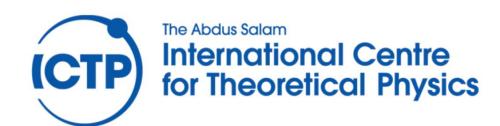
GPU Hardware & LA

Hatem Ltaief Principal Research Scientist, KAUST

Advanced School on High-Performance Computing and Applied AI for High-Resolution Regional Climate Modeling

September 8-19 2025





Nov'24 Top500 Highlights

- El Capitan becomes #1 and third ExaScale system ever
 - Frontier is #2 and Aurora #3
 - These three system are installed at different DOE laboratories
- Aurora and Frontier achieve over 10 Exaflop/s with mixed precision MxP)
- 3 new systems in TOP10 (#1 El Capitan, #5 HPC6, #10 Tuolumne)
- 8 NVIDIA Grace Hopper systems on the list
- 6 NVIDIA Grace Hopper and 3 AMD Zen-4 Genoa systems in top10 of Green500
- HPC systems are used longer and replaced less often
 - Technological limits lead to strong concentration at the top
- TOP500 shows further reduced growth-rates since 2017
 - End of Moore's Law -Very unlikely to achieve 10 Exascale(HPL) by 2030
 - However: New Workloads (AI) require new benchmarks!
 - Chinese systems are missing in the equation







Welcome to El Capitan, the new crown!



Welcome to El Capitan, the new crown!

HPE has delivered a highly capable AMD GPU-accelerated system





- System specifications:
 - Peak 2.7929 DP exaflops
 - Per node peak of 250.8 DP teraflops
 - ~42.3 FP8 exaflops
 - Peak power 34.8 MW
 - AMD MI300A APU 3D chiplet design w/AMD CDNA 3 GPU, "Zen 4" CPU, cache memory, HBM3
 - Slingshot interconnect

- HPE has provided several critical innovations
 - HPE and LLNL have worked with ORNL jointly on non-recurring engineering (NRE) activities
 - MI300A, world's first data center APU directly addresses multiple challenges
 - Uses TOSS software stack, enhanced with HPE software
 - El Capitan includes an innovative near node local storage solution: the "Rabbits"

Late binding of the processor solution has ensured El Capitan provides the best possible value









Under the hood...

AMD INSTINCT™ MI300A: The world's first data center APU



- 4th Gen AMD Infinity Architecture:
 AMD CDNA™ 3 and EPYC™ CPU "Zen 4" together
 - CPU cores and GPU compute units share a unified on-package pool of memory
- Groundbreaking 3D packaging
 - CPU | GPU | Cache | HBM
 - 24 Zen4 cores, 146B transistors, 128GB HBM3
- Designed for leadership memory bandwidth and application latency
- APU architecture designed for power savings
 - compared to discrete implementation



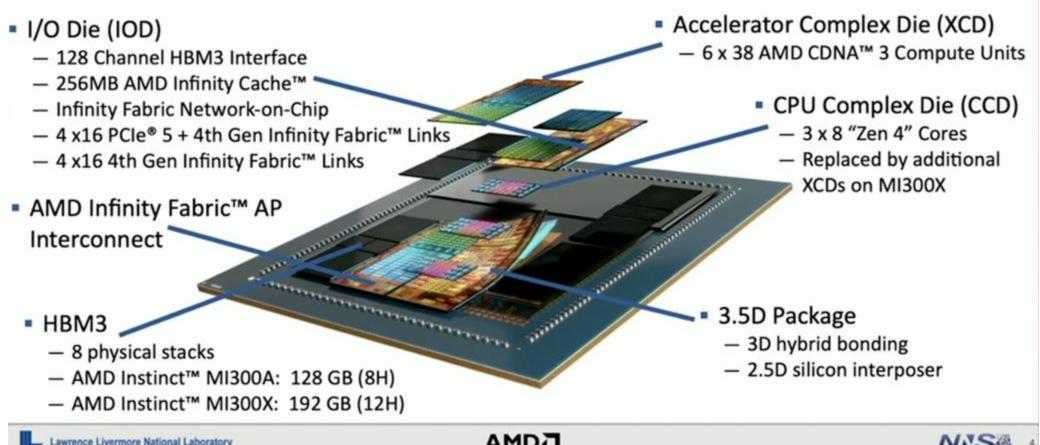




The Beast

AMD Instinct™ MI300 Modular Chiplet Package





Nvidia H100 "Hopper" SXM5 specs

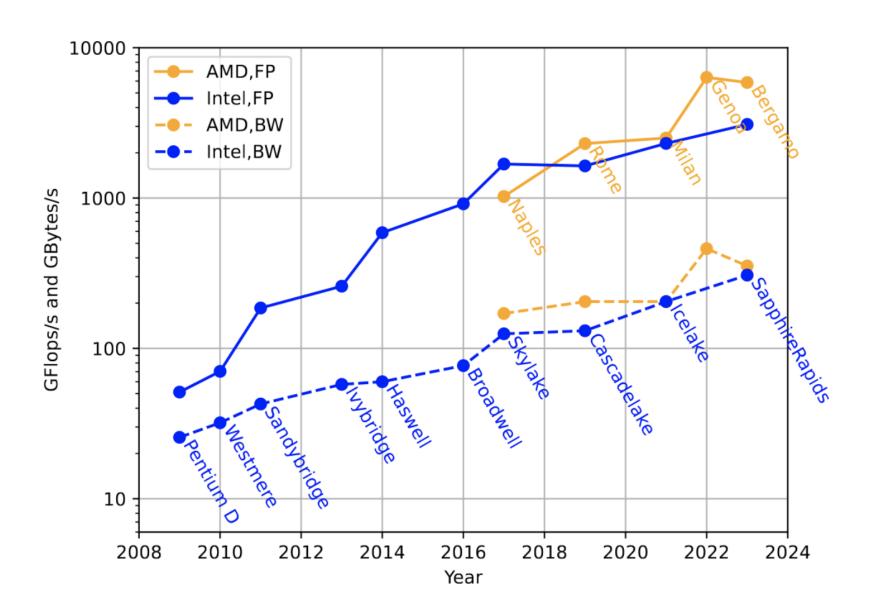
Architecture

- 80 B Transistors
- ~ 1.8 GHz clock speed
- ~ 144 "SM" units
 - 128 SP "cores" each (FMA)
 - 64 DP "cores" each (FMA)
 - 4 "Tensor Cores" each
 - 2:1 SP:DP performance
- ~ 34 TFlop/s DP peak (FP64)
- 50 MiB L2 Cache
- 80 GB HBM3
- MemBW ~ 3300 GB/s (theoretical)
- MemBW ~ 3000 GB/s (measured)





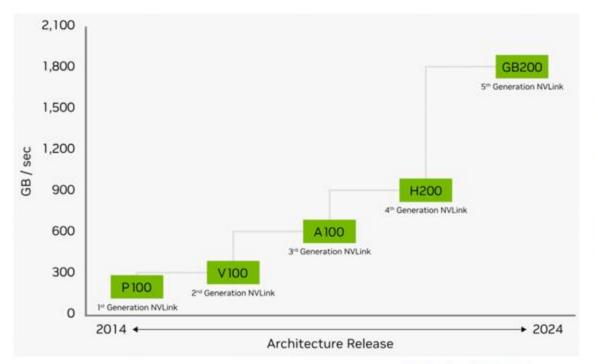
But we have a major bottleneck



8

But we have a major bottleneck

- High-performance interconnect for emerging dense GPU systems
 - Allows Load-Store operations between all GPUs



	Second Generation	Third Generation	Fourth Generation	Fifth Generation		
NVLink bandwidth per GPU	300GB/s	600GB/s	900GB/s	1,800GB/s		
Maximum Number of Links per GPU	6	12	Generation Generation OGB/s 900GB/s 1,800GB/s 12 18 18 VIDIA NVIDIA NVIDIA NVIDIA Blackwell			
Supported NVIDIA Architectures	NVIDIA Volta™ architecture	NVIDIA Ampere architecture	Hopper™	Blackwell		

NVLink Performance Trends

Courtesy: NVIDIA

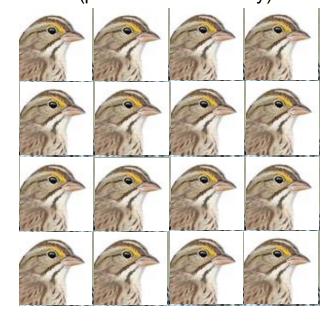
Specialization: Natures way of Extracting More Performance in Resource Limited Environment

Powerful General Purpose



Xeon, Power

Many Lighter Weight (post-Dennard scarcity)



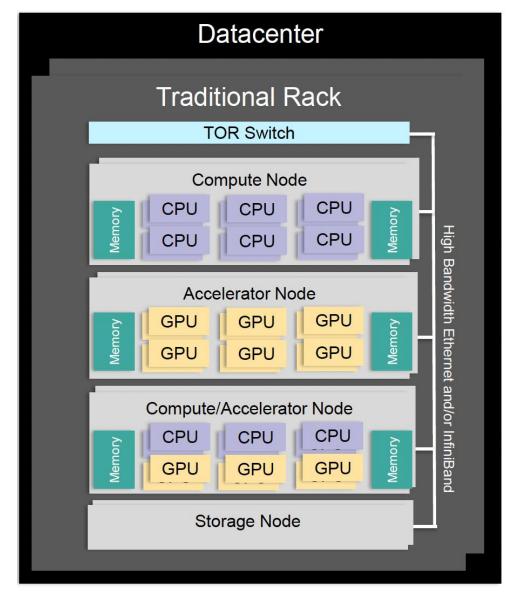
KNL, AMD, Cavium/Marvell, GPU

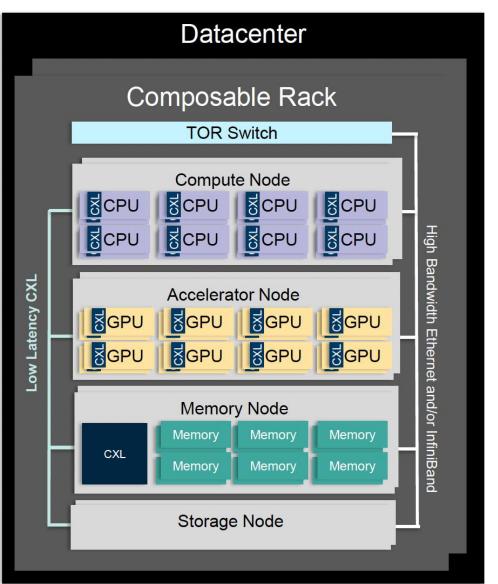
Many Different Specialized (Post-Moore Scarcity)



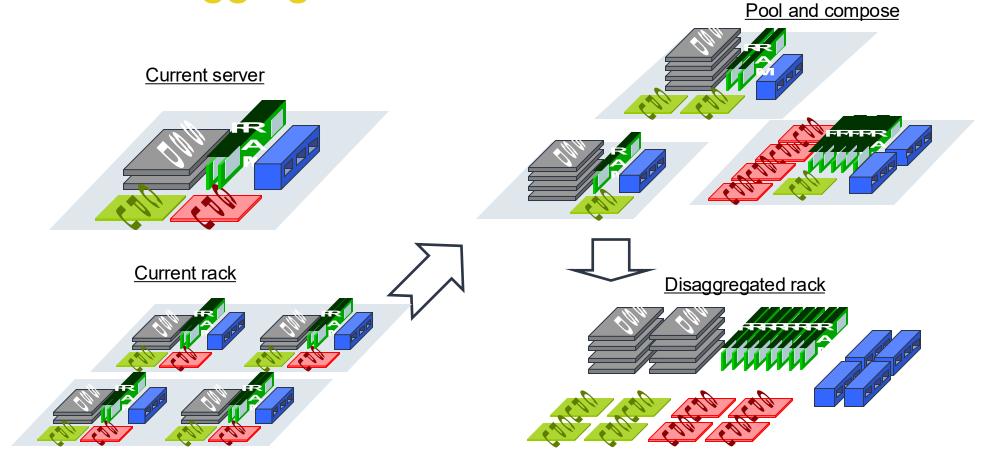
Apple, Google, Amazon Microsoft

You may then want to compose architectures!



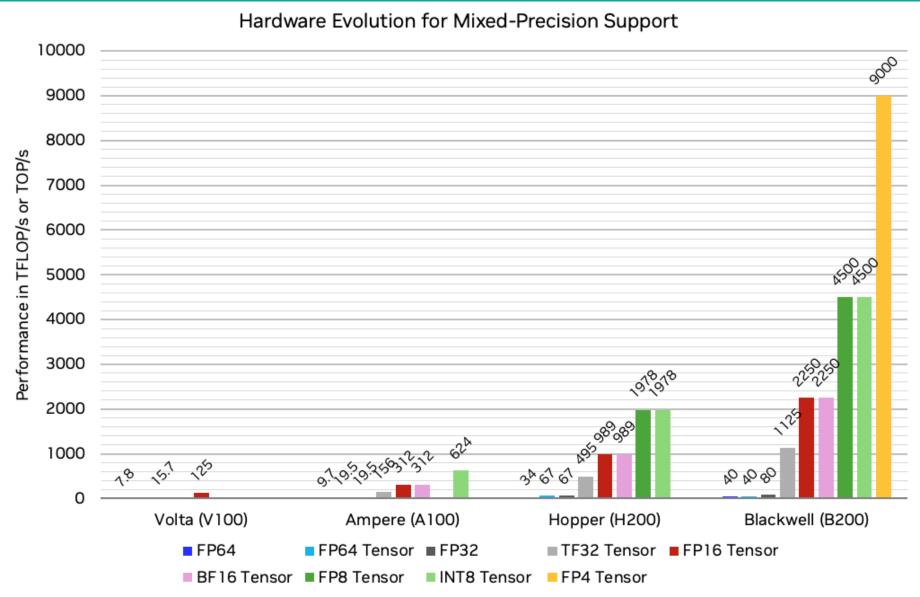


Or even disaggregate hardware resources!

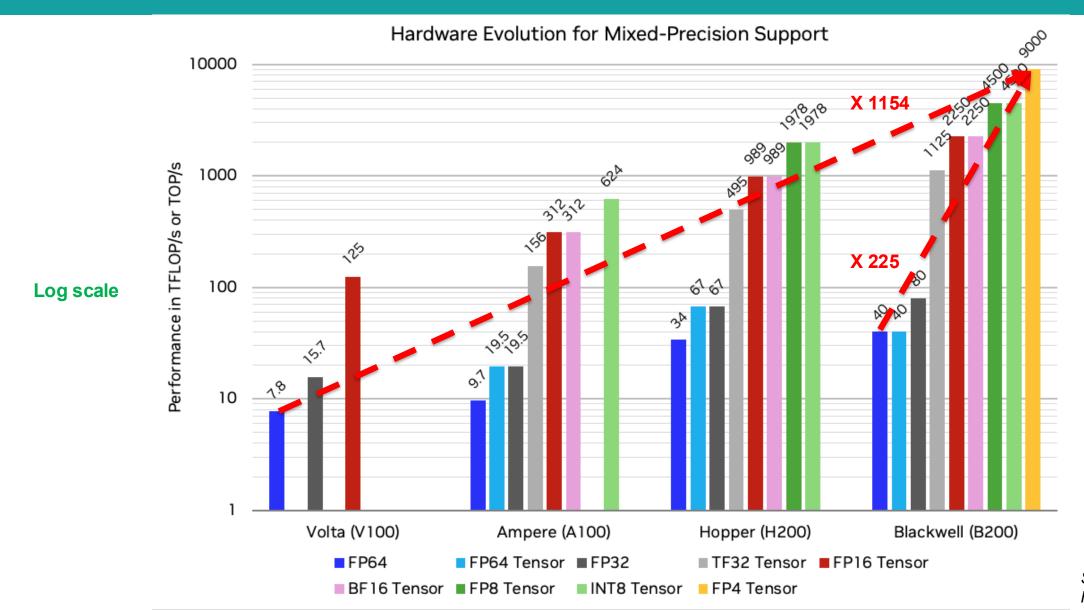


Current disaggregation solutions use Interconnect bandwidth (1 – 10 GB/s)
But this is significantly inferior to RAM bandwidth (100 GB/s – 1 TB/s)

Peak performance of four generations of NVIDIA GPUs

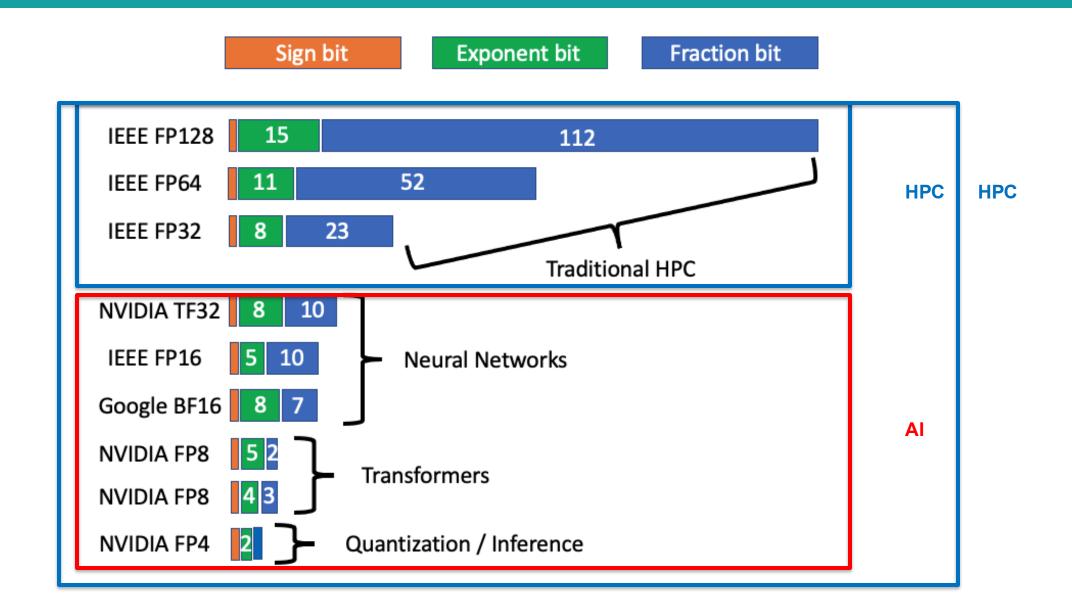


Peak performance of four generations of NVIDIA GPUs



Slide courtesy H. Bayraktar, NVIDIA

Feeling like a kid in a candy store



Motivations for Mixed Precisions (2)

IBM Cell Broadband Engine	Apple ARM Cortex-A9	NVIDIA Kepler K10, K20, K40, K80	NVIDIA Volta/Turing	NVIDIA Volta/Turing
14x	7x	3x	2x	16x
32 bits / 64 bits	32 bits / 64 bits	32 bits / 64 bits	32 bits / 64 bits	16 bits / 64 bits

Peak Performance in TF/s	V100 NVLink	A100 NVLink	H100 SXM	B200		
FP64	7.5	9.7	34	90		
FP32		19.5	67	180		
FP64 Tensor Core	15	19.5	67	40		
FP/TF32 Tensor Core	8x	156	495 30 x	1125		
FP16 Tensor Core	120	312	990	2250 225 x		
FP8/INT8 Tensor Core	=	624	1980	4500		
FP4 Tensor Core	-	-	-	9000		

The Landscape of Mixed Precision Hardware

•Mixed-Precision Startups and their hardware

- GraphCore
 - Colossus
- Habana
 - Labs Gaudi
- Cerebras
 - Wafer Scale Chip
- Blaize
 - Graph Streaming Processor
- Groq
 - Tensor Streaming Processor
- SambaNova
 - Cardinal
- Tenstorrent
 - Grayskull

NVIDIA mixed-precision hardware

- Pascal
 - FP16 units only
- Volta
 - Tensor Cores and FP16
- Turing
 - Tensor Cores and FP16
- Ampere
 - Tensor Cores for FP16 and FP64
- Hopper
 - Double-, single-, half-, and quarter-precision formats in scalar and tensor units

HPC is not the driver for hardware technology, AI/ML are!

Al and ML have been around for a long time as research efforts

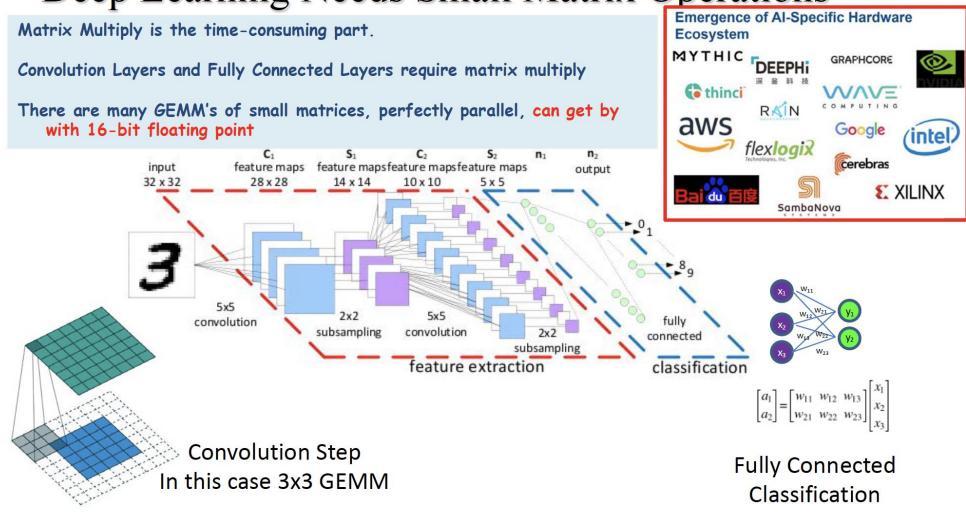
- ❖ Why now?
- Deluge of data (IoTs, Internet)
- Flops are free (hardware technology scaling)
- Development of new Al/ML algorithms (asynchronous, 2nd order methods, Federated Learning)
- Market! Market! Oh, did I say Market?!

Intelligence

ANNS, CNNS

Batching (not bashing!) Al workloads

Deep Learning Needs Small Matrix Operations



Motivations for Mixed Precisions (1)

- Less communication: reduce memory and network traffic
- Reduce memory footprint
- Increase throughput: more flops per seconds
- Reduce time-to-solution
- Reduce energy consumption
- More science per joule!

What if HPC algorithms could exploit these AI hw features?

- Use a mathematical technique
- Get an approximation in lower precision then use something like Newton's method to enhance accuracy
- Transfer less bytes, data transfer is expensive
 - Store data in primary storage in full precision
 - Transfer the data in short precision
 - Once in registers, compute in full precision
- Apply algebraic compression
- Combine all above

The HPL-MxP Benchmark

1. Generate random linear system Ax=b

- 2. Represent the matrix A in low precision (16-bit floating point)
- 3. Factor A in lower precision into LU by Gaussian elimination



- 4. Compute approximate solution with LU factors in low precision
- 5. Perform up to 50 iterations of refinement, e.g., GMRES to get accuracy up to 64-bit floating point
 - a. Use LU factors for preconditioning

Iterative refinement for dense systems, $Ax = b$, can we	ork this way.	
L U = lu(A)	Lower precision	$O(n^3)$
x = U\(L\b)	Lower precision	O(n ²)
GMRes preconditioned by the LU to solve Ax=b	FP64 precision	O(n ²)

6. Validate the answer is correct: scaled residual small $\frac{||Ax - b||}{||A||||x|| + ||b||} \times \frac{1}{n\epsilon} \le O(10)$

$$\frac{||Ax-b||}{||A||||x||+||b||} \times \frac{1}{n\epsilon} \le O(10)$$

7. Compute performance rate as $\frac{2}{3} \times \frac{n^3}{\text{time}}$

Algorithms Matter, Perhaps More Than Hardware! (1)

HPC algorithmic efficiency tracked by Poisson solvers

Consider a Poisson solve in a 3D $n \times n \times n$ box; natural ordering gives bandwidth of n^2

Year	Method	Reference	Storage	Flops
1947	GE (banded)	Von Neumann & Goldstine	<i>n</i> ⁵	n^7
1950	Optimal SOR	Young	n^3	$n^4 \log n$
1971/77	MILU-CG	Reid/Van der Vorst	n^3	$n^{3.5}\log n$
1984	Full MG	Brandt	n^3	n^3

If n = 64, this implies an overall reduction in flops of ~16 million *

^{*}Six months is reduced to 1 second (recall: 3.154 x 10⁷ seconds per year)

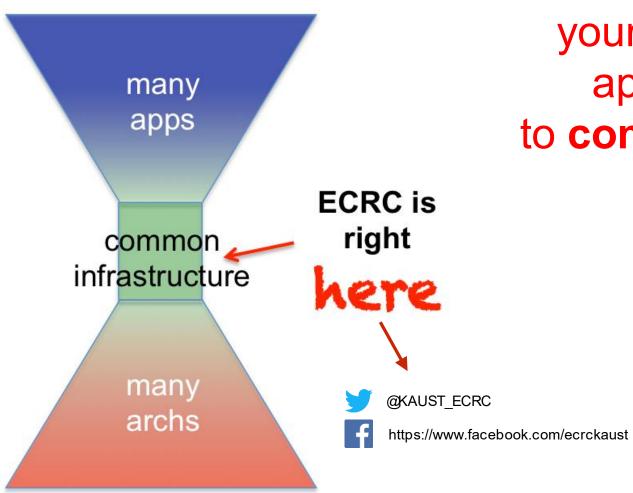
Algorithms Matter, Perhaps More Than Hardware! (2)

Algorithms improve exponents; Moore only adjusts the base

- To scale to extremes, one must start with algorithms with optimal asymptotic complexity, $O(N \log^p N)$, p = 0, 1, 2
- These are typically (not exclusively) recursively hierarchical
- Some such algorithms through the decades:

```
    Fast Fourier Transform (1960's): N^2 \to N \log N
    Multigrid (1970's): N^{4/3} \log N \to N
    Fast Multipole (1980's): N^2 \to N
    Sparse Grids (1990's): N^d \to N (\log N)^{d-1}
    \mathcal{H} matrices (2000's): N^3 \to k^2 N (\log N)^2
    MLMC (2000's): N^{3/2} \to N (\log N)^2
    Randomized matrix algorithms (2010's): N^3 \to N^2 \log k
    ??? (2020's): ??? → ???
```

Revisiting the Hourglass



Shifting
your I/O-bound
applications
to compute-bound

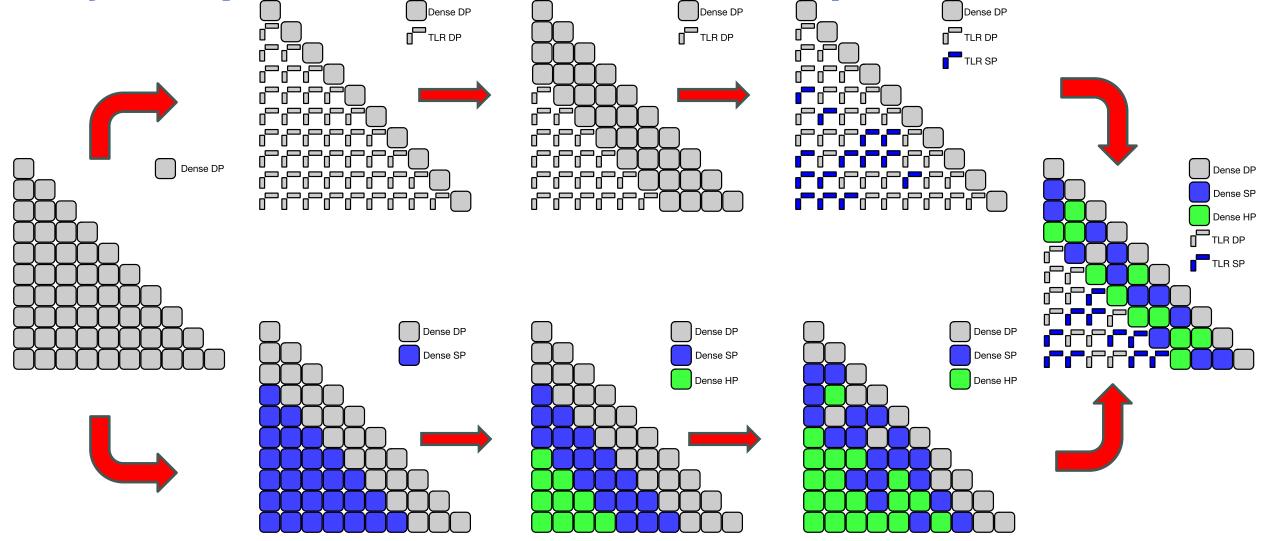
Reshaping Linear Algebra for Massively Parallel Architectures

- Enhance user-productivity using layers of abstraction
- Expose parallelism using fine-grained computations
- Achieve scalability using asynchronous executions
- Exploit data sparsity using low-rank approximations
- Maintain code portability using standard basic blocks

Are you willing to redesign your algorithm?

One possible productive solution: Matricization

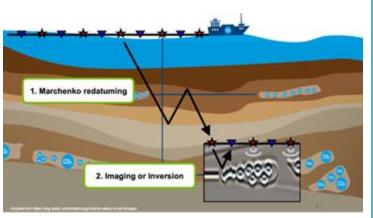
Computational efficiency through tuned approximation: A journey with tile low-rank and mixed precisions



- 1. Don't oversolve: maintain just enough accuracy for the application purpose
- 2. Economize on storage: no extra copies of the original matrix

Example of Accelerated Applications

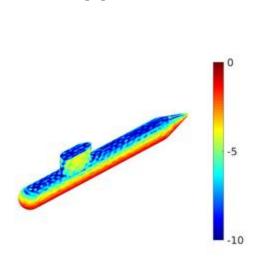
Seismic Imaging



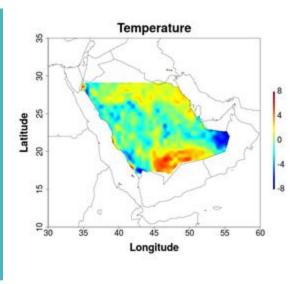
Computational Astronomy



Radar Applications



Climate/Weather Prediction



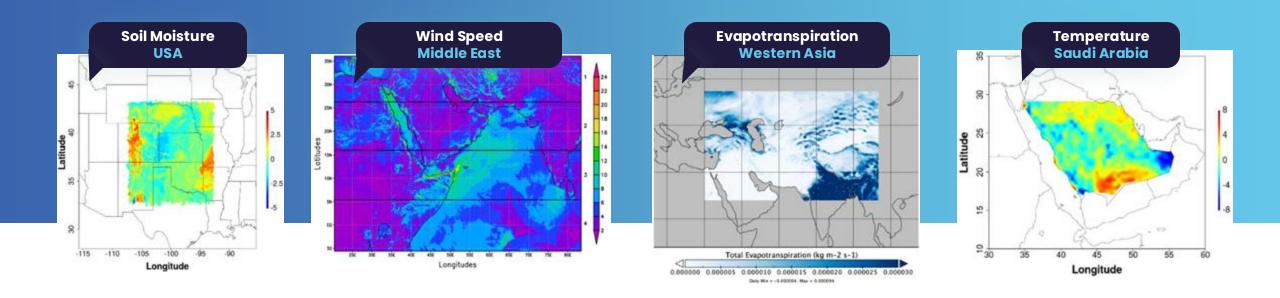
Memory: up to 63X smaller **Analytics**: up to 150X faster

Memory: up to 4X smaller **Analytics**: up to 100X faster

Memory: up to 4X smaller **Analytics**: up to 30X faster

Memory: up to 50X smaller **Analytics**: up to 12X faster

Compress to Impress



Memory
up to 50 X smaller

Analytics
up to 10 X faster

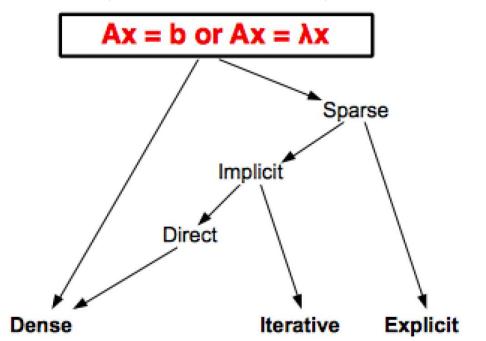
Storage
From \$750M to \$15M

Compute
From \$400M to \$40M

Linear Algebra 101

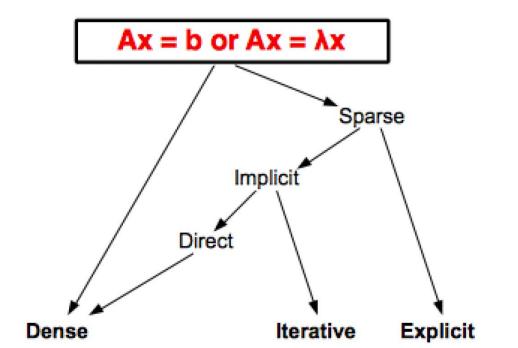
Critical component for many scientific applications:

- cardio-magnetism, wave guide propagation, image processing, quantum chemistry/physics, atomic structure calculations, electromechanics, geophysics/seismology, nonlinear mechanics, computational astronomy, computational fluid dynamics, geospatial statistics, climate/weather prediction, smart health, smart agriculture, smart satellite, etc...



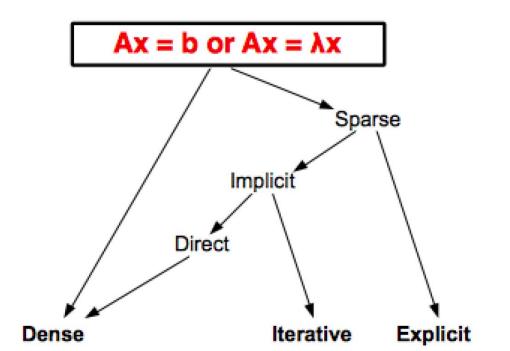
Linear Algebra 101

- Dense solvers: systems of linear equations, eigenvalue / singular value problems
- Sparse iterative solvers: sparse matrix-vector multiplication (SpMV)
- Sparse explicit solvers: stencil computations



Linear Algebra 101

- Dense solvers: systems of linear equations, eigenvalue / singular value problems
- Sparse iterative solvers: sparse matrix-vector multiplication (SpMV)
- Sparse explicit solvers: stencil computations



The Two Distinct Optimization Paths

- By using the existing hardware features (sometimes comes for free)
- By redesigning the numerical methods and optimizing the actual implementation (requires effort and time)

Separation of concerns:

- Abstracting the hardware complexity: dynamic runtime systems
- Novel Algorithmic challenges: numerical accuracy/stability

Why software libraries are so important?

- Basic blocks for large applications
- Highly-tuned by vendors if the software becomes mainstream
- Provide abstraction
- Impacting the scientific community

Survey on LA software

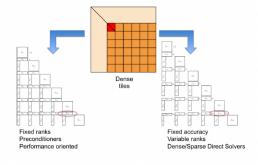
-															
Freely Available Software	for Linear Alg	gebra (Au	gust 20	021)											
Here is a list of freely avail web for solving problems i corrections.															
Send corrections and upday	gtes to Dalal.														
An old survey of Iterative I	Linear System S	olver Pack	tages c	an be found	at:										
http://www.netlib.org/utk/p	apers/iterative-s	survey/													
Γhanks,															
lack Dongarra and															
Dalal Sukkari															
															_
SUPPORT ROUTINES	License	Support	_	Туре	Language		Mode		Dense	Sparse			Last release date	Updated	Nev
		-	Real			Shared	Accel.	Dist	-					222	⊢
<u>Armadillo</u>	Mozilla	yes	X	X	C++	X	_		X	X			2018-06-26	X	⊢
Armas	LGPL	yes	X		C	X	_		X				2015-12-22		⊢
ATLAS	BSD like	yes	X	X	F77/F95/C	X			X				2018-10-05	X	⊢
BLAS	BSD	yes	X	X	F77/F95/C	X			X				2017-11-01		⊢
BLIS	New BSD	yes	X	X	F77/F95/C	X			X				2021-03-22	X	⊢
Blitz++	LGPLv3+	yes	X	X	C++	X			X				2019-08-01	X	⊢
BML	BSD	yes	X	X	F77/F95/C	X	X	X	X	X			2020-09-10		X
clBLAS	Apache	yes	X	X	C/C++	X	0		X				2017-01-18	X	⊢
GHOST	BSD	yes	X	X	C/C++	X	C/X	M	_	X			2020-09-03		X
GraphBLAS	Apache2	yes	X	X	C	X			X	X			2021-01-19	X	⊢
KBLAS	BSD	yes	X	X	C/C++	X	C	200	X				2017-11-15	X	_
KSVD	BSD	yes	X	1	C	X		M	SVD				2018-11-08		X
librsb	LGPLv3	yes	X	X	F77/F95/C/C++	X	_		⊢	X			2017-06-04	X	⊢
LINALG *	?	?							_				n/a		⊢
MR3-SMP	New BSD	yes	X	X	F77/F95/C	X			X				2013-06-24		⊢
MTL	Boost	yes	X	X	C++	X			X				2014-05-22		⊢
NEWMAT	Own	yes	X		C++	X			X				2008-11-20		⊢
NIST Sparse BLAS	PD	yes	X	X	C/C++	X			-	X			2009-04-27		⊢
<u>OpenBLAS</u>	BSD	yes	X	X	F77/F95/C	X			X				2020-12-12	X	⊢
PMRRR	New BSD	yes	X	X	F77/F95/C	X			X				2014-02-23		⊢
pOSKI	BSD	yes	X	X	F77/F95/C/C++	X			-	X			2012-04-27		⊢
PSBLAS	BSD	yes	X	X	F90	X		M		X			2020-06-30	X	⊢
QDWH	BSD	yes	X		C	X		M	X				2017-02-27		X
Scotch	CeCILL-C	yes			F77/F95/C	X		M	\vdash	X			2020-09-03		⊢
SparseLib++	PD	yes	X	X	C/C++	X			\vdash	X			2008-10-30		╙
Trilinos/Epetra	BSD	yes	X		F77/F95/C/C++	X		M	X				2015-05-07		

https://docs.google.com/spreadsheets/d/11ESR3uucNvVKEolcalP9gR7ApaOEILwmE5sAS-VRMOM/edit?gid=90156307#gid=90156307

A Look back to software evolution

Software infrastructure and algorithmic design follow hw evolution in time:

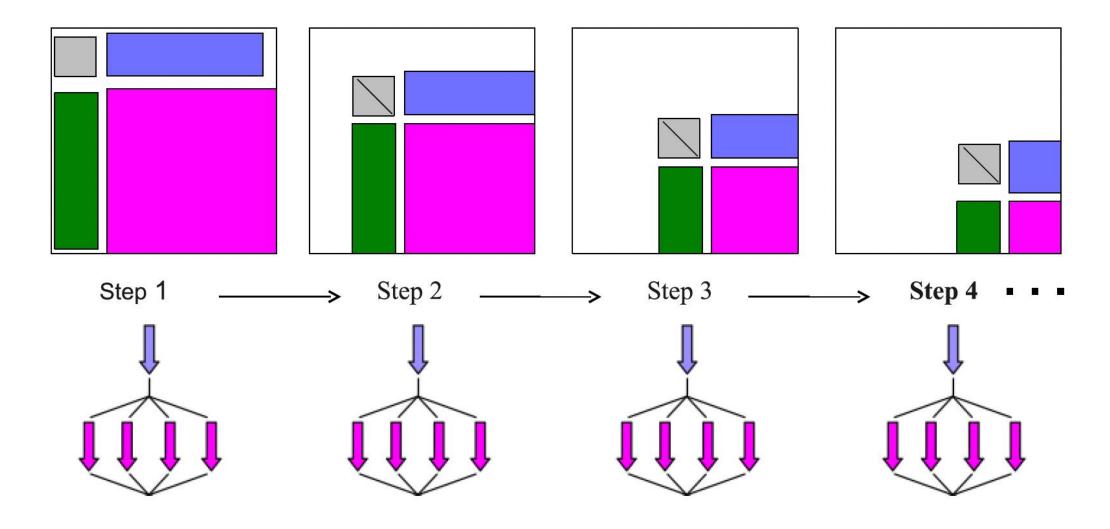
- 70's LINPACK, vector operations: Level-1 BLAS operation
- 80's LAPACK, block, cache-friendly: Level-3 BLAS operation
- 90's ScaLAPACK, distributed memory: PBLAS Message passing
- 00's:
 - PLASMA, MAGMA:
 x86 multicore + GPU, DAG scheduler
- 10's:
 - SLATE: Standard (MPI + OpenMP), Applications
- 20's:
 - HiCMA, numerical approximations: algebraic compression, mixed precisions



Facts on LAPACK / ScaLAPACK

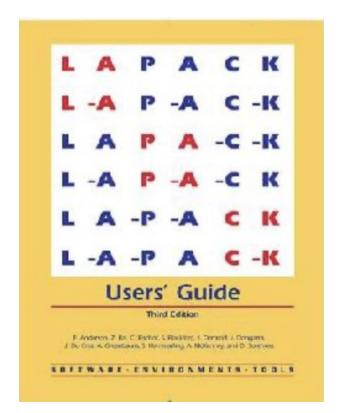
- Open-source packages (downloaded more than 60 million times)
- Large community contributors
- Integrated in open-source libraries (PETSc, SLEPc, MUMPS, CPMD, CP2K ...)
- Integrated in vendor numerical software (Mathworks, Intel, Cray, IBM, HP, Fujitsu ...)
- Critical library for many scientific application

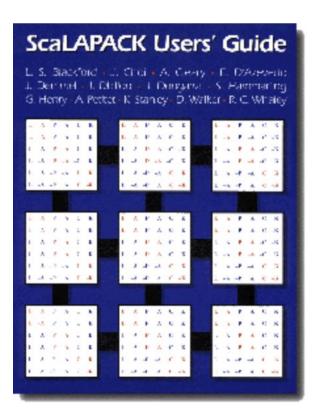
Block Algorithms: Fork-Join Paradigm



The Three Siblings

- BLAS: kernels for dense linear algebra
- LAPACK: sequential dense linear algebra
- ScaLAPACK: parallel distributed dense linear algebra





BLAS: Basic Linear Algebra Subroutines (BLAS)

• Level 1 BLAS Consider AXPY (y = alpha.x + y): 2n flops on 3n read/write operations Computational intensity = (2n)/(3n) = 2/3 Too low to run near peak speed (read/write dominates).

• Level 2 BLAS Standard library of 25 operations (mostly) on matrix/vector pairs "GEMV": $y = alpha \cdot A \cdot x + beta \cdot x$, "GER": $A = A + alpha \cdot x \cdot y^T$ Up to 4 versions of each (S/D/C/Z), 66 routines Why BLAS 2? They do $O(n^2)$ ops on $O(n^2)$ data So computational intensity still just $(2n^2)/(n^2) = 2$ OK for vector machines, but not for machine with cache memory.

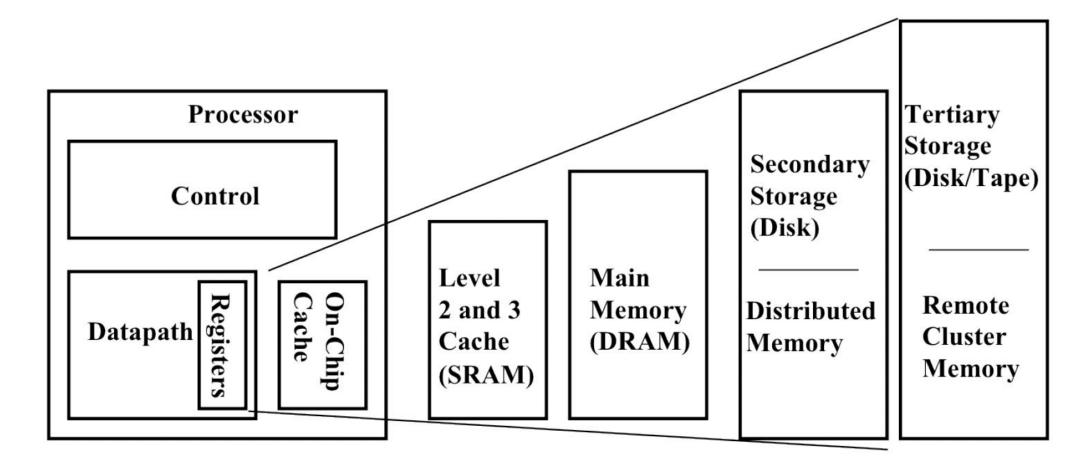
BLAS: Basic Linear Algebra Subroutines (BLAS)

• Level 3 BLAS Standard library of 9 operations (mostly) on matrix/matrix pairs "GEMM": $C = alpha \cdot A \cdot B + beta \cdot C$, $C = alpha \cdot A \cdot AT + beta \cdot C$ Up to 4 versions of each (S/D/C/Z), 30 routines Why BLAS 3? They do $O(n^3)$ ops on $O(n^2)$ data So computational intensity $(2n^3)/(4n^2) = n/2 - big$ at last!

Good for machines with caches and many memory hierarchy levels

Data Locality

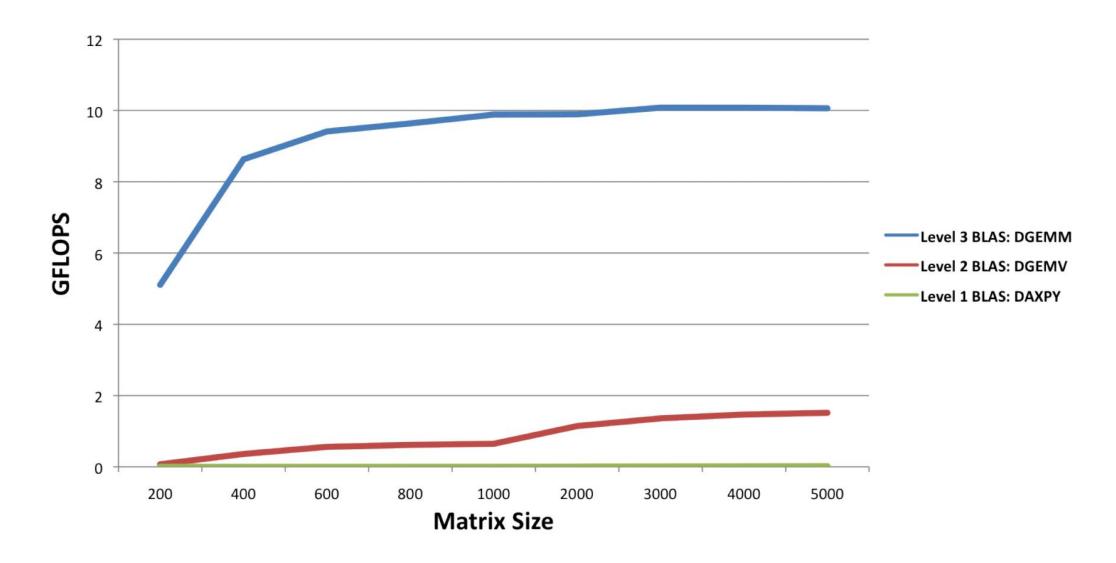
Can only do arithmetic on data at the top of the hierarchy



Why Higher Level BLAS?

BLAS	Memory Refs	Flops	Flops/ Memory Refs	
Level 1 y=y+αx	3n	2n	2/3	Registers L 1 Cache
Level 2 y=y+Ax	n ²	2n ²	2	L 2 Cache Local Memory
Level 3 C=C+AB	4n ²	2n ³	n/2	Remote Memory Secondary Memory

BLAS Performance



Linear Algebra Package (LAPACK)

- Algorithms we can turn into (nearly) 100% BLAS 3 Linear Systems: solve A.x = b for x Least Squares: choose x to minimize $||Ax b||_2$
- Algorithms that are only 50% BLAS 3 (so fa|r) "Eigenproblems": Find λ and x where $Ax = \lambda x$ Singular Value Decomposition (SVD): $(A^T.A).x = \sigma^2.x$
- Generalized problems (eg $A.x = \lambda B.x$)
- Error bounds for everything
- Lots of variants depending on A's structure (banded, $A = A^T$, etc)

Linear Algebra Package (LAPACK)

- LAPACK is in FORTRAN Column Major
- LAPACK is SEQUENTIAL
- LAPACK is a REFERENCE implementation

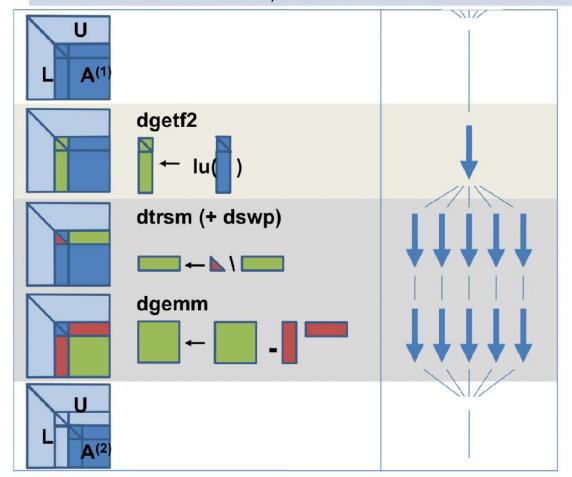
Fork-Join Paradigm

Parallelization of LU and QR.

Parallelize the update:

- Easy and done in any reasonable software.
- This is the 2/3n³ term in the FLOPs count.
- Can be done efficiently with LAPACK+multithreaded BLAS



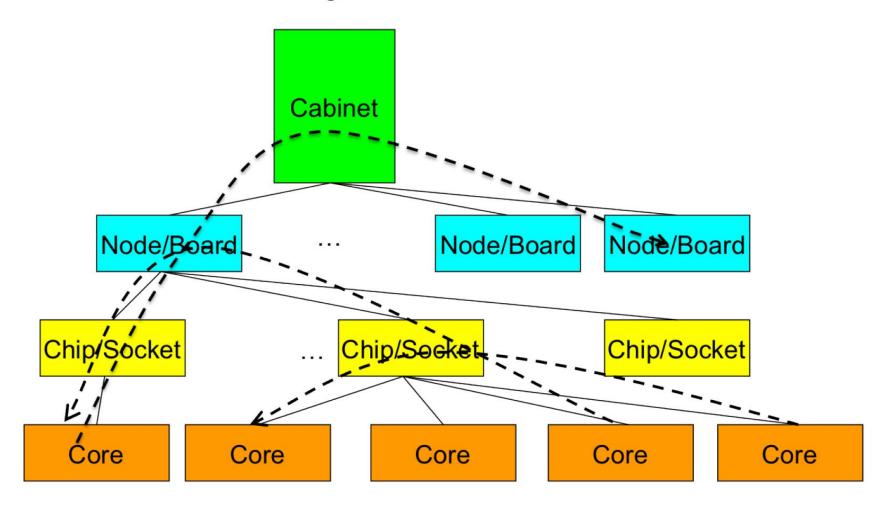


Scalable Linear Algebra Package (ScaLAPACK)

- Library of software dealing with dense & banded routines
- Distributed Memory MPI
- MIMD Computers and Networks of Workstations
- Clusters of SMPs
- Relies on LAPACK / BLAS and BLACS / MPI
- Includes PBLAS (Parallel BLAS)
- ScaLAPACK is in FORTRAN and C
- ScaLAPACK is for PARALLEL DISTRIBUTED
- ScaLAPACK is a REFERENCE implementation

Example of typical parallel machine

- Shared memory within a node
- Distributed within a single cabinet

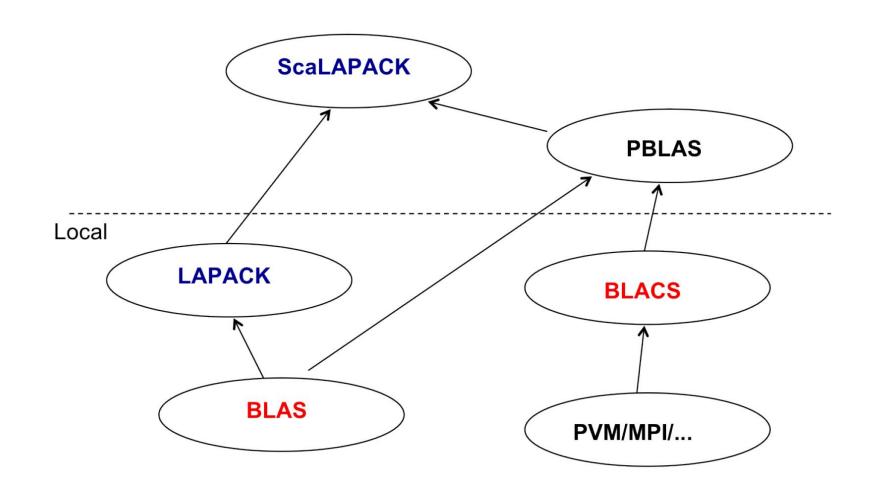


ScaLAPACK's Overall Structure

- Object based Array descriptor
 Contains information required to establish mapping between a global array entry and its corresponding process and memory location.

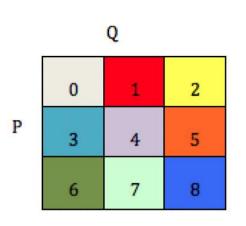
 Provides a flexible framework to easily specify additional data distributions or matrix types.
- Currently supports dense, banded matrix structure
- Using the concept of context

Putting them all together...



Distributed Data Layout

2D Block-Cyclic Data Distribution:



Processes Grid

A ₁₁	A ₁₂	A ₁₃	A ₁₄	A ₁₅
A ₂₁	A ₂₂	A ₂₃	A ₂₄	A ₂₅
A ₃₁	A ₃₂	A ₃₃	A ₃₄	A ₃₅
A41	A ₄₂	A ₄₃	A44	A ₄₅
A ₅₁	A ₅₂	A ₅₃	A ₅₄	A ₅₅

Logical View (Matrix)

A ₁₁	A ₁₄	A ₁₂	A ₁₅	A ₁₃
A ₄₁	A44	A ₄₂	A45	A ₄₃
A ₂₁	A ₂₄	A ₂₂	A ₂₅	A ₂₃
A ₅₁	A ₅₄	A ₅₂	A ₅₅	A ₅₃
A ₃₁	A ₃₄	A ₃₂	A ₃₅	A ₃₃

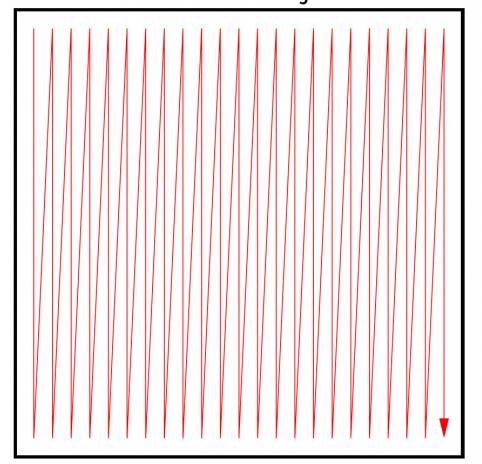
Local View (CPUs)

(R)Evolution

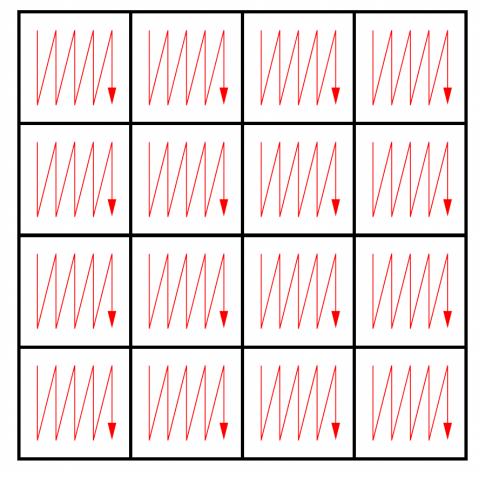
Software/Algorithms follow hardware evolution in time				
LINPACK (70's) (Vector operations)		Rely on - Level-1 BLAS operations		
LAPACK (80's) (Blocking, cache friendly)		Rely on - Level-3 BLAS operations		
ScaLAPACK (90's) (Distributed Memory)		Rely on - PBLAS Mess Passing		
PLASMA (00's) New Algorithms (many-core friendly)		Rely on - a DAG/scheduler - block data layout - some extra kernels		

Tile Data Layout Format

LAPACK: column-major format



PLASMA: tile format



PLASMA: Tile Algorithms

- Parallelism is brought to the fore
- May require the redesign of linear algebra algorithms
- Tile data layout translation
- Remove unnecessary synchronization points between Panel-Update sequences
- DAG execution where nodes represent tasks and edges define dependencies between them
- Dynamic runtime system environment QUARK + OpenMP

Example: Least-square solver

```
FOR k = 0..TILES-1

A[k][k], T[k][k] \leftarrow DGRQRT(A[k][k])

FOR m = k+1..TILES-1

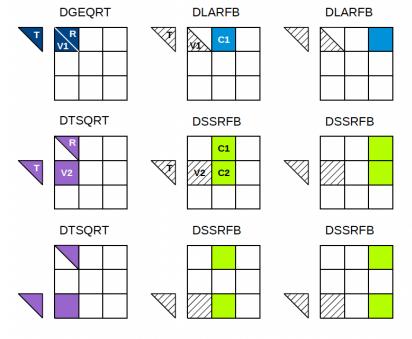
A[k][k], A[m][k], T[m][k] \leftarrow DTSQRT(A[k][k], A[m][k], T[m][k])

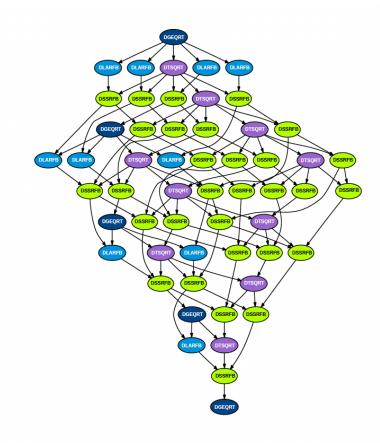
FOR n = k+1..TILES-1

A[k][n] \leftarrow DLARFB(A[k][k], T[k][k], A[k][n])

FOR m = k+1..TILES-1

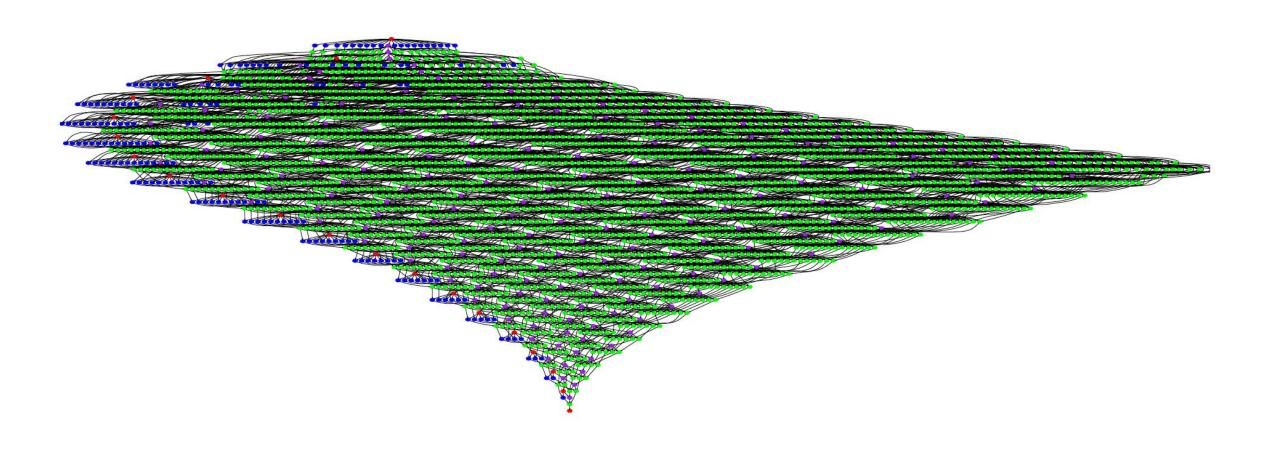
A[k][n], A[m][n] \leftarrow DSSRFB(A[m][k], T[m][k], A[k][n], A[m][n])
```





- Fine granularity;
- Tile algorithms;
- Productivity
- DAG scheduler framework.

DAG can be Large and Complex

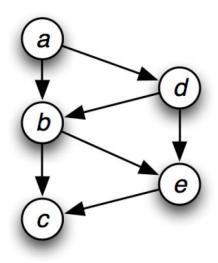


Dynamic Runtime System

- Conceptually similar to out-of-order processor scheduling because it has:
 - Dynamic runtime DAG scheduler
 - Out-of-order execution flow of fine-grained tasks
 - Task scheduling as soon as dependencies are satisfied
 - Producer-Consumer

DataFlow Programming

- Five decades **OLD** concept
- Programming paradigm that models a program as a directed graph of the data flowing between operations (cf. Wikipedia)
- Think "how things connect" rather than "how things happen"
- Assembly line
- Inherently parallel





SLATE-CPU Vs SLATE-GPU

