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Parallel Processing for Scientific Computing
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Five Important Concepts to Consider When Using Computing High Performance Systems at Scale

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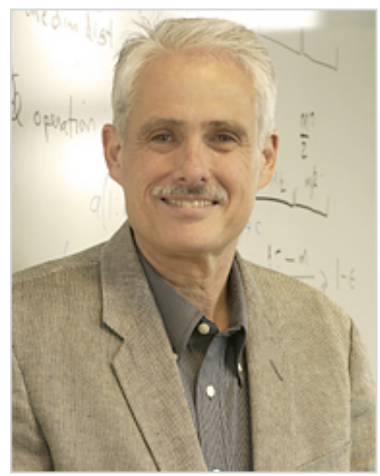
First, Thanks to My Mentors

Brian Smith

Cleve Moler

Jim Wilkinson

Gene Golub

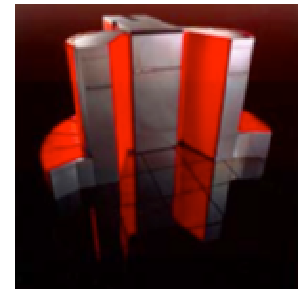


Ken Kennedy

And, Thanks to Many Colleagues

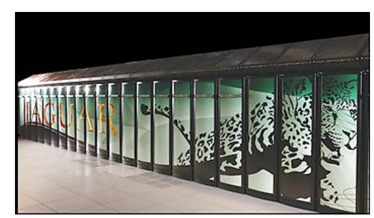
Looking at the Gordon Bell Prize

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



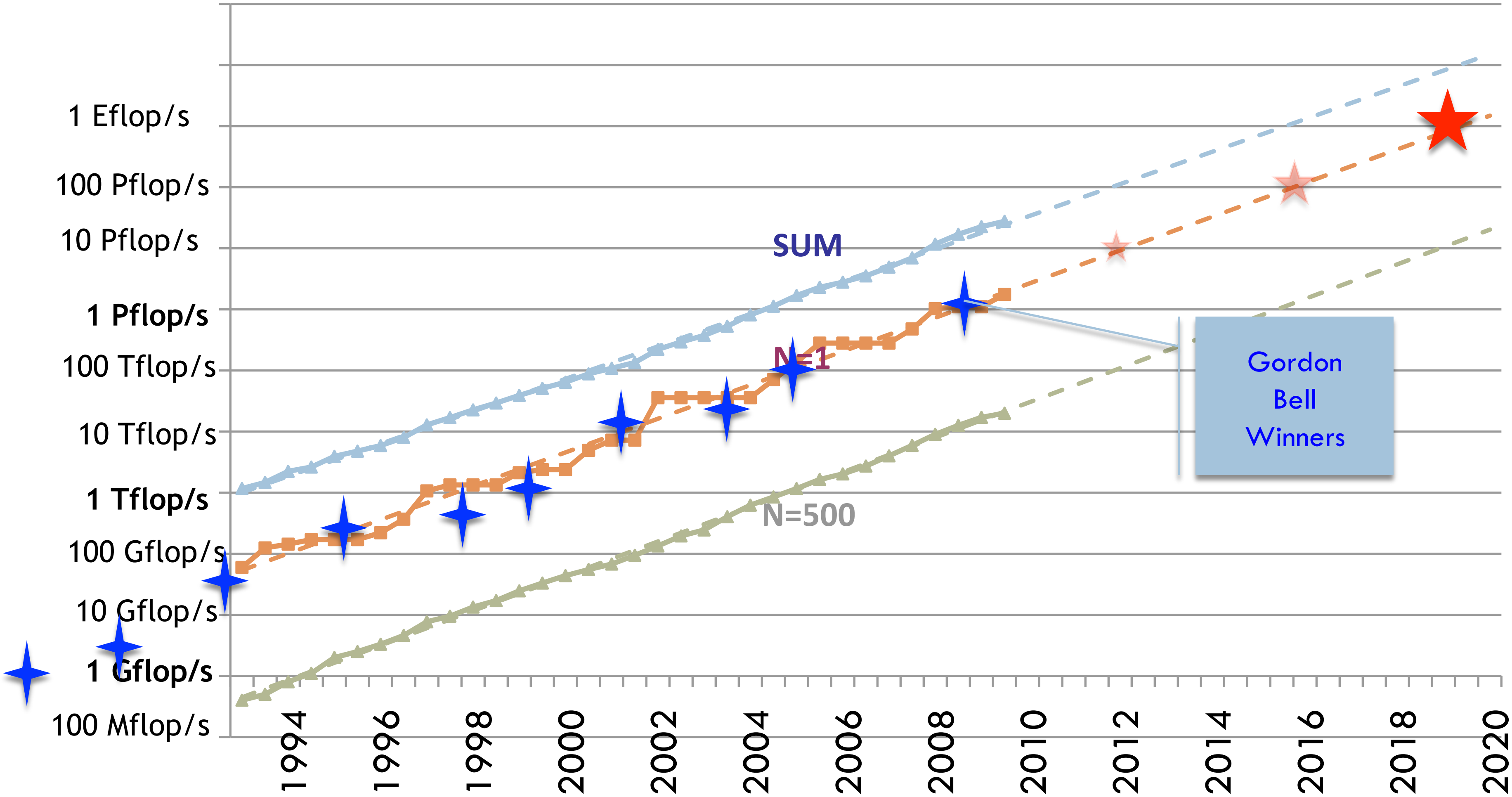
- 1 GFlop/s; 1988; Cray Y-MP; 8 Processors
  - Static finite element analysis

- 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; $1.5x10^5$ Processors
  - Superconductive materials



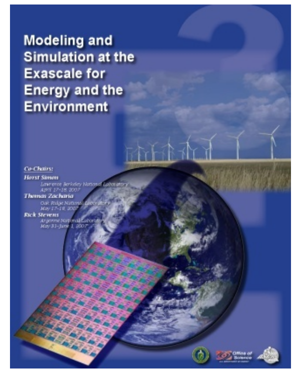
- 1 EFlop/s; ~2018; ?; $1x10^7$ Processors (10^9 threads)

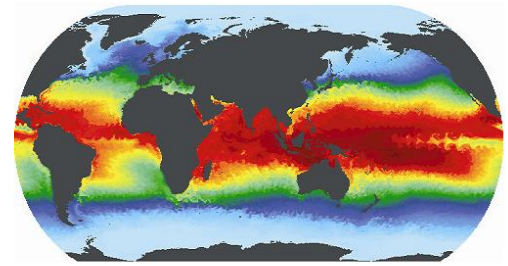
Performance Development in Top500

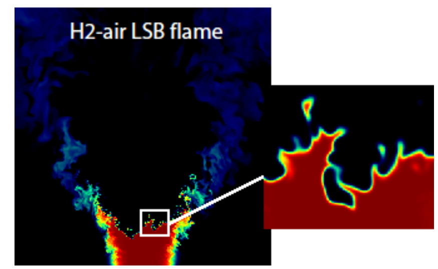


Process for Identifying Exascale Applications and Technology for DOE

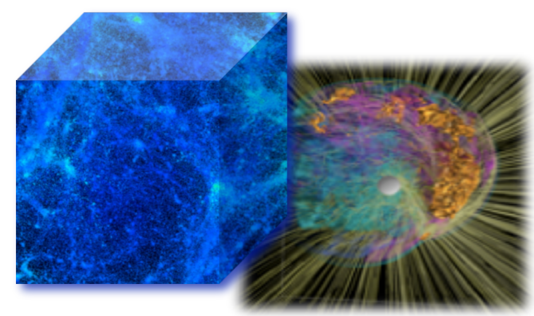
- **Town Hall Meetings April-June 2007**
- **Scientific Grand Challenges Workshops Nov, 2008 - Feb, 2010**
  - Climate Science (11/08),
  - High Energy Physics (12/08),
  - Nuclear Physics (1/09),
  - Fusion Energy (3/09),
  - Nuclear Energy (5/09),
  - Biology (8/09),
  - Material Science and Chemistry (8/09),
  - National Security (10/09)
  - Cross-cutting technologies (2/10)
- **Exascale Steering Committee**
  - "Denver" vendor NDA visits 8/2009
  - SC09 vendor feedback meetings
  - Extreme Architecture and Technology Workshop 12/2009
- **International Exascale Software Project**
  - Santa Fe, NM 4/2009; Paris, France 6/2009; Tsukuba, Japan 10/2009; Oxford 4/2010







MISSION IMPERATIVES



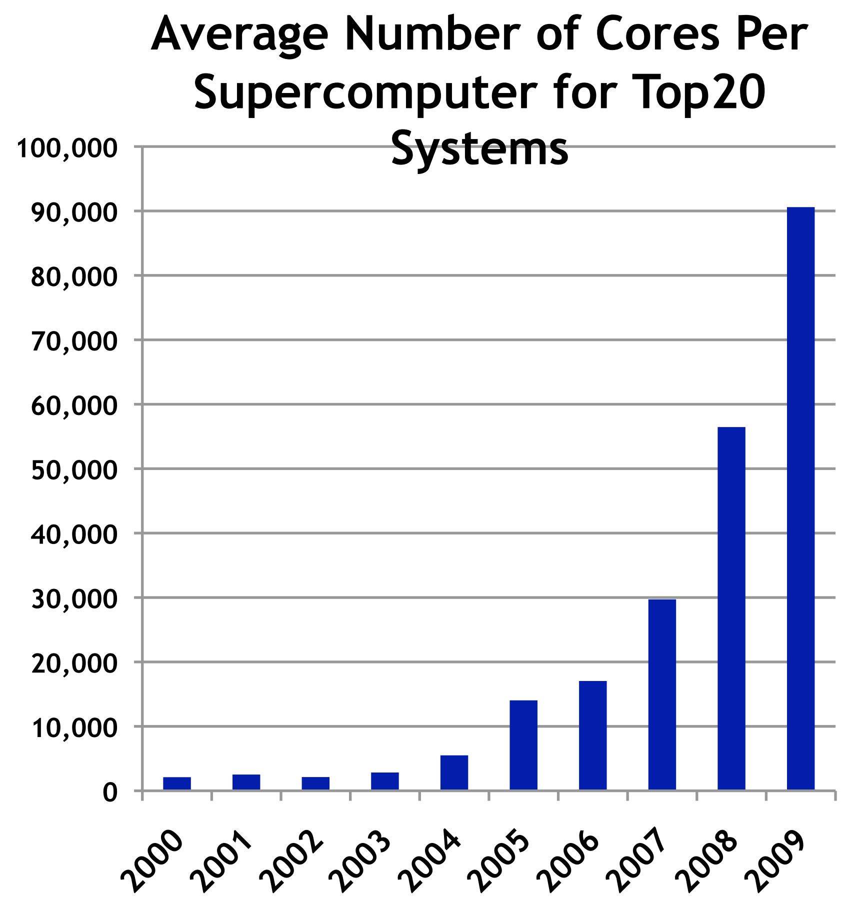
FUNDAMENTAL SCIENCE

Potential System Architecture

Systems	2009
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
IO	0.2 TB
MTTI	days

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



Software infrastructure does not exist today

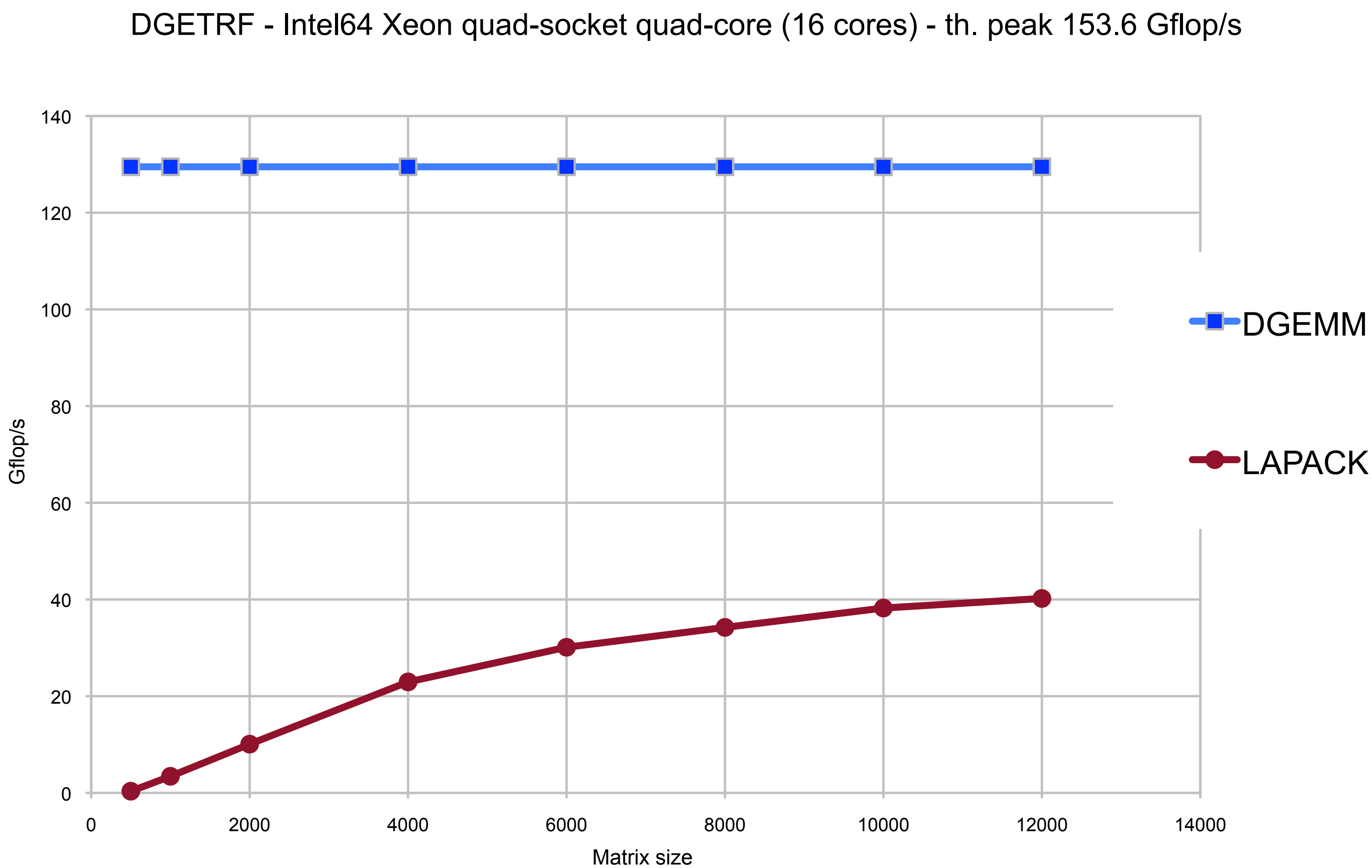
Major Changes to Software

- 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

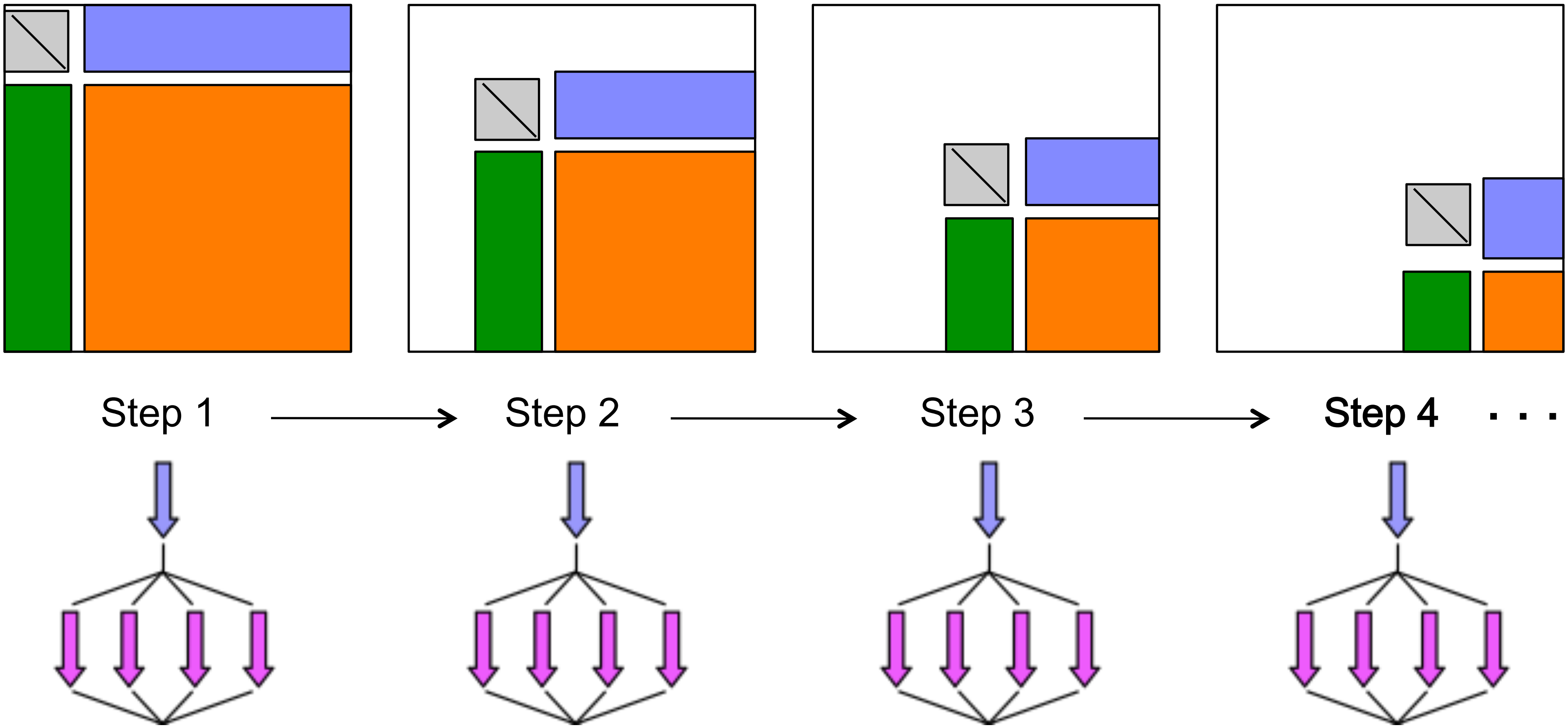
Five Important Features to Consider When Computing at Scale

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

LAPACK LU - Intel64 - 16 cores

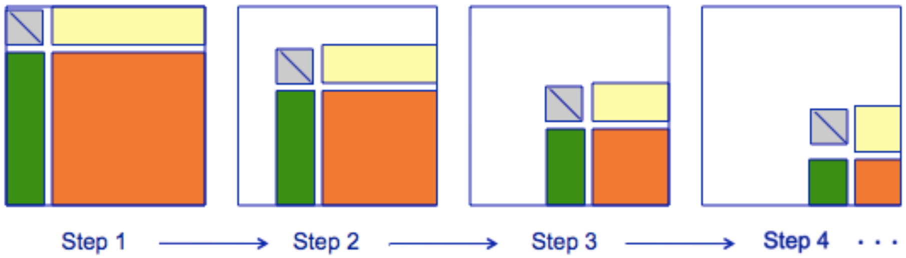


LAPACK LU

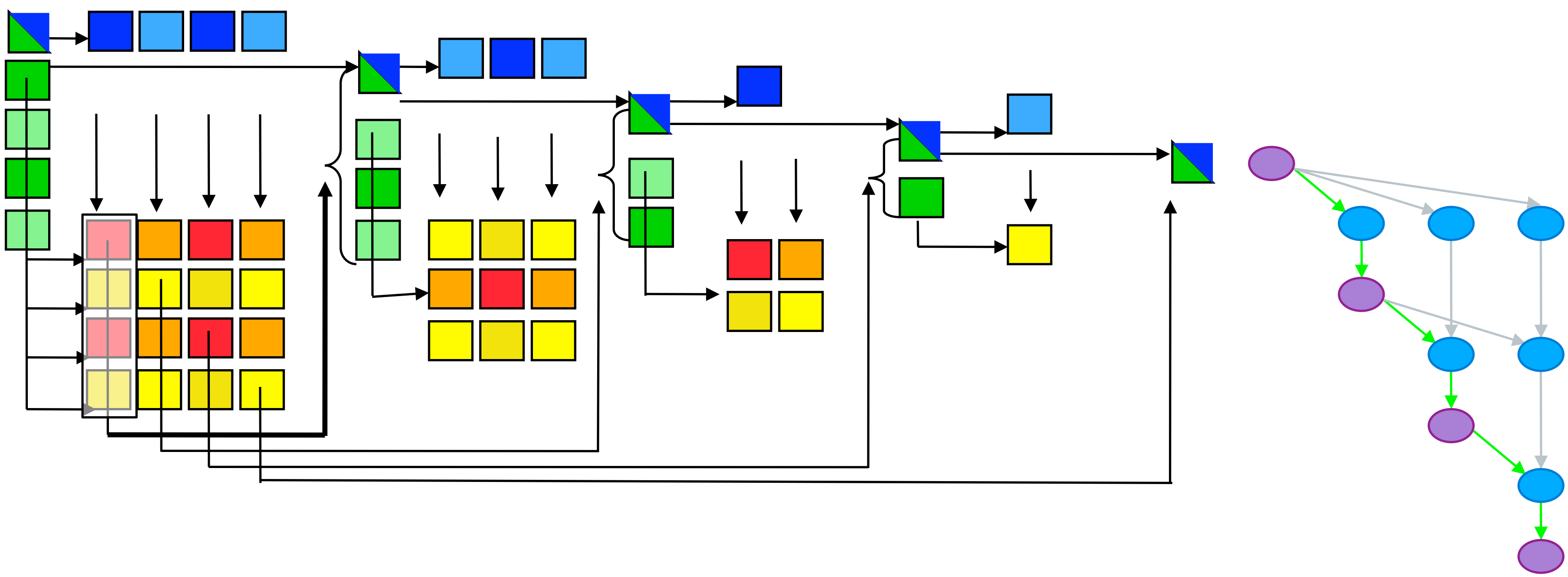


- **Fork-join, bulk synchronous processing**

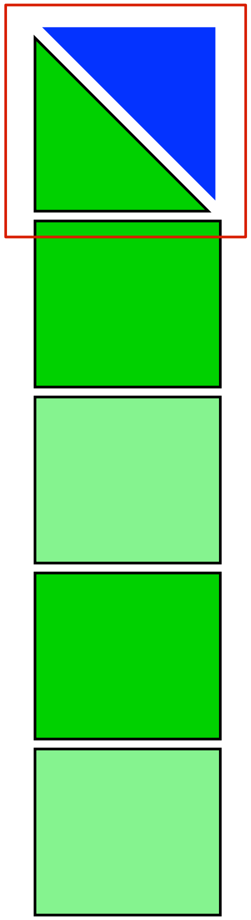
Parallel Tasks in LU



- Break into smaller tasks and remove dependencies

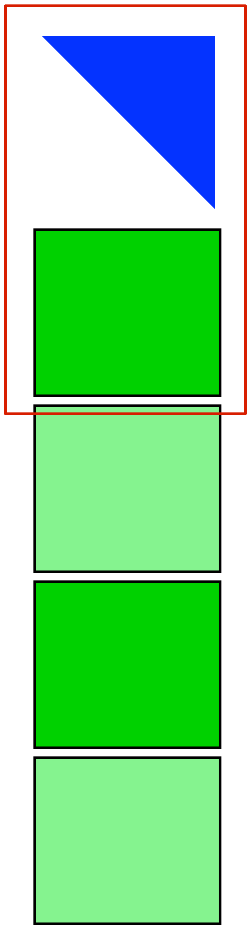


Parallel Tasks in LU



Step 1: LU of block 1,1 (w/partial pivoting)

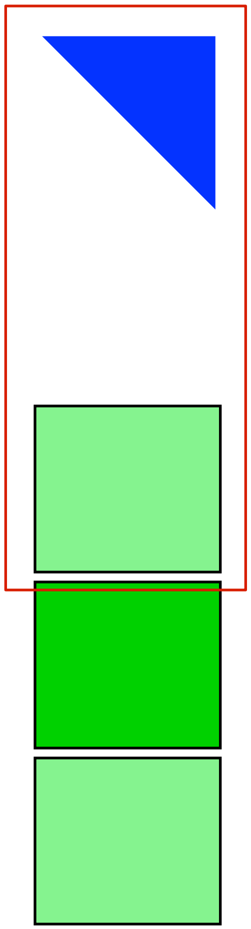
Parallel Tasks in LU



Step 1: LU of block 1,1 (w/partial pivoting)

Step 2: Use $U_{1,1}$ to zero $A_{1,2}$ (w/partial pivoting)

Parallel Tasks in LU



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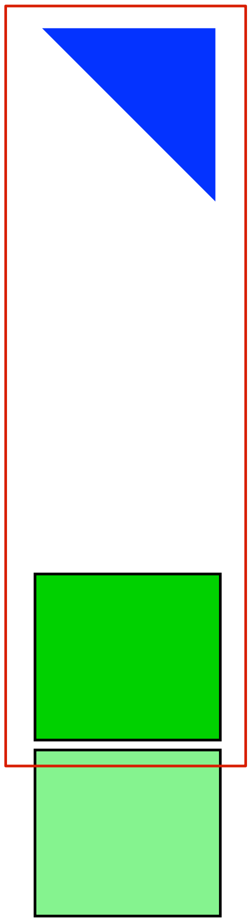
Parallel Tasks in LU



Step 1: LU of block 1,1 (w/partial pivoting)

Step 2: Use $U_{1,1}$ to zero $A_{1,2}$ (w/partial pivoting)

Step3: Use $U_{1,1}$ to zero $A_{1,3}$ (w/partial pivoting)

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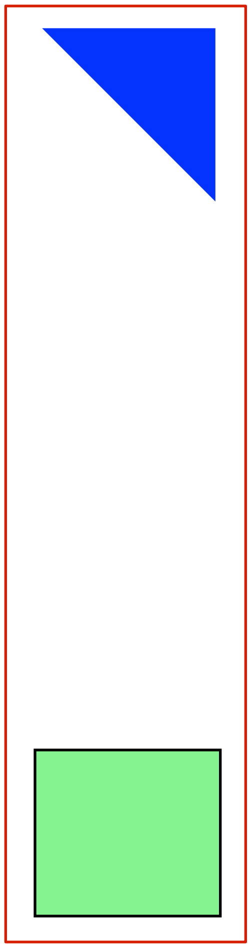
Parallel Tasks in LU



Step 1: LU of block 1,1 (w/partial pivoting)

Step 2: Use $U_{1,1}$ to zero $A_{1,2}$ (w/partial pivoting)

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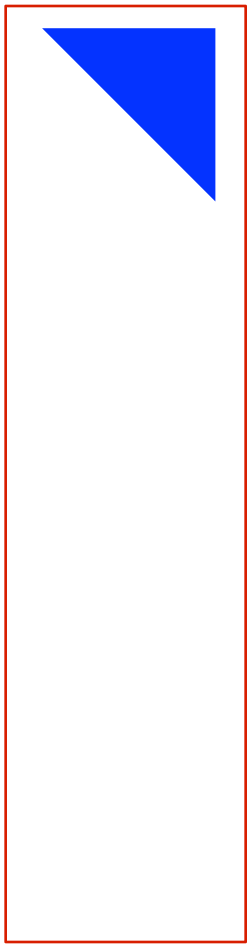
Parallel Tasks in LU



Step 1: LU of block 1,1 (w/partial pivoting)

Step 2: Use $U_{1,1}$ to zero $A_{1,2}$ (w/partial pivoting)

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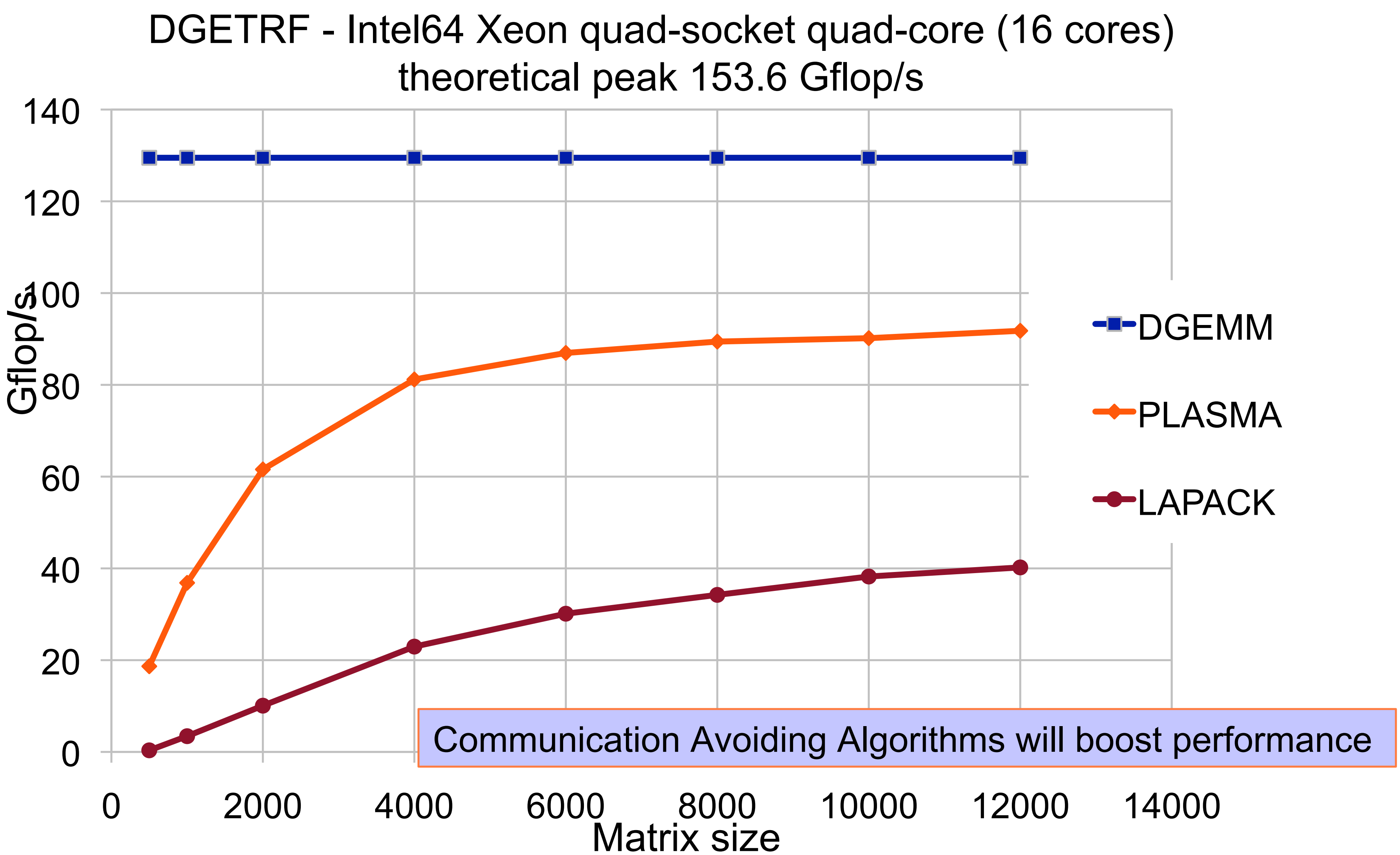
LU - Intel64 - 16 cores

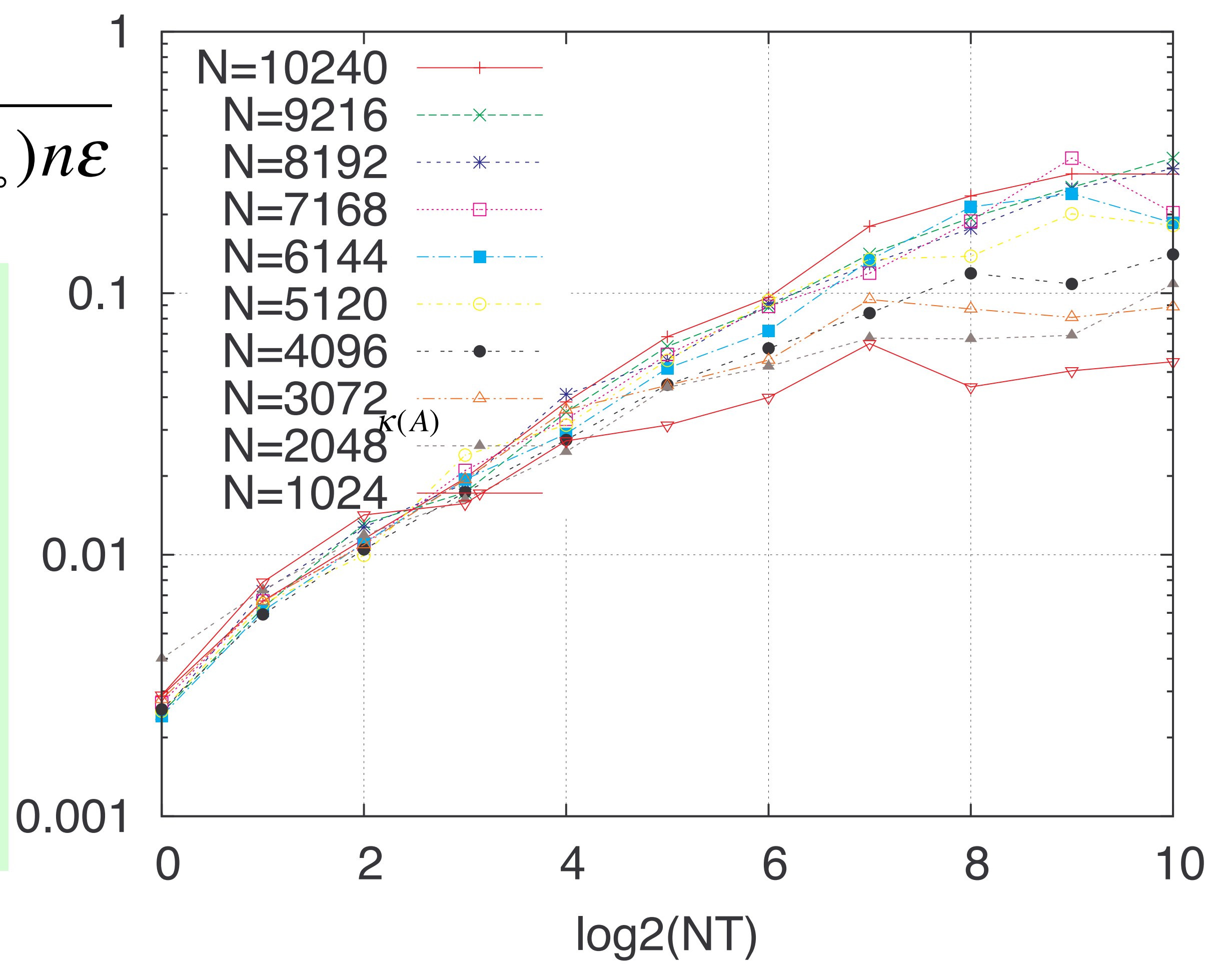


Residual from PLASMA's Tiled LU

$$\frac{\| Ax - b \|_\infty}{(\| A \|_\infty \| x \|_\infty + \| b \|_\infty) n\varepsilon}$$

Validation and verification

- Compute the answer fast with a possibly (but rarely) unreliable/ unstable algorithm
- Quickly check that the answer is ok (exception flags, small residual..)
- In the rare event of a problem, recompute carefully and slowly using classical approach



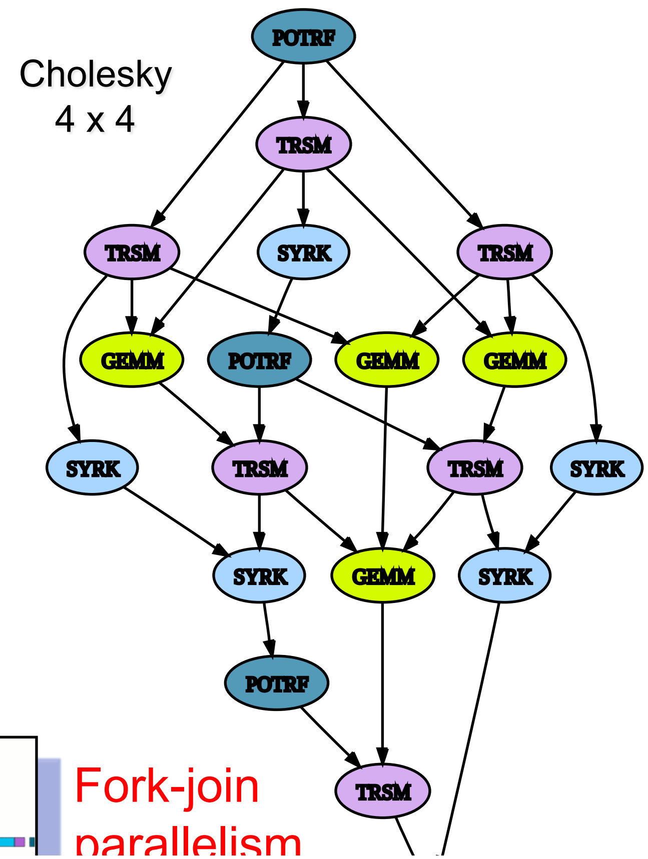
Random Matrices

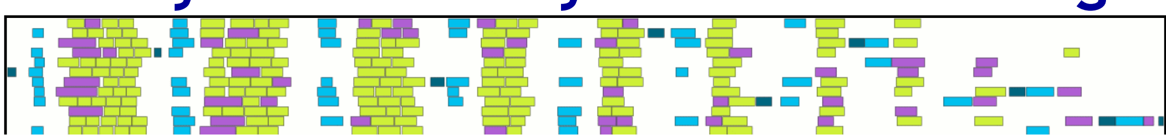
NT (Number of Tiles)

$\kappa(A) : 10^5 - 10^8$

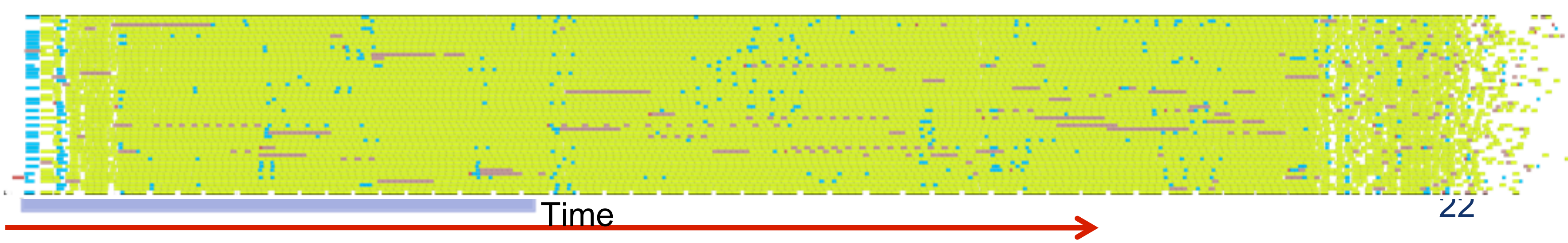
PLASMA: Parallel Linear Algebra s/w for Multicore Architectures

- **Objectives**
  - high utilization of each core
  - scaling to large number of cores
  - shared or distributed memory
- **Methodology**
  - DAG scheduling
  - explicit parallelism
  - implicit communication
  - Fine granularity / block data layout
- **Arbitrary DAG with dynamic scheduling**





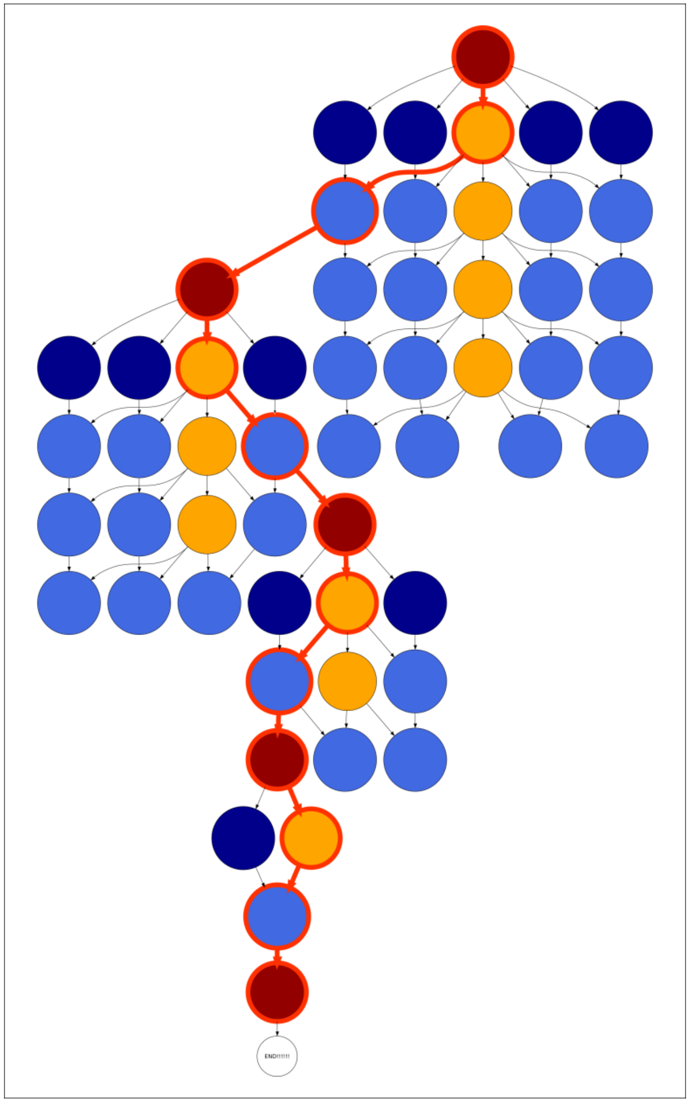
Fork-join parallelism



Time

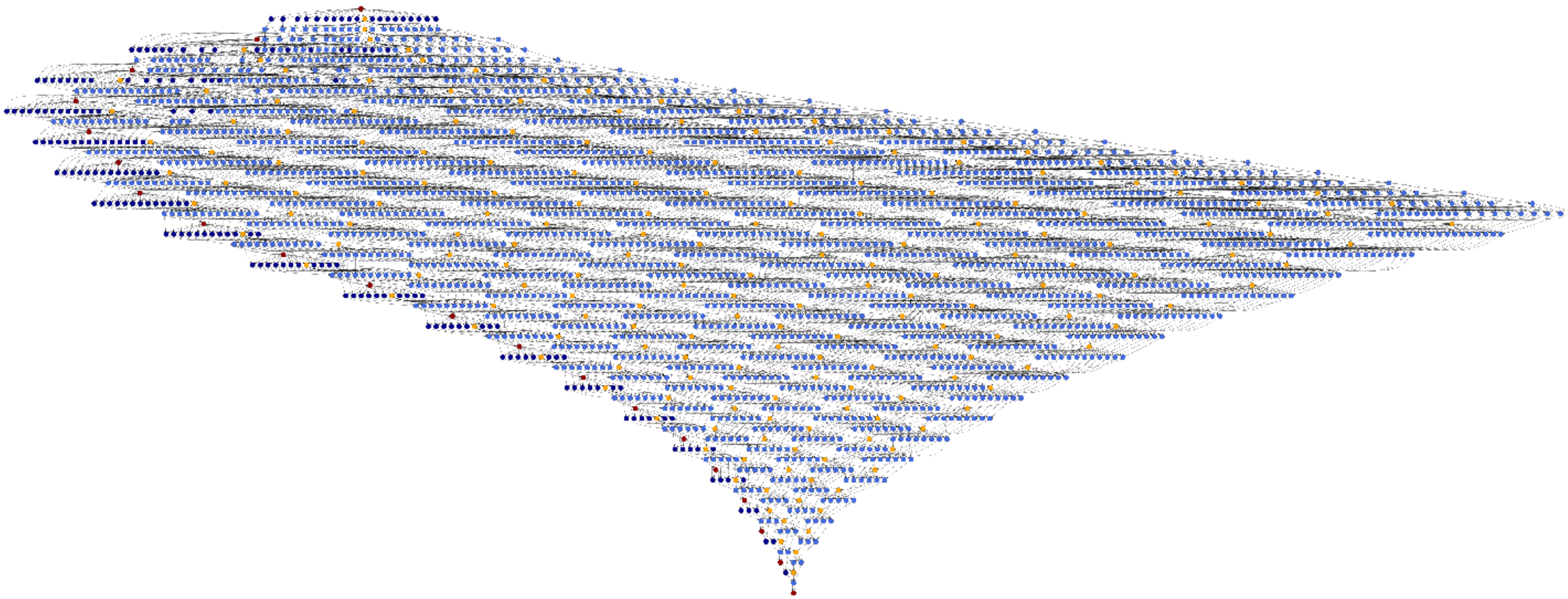
If We Had A Small Matrix Problem

- 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



The DAGs are Large

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



- For a large matrix say $O(10^6)$ the DAG is huge
- Many challenges for the software

- **www.exascale.org**

INTERNATIONAL
EXASCALE
SOFTWARE PROJECT

ROADMAP

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If you are wondering what's beyond ExaFlops

Mega, Giga, Tera, Peta, Exa, Zetta …

10^{3}	kilo
10^{6}	mega
10^{9}	giga
10^{12}	tera
10^{15}	peta
10^{18}	exa
10^{21}	zetta

10^{24}	yotta
10^{27}	xona
10^{30}	weka
10^{33}	vunda
10^{36}	uda
10^{39}	treda
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