

Impact of Architecture and Technology for Extreme Scale on Software and Algorithm Design

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H. Meuer, H. Simon, E. Strohmaier, & JD

Listing of the 500 most powerful Computers in the World
Yardstick: Rmax from LINPACK MPP

Ax=b, dense problem

- Updated twice a year



SC'xy in the States in November Meeting in Germany in June

- All data available from www.top500.org



Processors Used in the Top500 Systems



AMD 10% IBM 8%

Today's Multicores 99% of Top500 Systems Are Based on Multicore

Of the Top500, 499 are multicore.



Sun Niagra2 (8 cores)



IBM Power 7 (8 cores)



AMD MagnyCours (12 cores)



Intel Xeon(8 cores)



Intel Knight's Corner (40 cores)







Fujitsu Venus (8 cores)



IBM BG/P (4 cores)









Countries / System Share



7 systems in the Italy

• June 2010: The TOP10

Rank	Site	Computer	Country Cores		Rmax [Pflops]	% of Peak
1	DOE / OS Oak Ridge Nat Lab	Jaguar / Cray Cray XT5si×Core 2.6 GHz	USA	224,162	1.76	75
2	Nat. Supercomputer Center in Shenzhen	Nebulea / Dawning / TC3600 Blade, Intel X5650, Nvidia C2050 GPU	China	120,640	1.27	43
3	DOE / NNSA Los Alamos Nat Lab	Roadrunner / IBM BladeCenterQS22/LS21	USA	122,400	1.04	76
4	NSF / NICS / U of Tennessee	Kraken/ Cray Cray XT5sixCore 2.6 GHz	USA	98,928	.831	81
5	ForschungszentrumJueli ch (FZJ)	Jugene / IBM Blue Gene/P Solution	Germany	294,912	.825	82
6	NASA / Ames Research Center/NAS	Pleiades / SGI SGI Altix ICE 8200EX	USA	56,320	.544	82
7	National SC Center in Tianjin / NUDT	Tianhe-1 / NUDT TH-1 / IntelQC + AMD ATI Radeon 4870	China	71,680	.563	46
8	DOE / NNSA Lawrence Livermore NL	BlueGene/L IBM eServerBlue Gene Solution	USA	212,992	.478	80
9	DOE / OS Argonne Nat Lab	Intrepid / IBM Blue Gene/P Solution	USA	163,840	.458	82
10	DOE / NNSA Sandia Nat Lab	Red Sky / Sun / SunBlade 6275	USA	42,440	.433	87

• June 2010: The TOP10

Rank	Site	Computer	Country	Cores	Rmax [Pflops]	% of Peak	Power [MW]	MFlops /Watt
1	DOE / OS Oak Ridge Nat Lab	Jaguar / Cray Cray XT5sixCore 2.6 GHz	USA	224,162	1.76	75	7.0	251
2	Nat. Supercomputer Center in Shenzhen	Nebulea / Dawning / TC3600 Blade, Intel X5650, Nvidia C2050 GPU	China	120,640	1.27	43	2.58	493
3	DOE / NNSA Los Alamos Nat Lab	Roadrunner / IBM BladeCenterQS22/LS21	USA	122,400	1.04	76	2.48	446
4	NSF / NICS / U of Tennessee	Kraken/ Cray Cray XT5sixCore 2.6 GHz	USA	98,928	.831	81	3.09	269
5	ForschungszentrumJueli ch (FZJ)	Jugene / IBM Blue Gene/P Solution	Germany	294,912	.825	82	2.26	365
6	NASA / Ames Research Center/NAS	Pleiades / SGI SGI Altix ICE 8200EX	USA	56,320	.544	82	3.1	175
7	National SC Center in Tianjin / NUDT	Tianhe-1 / NUDT TH-1 / IntelQC + AMD ATI Radeon 4870	China	71,680	.563	46	1.48	380
8	DOE / NNSA Lawrence Livermore NL	BlueGene/L IBM eServerBlue Gene Solution	USA	212,992	.478	80	2.32	206
9	DOE / OS Argonne Nat Lab	Intrepid / IBM Blue Gene/P Solution	USA	163,840	.458	82	1.26	363
10	DOE / NNSA Sandia Nat Lab	Red Sky / Sun / SunBlade 6275	USA	42,440	.433	87	2.4	180

#1 ORNL's Newest System Jaguar XT5



Recently upgraded to a 2 Pflop/s system with more than 224K cores using AMD's 6 Core chip.

Peak performance	2.332 PF
System memory	300 TB
Disk space	10 PB
Disk bandwidth	240+ GB/s
Interconnect bandwidth	374 TB/s





#2 – National Supercomputer Center in Shenzhen, China – Dawning Integrator

Nebulae

- Hybrid system, commodity + GPUs
- Theoretical peak 2.98Pflop/s
- Linpack Benchmark at 1.27 Pflop/s
- 4640 nodes, each node:
 2 Intel 6-core Xeon5650 + Nvidia
 Fermi C2050 GPU (each 14 cores)
 - >120,640 cores
 - >Infiniband connected



>500 MB/s peak per link and 8 GB/s

Commodity plus Accelerators





Looking at the Gordon Bell Prize

(Recognize outstanding achievement in high-performance computing applications and encourage development of parallel processing)

- I GFlop/s; 1988; Cray Y-MP; 8 Processors
 - Static finite element analysis
- 1 TFlop/s; 1998; Cray T3E; 1024 Processors
 - Modeling of metallic magnet atoms, using a variation of the locally self-consistent multiple scattering method.





- □ 1 PFlop/s; 2008; Cray XT5; 1.5x10⁵ Processors
 - Superconductive materials



□ 1 EFlop/s; ~2018; ?; 1×10^7 Processors (10⁹ threads)

Performance Development in Top500



Potential System Architecture with a cap of \$200M and 20MW

Systems	2010
System peak	2 Pflop/s
Power	6 MW
System memory	0.3 PB
Node performance	125 GF
Node memory BW	25 GB/s
Node concurrency	12
Total Node Interconnect BW	3.5 GB/s
System size (nodes)	18,700
Total concurrency	225,000
Storage	15 PB
ΙΟ	0.2 TB
MTTI	days

Potential System Architecture with a cap of \$200M and 20MW

Systems	2010	2018
System peak	2 Pflop/s	1 Eflop/s
Power	6 MW	~20 MW
System memory	0.3 PB	32 - 64 PB [.03 Bytes/Flop]
Node performance	125 GF	1,2 or 15TF
Node memory BW	25 GB/s	2 - 4TB/s [.002 Bytes/Flop]
Node concurrency	12	O(1k) or 10k
Total Node Interconnect BW	3.5 GB/s	200-400GB/s (1:4 or 1:8 from memory BW)
System size (nodes)	18,700	O(100,000) or O(1M)
Total concurrency	225,000	O(billion) [O(10) to O(100) for latency hiding]
Storage	15 PB	500-1000 PB (>10x system memory is min)
ΙΟ	0.2 TB	60 TB/s (how long to drain the machine)
MTTI	days	O(1 day)

Potential System Architecture with a cap of \$200M and 20MW

Systems	2010	2018	Difference Today & 2018	
System peak	2 Pflop/s	1 Eflop/s	O(1000)	
Power	6 MW	~20 MW		
System memory	0.3 PB	32 - 64 PB [.03 Bytes/Flop]	O(100)	
Node performance	125 GF	1,2 or 15TF	O(10) - O(100)	
Node memory BW	25 GB/s	2 - 4TB/s [.002 Bytes/Flop]	O(100)	
Node concurrency	12	O(1k) or 10k	O(100) - O(1000)	
Total Node Interconnect BW	3.5 GB/s	200-400GB/s (1:4 or 1:8 from memory BW)	O(100)	
System size (nodes)	18,700	O(100,000) or O(1M)	O(10) - O(100)	
Total concurrency	225,000	O(billion) [O(10) to O(100) for latency hiding]	O(10,000)	
Storage	15 PB	500-1000 PB (>10x system memory is min)	O(10) - O(100)	
ΙΟ	0.2 TB	60 TB/s (how long to drain the machine)	O(100)	
MTTI	days	O(1 day)	- O(10)	

Exascale (10¹⁸ Flop/s) Systems: Two possible paths

- Light weight processors (think BG/P)
 - ~1 GHz processor (10⁹)
 - ~1 Kilo cores/socket (10³)
 - ~1 Mega sockets/system (10⁶)
- Hybrid system (think GPU based)
 - ~1 GHz processor (10⁹)
 - ~10 Kilo FPUs/socket (10⁴)
 - ~100 Kilo sockets/system (10⁵)

Factors that Necessitate Redesign of Our Software

- Steepness of the ascent from terascale to petascale to exascale
- Extreme parallelism and hybrid design
 - Preparing for million/billion way parallelism
- Tightening memory/bandwidth bottleneck
 - Limits on power/clock speed implication on multicore
 - Reducing communication will become much more intense
 - Memory per core changes, byte-to-flop ratio will change
- Necessary Fault Tolerance
 - MTTF will drop
 - Checkpoint/restart has limitations







- Number of cores per chip will double every two years
- Clock speed will not increase (possibly decrease) because of Power

- Need to deal with systems with millions of concurrent threads
- Need to deal with inter-chip parallelism as well as intra-chip parallelism

Major Changes to Software

- Must rethink the design of our software
 - Another disruptive technology
 - Similar to what happened with cluster computing and message passing
 - Rethink and rewrite the applications, algorithms, and software
- Numerical libraries for example will change
 - For example, both LAPACK and ScaLAPACK will undergo major changes to accommodate this

Future Computer Systems

- Most likely be a hybrid design
- Think standard multicore chips and accelerator (GPUs)
- Today accelerators are attached
- Next generation more integrated
- Intel's Larrabee? Now called "Knights Corner" and "Knights Ferry" to come.
 - 48 x86 cores
- AMD's Fusion in 2011 2013
 - Multicore with embedded graphics ATI
- Nvidia's plans?











Five Important Software Features to Consider When Computing at Scale

- **1.** Effective Use of Many-Core and Hybrid architectures
 - Break fork-join parallelism
 - Dynamic Data Driven Execution
 - Block Data Layout
- **2.** Exploiting Mixed Precision in the Algorithms
 - Single Precision is 2X faster than Double Precision
 - With GP-GPUs 10x
 - Power saving issues
- 3. Self Adapting / Auto Tuning of Software
 - Too hard to do by hand
- 4. Fault Tolerant Algorithms
 - With 1,000,000's of cores things will fail
- **5.** Communication Reducing Algorithms
 - For dense computations from O(n log p) to O(log p) communications
 - Asynchronous iterations
 - GMRES k-step compute (x, Ax, A²x, ... A^kx)

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Fork-join, bulk synchronous processing 28



Parallel Tasks in LU/LL^T/QR



• Break into smaller tasks and remove dependencies



* LU does block pair wise pivoting

PLASMA: Parallel Linear Algebra s/w ICLUT for Multicore Architectures

POTRI

TRSM

SYRK

POTRF

TRSM

SYRK

GEMM

GEMM

TRSM

GEMM

TRSM

SYRK

SYRK

Cholesky 4 x 4

TRSM

GRMM

SYRK

Objectives

- High utilization of each core
- Scaling to large number of cores
- Shared or distributed memory

Methodology

- Dynamic DAG scheduling
- Explicit parallelism
- Implicit communication
- Fine granularity / block data layout

Arbitrary DAG with dynamic scheduling



Communication Avoiding Algorithms

- Goal: Algorithms that communicate as little as possible
- Jim Demmel and company have been working on algorithms that obtain a provable minimum communication.
- Direct methods (BLAS, LU, QR, SVD, other decompositions)
 - Communication lower bounds for *all* these problems
 - Algorithms that attain them (*all* dense linear algebra, some sparse)
 - Mostly not in LAPACK or ScaLAPACK (yet)
- Iterative methods Krylov subspace methods for Ax=b, $Ax=\lambda x$
 - Communication lower bounds, and algorithms that attain them (depending on sparsity structure)
 - Not in any libraries (yet)
- For QR Factorization they can show:
























• We have a *mxn*matrix *A* we want to reduce to upper triangular form.





• We have a *mxn*matrix *A* we want to reduce to upper triangular form.



 $A = Q_1 Q_2 Q_3 R = QR$















Communication Reducing QR Factorization



Challenges of using GPUs

- High levels of parallelism
 Many GPU cores, serial kernel execution

 [e.g. 240 in theNvidia Tesla; up to 512 in Fermi to have concurrent kernel execution]
- Hybrid/heterogeneous architectures
 Match algorithmic requirements to architectural strengths

[e.g. small, non-parallelizable tasks to run on CPU, large and parallelizable on GPU]

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 Compute vs communication gap Exponentially growing gap; persistent challenge
 [Processor speed improves 59%, memory bandwidth 23%, latency 5.5%]
 [on all levels, e.g. a GPU Tesla C1070 (4 x C1060) has compute power of O(1,000) Gflop/s but GPUs communicate through the CPU using O(1) GB/s connection]



 Match algorithmic requirements to architectural strengths of the hybrid components
 Multicore: small tasks/tiles
 Accelerator: large data parallel tasks



- e.g. split the computation into tasks; define critical path that "clears" the way for other large data parallel tasks; proper schedule the tasks execution
- Design algorithms with well defined "search space" to facilitate auto-tuning



Hardware

- •HOST: Two-dual core AMD Opteron 1.8GHz, 2GB memory
- •DEVICE:
 - -4 GPU TESLA C1070 1.44GHz
 - –240 computing cores per GPU
 - -4GB memory per GPU
 - -Single precision floating point performance (NVIDIA PEAK): 4.14 Tflop/s
 - -Memory bandwidth: 408 GB/s
 - -System interface: PCIexpress
- Memory limitations prevented runs on larger sizes







Performance of Single Precision on Conventional and GPU's

 Realized have the similar situation on our commodity processors.



NVIDIA.

NVIDIA Tesla



- That is, SP is 2X as fast as DP on many systems
- The Intel Xeon and AMD Opteron have SSE3
 - 2 flops/cycle DP
 - 4 flops/cycle SP
- IBM PowerPC has AltiVec
 - 8 flops/cycle SP
 - 4 flops/cycle DP
 - No DP on AltiVec

Best case reality: 240 mul-adds per clock

Just able to do the mul-add so 2/3 or 624 Gflop/s of theoretical peak

All this is single precision

Double precision is 78 Gflop/s peak (Factor of 8 from SP; exploit mixed prec)

Single precision is faster because:

- •Operations are faster
- Reduced data motion
- •Larger blocks gives higher locality in cache

Idea Goes Something Like This...

- Exploit 32 bit floating point as much as possible.
 - Especially for the bulk of the computation
- Correct or update the solution with selective use of 64 bit floating point to provide a refined results
- Intuitively:
 - Compute a 32 bit result,
 - Calculate a correction to 32 bit result using selected higher precision and,
 - Perform the update of the 32 bit results with the correction using high precision.

Mixed-Precision Iterative Refinement

- Iterative refinement for dense systems, Ax = b, can work this way.
 - L U = lu(A)SINGLEO(n^3) x = L\(U\b)SINGLEO(n^2) r = b - AxDOUBLEO(n^2) WHILE || r || not small enough z = L\(U\r) x = x + zDOUBLEO(n^1) r = b - AxDOUBLEO(n^2) END
 - Wilkinson, Moler, Stewart, & Higham provide error bound for SP fl pt results when using DP fl pt.

²)

Mixed-Precision Iterative Refinement

Iterative refinement for dense systems, Ax = b, can work this way.

```
L U = lu(A)SINGLEO(n^3)

x = L\(U\b)SINGLEO(n^2)

r = b - AxDOUBLEO(n^2)

WHILE || r || not small enough

z = L\(U\r) SINGLEO(n^2)

x = x + zDOUBLEO(n^1)

r = b - AxDOUBLEO(n^2)

END
```

- Wilkinson, Moler, Stewart, & Higham provide error bound for SP fl pt results when using DP fl pt.
- It can be shown that using this approach we can compute the solution to 64-bit floating point precision.
 - Requires extra storage, total is 1.5 times normal;
 - O(n³) work is done in lower precision
 - O(n²) work is done in high precision
 - Problems if the matrix is ill-conditioned in sp; O(10⁸)



Results for Mixed Precision Iterative Refinement for Dense Ax = b

- Single precision is faster than DP because:
 - Higher parallelism within floating point units
 - 4 ops/cycle (usually) instead of 2 ops/cycle
 - Reduced data motion
 - 32 bit data instead of 64 bit data
 - Higher locality in cache
 - More data items in cache





Matrix size Tesla C2050, 448 CUDA cores (14 multiprocessors x 32) @ 1.15 GHz., 3 GB memory, connected through PCIe to a quad-core Intel @2.5 GHz.





Matrix size Tesla C2050, 448 CUDA cores (14 multiprocessors x 32) @ 1.15 GHz.,

3 GB memory, connected through PCIe to a quad-core Intel @2.5 GHz.

Sparse Direct Solver and Iterative Refinement

MUMPS package based on multifrontal approach which generates small dense matrix multiplies



Sparse Iterative Methods (PCG)

Outer/Inner Iteration

Outer iterations using 64 bit floating point

Inner iteration: In 32 bit floating point



Outer iteration in 64 bit floating point and inner iteration in 32 bit floating point



Mixed Precision Computations for Sparse Inner/Outer-type Iterative Solvers



Speedups for mixed precision Inner SP/Outer DP (SP/DP) iter. methods vs DP/DP (CG², GMRES², PCG², and PGMRES² with diagonal prec.)

Iterations for mixed precision SP/DP iterative methods vs DP/DP

> Machine: Intel Woodcrest (3GHz, 1333MHz bus)

Stopping criteria: Relative to r_0 residual reduction (10⁻¹²)

Intriguing Potential

- Exploit lower precision as much as possible
 - Payoff in performance
 - Faster floating point
 - Less data to move
- Automatically switch between SP and DP to match the desired accuracy
 - Compute solution in SP and then a correction to the solution in DP
- Potential for GPU, FPGA, special purpose processors
 - Use as little you can get away with and improve the accuracy
- Applies to sparse direct and iterative linear systems and Eigenvalue, optimization problems, where Newton's method is used. $x_{i+1} = x_i - \frac{f(x_i)}{f'(x_i)}$

$$x_{i+1} - x_i = -\frac{f(x_i)}{f'(x_i)}$$

Correction = - A (b - Ax)







- Hardware has changed dramatically while software ecosystem has remained stagnant
 - Need to exploit new hardware trends (e.g., manycore, heterogeneity) that cannot be handled by existing software stack, memory per socket trends
 - Emerging software technologies exist, but have not been fully integrated with system software, e.g., UPC, Cilk, CUDA, HPCS
 - Community codes unprepared for sea change in architectures
 - No global evaluation of key missing components



Improve the world's simulation and modeling capability by improving the coordination and development of the HPC software environment

Workshops:

Build an international plan for coordinating research for the next generation <u>open source software</u> for scientific high-performance computing

www.exascale.org

International Community Effort



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- We believe this needs to be an international collaboration for various reasons including:
 - The scale of investment
 - The need for international input on requirements
 - US, Europeans, Asians, and others are working on their own software that should be part of a larger vision for HPC.
 - No global evaluation of key missing components
 - Hardware features are uncoordinated with software development





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- Jack Dongarra, UTK & ORNL
- Pete Beckman, ANL
- Patrick Aerts, NWO Netherlands
- Franck Cappello, INRIA, France
- Thom Dunning, NCSA
- Thomas Lippert, Juelich, Germany
- Satoshi Matsuoka, TiTech, Japan
- Paul Messina, ANL
- Anne Trefethen, Oxford, UK
- Mateo Valero, BSC, Spain



- The IESP software roadmap is a planning instrument designed to enable the international HPC community to improve, coordinate and leverage their collective investments and development efforts.
- After we determine what needs to be accomplished, our task will be to construct the organizational structures suitable to accomplish the work





www.exascale.org



European Exascale Software Initiative - EESI

- A detailed evaluation of how Europe is positioned, its strengths and weaknesses, in the overall international HPC landscape and competition
 - Are European stakeholders willing/able to build an exa-scale prototype/by when?
 - Actors/users/projects

A European and international vision and roadmap

- Why is exa-scale initiatives important? Who cares? Impact?
 - Scientific
 - Economic
 - Social benefits

Dissemination actions

- Visibility of EESI: who is the potential target public?
 - R&D stakeholders
 - EC and national policy-makers
 - Society as a whole

Identification of opportunities of worldwide collaborations

- European position inside IESP: who's doing/deciding what?
- Contribution to the international dialogs: mutual benefits!

EC and G8 Related

- G8 has a call out for "Interdisciplinary Program on Application Software towards Exascale Computing for Global Scale Issues"
 - IO million € over three years
 - An initiative between Research Councils from Canada, France, Germany, Japan, Russia, the UK, and the USA
 - 78 preproposals submitted, 25 selected, expect to fund 6-10
 - Full proposals due August 25th
- EC FP7: Exascale computing, software and simulation
 - Announcement due September 28, 2010
 - 25 million €
 - 2 or 3 integrated project to be funded

If you are wondering what's beyond ExaFlops

Mega, Giga, Tera, Peta, Exa, Zetta ... 10³ kilo 10⁶ mega 10⁹giga 10¹²tera

10¹⁵peta 10¹⁸exa 10²¹zetta 10²⁴yotta 10²⁷xona 10³⁰weka 10³³vunda 10³⁶uda 10³⁹treda 10⁴²sorta **10**⁴⁵**rinta** 10⁴⁸quexa 10⁵¹pepta 10⁵⁴ocha 10⁵⁷nena 10⁶⁰minga 10⁶³luma



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ROADMAP

Jack Dorgania Alok Choudhary Pete Beckman Sudip Dosanjh Al Geist Terry Moore Jean-Claude Andre BIII Groop Robert Harrison Jean-Yves Berthou Taisuko Boku Mark Horold Franck Cappello Michael Heroux Barbara Chapman Adolfy Holsle Xuebin Chi Koh Hotta

Yutaka Ishikawa Fred Jehnson Sanjay Kalo Richard Kenway Bill Kramer Josus Labarta Bob Lucas Barney Maccabe Satoshi Matsuoka

Paul Messina Dend Mohr Matthias Muellar Wolfgang Nagai Hiroshi Nakashima Michaol E. Papks Dan Read Mitsuhisa Sato Ed Seidel

John Shalf Devid Skinner Thomas Sterling Rick Stevens William Tang John Taylor Rajeev Thakur Anne Trefethen Marc Snir

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Aad van der Steen Fred Streitz Bob Sugar Shinji Sumimoto Jeffrey Vettar Robort Wieniswski Kathy Yelick





- Major Challenges are ahead for extreme computing
 - Power
 - Parallelism
 - Hybrid
 - Fault Tolerance
 - In and many others not discussed here
- We will need completely new approaches and technologies to reach the Exascale level
- This opens up many new opportunities for applied mathematicians


• "We can only see a short distance ahead, but we can see plenty there that needs to be done."

Alan Turing (1912–1954)

Shackleton's Quote on Exascale



Ernest Shackleton's 1907 ad in London's Times, recruiting a crew to sail with him on his exploration of the South Pole

"Wanted. Men/women for hazardous architectures. Low wages. Bitter cold. Long hours of software development. Safe return doubtful. Honor and recognition in the event of success."



One-Sided Dense Matrix Factorizations (LU, QR, and Cholesky) from MAGMA



CUDA implementation:

- •a_ref points to the GPU memory
- GPU kernels are started asynchronously which results in overlapping

the GPU sgemm with transferring T to the CPU, factoring it, and sending the result back to the GPU

•For full details see http://www.cs.utk.edu/~tomov/magma/spotrf_gpu.cpp

Communication Reducing Iterative Methods

- Take k-steps of Krylov subspace method
 - GMRES, CG, Lanczos, Arnoldi
 - Assume matrix "well-partitioned," with modest surface-to-volume ratio
 - Parallel implementation
 - Conventional: O(k log p) messages
 - New: O(log p) messages optimal
 - Serial implementation
 - Conventional: O(k) moves of data from slow to fast memory
 - New: O(1) moves of data optimal
 - Can incorporate some preconditioners
 - Need to be able to "compress" interactions between distant i, j
 - Hierarchical, semiseparable matrices ...
 - Lots of speed up possible (modeled and measured)
 - Price: some redundant computation

Minimizing Communication of to solve Ax=b

- GMRES: find x in span{b,Ab,...,A^kb} minimizing || Ax-b ||₂
- Cost of k steps of standard GMRES vs new GMRES

```
Standard GMRES
for i=1 to k
w = A · v(i-1)
MGS(w, v(0),...,v(i-1))
update v(i), H
endfor
solve LSQ problem with H
```

```
Sequential: #words_moved =
O(k·nnz) from SpMV
```

```
+ O(k<sup>2</sup>•n) from MGS
Parallel: #messages =
O(k) from SpMV
+ O(k<sup>2</sup> · log p) from MGS
```

Communication-avoiding GMRES $W = [v, Av, A^2v, ..., A^kv]$ [Q,R] = TSQR(W) ... "Tall Skinny QR"Build H from R, solve LSQ problem GMRE

```
Sequential: #words_moved =
O(nnz) from SpMV
+ O(k·n) from TSQR
Parallel: #messages =
O(1) from computing W
+ O(logp) from TSQR
```

•Numerical issue with potential loss of precision from computing W from power method.



Rank	Site	Manufact.	Computer	Cores	Rmax Gflop/s
70	CINECA	IBM	Power 575, p6 4.7 GHz, Infiniband	5376	78680
129	Telecom	IBM	BladeCenter HS22 Cluster, Xeon QC GT 2.53 GHz, GigEthernet	8048	45528
211	CILEA	HP	Cluster Platform 3000 BL2x220, X56xx 3.0 Ghz, Infiniband QDR	4032	35665
295	Energy Company (A)	IBM	BladeCenter HS22 Cluster, Xeon QC X56xx 2.66 GHz, Infiniband	3408	31310
296	Energy Company (A)	IBM	BladeCenter HS22 Cluster, Xeon QC X56xx 2.66 GHz, Infiniband	3408	31310
297	Energy Company (A)	IBM	BladeCenter HS22 Cluster, Xeon QC X56xx 2.66 GHz, Infiniband	3408	31310
404	Sardegna Ricerche	HP	Cluster Platform 3000 BL460c G1, Xeon E5440 2.83 GHz, Infiniband	3088	27708

DP Cholesky with Multiple GPUs



How to Code for GPUs?

Complex question

 Language, programming model, user productivity, etc

Recommendations

Use CUDA / OpenCL

[already demonstrated benefits in many areas; data-based parallelism; move to support taskbased]

Use GPU BLAS

[high level; available after introduction of shared memory -

can do data reuse; leverage existing developments]

Use Hybrid Algorithms

[currently GPUs - massive parallelism but serial kernel execution;

hybrid approach - small non-parallelizable tasks on the CPU, large parallelizable tasks on the GPU



GPU vs CPU GEMV

3000

2000

4000

Matrix size

5000

70

60

50

40

30

20

10

0

1000

GFlop/s

GPU vs CPU GEMM

81/29

6000

7000

GPU SGEMV

GPU DGEMV

CPU SGEMV

∇ CPU DGEMV



GPUs: excelling in graphics rendering

Scene streams model of data	Graphics pipelined computation		Final image					
Repeated fast over and over: e.g. TV refresh rate is 30 fps; limit is 60 fps								
	C n	Currently, car nultithreaded	n be viewed as I multicore veo	3 xtor units				

This type of computation:

- Requires enormous computational power
- Allows for high parallelism
- Needs high bandwidth vs low latency

(as low latencies can be compensated with deep graphics pipeline)

Obviously, this pattern of computation is common with many other applications

Moore's Law Reinterpreted

- Number of cores per chip doubles every 2 year, while clock speed decreases (not increases).
 - Need to deal with systems with millions of concurrent threads
 - Future generation will have billions of threads!
 - Need to be able to easily replace inter-chip parallelism with introchip parallelism
- Number of threads of execution doubles every 2 year



Potential System Architectures

Systems	2009		
System peak	2 Pflop/s		
System memory	0.3 PB		
Node performance	125 Gflop/s		
Node memory BW	25 GB/s		
Node concurrency	12		
Interconnect BW	1.5 GB/s		
System size (nodes)	18,700		
Total concurrency	225,000		
Storage	15 PB		
10	0.2 TB/s		
MTTI	days		
Power	7 MW		



- For the last decade or more, the research investment strategy has been overwhelmingly biased in favor of hardware.
- This strategy needs to be rebalanced barriers to progress are increasingly on the software side.
- Moreover, the return on investment is more favorable to software.
 - Hardware has a half-life measured in years, while software has a half-life measured in decades.
- High Performance Ecosystem out of balance
 - Hardware, OS, Compilers, Software, Algorithms, Applications
 - No Moore's Law for software, algorithms and applications



Employment opportunities for post-docs in the PLASMA/MAGMA projects

PLASMA Parallel Linear Algebra Software for Multicore Architectures

http://icl.cs.utk.edu/plasma/

MAGMA Matrix Algebra on GPU and Multicore Architectures http://icl.cs.utk.edu/magma/

Emmanuel Agullo, Jim Demmel, Jack Dongarra, BilelHadri,Jakub Kurzak, Julie&JulienLangou,Hatem Ltaief,PiotrLuszczek, Stan Tomov





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Strong scaling: fixed problem size.

- Data on each node decreases as the number of nodes increases
- Weak scaling: fixed the data size on each node.
 - Problem size increases as the number of node increases.

Review: two definitions of scalability

"Strong scaling"

- execution time decreases in inverse proportion to the number of processors
- fixed size problem overall
- often instead graphed as reciprocal, "speedup"

"Weak scaling"

- execution time remains constant, as problem size and processor number are increased in proportion
- fixed size problem per processor
- Various sub-types of weak-scaling "memory bound", etc. (see Kumar et



Symmetric Positive Definite

Cholesky-GPU Intel (R) Xeon (R) E5410 2.33 GHz (8 Core) GForce GTX 280 1.3 GHz (240 Core)





- Projections
 - Performance
 - Memory
- Async
 - Break fork-join
 - DAGs
 - New algorithms numerical issues
 - Communication avoiding
 - Chaotic iteration
- Mixed precision
 - Iter refine
 - precond
- Hybrid
 - balance
 - autotune
- FT
 - Number of approaches



- Available through MAGMA's homepage <u>http://icl.cs.utk.edu/magma/</u>
- Included are the 3 one-sided matrix factorizations
- Iterative Refinement Algorithm (Mixed Precision)
- Standard (LAPACK) data layout and accuracy
- Two LAPACK-style interfaces
 - CPU interface: both input and output are on the CPU
 - GPU interface: both input and output are on the GPU
- This release is intended for single GPU



- The IESP software roadmap is a planning instrument designed to enable the international HPC community to improve, coordinate and leverage their collective investments and development efforts.
 - After we determine what needs to be accomplished, our task will be to construct the organizational structures suitable to accomplish the work

Diskless Checkpointing 1/2

Principle: Compute a checksum of the processes' memory and store it on spare processors

Advantage: does not require ckpt on stable storage.



A) Every process saves a copy of its local state of in memory or local disc

B) Perform a global bitstream or floating point operation on all saved local states

All processes restore its local state from the one saved in memory or local disc

Diskless Checkpointing 2/2

Could be done at application and system levels

•Process data could be considered (and encoded) either as bit-streams or as floating point numbers. Computing the checksum from bit-streams uses operations such as parity. Computing checksum from floating point numbers uses operations such as addition

•Can survive multiple failures of arbitrary patterns Reed Solomon for bit-streams and weighted checksum for floating point numbers (sensitive to round-off errors).

•Work with with incremental ckpt.





•Need spare nodes and double the memory occupation (to survive failures during ckpt.) --> increases the overall cost and #failures

Need coordinated checkpointing or message logging protocol

Need very fast encoding & reduction operations

Need automatic Ckpt protocol or program modifications



Challenge: experiment more Diskless CKPT and in very large machines (current result are for ~1000 CPUs)

Algorithmic Based Fault Tolerance"

In 1984, Huang and Abraham, proposed the ABFT to detect and correct errors in some matrix operations on systolic arrays.

ABFT encodes data & redesign algo. to operate on encoded data. Failure are detected and corrected off-line (after execution).

ABFT variation for on-line recovery (runtime detects failures + robust to failures):

•Similar to Diskless ckpt., an extra processor is added, Pi+1, store the checksum of data: (vector X and Y in this case) Xc = X1 + ... + Xp, Yc = Y1 + ... + Yp. Xf = [X1, ... Xp, Xc], Yf = [Y1, ... Yp, Yc],

• Operations are performed on Xf and Yf instead of X and Y : Zf=Yf+Zf

- Compared to diskless checkpointing, the memory AND CPU of Pc take part of the computation):
- No global operation for Checksum!
- No local checkpoint!

	P1	P2	P3	P4	Pc
т	X1	X2	X3	X4	Xc
т	Y1	Y2	Y3	Y4	Yc
=	Z1	Z2	Z3	Z4	Zc

Works for many Linear Algebra operations:Matrix Multiplication: $A * B = C \rightarrow Ac * Br = Cf$ LU Decomposition: $C = L * U \rightarrow Cf = Lc * Ur$ Addition: $A + B = C \rightarrow Af + Bf = Cf$ Scalar Multiplication: c * Af = (c * A)fTranspose: AfT = (AT)fCholesky factorization & QR factorization

"Naturally fault tolerant algorithm"

Natural fault tolerance is the ability to tolerate failures through the mathematical properties of the algorithm itself, without requiring notification or recovery.

The algorithm includes natural compensation for the lost information.

For example, an iterative algorithm may require more iterations to converge, but it still converges despite lost information

Assumes that a maximum of 0.1% of tasks may fail

Ex1 : Meshless iterative methods+chaotic relaxation (asynchronous iterative methods)

> This algorithm share some features with SelfStabilization algorithms: detection of termination is very hard! →it provides the max « eventually »... BUT, it does not tolerate Byzantine faults (SelfStabilization does for transient failures + acyclic topology)







Proactive Migration

Principle: predict failures and migrate processes before failures

•Prediction models are based on the analysis of correlations between non fatal and fatal errors, and temporal and spatial correlations between failure events.

Results on the 100 first days of BlueGene/L demonstrate good failure
 Proactive migration may help to significantly increase the checkpoint
 tr interval.

Results are lacking concerning real time predictions and actual benefits of migration in real conditions

•Migration has a cost (need to checkpoint and log or delay messages)

•What to migrate?

•Virtual Machine, Process checkpoint?

•Only application state (user checkpoint)?

Challenge: Analyze more traces, Identify more correlations, Improve predictive algorithms

Fault Recovery Options

- Saved State
 - Restart from checkpoint file
 - Restart from **local** checkpoint
 - Recalculate lost data from inmemory checkpoint (RAID like)

No Checkpoint

- Lossy recalculation of lost data
- Recalculate lost data from initial and remaining data
- Replicate computation across system
- Reassign lost work to another resource
- Use natural fault tolerant algorithms





Hard errors – permanent component failure either HW or SW (hung or crash)

Soft errors – transient errors, a blip or short term failure of either HW or SW

Silent errors – undetected errors either hard or soft, due to lack of detectors for a component or inability to detect (transient effect too short). Real danger is that answer may be incorrect but the user wouldn't know.

HW (node and interconnect)resilience needed to reduce Silent errors – Either turn them into Hard or Soft errors or fix them

Potential System Architecture

Systems	2009	2018
System peak	2 Pflop/s	1 Eflop/s
Power	6 MW	~20 MW
System memory	0.3 PB	32 - 64 PB
Node performance	125 GF	1,2 or 15TF
Node memory BW	25 GB/s	2-4TB/s
Node concurrency	12	O(1k) or 10k
Total Node Interconnect BW	3.5 GB/s	200-400GB/s (1:4 or 1:8 from memory BW)
System size (nodes)	18,700	O(100,000) or O(1M)
Total concurrency	225,000	O(billion) [O(10) to O(100) for latency hiding]
Storage	15 PB	500-1000 PB (>10x system memory is min)
10	0.2 TB	60 TB/s (how long to drain the machine)
MTTI	days	O(0.1 day)



- panel factorization
- > updating the trailing submatrix
- > merge the domains





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- panel factorization
- > updating the trailing submatrix
- > merge the domains
- Final R computed





Rank	Site	Computer	Country	Cores	Rmax [Pflops]	% of Peak
1	DOE / OS Oak Ridge Nat Lab	Jaguar / Cray Cray XT5sixCore 2.6 GHz	USA	224,162	1.76	75
2	Nat. Supercomputer Center in Shenzhen	Nebulea / Dawning / TC3600 Blade, Intel X5650, Nvidia C2050 GPU	China	120,640	1.27	43
3	DOE / NNSA Los Alamos Nat Lab	Roadrunner / IBM BladeCenterQS22/LS21	USA	122,400	1.04	76
4	NSF / NICS / U of Tennessee	Kraken/ Cray Cray XT5sixCore 2.6 GHz	USA	98,928	.831	81
5	ForschungszentrumJueli ch (FZJ)	Jugene / IBM Blue Gene/P Solution	Germany	294,912	.825	82
6	NASA / Ames Research Center/NAS	Pleiades / SGI SGI Altix ICE 8200EX	USA	56,320	.544	82
7	National SC Center in Tianjin / NUDT	Tianhe-1 / NUDT TH-1 / IntelQC + AMD ATI Radeon 4870	China	71,680	.563	46
8	DOE / NNSA Lawrence Livermore NL	BlueGene/L IBM eServerBlue Gene Solution	USA	212,992	.478	80
9	DOE / OS Argonne Nat Lab	Intrepid / IBM Blue Gene/P Solution	USA	163,840	.458	82
10	DOE / NNSA Sandia Nat Lab	Red Sky / Sun / SunBlade 6275	USA	42,440	.433	87



Rank	Site	Computer	Country	Cores	Rmax [Pflops]	% of Peak	Power [MW]	MFlops /Watt
1	DOE / OS Oak Ridge Nat Lab	Jaguar / Cray Cray XT5sixCore 2.6 GHz	USA	224,162	1.76	75	7.0	251
2	Nat. Supercomputer Center in Shenzhen	Nebulea / Dawning / TC3600 Blade, Intel X5650, Nvidia C2050 GPU	China	120,640	1.27	43	2.58	493
3	DOE / NNSA Los Alamos Nat Lab	Roadrunner / IBM BladeCenterQS22/LS21	USA	122,400	1.04	76	2.48	446
4	NSF / NICS / U of Tennessee	Kraken/ Cray Cray XT5sixCore 2.6 GHz	USA	98,928	.831	81	3.09	269
5	ForschungszentrumJueli ch (FZJ)	Jugene / IBM Blue Gene/P Solution	Germany	294,912	.825	82	2.26	365
6	NASA / Ames Research Center/NAS	Pleiades / SGI SGI Altix ICE 8200EX	USA	56,320	.544	82	3.1	175
7	National SC Center in Tianjin / NUDT	Tianhe-1 / NUDT TH-1 / IntelQC + AMD ATI Radeon 4870	China	71,680	.563	46	1.48	380
8	DOE / NNSA Lawrence Livermore NL	BlueGene/L IBM eServerBlue Gene Solution	USA	212,992	.478	80	2.32	206
9	DOE / OS Argonne Nat Lab	Intrepid / IBM Blue Gene/P Solution	USA	163,840	.458	82	1.26	363
10	DOE / NNSA Sandia Nat Lab	Red Sky / Sun / SunBlade 6275	USA	42,440	.433	87	2.4	180





• Break into smaller tasks and remove dependencies



Communication Avoiding QR Example



A. Pothen and P. Raghavan. Distributed orthogonal factorization. In *The 3rd Conference on Hypercube Concurrent Computers and Applications, volume II, Applications,* pages 1610–1620, Pasadena, CA, Jan. 1988. ACM. Penn. State.







Parallel Tasks in LU/LL^T/QR



- Break into smaller tasks and remove dependencies
- Tile LU factorization on a square matrix with 5 x 5 tiles. Each tile is of size bxb and corresponds to a fine grain task. The arcs show the data dependencies between the tasks.









#3 LANL Roadrunner A Petascale System in 2008



Dual Core Opteron Chip