OpenMP
Plasmas/ Magnetosphere	PPM – 7/2/12	8,256	Fortran, MPI +OpenMP

Area	Code	Run Scale	Method
Molecular Dynamics	NAMD	768	Cuda
Quantum Monte- Carlo	QMCPACK	700	Cuda
Quantum Chromodynamics	CHROMA	768	Cuda
Quantum Chemistry	GAMESS	1,536	OpenACC

Composite System SPP – <u>1.31 PF/s</u>

- x86 SPP Contribution 1.10 PF/s
- Kepler SPP Contribution 0.21 PF/s





SPP Metric Definition for BW

- SPP metric is a geometric mean of per node performance rates for a suite of applications, each running in dedicated mode on a 1/5 to a 1/2 of the full number of compute nodes on the Blue Waters system, multiplied by the total number of compute nodes in the system.
- Each set of nodes of a given type is has the SPP contribution calculated independently and those sustained measures are summed to obtain the full system SPP value.
 - More precisely, for a given set of benchmark codes, the performance rate of the i-th code expressed in units of GFLOPS per node of type a, P_{α,i}, is calculated by dividing the reference FLOP count for that benchmark by the number of nodes of that type used to run the problem and by the total wall clock time for that run.
 - For a given number of nodes of a given type α , N_{α} , the contribution to the SSP from nodes of type a is the geometric mean of $P_{\alpha,i}$ over all applications, multiplied by N_{α} .
 - The total SSP is the sum of the contributions for each node type. For Blue Waters, α is two for the XE and XK node types. N_{XE} = 22640 and N_{xk}= 4224.
 - The number of GFLOPS per node was computed for the i-th benchmark running on the XE nodes, P_{XE6,i} and the jth benchmark running on the XK nodes, P_{XK7,j}.
 - The contribution to the SSP for a given node type is the geometric mean of the P_{{XE6,XK7},i or j} values times the corresponding numbers of nodes of each type in the full system.
 - Thus, the total SSP of the XE/XK system is:
 - SSP = Geometric Mean for all i ($P_{XE6,i}$) × N_{XE6} + Geometric Mean for all j ($P_{XK7,j}$) × N_{XK7}





Additional SPP Test Results

- Three Full Scale NSF applications defined as problems
 - NAMD, MILC, P3DNS
- Full Scale SPP XE Codes
 - In addition to the NSF Petascale tests, 4 SPP tests ran above 1 PF using the full XE node section of the system
 - Two of the four ran above 1.2 PF
 - Scale ranges from 21,417 to 22,528 nodes
- SPP XK codes x86 to Kepler Speed ups
 - Four XK SPP codes all show a runtime improvement between 3.1-4.9x over x86 version running at same scale.
 - Scale ranges from 700 to 1,536 nodes
 - Three codes were CUDA implementation, 1 code was an OpenACC implementations







Example for SPP - NSF Workload Blue Waters & Titan Computing Systems

System Attribute (2012)

UIUC/NCSA Blue Waters

DOE/ORNL Titan

Vendor(s) Processors	Cray/AMD/NVIDIA Interlagos 2.3 GHz/Kepler K20X	Cray/AMD/NVIDIA Interlagos 2.1 GHz /Kepler K20X
Total Peak Performance (PF/s) Total Peak Performance (CPU/GPU)	<i>13.1</i> 7.6/5.5	27.11 2.63/24.5
Number of Nodes	27,648	19,200
Number of CPU Modules (8 cores/Module) Number of GPU Chips	49,504 4,224	18,688 18,688
SPP Sustained Performance (PF/s)	1.31	0.64
Amount of CPU Memory (TB)	1,660	710
nterconnect Dimensions	Gemini 3-D Torus 24x24x24	Gemini 3-D Torus 25x16x24
Amount of Usable On-line Disk Storage (PB) 2013 upgrade Sustained Disk Transfer (TB/sec) 2013 upgrade	26 1.2	>10 ~40 shared 0.245 ~1 shared
Amount of Near-line/Archival Storage (Usable/Ma 2013 upgrade	ximum) (PB) 300/400	125/250 150/300
Protection from single point of tape failure Sustained Tape Transfer (GB/sec)	Yes 88	No 18







Leval

The proposed deployment time and SSP of two systems

SSP performance chart after periods are aligned. For clarity $\tau_{2,k}$ replaces $\tau_{2,k}$





Value and Price Performance

- 1. Determine the *Potency* of the system how well will the system perform the expected work over some time period
 - Potency is the sum, over the specified time, of the product of a system's SSP and the time period of that SSP over some time period
 - Different SSPs for different periods
 - Different SSPs for different types of computation units (heterogeneous)

$$Potency_{s} = \sum_{k=1}^{K_{s}} SSP_{s,k} * \left[\min(\tau_{s,k+1}, \tau_{max}) - \min(\tau_{s,k}, \tau_{max}) \right] \forall \tau_{s,k} \leq \tau_{max}$$

- 2. Determine the Cost of systems
 - Cost can be any resource units (\$, Watts, space...) and with any complexity (Initial, TCO,...)

$$Cost_{s} = \sum_{k=1}^{K_{s}} \sum_{l=1}^{L_{s,k}} c_{s,k,l}$$

- 3. Determine the Value of the system
 - Value is the potency divide by a cost function

$$Value_s = \frac{Potency_s}{Cost}$$

4. If needed, compare the value of different system alternatives





SSP Method

- Used in different forms
 - NSF Blue Waters SPP 2011-2012
 - Codes and test cases at different scale close to release
 - DOE

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- NERSC 1998-2017
 - https://www.nersc.gov/research-and-development/performance-andmonitoring-tools/sustained-system-performance-ssp-benchmark/
- Los Alamos + NERSC + Sandia Trinity 2015/2016
 - https://www.nersc.gov/systems/trinity-nersc-8-rfp/nersc-8-trinitybenchmarks/ssp/
- Australian Meteorology Office 2000-present
- DOD Modernization Office (ERDC, ARL, AFWL, NAVO, MHPCC) 2000-present











CRAY

Stay True to the Mission

BW Focus on Sustained Performance

- Blue Water's and NSF are focusing on sustained performance
- We intentionally choose not the list Blue Waters on the Top500 List.
- *Sustained* is the computer's useful, consistent performance on a broad range of applications that scientists and engineers use every day.
 - Time to solution for a given amount of work is the important metric not hardware Ops/s
 - Work is categorized regardless of scale ofr implementation so tests should approximate this as closely as possible
 - Sustained performance (and therefore 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 large 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
 - Explore new tools, programming models, and libraries to help applications get the most from the system







There is Life Beyond the Top500



Top500 values do not correlate with vs measured System Sustained Performance - 13 years of systems at NERSC show this trend

TOP500 is dominated by who has the most money to spend–not what system is the best.





BLUE WATERS SUSTAINED PETASCALE COMPUTING



There is Life Beyond the Top500

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NCSA

	Top News from Leading HPC Solution Providers						
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UDUCATION IN A MACHINE IN A M	he TOP500 list – nor will it be taking pa	art in the HPC					
Challenge (HPCC) awards. While Digital unknown number of classified a	le it's generally understood that there a and commercial systems that don't shi	are an					
Manufacturing report list, this is the first time an ope	en science system has opted out in sud	ich a fashion.					
According to the folks at the N	National Center for Supercomputing Ap	pplications VISUA	AL ANALYTICS				
HPC (NCSA), there's a good reason	for this. In the days leading up to the	24th annual See you	r data for all it's worth.				
JAPAN Supercomputing Conference (S Waters Project Director Bill Kra	amer to find out what went into this de	lecision.					
	FISCAL FOR						





Community is at a tipping point

- Wide spread understanding HPL is not an effective measure of system potential
 - Not representative of many applications e.g. John McCalpin presented a study of correlation between applications and Linpack.
 - The correlation coefficient was 0.15.
 - The slope of the best-fit line was 0.1;
 - Conclusion Doubling Linpack performance corresponded to 10% increase in application performance.
 - New HPCG benchmark proposed
 - Jack Dongarra and Mike Heroux
 - SANDIA REPORT SAND2013-4744 June 2013
 - https://software.sandia.gov/hpcg/doc/HPCG-Benchmark.pdf
 - New Beta Implementation Just release
 - Michael A. Heroux, Jack Dongarra and Piotr Luszczek
 - SAND2013- 8752 October 2013
 - https://software.sandia.gov/hpcg/doc/HPCG-Specification.pdf
- Regardless of the measure a problem remains of a single test combined with a non-peer reviewed list – see future slides
- Workshops may be formed to improve the HPCG approach




- 1. Require (estimated) cost data be posted for every system listed
- 2. Do not allow a system to be listed until it is fully accepted and performing its mission
- 3. Require a complete description for every system listed to give information about the investment balance
- **4**. Move from weak scaling to strong scaling Linpack
 - Could use size classes as NPBs do to address large range of system scale





Revolutionary Improvements - Align Our Community Metric To Best Practices In Benchmarking

- Combining the criteria from (Smith, 1988) and (Lilja, 2000) provides the following list of good attributes for benchmarks
- <u>Proportionality</u> a linear relationship between the metric used to estimate performance and the actual performance. In other words, if the metric increases by 20%, then the real performance of the system should be expected to increase by a similar proportion.
 - A scalar performance measure for a set of benchmarks expressed in units of time should be directly proportional to the total time consumed by the benchmarks.
 - A scalar performance measure for a set of benchmarks expressed as a rate should be inversely proportional to the total time consumed by the benchmarks.
- <u>Reliability</u> means if the metric shows System A is faster than System B, it would be expected that System A outperforms System B in a real workload represented by the metric.
- <u>Consistency</u> so that the definition of the metric is the same across all systems and configurations.
- <u>Independence</u> so the metric is not influenced by outside factors such as a vendor putting in special instructions that just impact the metric and not the workload.
- <u>Ease of use</u> so the metric can be used by more people.
- <u>Repeatability</u> meaning that running the test for the metric multiple times should produce close to the same result.





David Bailey – 12 Ways to Fool the Masses – 1991

- 1. Quote only 32-bit performance results, not 64-bit results.
- 2. <u>Present performance figures for an inner kernel, and then</u> represent these figures as the performance of the entire application.
- 3. Quietly employ assembly code and other low-level language constructs.
- 4. Scale up the problem size with the number of processors, but omit any mention of this fact.
- 5. Quote performance results projected to a full system.
- 6. Compare your results against scalar, unoptimized code on conventional systems.
- 7. When direct run time comparisons are required, compare with an old code on an obsolete system.
- 8. If Mflop/s rates must be quoted, base the operation count on the parallel implementation, not on the best sequential implementation.
- 9. Quote performance in terms of processor utilization, parallel speedups or Mflop/s per dollar.
- 10. Mutilate the algorithm used in the parallel implementation to match the architecture.
- 11. Measure parallel run times on a dedicated system, but measure conventional run times in a busy environment.
- 12. If all else fails, show pretty pictures and animated videos, and don't talk about performance.

David's Update for 2011

- A. Cite performance rates for a run with only one processor core active in a shared-memory multi-core node. For example, cite performance on 1024 cores, even though the code was run on 1024 nodes, wasting 15 out of 16 cores on each node.
- B. Cite performance rates only for a core algorithms (such as FFT or LU decomposition), even though the paper mentions one or more full-scale applications that were done on the system.
- C. List only the best performance figure in the paper, even though the run was made numerous times.
- D. Employ special hardware, operating system or compiler settings that are not appropriate for real-world usage.
- E. Define "scalability" as successful execution on a large number of CPUs, regardless of performance.
- http://crd.lbl.gov/~dhbailey/dhbtalks/dhb-12ways.pdf



Create A New, Meaningful Suite Of Benchmarks

- Many benchmark suites that were held in high regard (Livermore Loops, NPBs, SPEC) over time are suites of pseudo and/or full applications.
- While the best case for any benchmark is to be a statistically representative sample of real workload, in realty, this is not possible for community tests.
- **SERPOP** (Sample Estimation of Relative Performance of Programs) method is best suited for a generalized test.
 - A sample of a workload is selected to represent a workload. However, the sample is not random and cannot be considered a statistical sample.
 - SERPOP methods occur frequently in performance analysis and reflect very meaning measures that span individual communities.
 - In SERPOP analysis, the workload is related to SERPOP tests, but does not indicate the frequency of usage or other characteristics of any individual workload.
- Many common benchmark suites—including SPEC, TCP and NPB, as well as many acquisition test suites—are SERPOP.

Mashey, John R. "War of the Benchmark Means: Time for a Truce." ACM SIGARCH Computer Architecture News (Association for Computing Machinery) 32, no. 4 (September 2004)





- Multiple Benchmarks not just one
 - Will lose its uniqueness over time
- Compositing Function is necessary
 - SPP
 - Decathlon
 - Flexibly defined sets of criteria HPC Sabernetics





Decathlon Measuring Method

- Proposed by Authors: Satoshi Matsuoka (Tokyo Tech./NII/Riken AICS), William Kramer (NCSA), Daisuke Takahashi (University of Tsukuba)
- 10 tests
 - 10 individual event winners
 - 1 overall winner
- Goal is each test has equal influence in overall best score
- Example The 2001 IAAF points tables use the following formulae (
 - Points = INT(A(B P)^C) for tests where faster time produces a better score
 - Points = INT(A(P B)^C) for tests where greater distance or height produces a better score)
- A, B and C are parameters that vary by discipline and a set according normalized performance aspects of the period
- P is the performance by the test, measured in time or amounts







The HPC Decathlon Assessment Measure Desired Characteristics

- Proportionality
- Scalability
- Reasonable Execution Time
- Reliability
- Consistency
- Independence
- Repeatability
- Verifiabiliy
- Ease of use
- Succinctness of the Rules
- Algorithmic Specification and not Code
- Availability of Efficient, Parallel, and Scalable Reference Implementation
- Single Value Metric Result

- Orthogonality.
- Community agreement and participation
- Maintainability
- Longevity: that allows comparisons of machines of current and past generations and properties of systems to come
- Governance to be able to fairly and responsibly judge the rules applicability
- Composibility
 - should be technically meaningful
 - agreeable by the community,
 - should be changeable in a documented fashion to derive a metric favoring a particular type of workload can be synthesized for respective domains, changes over time, etc.





Reaching Community Consensus

- Determine Key issues pro and cons, ROI, etc.
 - Full Applications, Mini-applications, kernels
 - Scales and Scaling
 - Sizes
 - Weak vs Strong
 - Explainability
 - Distributions
- Community Ownership
 - Lists must be transparent and community managed
 - Peer Review
 - Professional Society Endorsement
 - Conflict of Interest Avoidance
 - Application Domain Relationships
- Revitialized every 5 years.







Summary – Let US Be Guided by What Users Want and Need From @Scale Systems

- <u>P</u>erformance -
 - How fast will a system process work if everything is working really well
 - Establishes a system's potential to do productive work
- <u>Effectiveness</u>
 - The likelihood users can get the system to do their work when they need it
- <u>R</u>eliability
 - The likelihood the system is available to do the work
- <u>C</u>onsistency
 - How often will the system process the same or similar work correctly and in the length of same time
- <u>U</u>sability
 - How easy is it for users to get the system to process their work as fast as possible

We need good PERCU metrics to assess complete systems for the science impact view point Cost and other "business factors" are also part of a decision making







Questions







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The work described is achievable through the efforts of the many other on different teams.