An Overview of High Performance Computing and Challenges for the Future

Jack Dongarra INNOVATIVE COMPUTING LABORATORY



University of Tennessee Oak Ridge National Laboratory University of Manchester



- Quick look at High Performance Computing
 - Top500
- Challenges for Math Software
 - Linear Algebra Software for Multicore and Beyond





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







Performance Development & Projections





Performance Development & Projections

LANL Roadrunner A Petascale System in 2008



Dual Core Opteron Chip

Top10 of the June 2008 List

	Computer	Rmax [TF/s]	Rmax / Rpeak	Installation Site	Country	#Cores
1	IBM / Roadrunner BladeCenter QS22/LS21	1,026	75%	DOE/NNSA/LANL	USA	122,400
2	IBM / BlueGene/L eServer Blue Gene Solution	478	80%	DOE/NNSA/LLNL	USA	212,992
3	IBM / Intrepid Blue Gene/P Solution	450	81%	DOE/OS/ANL	USA	163,840
4	SUN / Ranger SunBlade x6420	326	65%	NSF/TACC	USA	62,976
5	CRAY / Jaguar Cray XT4 QuadCore	205	79%	DOE/OS/ORNL	USA	30,976
6	IBM / JUGENE Blue Gene/P Solution	180	81%	Forschungszentrum Juelich (FZJ)	Germany	65,536
7	SGI / Encanto SGI Altix ICE 8200	133.2	77%	New Mexico Computing Applications Center	USA	14,336
8	HP / EKA Cluster Platform 3000 BL460c	132.8	77%	Computational Research Lab, TATA SONS	India	14,384
9	IBM / Blue Gene/P Solution	112	81%	IDRIS	France	40,960
10	SGI / Altix ICE 8200EX	106	86%	Total Exploration Production	France	10,240

Top10 of the June 2008 List

	Computer	Rmax [TF/s]	Rmax / Rpeak	Installation Site	Country	#Cores	Power [MW]	MFlops/ Watt
1	IBM / Roadrunner BladeCenter QS22/LS21	1,026	75%	DOE/NNSA/LANL	USA	122,400	2.35	437
2	IBM / BlueGene/L eServer Blue Gene Solution	478	80%	DOE/NNSA/LLNL	USA	212,992	2.33	205
3	IBM / Intrepid Blue Gene/P Solution	450	81%	DOE/OS/ANL	USA	163,840	1.26	357
4	SUN / Ranger SunBlade x6420	326	65%	NSF/TACC	USA	62,976	2.00	163
5	CRAY / Jaguar Cray XT4 QuadCore	205	79%	DOE/OS/ORNL	USA	30,976	1.58	130
6	IBM / JUGENE Blue Gene/P Solution	180	81%	Forschungszentrum Juelich (FZJ)	Germany	65,536	0.50	357
7	SGI / Encanto SGI Altix ICE 8200	133.2	77%	New Mexico Computing Applications Center	USA	14,336	0.86	155
8	HP / EKA Cluster Platform 3000 BL460c	132.8	77%	Computational Research Lab, TATA SONS	India	14,384	0.79	169
9	IBM / Blue Gene/P Solution	112	81%	IDRIS	France	40,960	0.32	357
10	SGI / Altix ICE 8200EX	106	86%	Total Exploration Production	France	10,240	0.44	240

ORNL/UTK Computer Power Cost Projections 2007-2012

- Over the next 5 years ORNL/UTK will deploy 2 large Petascale systems
- Using 4 MW today, going to 15MW before year end
- By 2012 could be using more than 50MW!!
- Cost estimates based on \$0.07 per KwH

Power becomes the architectural driver for future large systems



Cost Per Year Includes both DOE and NSF systems.

Something's Happening Here...



- In the "old days" it was: each year processors would become faster
- Today the clock speed is fixed or getting slower
- Things are stilldoubling every18 -24 months
- Moore's Law reinterpretated.
 - Number of cores double every 18-24 months



• What is multicore?



- A multicore chip is a single chip (socket) that combines two or more independent processing units that provide independent threads of control
- Why multicore?
 - The race for ever higher clock speeds is over.
 - In the old days, new the chips where faster
 - Applications ran faster on the new chips
 - Today new chips are not faster, just have more processors per chip
 - Applications and software must use those extra processors to become faster



- Power \propto Voltage² x Frequency (V²F)
- Frequency ~ Voltage

 Power «Frequency³ 								
	Cores	V	Freq	Perf	Power	PE (Bops/W	att)	
Superscalar	1	1	1	1	1	1		
"New" Superscalar	1X	1.5X	1.5X	1.5X	3.3X	0.45X		
							1	



- Power \propto Voltage² x Frequency (V²F)
- Frequency ~ Voltage



50% more performance with 20% less power

Preferable to use multiple slower devices, than one superfast device



And then there's the GPU's NVIDIA's Tesla T10P

- T10P chip
 - 240 cores; 1.5 GHz
 - Tpeak 1 Tflop/s 32 bit floating point
 - Tpeak 100 Gflop/s 64 bit floating point
- S1070 board
 - 4 T10P devices;
 - 700 Watts
- C1060 card
 - 1 T10P; 1.33 GHz
 - 160 Watts
 - Tpeak 887 Gflop/s 32 bit floating point
 - Tpeak 88.7 Gflop/s 64 bit floating point









What's Next? Multicore to Manycore



Coding for an Abstract Multicore

Parallel software for multicores should have two characteristics:

- Fine granularity:
 - High level of parallelism is needed
 - Cores will probably be associated with relatively small local memories. This requires splitting an operation into tasks that operate on small portions of data in order to reduce bus traffic and improve data locality.
- Asynchronicity:
 - As the degree of thread level parallelism grows and granularity of the operations becomes smaller, the presence of synchronization points in a parallel execution seriously affects the efficiency of an algorithm.

ManyCore - Parallelism for the Masses

- We are looking at the following concepts in designing the next numerical library implementation
 - Dynamic Data Driven Execution
 - Self Adapting
 - Block Data Layout
 - Mixed Precision in the Algorithm
 - Exploit Hybrid Architectures
 - Fault Tolerant Methods

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

Software/Algorithms follow hardware evolution in time



Software/Algorithms follow hardware evolution in time					
LINPACK (70's) (Vector operations)		Rely on - Level-1 BLAS operations			
LAPACK (80's) (Blocking, cache friendly)		Rely on - Level-3 BLAS operations			

Software/Algorithms follow hardware evolution in time						
LINPACK (70's) (Vector operations)		Rely on - Level-1 BLAS operations				
LAPACK (80's) (Blocking, cache friendly)		Rely on - Level-3 BLAS operations				
ScaLAPACK (90's) (Distributed Memory)		Rely on - PBLAS Mess Passing				

Parallel Linear Algebra Software for Multicore Architectures (PLASMA)



Those new algorithms

- have a very low granularity, they scale very well (multicore, petascale computing, ...)
- removes a lots of dependencies among the tasks, (multicore, distributed computing)
- avoid latency (distributed computing, out-of-core)
- rely on fast kernels

Those new algorithms need new kernels and rely on efficient scheduling algorithms.









Achieving Fine Granularity

Fine granularity may require novel data formats to overcome the limitations of BLAS on small chunks of data.

Column-Major



Achieving Fine Granularity

Fine granularity may require novel data formats to overcome the limitations of BLAS on small chunks of data.

Column-Major



Block data layout



LU – 16 Core (8 Socket - Dual Core Opteron 2.2 GHz)

1. LAPACK (BLAS Fork-Join Parallelism) 2. ScaLAPACK (Mess Pass using mem copy)



Problem Size



QR -- quad-socket, dual-core Opteron





Cholesky on the CELL





CELL Cholesky – 8 cores



Single precision results on the Cell

Ç

If We Had A Small Matrix Problem

- We would generate the DAG, find the critical path and execute it.
- DAG too large to generate ahead of time
 - Not explicitly generate
 - Dynamically generate the DAG as we go
- Machines will have large number of cores in a distributed fashion
 - Will have to engage in message passing
 - Distributed management
 - Locally have a run time system





 Here is the DAG for the QR factorization on a 20 x 20 matrix



- For a large matrix say O(10⁶) the DAG is huge
- Many challenges for the software

Each Node or Core Will Have A Run Time System



BIN 1



- some dependencies satisfied
- waiting for all dependencies
- all dependencies satisfied
- some data delivered
- waiting for all data





- all data delivered
- waiting for execution

Performance of Single Precision on Conventional Processors

- Realized have the similar situation on our commodity processors.
 - That is, SP is 2X as fast as DP on many systems
- The Intel Pentium and AMD Opteron have SSE2
 - 2 flops/cycle DP
 - 4 flops/cycle SP
- IBM PowerPC has AltiVec
 - 8 flops/cycle SP
 - 4 flops/cycle DP
 - No DP on AltiVec

	Size	SGEMM/ DGEMM	Size	SGEMV/ DGEMV
AMD Opteron 246	3000	2.00	5000	1.70
UltraSparc-lle	3000	1.64	5000	1.66
Intel PIII Coppermine	3000	2.03	5000	2.09
PowerPC 970	3000	2.04	5000	1.44
Intel Woodcrest	3000	1.81	5000	2.18
Intel XEON	3000	2.04	5000	1.82
Intel Centrino Duo	3000	2.71	5000	2.21

Single precision is faster because:

- Higher parallelism in SSE/vector units
- Reduced data motion
- Higher locality in cache



32 or 64 bit Floating Point Precision?

- A long time ago 32 bit floating point was used
 - Still used in scientific apps but limited
- Most apps use 64 bit floating point
 - Accumulation of round off error
 - A 10 TFlop/s computer running for 4 hours performs > 1 Exaflop (10¹⁸) ops.
 - Ill conditioned problems
 - IEEE SP exponent bits too few (8 bits, 10^{±38})
 - Critical sections need higher precision
 - Sometimes need extended precision (128 bit fl pt)
 - However some can get by with 32 bit fl pt in some parts
- Mixed precision a possibility
 - Approximate in lower precision and then refine or improve solution to high precision.



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 = Iu(A)	O (n ³)
x = L\(U\b)	O (<i>n</i> ²)
r = b - Ax	O (<i>n</i> ²)
WHILE r not small enough	
z = L (U r)	O(n ²)
x = x + z	 O (<i>n</i> ¹)
r = b - Ax	O (<i>n</i> ²)
END	

 Wilkinson, Moler, Stewart, & Higham provide error bound for SP fl pt results when using DP fl pt.

Mixed-Precision Iterative Refinement

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

L U = Iu(A)	SINGLE	O (n ³)
x = L\(U\b)	SINGLE	O (<i>n</i> ²)
r = b - Ax	DOUBLE	O (<i>n</i> ²)
WHILE r not small enough	l	
z = L (U r)	SINGLE	O (n ²)
$\mathbf{x} = \mathbf{x} + \mathbf{z}$	DOUBLE	O (n ¹)
r = b - Ax	DOUBLE	O (<i>n</i> 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; $O(10^8)$

Results for Mixed Precision Iterative Refinement for Dense Ax = b



	Architecture (BLAS)
1	Intel Pentium III Coppermine (Goto)
2	Intel Pentium III Katmai (Goto)
3	Sun UltraSPARC IIe (Sunperf)
4	Intel Pentium IV Prescott (Goto)
5	Intel Pentium IV-M Northwood (Goto)
6	AMD Opteron (Goto)
7	Cray X1 (libsci)
8	IBM Power PC G5 (2.7 GHz) (VecLib)
9	Compaq Alpha EV6 (CXML)
10	IBM SP Power3 (ESSL)
11	SGI Octane (ATLAS)

- Single precision is faster than DP because:
 - Higher parallelism within vector 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

Results for Mixed Precision Iterative Refinement for Dense Ax = b



	Architecture (BLAS)
1	Intel Pentium III Coppermine (Goto)
2	Intel Pentium III Katmai (Goto)
3	Sun UltraSPARC IIe (Sunperf)
4	Intel Pentium IV Prescott (Goto)
5	Intel Pentium IV-M Northwood (Goto)
6	AMD Opteron (Goto)
7	Cray X1 (libsci)
8	IBM Power PC G5 (2.7 GHz) (VecLib)
9	Compaq Alpha EV6 (CXML)
10	IBM SP Power3 (ESSL)
11	SGI Octane (ATLAS)

Architecture (BLAS-MPI)	# procs	п	DP Solve /SP Solve	DP Solve /Iter Ref	# iter
AMD Opteron (Goto – OpenMPI MX)	32	22627	1.85	1.79	6
AMD Opteron (Goto – OpenMPI MX)	64	32000	1.90	1.83	6

- Single precision is faster than DP because:
 - Higher parallelism within vector 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



Sparse Direct Solver and Iterative ICL UT" Refinement

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



Tim Davis's Collection, n=100K - 3M

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



Cray XD-1 (OctigaBay Systems)

Experiments with Field Programmable Gate Array (FPGA) Specify arithmetic precision



Mixed Precision Iterative Refinement - FPGA Performance Test - Junging Sun et al

Characteristics of multiplier on an FPGA* (using DSP48)

Data Formats	DSP48s	Frequency (MHz)	GFLOPs
s52e11 (double)	16/96	237	1.42
s51e11	16/96	238	1.43
s50e11	9/96	245	2.61
s34e8	9/96	289	3.08
s33e8	4/96	292	7.01
s23e8 (single)	4/96	339	8.14
s17e8	4/96	370	8.88
s16e8	1/96	331	31.78
s16e7	1/96	352	33.79
s13e7	1/96	336	32.26



* XC4LX160-10

TENNESSEE ADVANCED COMPUTING LABORATORY



Mixed Precision Iterative Refinement Random Matrix Test - Junging Sun et al

Refinement iterations for customized formats (sXXe11). Random matrices (average number of iterations/random matrices)

More Bits

			_	_	_	
Mantissa Bits Problem Size	12	16	23	31	48	52
128	8.9	4	2	1	1	0
256	11.1	5.1	2.1	1	1	0
512	19.7	6.1	2.5	1	1	0
1024	28	6.3	2.6	1	1	0
2048	-	9.3	3	1.3	1	0
4096	-	13.3	3.1	1.43	1	0





TENNESSEE ADVANCED COMPUTING LABORATORY



Mixed Precision Hybrid Direct Solver - Profiled Time* on Cray-XD1 - Junging Sun et al



■ LU ■ communication □ triangular solvers □ Refinement

* For a 128x128 matrix

High Performance Mixed-Precision Linear Solver for FPGAs, Junqing Sun, Gregory D. Peterson, Olaf Storaasli, To appear IEEE TPDC

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
 - What about 16 bit floating point?
 - 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. $f(x_i) = x_i - \frac{f(x_i)}{f'(x_i)}$

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

Correction = -A(b - Ax)

Conclusions

- 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



Marc Baboulin UCoimbra Alfredo Buttari, ENS/INRIA Bilel Hadri, UTK Julien Langou, UColorado Julie Langou, UTK Hatem Ltaief, UTK Piotr Luszczek, MathWorks Jakub Kurzak, UTK Stan Tomov, UTK







©2007 Google

PLASMA Collaborators

- U Tennessee, Knoxville
 - Jack Dongarra, Julie Langou, Stan Tomov, Jakub Kurzak, Hatem Ltaief, Alfredo Buttari, Julien Langou, Piotr Luszczek, Marc Baboulin
- UC Berkeley
 - Jim Demmel, Ming Gu, W. Kahan, Beresford Parlett, Xiaoye Li, Osni Marques, Yozo Hida, Jason Riedy, Vasily Volkov, Christof Voemel, David Bindel
- Other Academic Institutions
 - UC Davis, CU Denver, Florida IT, Georgia Tech, U Maryland, North Carolina SU, UC Santa Barbara, UT Austin, LBNL
 - TU Berlin, ETH, U Electrocomm. (Japan), FU Hagen, U Carlos III Madrid, U Manchester, U Umeå, U Wuppertal, U Zagreb, UPC Barcelona, ENS Lyon, INRIA
- Industrial Partners
 - Cray, HP, Intel, Interactive Supercomputing, MathWorks, NAG, NVIDIA, Microsoft