

An Overview of High Performance Computing and Experiments with Energy Savings and Short Precision

Jack Dongarra

University of Tennessee Oak Ridge National Laboratory University of Manchester

1

1/30/18



- Overview of High Performance Computing
- With Extreme Computing the "rules" for computing have changed





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 OF HPC OVER THE LAST 25 YEARS FROM THE TOP500



TOP 500



PERFORMANCE DEVELOPMENT



5

State of Supercomputing in 2018

- Pflops (> 10¹⁵ Flop/s) computing fully established with 181 systems.
- Three technology architecture possibilities or "swim lanes" are thriving.
 - Commodity (e.g. Intel)
 - Commodity + accelerator (e.g. GPUs) (101 systems)
 - Special purpose lightweight cores (e.g. IBM BG, ARM, Knights Landing, TaihuLight, PEZY-SC2)
- Interest in supercomputing is now worldwide, and growing in many new markets (~50% of Top500 computers are in industry).
- Exascale (10¹⁸ Flop/s) projects exist in many countries and regions.
- Intel processors largest share, 94% followed by AMD, 1%.



Countries Share





US has fallen to the lowest point since the TOP500 list was created. China has 35% of the performance US has 30% of the performance

7



November 2017: The TOP 10 Systems

Rank	Site	Computer	Country	Cores	Rmax [Pflops]	% of Peak	Power [MW]	GFlops/ Watt	-
1	National Super Computer Center in Wuxi	Sunway TaihuLight, SW26010 (260C) + Custom	China	10,649,000	93.0	74	15.4	6.04	

TaihuLight is Equal to Sum of All Top500 Systems in Japan

TaihuLight is about 1/3 the Sum of the other Asian Machines in Top500

	4	Japan Agency Marine-Earth S&T	ExaScalar ZettaScaler-2.2 Xeon (16c) + PEZY-SC2 (2048C)	Japan	19,840,000	19.1	67	1.35	14.1
	5	DOE / OS Oak Ridge Nat Lab	Titan, Cray XK7, AMD (16C) + Nvidia Kepler GPU (14C) + Custom	USA	560,640	17.6	65	8.21	2.14
	6	DOE / NNSA L Livermore Nat Lab	Sequoia, BlueGene/Q (16C) + custom	USA	1,572,864	17.2	85	7.89	2.18
	7	DOE / NNSA / Los Alamos & Sandia	Trinity, Cray XC40,Xeon Phi (68C) + Custom	USA	979,968	14.1	80	3.84	3.67
	8	DOE / OS L Berkeley Nat Lab	Cori, Cray XC40, Xeon Phi (68C) + Custom	USA	622,336	14.0	50	3.94	3.65
	9	Joint Center for Advanced HPC	Oakforest-PACS, Fujitsu Primergy CX1640, Xeon Phi (68C) + Omni-Path	Japan	558,144	13.6	54	2.72	4.98
	10	RIKEN Advanced Inst for Comp Sci	K computer Fujitsu SPARC64 VIIIfx (8C) + Custom	Japan	705,024	10.5	93	12.7	.827
1	500	Flemish Supercomputer	r Intel (14C)		16128	.548	88		



 HPL (Top500) based on solving
 HPCG based on solving a a dense matrix problem.

A x = b

- > A is dense (full of nonzeros)
- > Use a direct solver
- Gaussian Eli. w/partial pivoting
- > Main driver is matrix multiply
- > Matrix random



07

- sparse matrix problem.
 - A x = b
 - > A is sparse (mainly zeros)
 - >Use an iterative solver
 - Conjugate Gradient Method
 - > Main driver is matrix vector ops
 - > Matrix from a synthetic discretized 3D PDE



	Rank	Site	Computer	Cores	HPL Rmax (Pflop/s)	TOP500 Rank	HPCG (Pflop/s)	Fraction of Peak
2017	1	RIKEN Advanced Institute fo Computational Science Japan	r K computer – , SPARC64 VIIIfx 2.0GHz, Tofu interconnect, Fujitsu	705,024	10.51	10	0.603	5.3%
ber	2	NSCC / Guangzhou China	Tianhe-2 (MilkyWay-2) – TH-IVB-FEP Cluster, Intel Xeon 12C 2.2GHz, TH Express 2, Intel Xeon Phi 31S1P 57-core, NUDT	3,120,000	33.86	2	0.580	1.1%
em	3	DOE/NNSA/LANL/SNL USA	Trinity – Cray XC40, Intel Xeon E5-2698 v3 300160C 2.3GHz, Aries, Cray	979,072	14.13	7	0.546	1.8%
rk Nov	4	Swiss National Supercomputing Centre (CSCS) Switzerland	Piz Daint – Cray XC50, Intel Xeon E5-2690v3 12C 2.6GHz, Cray Aries, NVIDIA Tesla P100 16GB, Cray	361,760	19.59	3	0.486	1.9%
Benchmai	5	National Supercomputing Center in Wuxi China	Sunway TaihuLight – Sunway MPP, SW26010 260C 1.45GHz, Sunway, NRCPC	10,649,600	93.01	1	0.481	0.4%
	6	Joint Center for Advanced High Performance Computing Japan	Oakforest-PACS – PRIMERGY CX600 M1, Intel Xeon Phi Processor 7250 68C 1.4GHz, Intel Omni-Path Architecture, Fujitsu	557,056	13.55	9	0.385	1.5%
U U	7	DOE/SC/LBNL/NERSC USA	Cori – XC40, Intel Xeon Phi 7250 68C 1.4GHz, Cray Aries, Cray	632,400	13.83	8	0.355	1.3%
노	8	DOE/NNSA/LLNL USA	Sequoia – IBM BlueGene/Q, PowerPC A2 1.6 GHz 16-core, 5D Torus, IBM	1,572,864	17.17	6	0.330	1.6%
	9	DOE/SC/Oak Ridge Nat Lab USA	Titan – Cray XK7, Opteron 6274 16C 2.200GHz, Cray Gemini interconnect, NVIDIA K20x, Cray	560,640	17.59	5	0.322	1.2%
	10	GSIC Center, Tokyo Institute of Technology Japan	TSUBAME3.0 – SGI ICE XA (HPE SGI 8600), IP139-SXM2, Intel Xeon E5-2680 v4 15120C 2.9GHz, Intel Omni-Path Architecture, NVIDIA TESLA P100 SXM2 with NVLink, HPE	136,080	12.12	13	0.189	1.6%

Exascale Race/Technologies Projected Exascale Dates and Suppliers

 U.S. Sustained ES: 2023 Peak ES: 2021 Vendors: U.S. Processors: U.S. (some ARM?) Initiatives: NSCI/ECP Cost: \$300-600M per system, plus heavy R&D investments 	 EU Sustained ES: 2022-2023 Peak ES: 2021 Vendors: U.S., Europe Processors: Likely ARM Initiatives: EuroHPC Cost: \$300-\$350M per system, plus heavy R&D investments
 China Sustained ES: 2021-2022 Peak ES: 2020 Vendors: Chinese Processors: Chinese (plus U.S.?) 13th 5-Year Plan Cost: \$350-500M per system, plus heavy R&D 	 Japan Sustained ES: 2022 Peak ES: Likely as a Al/ML/DL system Vendors: Japanese Processors: Japanese Cost: \$800M-\$1B, this includes both 1 system and the R&D costs, will also do many smaller size systems

Sustained ES on a single 64-bit real application

Exascale Race/Technologies

Projected Exascale Investment Levels (In Addition to System Purchases)

U.S. \$1 to \$2 billion a year in R&D

- Investments by both governments & vendors
- Plans are to purchases multiple exascale systems each year

EU 🚺

- About 5 billion euros in totalInvestments in multiple exascale
- and pre-exascale systems
- Investments mostly by country governments with a little from the EU

China

- Over \$1 billion a year in R&D
- Investments by both governments & vendors
- Plans are to purchases multiple exascale systems each year
- Already investing in 3 preexascale systems starting in late 2018

Japan |

- Planned investment of just over \$1billion* (over 5 years) for both the R&D and purchase of 1 exascale system
- To be followed by a number of smaller systems ~\$100M to \$150M each
- Creating a new processor and a new software environment

* Note that this includes both the system and R&D

© Hyperion Research



- China plans for Exascale 2020
 - Three separate developments in HPC; "Anything but from the US"
 - Wuxi
 - Upgrade the ShenWei O(100) Pflops all Chinese
 - National University for Defense Technology
 - Tianhe-2A O(100) Pflops will be Chinese ARM processor + accelerator
 - Sugon CAS ICT
 - X86 based; collaboration with AMD
- US DOE Exascale Computing Program 7 Year Program
 - Initial exascale system based on advanced architecture and delivered in 2021
 - Enable capable exascale systems, based on ECP R&D, delivered in 2022 and deployed in 2023







Exascale

- 50X the performance of today's 20 PF systems
- 20-30 MW power
- \leq 1 perceived fault /week
- SW to support broad range of apps

Next Big Systems in the US DOE

- Oak Ridge Lab and Lawrence Livermore Lab to receive IBM and Nvidia based systems
 - IBM Power 9 + Nvidia Volta V100
 - Installation started but not completed until 2018
 - 5-10 times Titan on apps
 - 4,600 nodes, each containing six 7.5-teraflop NVIDIA V100 GPUs, and two IBM Power9 CPUs, its aggregate peak performance should be > 200 petaflops.
 - ORNL June 2018 fully ready (Top500 number)
- In 2021 Argonne Lab to receive Intel based system
 - Exascale systems, based on a Future Intel proc, not Knights Hill
 - Aurora 21
 - Balanced architecture to support three pillars
 - Large-scale Simulation (PDEs, traditional HPC)
 - Data Intensive Applications (science pipelines)
 - Deep Learning and Emerging Science AI
 - Integrated computing, acceleration, storage
 - Towards a common software stack





14

US Department of Energy Exascale Computing Program has formulated a holistic approach that uses co-design and integration to achieve capable exascale

Application Development Software Technology		Hardware Technology	Exascale Systems
Science and mission applications	Scalable and productive software stack	Hardware technology elements	Integrated exascale supercomputers
	Correctness Visualization Data Analysis Applications Co-Design Programming models, development environment, and runtimes Math libraries and Frameworks Tools System Software, resource management threading, scheduling, Memory untoritoring, and control Memory and Burst buffer Data management VO and file system Node OS, runtimes Hardware interface		
EC	CP's work encompasses app chitectures, and workforce de	lications, system software, h evelopment	ardware technologies and



15 Exascale Computing Project, www.exascaleproject.org

Machine Learning in Computational Science

Many fields are beginning to adopt machine learning to augment modeling and simulation methods

- Climate
- Biology
- Drug Design
- Epidemology
- Materials
- Cosmology
- High-Energy Physics







Deep Learning Needs Small Matrix Operations

Matrix Multiply is the time consuming part.

Convolution Layers and Fully Connected Layers require matrix multiply

There are many GEMM's of small matrices, perfectly parallel, can get by with 16-bit floating point



EEE 754 Half Precision (16-bit) Floating Pt Standard

A lot of interest driven by "machine learning"



intel [®] INTEL [®] XE	ON PHI™
UP TO DIRECT 4000GB ACCESS VS TOCOL WITH A CAU!	NEAR LINEAR SCALING 31X REDUCTION IN WHEN SCALING TO 32 NORES ²
KNIGHTS MILL Next Gen Xeon Phi AX DEEP LEARNING DEEF LEARNING	INTEL XEON PHI RESULTS NOV'16 TOP500 LIST +45 80% NEW
	18 / 57

	AMD Rad		
	Instinct MI6	Instinct MI8	Instinct MI25
Memory Type	16GB GDDR5	4GB HBM	"High Bandwidth Cache and Controller"
Memory Bandwidth	224GB/sec	512GB/sec	?
Single Precision	5.7 TELOPS	8.2 TELOPS	12.5 TFLOPS
Half Precision (FP16)	5.7 TFLOPS	8.2 TFLOPS	25 TFLOPS
TDP	<150W	<175W	<3000
Cooling	Passive	Passive (SFF)	Passive
GPU	Polaris 10	Fiji	Vega
Manufacturing Process	GloFo 14nm	TSMC 28nm	?

Tesla Product	Tesla K40	Tesla M40	Tesla P100	Tesla V100	
GPU	GK110 (Kepler)	GM200 (Maxwell)	GP100 (Pascal)	GV100 (Volta)	
SMs	15	24	56	80	
TPCs	15	24	28	40	
FP32 Cores / SM	192	128	64	64	
FP32 Cores / GPU	2880	3072	3584	5120	
FP64 Cores / SM	64	4	32	32	
FP64 Cores / GPU	960	96	1792	2560	
Tensor Cores / SM	NA	NA	NA	8	
Tensor Cores / GPU	NA	NA	NA	640	
GPU Boost Clock	810/875 MHz	1114 MHz	1480 MHz	1455 MHz	
Peak FP32 TFLOP/s*	5.04	6.8	10.6	15	
Peak ED64 TELOP / 3	1.68	2.1	5.3	7.5	
Peak Tensor Core TFLOP/s [*]	NA	NA	NA	120	>



Today many precisions to deal with

Туре	Size	Range	$u = 2^{-t}$
half	16 bits	10 ^{±5}	$2^{-11}\approx 4.9\times 10^{-4}$
single double	32 bits 64 bits	10 ^{±38} 10 ^{±308}	$\begin{array}{l} 2^{-24} \approx 6.0 \times 10^{-8} \\ 2^{-53} \approx 1.1 \times 10^{-16} \end{array}$
quadruple	128 bits	10 ^{±4932}	$2^{-113}\approx9.6\times10^{-35}$

 Note the number range with half precision (16 bit fl.pt.)



1/30/18





- 64 bit floating point (FMA): 7.5 Tflop/s
- 32 bit floating point (FMA): 15 Tflop/s
- 16 bit floating point (FMA): 30 Tflop/s
- 16 bit floating point with Tensor core: 120 Tflop/s

Mixed Precision Matrix Math 4x4 matrices



07

VOLTA TENSOR OPERATION



Also supports FP16 accumulator mode for inferencing





Study of the Matrix Matrix multiplication kernel on Nvidia V100



Study of the Matrix Matrix multiplication kernel on Nvidia V100



dgemm achieve about 6.4 Tflop/s sgemm achieve about 14 Tflop/s hgemm achieve about 27 Tflop/s Tensor cores gemm reach about 85 Tflop/s

Matrix matrix multiplication GEMM

+β

В

С

 $= \alpha | A$

С

Study of the Matrix Matrix multiplication kernel on Nvidia V100



dgemm achieve about 6.4 Tflop/s sgemm achieve about 14 Tflop/s hgemm achieve about 27 Tflop/s Tensor cores gemm reach about 85 Tflop/s

Matrix matrix multiplication GEMM

 $C = \alpha \quad A \quad B + \beta \quad C$

Study of the rank k update used by the LU factorization algorithm on Nvidia V100



 In LU factorization need matrix multiple but operations is a rank-k update computing the Schur complement

	=		+	×	
--	---	--	---	---	--



Leveraging half precision for HPC Mixed Precision Methods

- Mixed precision, use the lowest precision required to achieve a given accuracy outcome
 - Improves runtime, reduce power consumption, lower data movement
 - Reformulate to find correction to solution, rather than solution; Δx rather than x.

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

Use Mixed Precision algorithms

>Achieve higher performance \rightarrow faster time to solution

➤Reduce power consumption reduce power consumption by decreasing the execution time → Energy Savings !!!

Reference:

A. Haidar, P. Wu, S. Tomov, J. Dongarra,

Investigating Half Precision Arithmetic to Accelerate Dense Linear System Solvers,

SC-17, ScalA17: 8th Workshop on Latest Advances in Scalable Algorithms for Large-Scale Systems, ACM, Denver, Colorado, November 12-17, 2017.

Idea: use low precision to compute the expensive flops (LU $O(n^3)$) and then iteratively refine the solution in order to achieve the FP64 arithmetic

Iterative refinement for dense systems, Ax = b, can work th L U = lu(A) x = U\(L\b) r = b - Ax	is way.	lower precision lower precision FP64 precision	<mark>O(n³)</mark> O(n²) O(n²)
<pre>WHILE r not small enough 1. find a correction "z" to adjust x that satisfy Az=r solving Az=r could be done by either:</pre>	Classical Iterative Refinement Iterative Refinement using GMRes	lower precision lower precision FP64 precision FP64 precision	O(n²) O(n²) O(n¹) O(n²)

- > 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.









Flops = $2n^3/(3 \text{ time})$ meaning twice higher is twice faster

- solving Ax = b using FP64 LU
- solving Ax = b using FP32 LU and iterative refinement to achieve FP64 accuracy
- solving Ax = b using FP16 LU and iterative refinement to achieve FP64 accuracy

Matrices generated with positive λ and arithmetic distribution of its singular values $\sigma_i = 1 - (\frac{i-1}{n-1})(1 - \frac{1}{cond})$ and where its condition number is equal to 10^2 .



Flops = $2n^3/(3 \text{ time})$ meaning twice higher is twice faster

- solving Ax = b using FP64 LU
- solving Ax = b using FP32 LU and iterative refinement to achieve FP64 accuracy
- solving Ax = b using FP16 LU and iterative refinement to achieve FP64 accuracy
- solving Ax = b using FP16 Tensor Cores LU and iterative refinement to achieve FP64 accuracy

Matrices generated with positive λ and arithmetic distribution of its singular values $\sigma_i = 1 - (\frac{i-1}{n-1})(1 - \frac{1}{cond})$ and where its condition number is equal to 10^2 .









Flops = $2n^3/(3 \text{ time})$ meaning twice higher is twice faster

- solving Ax = b using FP64 LU
- solving Ax = b using FP32 LU and iterative refinement to achieve FP64 accuracy
- solving Ax = b using FP16 LU and iterative refinement to achieve FP64 accuracy

Matrices generated with positive λ and clustered distribution of its singular values $\sigma_i = (1, \dots, 1, \frac{1}{cond})$ and where its condition number is equal to 10^2 .



Flops = $2n^3/(3 \text{ time})$ meaning twice higher is twice faster

- solving Ax = b using FP64 LU
- solving Ax = b using FP32 LU and iterative refinement to achieve FP64 accuracy
- solving Ax = b using FP16 LU and iterative refinement to achieve FP64 accuracy
- solving Ax = b using FP16 Tensor Cores LU and iterative refinement to achieve FP64 accuracy

Matrices generated with positive λ and clustered distribution of its singular values $\sigma_i = (1, \dots, 1, \frac{1}{cond})$ and where its condition number is equal to 10^2 .

Use Mixed Precision algorithms

>Achieve higher performance \rightarrow faster time to solution

Reduce power consumption reduce power consumption by decreasing the execution time -> Energy Savings !!!





Leveraging Half Precision in HPC Power awareness Mixed precision



Mixed precision techniques can provide a large gain in energy efficiency

 Power consumption of the FP64 algorithm to solve Ax=b for a matrix of size 34K, it achieve 5.5 Tflop/s and requires about 2021 joules providing about 14 Gflops/Watts.

Power consumption of the mixed precision FP32→64 algorithm to solve Ax=b for a matrix of size 34K, it achieve 10.7 Tflop/s and requires about 1041 joules providing about 30 Gflops/Watts.

Matrices generated with positive λ and arithmetic distribution of its singular values $\sigma_i = 1 - (\frac{i-1}{n-1})(1 - \frac{1}{cond})$ and where its condition number is equal to 10^2 .

Leveraging Half Precision in HPC Power awareness Mixed precision



Mixed precision techniques can provide a large gain in energy efficiency

- Power consumption of the FP64 algorithm to solve Ax=b for a matrix of size 34K, it achieve 5.5 Tflop/s and requires about 2021 joules providing about 14 Gflops/Watts.
- Power consumption of the mixed precision FP32→64 algorithm to solve Ax=b for a matrix of size 34K, it achieve 10.7 Tflop/s and requires about 1041 joules providing about 30 Gflops/Watts.
- Power consumption of the mixed precision FP16→64 algorithm to solve Ax=b for a matrix of size 34K, it achieve 16.8 Tflop/s and requires about 609 joules providing about 48 Gflops/Watts.

Matrices generated with positive λ and arithmetic distribution of its singular values $\sigma_i = 1 - (\frac{i-1}{n-1})(1 - \frac{1}{cond})$ and where its condition number is equal to 10^2 .

Leveraging Half Precision in HPC Power awareness Mixed precision



Matrices generated with positive λ and arithmetic distribution of $\sigma_i = 1 - (\frac{i-1}{n-1})(1 - \frac{1}{cond})$ and where its condition number is equal

Mixed precision techniques can provide a large gain in energy efficiency

- Power consumption of the FP64 algorithm to solve Ax=b for a matrix of size 34K, it achieve 5.5 Tflop/s and requires about 2021 joules providing about 14 Gflops/Watts.
- Power consumption of the mixed precision FP32→64 algorithm to solve Ax=b for a matrix of size 34K, it achieve 10.7 Tflop/s and requires about 1041 joules providing about 30 Gflops/Watts.
- Power consumption of the mixed precision FP16→64 algorithm to solve Ax=b for a matrix of size 34K, it achieve 16.8 Tflop/s and requires about 609 joules providing about 48 Gflops/Watts.
- Power consumption of the mixed precision FP16→64 TC algorithm using Tensor Cores to solve Ax=b for a matrix of size 34K, it achieve 24 Tflop/s and requires about 470 joules providing about 74 Gflops/Watts.



Critical Issues and Challenges at Peta & Exascale for Algorithm and Software Design

- Synchronization-reducing algorithms
 - Break Fork-Join model
- Communication-reducing algorithms
 - Use methods which have lower bound on communication
- Mixed precision methods from FP16 to FP64
 - Leverage speed of lower precision but retain the accuracy of higher precision
- Autotuning
 - Today's machines are too complicated, build "smarts" into software to adapt to the hardware
- Fault resilient algorithms
 - Implement algorithms that can recover from failures/bit flips
- Reproducibility of results
 - Today we can't guarantee this, without a penalty. We understand the issues, but some of our "colleagues" have a hard time with this.

Collaborators and Support

MAGMA team

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

PLASMA team

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

Collaborating partners

University of Tennessee, Knoxville University of California, Berkeley University of Colorado, Denver **University of Manchester**







Rutherford Appleton Laboratory



University of Manchester



The MathWorks







