Algorithmic Adaptations to Extreme Scale

David Keyes, Applied Mathematics & Computational Science

Director, Extreme Computing Research Center (ECRC)

King Abdullah University of Science and Technology

Just a few of the tie-ins to ATPESC …

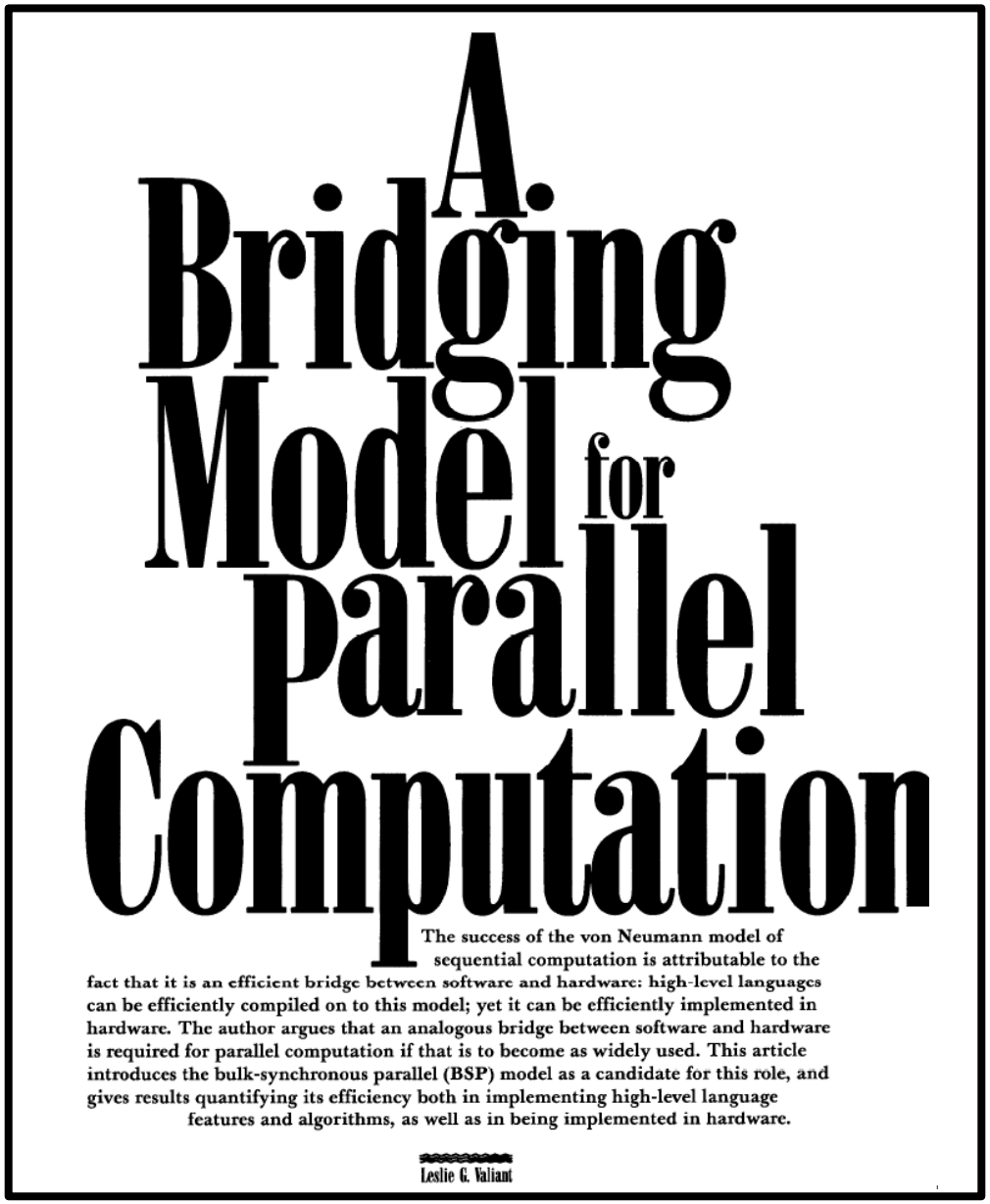
- **Jim**
  - **Premium on communication reduction**
  - **Models to know what is achievable; quantifying trade-offs between communication saved versus extra memory and flops**
- **Sherry**
  - **Hierarchical exploitation of effective low rank**
- **Rob**
  - **Multilevel methods**
- **Barry and Carol**
  - **Newton methods**
- **FastMath panel**
  - **Planning for extreme scale in solvers**
- **Jack**
  - **DAG-based synchronization reduction and concurrency improvement**


Energy-aware
generation
BSP
generation

Bulk Synchronous Parallelism

Leslie Valiant, Harvard

2010 Turing Award Winner



A Bridging Model for Parallel Computation

The success of the von Neumann model of sequential computation is attributable to the fact that it is an efficient bridge between software and hardware: high-level languages can be efficiently compiled on to this model; yet it can be efficiently implemented in hardware. The author argues that an analogous bridge between software and hardware is required for parallel computation if that is to become as widely used. This article introduces the bulk-synchronous parallel (BSP) model as a candidate for this role, and gives results quantifying its efficiency both in implementing high-level language features and algorithms, as well as in being implemented in hardware.

Leslie G. Valiant

Comm. of the ACM, 1990

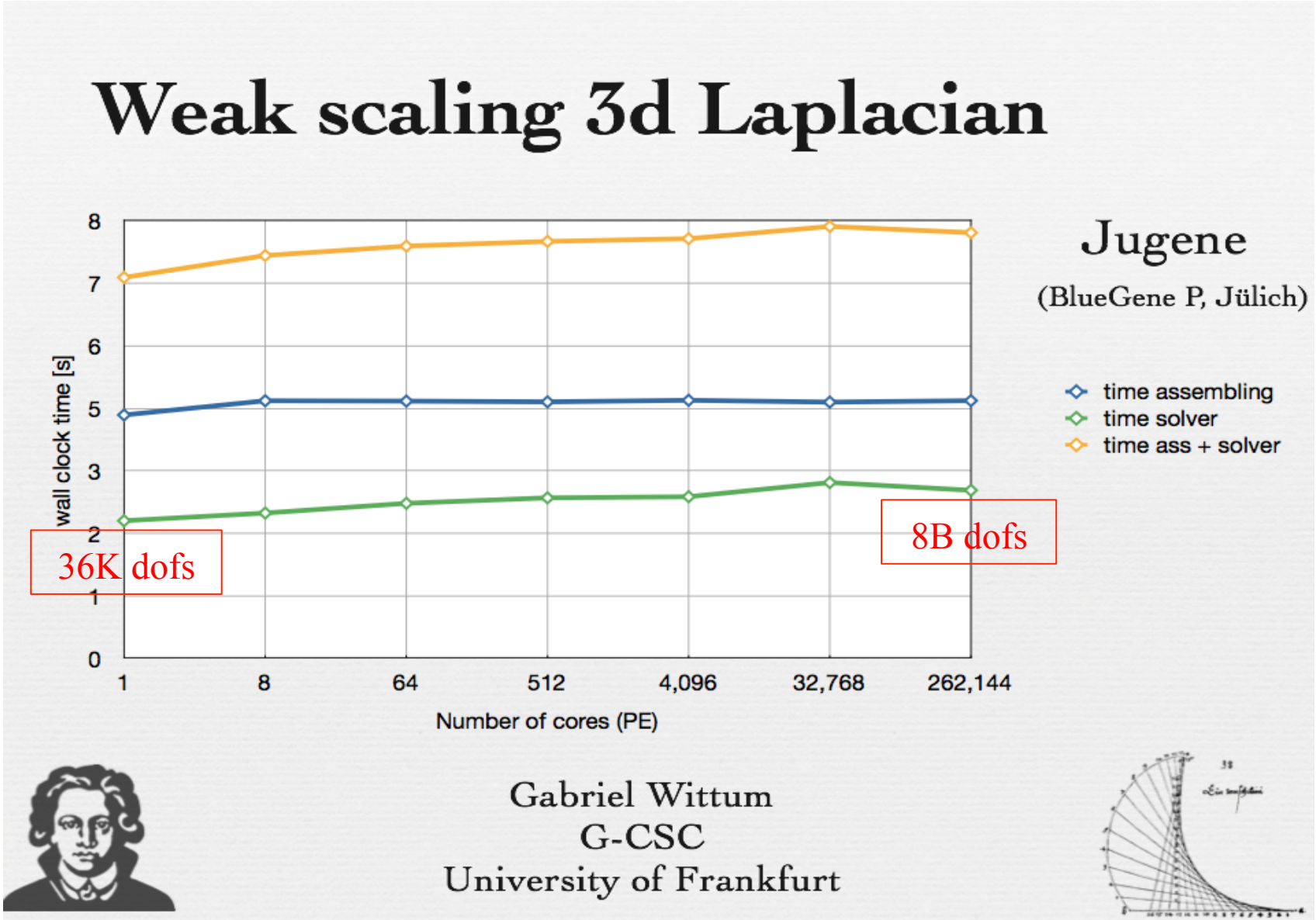
BSP has an impressive legacy

By the Gordon Bell Prize, performance on *real applications* (e.g., mechanics, materials, petroleum reservoirs, etc.) has improved *more* than a million times in two decades. Simulation *cost per performance* has improved by nearly a million times.

Gordon Bell Prize: Peak Performance Year	Gigaflop/s delivered to applications
1988	1
1998	1,020
2008	1,350,000

Gordon Bell Prize: Price Performance Year	Cost per delivered Gigaflop/s
1989	$2,500,000
1999	$6,900
2009	$8

Synchronous hierarchical algorithms underlie BSP scaling of PDE applications



Extrapolating exponentials eventually fails

- Scientific computing at a crossroads w.r.t. extreme scale
- Proceeded steadily for decades from giga- (1988) to tera- (1998) to peta- (2008) with
  - *same* BSP programming model
  - *same* assumptions about who (hardware, systems software, applications software etc.) is responsible for what (resilience, performance, processor mapping, etc.)
  - *same* classes of algorithms (*cf.* 25 yrs. of Gordon Bell Prizes)
- Exa- is qualitatively different and looks more difficult
  - but we once said that about message passing
- Core numerical analysis and scientific computing will confront exascale to maintain sponsor relevance
  - not a "distraction," but an intellectual stimulus
  - potentially big gains in adapting to new hardware environment
  - the journey will be as fun as the destination

Part of campaign to provide less synchronous alternatives, in *Supercomput. Front. Innov.* 1(1)

Communication Complexity of the Fast Multipole Method and its Algebraic Variants

Rio Yokota[1], *George Turkiyyah*[1], *David Keyes*[1]

A combination of hierarchical tree-like data structures and data access patterns from fast multipole methods and hierarchical low-rank approximation of linear operators from $\mathcal{H}$-matrix methods appears to form an algorithmic path forward for efficient implementation of many linear algebraic operations of scientific computing at the exascale. The combination provides asymptotically optimal computational and communication complexity and applicability to large classes of operators that commonly arise in scientific computing applications. A convergence of the mathematical theories of the fast multipole and $\mathcal{H}$-matrix methods has been underway for over a decade. We recap this mathematical unification and describe implementation aspects of a hybrid of these two compelling hierarchical algorithms on hierarchical distributed-shared memory architectures, which are likely to be the first to reach the exascale. We present a new communication complexity estimate for fast multipole methods on such architectures. We also show how the data structures and access patterns of $\mathcal{H}$-matrices for low-rank operators map onto those of fast multipole, leading to an algebraically generalized form of fast multipole that compromises none of its architecturally ideal properties.

Keywords: communication complexity, hierarchical low-rank approximation, fast multipole methods, H-matrices, sparse solvers.

Main challenge going forward for BSP

- **Almost all "good" algorithms in linear algebra, differential equations, integral equations, signal analysis, etc., require frequent synchronizing global communication**
  - **inner products, norms, and fresh global residuals are "addictive" idioms**
  - **tends to hurt efficiency beyond 100,000 processors**
  - **can be fragile for smaller concurrency, as well, due to algorithmic load imbalance, hardware performance variation, etc.**
- **Concurrency is heading into the billions of cores**
  - **already 3 million on the most powerful system today**

Conclusions, up front

- **Plenty of ideas exist to adapt or substitute for favorite solvers with methods that have**
  - **reduced synchrony (in frequency and/or span)**
  - **greater arithmetic intensity**
  - **greater SIMD-style shared-memory concurrency**
  - **built-in resilience ("algorithm-based fault tolerance" or ABFT) to arithmetic faults or lost/delayed messages**
- **Programming models and runtimes may have to be stretched to accommodate**
- **Everything should be on the table for trades, beyond disciplinary thresholds ➔ "co-design"**

Bad news/good news (1)

- **One will have to explicitly control more of the data motion**
  - **carries the highest energy cost in the exascale computational environment**
- **One finally will get the privilege of controlling the *vertical* data motion**
  - ***horizontal* data motion under control of users already**
  - **but vertical replication into caches and registers was (until recently with GPUs) mainly scheduled and laid out by hardware and runtime systems, mostly invisibly to users**

Bad news/good news (2)

- **"Optimal" formulations and algorithms may lead to poorly proportioned computations for exascale hardware resource balances**
  - **today's "optimal" methods presume flops are expensive and memory and memory bandwidth are cheap**
- **Architecture may lure scientific and engineering users into more arithmetically intensive formulations than (mainly) PDEs**
  - **tomorrow's optimal methods will (by definition) evolve to conserve whatever is expensive**

Bad news/good news (3)

- Fully hardware-reliable executions may be regarded as too costly/synchronization-vulnerable
- Algorithmic-based fault tolerance (ABFT) will be cheaper than hardware and OS-mediated reliability
  - developers will partition their data and their program units into two sets
    - a small set that must be done reliably (with today's standards for memory checking and IEEE ECC)
    - a large set that can be done fast and unreliably, knowing the errors can be either detected, or their effects rigorously bounded
- Examples already in direct and iterative linear algebra
- Anticipated by Von Neumann, 1956 ("Synthesis of reliable organisms from unreliable components")

Bad news/good news (4)

- **Default use of (uniform) high precision in nodal bases on dense grids may end, as wasteful of storage and bandwidth**
  - **representation of a smooth function in a hierarchical basis or on sparse grids requires fewer bits than storing its nodal values, for equivalent accuracy**
  - **we will have to compute and communicate "deltas" between states rather than the full state quantities, as when double precision was once expensive (e.g., iterative correction in linear algebra)**
  - **a generalized "combining network" node or a smart memory controller may remember the last address, but also the last values, and forward just the deltas**
- **Equidistributing errors properly to minimize resource use will lead to innovative error analyses in numerical analysis**

Bad news/good news (5)

- **Fully deterministic algorithms may be regarded as too synchronization-vulnerable**
  - **rather than wait for missing data, we may predict it using various means and continue**
  - **we do this with increasing success in problems without models ("big data")**
  - **should be fruitful in problems coming from continuous models**
  - **"apply machine learning to the simulation machine"**
- **A rich numerical analysis of algorithms that make use of statistically inferred "missing" quantities may emerge**
  - **future sensitivity to poor predictions can often be estimated**
  - **numerical analysts will use statistics, signal processing, ML, etc.**

Caveats

- **This talk is not a full algorithmic picture, but some "pixels" out of that big picture**
  - **… a point of light here, a point of light there…**
  - **a full picture will emerge progressively**
- **Algorithms people may be able to ignore the hardware-based disruption of numerical computing for another ~5 years and let the programming environment shake out**
  - **but why postpone the inevitable?**
  - **should offer fun for everyone**

Background of this talk:

www.exascale.org/iesp

INTERNATIONAL EXASCALE SOFTWARE PROJECT ROADMAP 1.0

Jack Dongarra, Pete Beckman, Terry Moore, Patrick Aerts, Giovanni Aloisio, Jean-Claude Andre, David Barkai, Jean-Yves Berthou, Taisuke Boku, Bertrand Braunschweig, Franck Cappello, Barbara Chapman, Xuebin Chi

Alok Choudhary, Sudip Dosanjh, Thom Dunning, Sandro Fiore, Al Geist, Bill Gropp, Robert Harrison, Mark Hereld, Michael Heroux, Adolfy Hoisie, Koh Hotta, Yutaka Ishikawa, Fred Johnson

Sanjay Kale, Richard Kenway, David Keyes, Bill Kramer, Jesus Labarta, Alain Lichnewsky, Thomas Lippert, Bob Lucas, Barney Maccabe, Satoshi Matsuoka, Paul Messina, Peter Michielse, Bernd Mohr

Matthias Mueller, Wolfgang Nagel, Hiroshi Nakashima, Michael E. Papka, Dan Reed, Mitsuhisa Sato, Ed Seidel, John Shalf, David Skinner, Marc Snir, Thomas Sterling, Rick Stevens, Fred Streitz

Bob Sugar, Shinji Sumimoto, William Tang, John Taylor, Rajeev Thakur, Anne Trefethen, Mateo Valero, Aad van der Steen, Jeffrey Vetter, Peg Williams, Robert Wisniewski, Kathy Yelick

SPONSORS

Office of Science U.S. Department of Energy, NSF, ANR, CEA, CEPMIA, CRAY, EDF, EPSRC Engineering and Physical Sciences Research Council, FUJITSU, INRIA, GENCI, NVIDIA, RIKEN, 東京大学 The University of Tokyo

The International Exascale Software Roadmap,

J. Dongarra, P. Beckman, et al., *International Journal of High Performance Computer Applications* **25**(1), 2011, ISSN 1094-3420.

What we have heard from IESP meetings:

- **Draconian reduction required in power per flop and per byte will make computing and copying data less reliable**
  - **voltage difference between "0" and "1" will be reduced**
  - **circuit elements will be smaller and subject to greater physical noise per signal**
  - **there will be more errors that must be caught and corrected**
- **Power may be cycled off and on or clocks slowed and speeded**
  - **based on compute schedules (user-specified or software adaptive)**
  - **based on cooling capacity (hardware adaptive)**
  - **makes per node performance rate unreliable**

What we believe

- **Expanding the number of nodes (processor-memory units) beyond 10^6 would *not* a serious threat to algorithms that lend themselves to well-amortized precise load balancing**
  - **provided that the nodes are performance reliable**
- **The real challenge is usefully expanding the number of cores on a node to 10^3**
  - **must be done while memory and memory bandwidth per node expand by (at best) ten-fold less (basically "strong" scaling)**
  - **don't need to wait for full exascale systems to experiment in this regime – the battle is fought on individual shared-memory nodes**

Philosophy

- **Algorithms must adapt to span the gulf between demanding applications and austere architectures**
  - **full employment for computer scientists and computational scientists and engineers**
  - **see, e.g., recent postdoc announcements from**
    - **Berkeley (8),**
    - **Oak Ridge (3), and**
    - **IBM (10)**

  for porting computational science applications to extreme scale

Motivation for algorithmic attention

- **High performance with high(-est possible) productivity on "the multis":**
  - **Multi-scale, multi-physics problems in multi-dimensions**
  - **Using multi-models and/or multi-levels of refinement**
  - **Exploiting polyalgorithms in adaptively multiple precisions in multi-protocol hybrid programming styles**
  - **On multi-core, massively multi-processor systems**
  - **Requiring a multi-disciplinary approach**

Can't cover all this in an hour, but we ask:

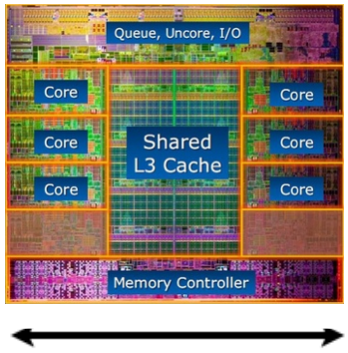
Given the architectural stresses, how can new algorithms help?

Why exa- is different

Which steps of FMADD take more energy?

64-bit floating-point fused multiply add **or** moving four 64-bit operands 20 mm across the die

```
      934,569.299814557                    input
x          52.827419489135904              input
-----------------------------
= 49,370,884.442971624253823
+           4.20349729193958               input
-----------------------------
= 49,370,888.64646892                      output
```



20 mm

(Intel Sandy Bridge, 2.27B transistors)

Going across the die will require an order of magnitude more!

DARPA study predicts that by 2019:

- **Double precision FMADD flop: 11pJ**
- **cross-die per word access (1.2pJ/mm): 24pJ (= 96pJ overall)**

Today's power costs per operation

Operation	approximate energy cost
DP FMADD flop	100 pJ
DP DRAM read-to-register	4800 pJ
DP word transmit-to-neighbor	7500 pJ
DP word transmit-across-system	9000 pJ

Remember that a *pico* (10^{-12}) of something done *exa* (10^{18}) times per second is a *mega* (10^{6})-somethings per second

- **100 pJ at 1 Eflop/s is 100 MW (for the flop/s only!)**
- **1 MW-year costs about $1M ($0.12/KW-hr × 8760 hr/yr)**
  - **We "use" 1.4 KW continuously, so 100MW is 71,000 people**

projections c/o J. Shalf (LBNL)

Why exa- is different

Moore's Law (1965) does not end but Dennard's MOSFET scaling (1972) does

Table 1
Scaling Results for Circuit Performance

Device or Circuit Parameter	Scaling Factor
Device dimension t_{ox}, L, W	$1/\kappa$
Doping concentration N_a	κ
Voltage V	$1/\kappa$
Current I	$1/\kappa$
Capacitance $\epsilon A/t$	$1/\kappa$
Delay time/circuit VC/I	$1/\kappa$
Power dissipation/circuit VI	$1/\kappa^2$
Power density VI/A	1

Table 2
Scaling Results for Interconnection Lines

Parameter	Scaling Factor
Line resistance, $R_L = \rho L/Wt$	κ
Normalized voltage drop IR_L/V	κ
Line response time $R_L C$	1
Line current density I/A	κ

Robert Dennard, IBM
(inventor of DRAM, 1966)

Eventually processing is limited by transmission, as known for > 4 decades

What will first "general purpose" exaflop/s machines look like?

- ***Hardware*: many potentially exciting paths beyond today's CMOS silicon-etched logic, but not commercially at scale within the decade**
- ***Software*: many ideas for general-purpose and domain-specific programming models beyond "MPI + X", but not penetrating the mainstream CS&E workforce for the next few years**
  - **"X" is OpenMP, CUDA, OpenACC, etc., or MPI, *itself***

Some exascale architecture themes

- **Clock rates cease to increase while arithmetic capacity continues to increase dramatically w/concurrency consistent with Moore's Law**
- **Memory storage capacity diverges exponentially below arithmetic capacity**
- **Transmission capacity (memory BW and network BW) diverges exponentially below arithmetic capacity**
- **Mean time between hardware interrupts shortens**
- **➔ Billions of $ € £ ¥ of scientific software worldwide hangs in the balance until better algorithms arrive to span the architectural gap**

Required software

Model-related

- Geometric modelers
- Meshers
- Discretizers
- Partitioners
- Solvers / integrators
- Adaptivity systems
- Random no. generators
- Subgridscale physics
- Uncertainty quantification
- Dynamic load balancing
- Graphs and combinatorial algs.
- Compression

Development-related

- Configuration systems
- Source-to-source translators
- Compilers
- Simulators
- Messaging systems
- Debuggers
- Profilers

High-end computers come with little of this stuff. Most has to be contributed by the user community

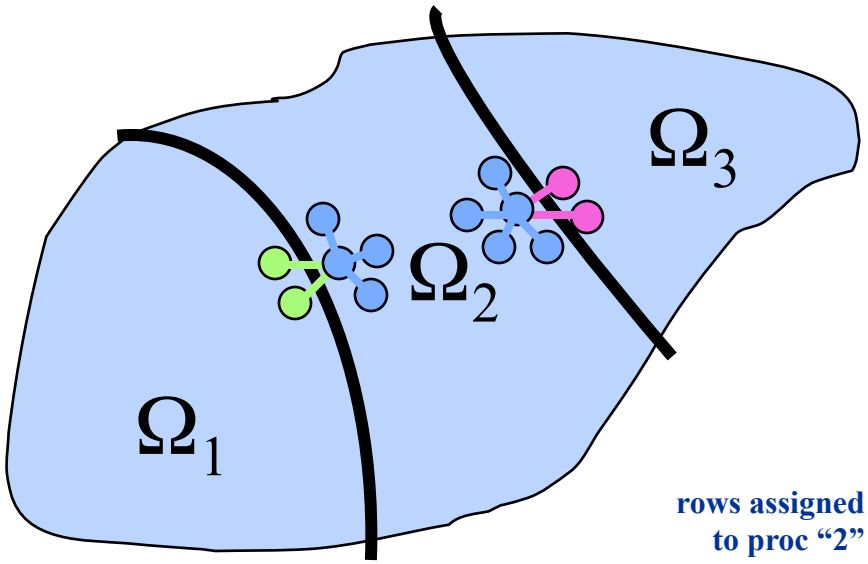
Production-related

- Dynamic resource management
- Dynamic performance optimization
- Authenticators
- I/O systems
- Visualization systems
- Workflow controllers
- Frameworks
- Data miners
- Fault monitoring, reporting, and recovery

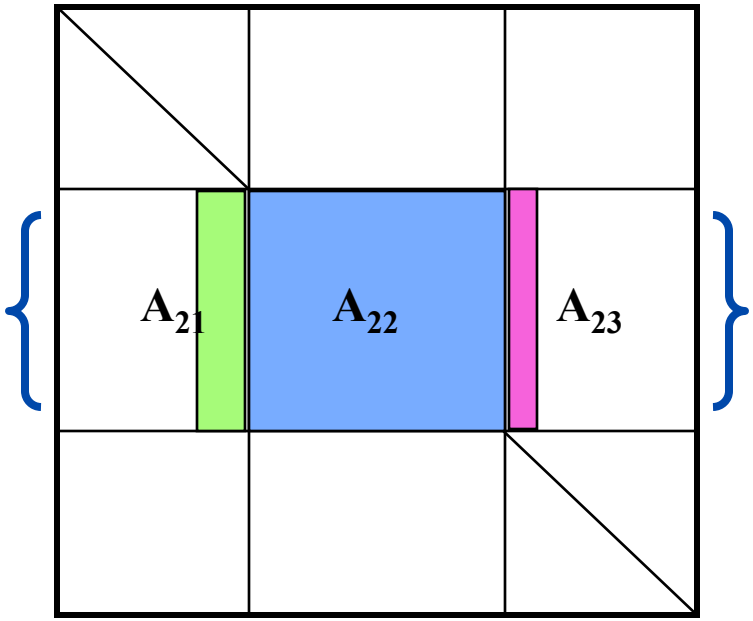
How are most simulations implemented at the petascale today?

- **Iterative methods based on data decomposition and message-passing**
  - **all data structures are distributed**
  - **each individual processor works on a subdomain of the original**
  - **exchanges information at its boundaries with other processors that own portions with which it interacts causally, to evolve in time or to establish equilibrium**
  - **computation and neighbor communication are both fully parallelized and their ratio remains constant in weak scaling**
- **The programming model is BSP/SPMD/CSP**
  - **Bulk Synchronous Programming**
  - **Single Program, Multiple Data**
  - **Communicating Sequential Processes**

BSP parallelism w/ domain decomposition



rows assigned
to proc "2"



Partitioning of the grid induces block structure on the system matrix (Jacobian)

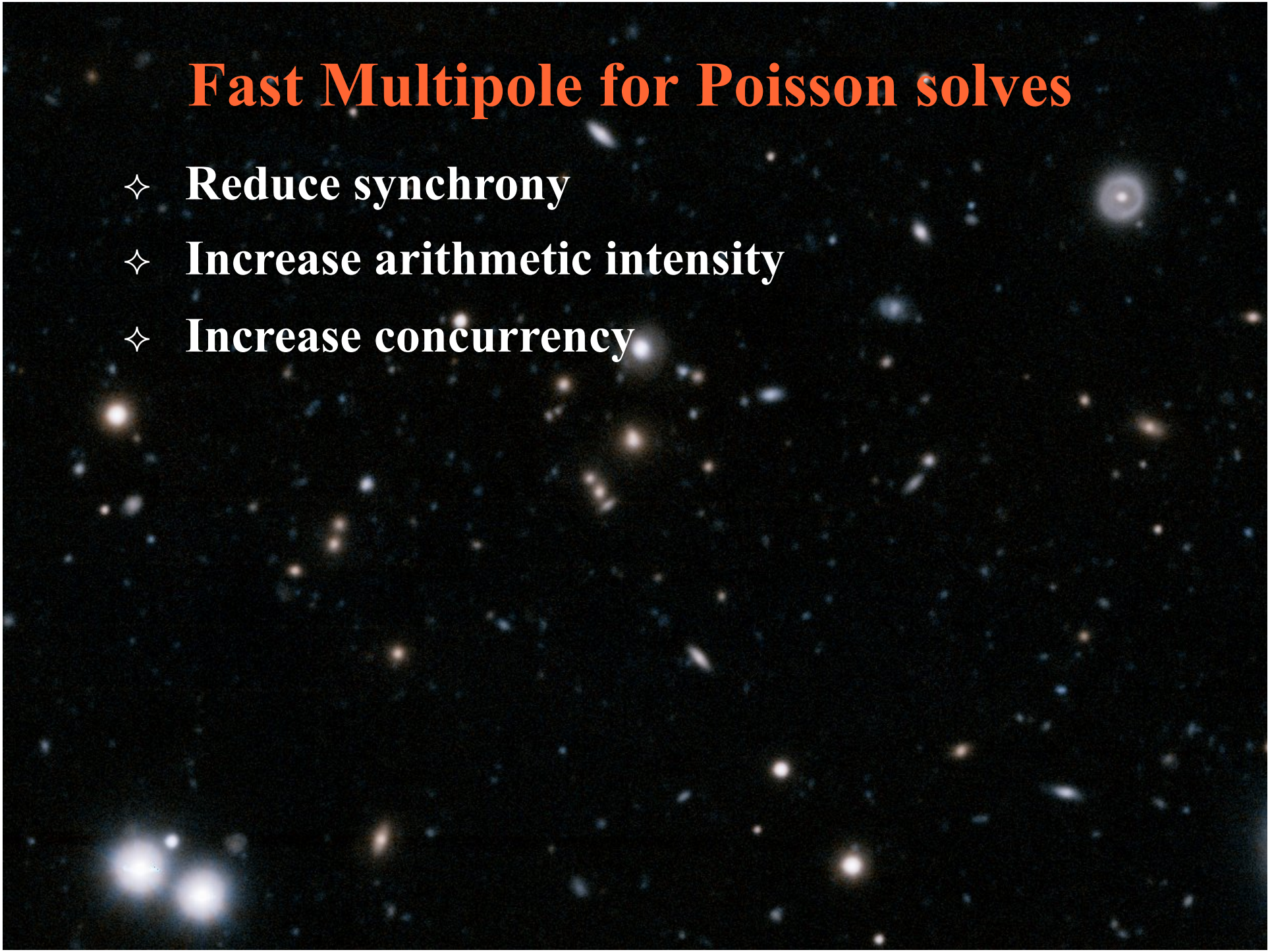
Recap of algorithmic agenda

- **New formulations with**
  - **greater arithmetic intensity (flops per byte moved into and out of registers and upper cache)**
    - **including assured accuracy with (adaptively) less floating-point precision**
  - **reduced synchronization and communication**
    - **less frequent *and/or* less global**
  - **greater SIMD-style thread concurrency for accelerators**
  - **algorithmic resilience to various types of faults**
- **Quantification of trades between limiting resources**
- ***Plus* all of the exciting analytical agendas that exascale is meant to exploit**
  - **"post-forward" problems: data assimilation, parameter inversion, uncertainty quantification, optimization, etc.**

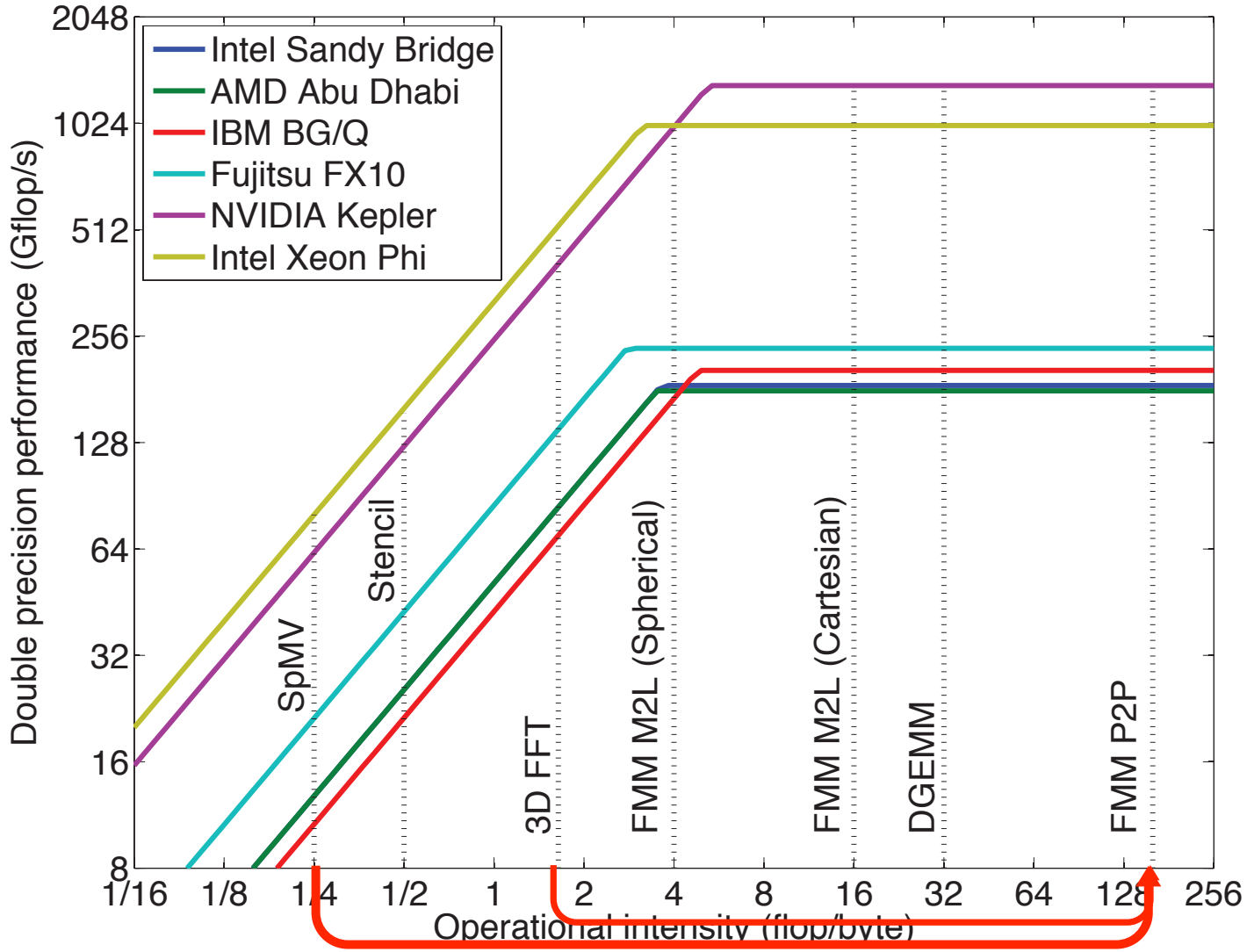
Some algorithmic "points of light"

Next section flashes six "points of light" that accomplish one or more of these agendas

- Fast Multipole for Poisson solves
- Algebraic Fast Multipole for variable coefficient equilibrium problems
- Nonlinear preconditioning for Newton's method
- DAG-based data flow for dense linear algebra
- GPU implementations of dense linear algebra
- New programming paradigms for PDE codes

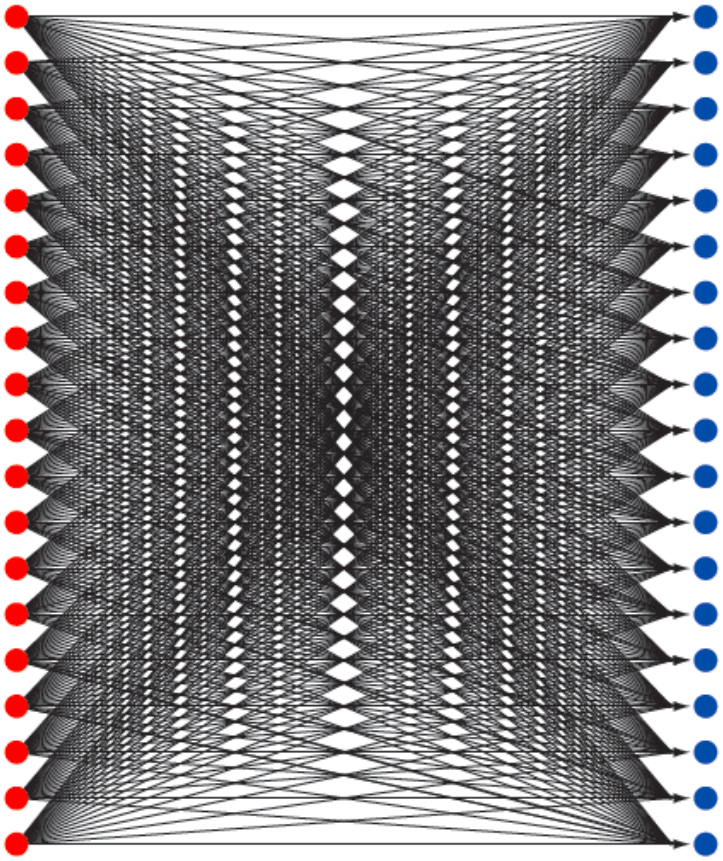

Fast Multipole for Poisson solves
Reduce synchrony
Increase arithmetic intensity
Increase concurrency

Arithmetic intensity of numerical kernels

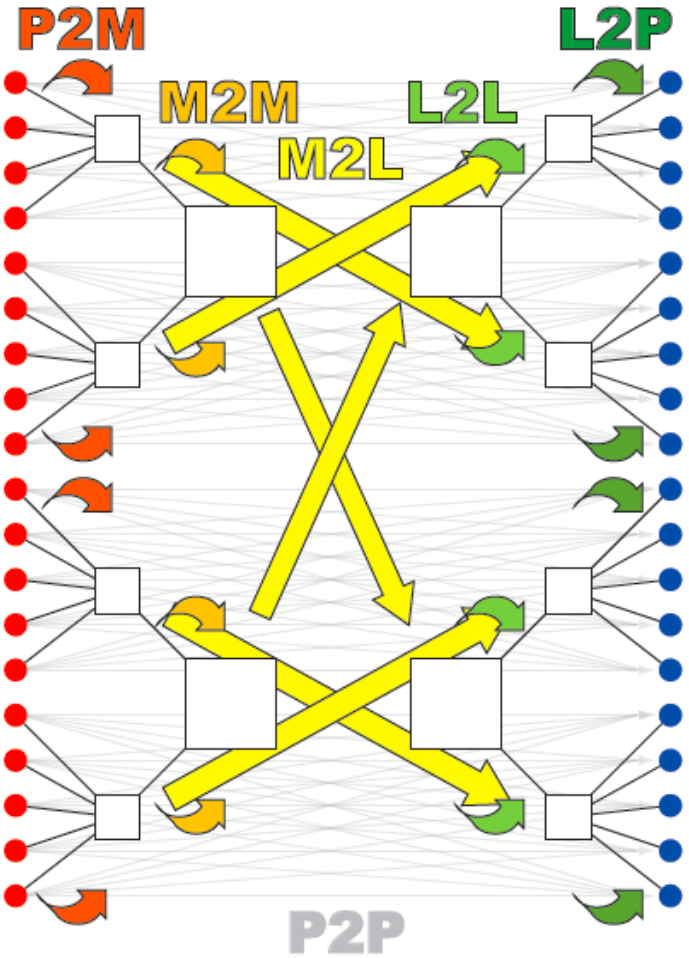


c/o R. Yokota, KAUST, *et al.*

Hierarchical interactions of Fast Multipole



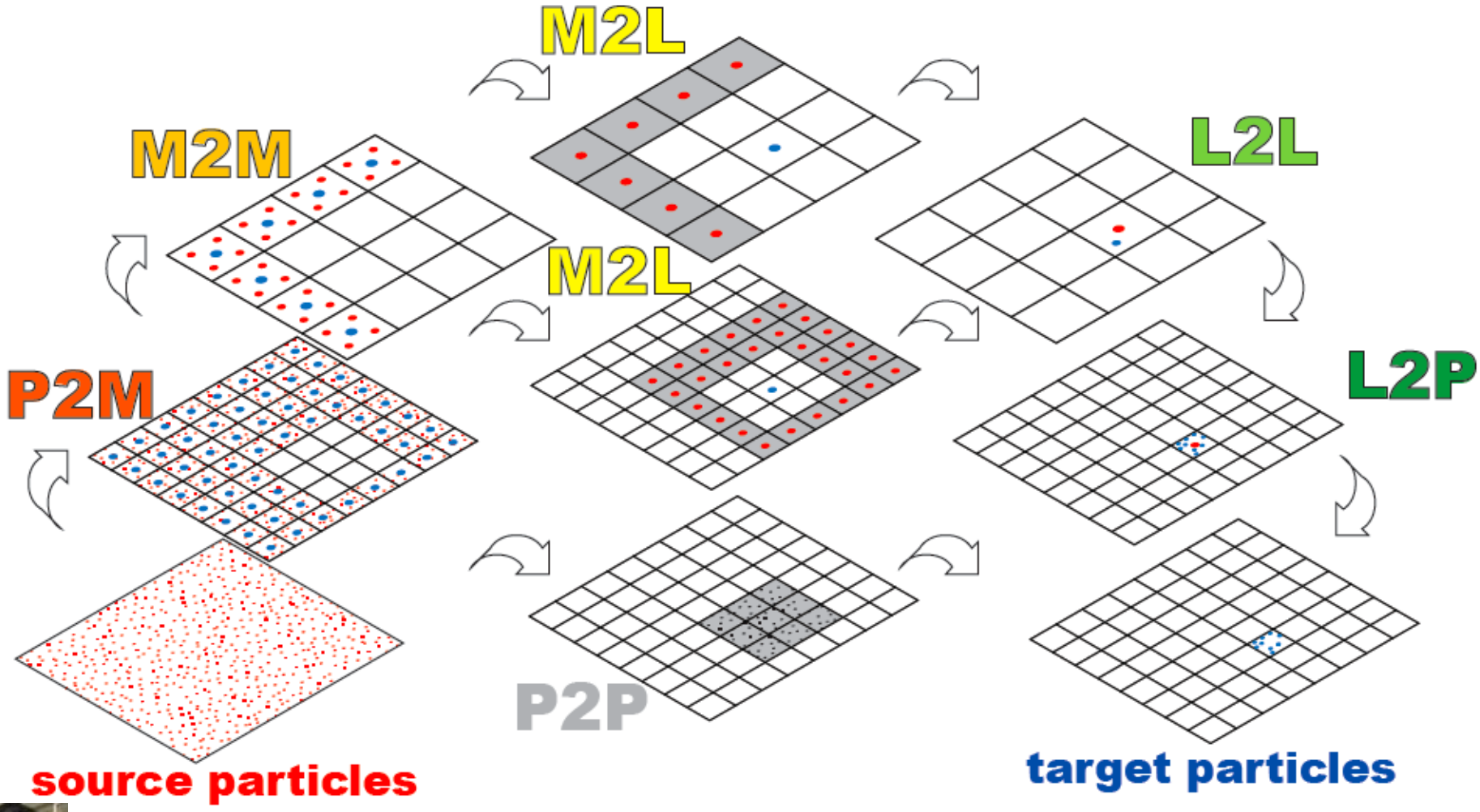
(a) Direct method



(b) Fast Multipole Method

c/o R. Yokota, KAUST, *et al.*

Geometrical structure of Fast Multipole



c/o R. Yokota, KAUST, *et al.*

Synchronization reduction – FMM

- **Within an FMM application, data pipelines of different types and different levels can be executed asynchronously**
  - **FMM simply adds up (hierarchically transformed) contributions**
  - **e.g., P2P and P2M -> *M2M* -> M2L -> *L2L* -> L2P**
- **Geographically distinct targets can be updated asynchronously**

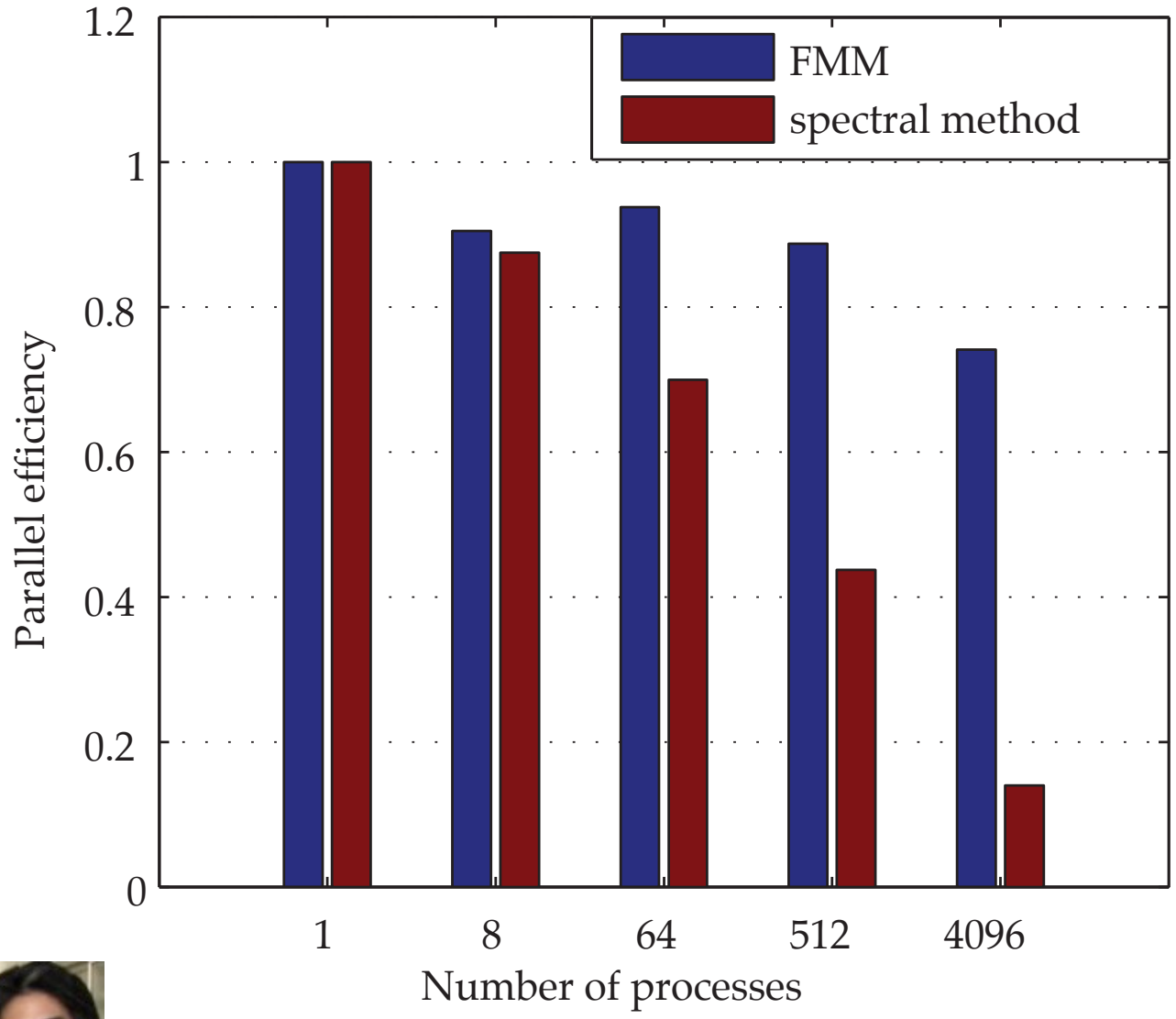
Salient features of FMM

- **High arithmetic intensity**
- **No all-to-all communication**
- ***O*(log *P*) messages**
  - **with high concurrency and asynchrony among themselves**
- **Up to *O*(*N*) arithmetic concurrency**
- **Tunable granularity in the sense of "*h-p*"**
  - **based on analytic "admissibility condition"**
- **Inside 8 Gordon Bell Prizes, 1997-2012**
- **Many effective implementations on GPUs**
- ***Fragile* (based on analytical forms of operators)**

Communication complexity of FMM

	Reference	Processes		Data per Process		Communication complexity
1998	Teng [32]	$\mathcal{O}(P)$		$\mathcal{O}\left((N/P)^{2/3}(\log N+\mu)^{1/3}\right)$		$\mathcal{O}\left(P(N/P)^{2/3}(\log N+\mu)^{1/3}\right)$
2009	Lashuk *et al.* [27]	$\mathcal{O}(\sqrt{P})$		$\mathcal{O}\left((N/P)^{2/3}\right)$		$\mathcal{O}\left(\sqrt{P}(N/P)^{2/3}\right)$
2014	Ibeid *et al.* [21]	Global	Local	Global	Local	Global + Local
		$\mathcal{O}(\log P)$	$\mathcal{O}(1)$	$\mathcal{O}(1)$	$\mathcal{O}\left((N/P)^{2/3}\right)$	$\mathcal{O}\left(\log P+(N/P)^{2/3}\right)$

FMM vs. FFT in processor scaling



Weak scaling of a vortex-formulation 3D Navier-Stokes code simulating decaying isotropic turbulence, referenced to the pseudo-spectral method, which uses FFT.

FFT: 14% parallel efficiency at 4096 processes, no GPU use.

FMM: 74% going from one to 4096 processes at one GPU per MPI process, 3 GPUs per node.

Largest problem corresponds to a 4096^3 mesh, i.e., almost 69 billion points (about 17 million points per process).

Run on the TSUBAME 2.0 system of the Tokyo Institute of Technology.

c/o R. Yokota, KAUST, *et al.*

FMM as preconditioner

- **FMM is a solver for free-space problems for which one has a Green's function**
- **For finite boundaries, FMM combines with BEM**
- **FMM and BEM have controllable truncation accuracies; can precondition other, different discretizations of the same PDE**
- **Can be regarded as a preconditioner for "nearby" problems, e.g., ∇^2 for $\nabla \cdot (1 + \varepsilon(\vec{x}))\nabla$**

FMM's role in solving PDEs

$$u = \int_\Gamma \frac{\partial u}{\partial n} G d\Gamma - \int_\Gamma u \frac{\partial G}{\partial n} d\Gamma + \int_\Omega f G d\Omega \quad \text{in } \Omega$$

BEM FMM

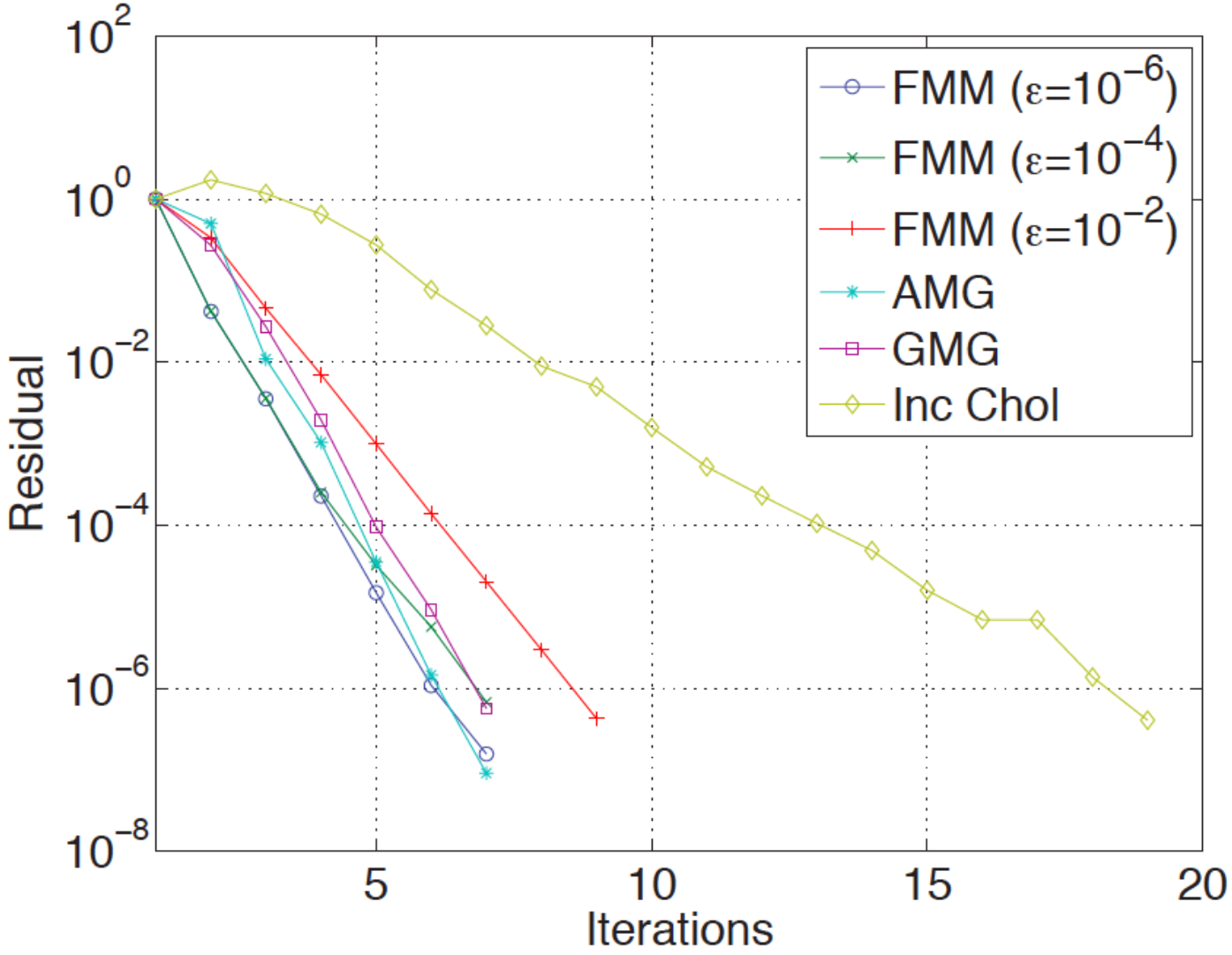
$$N_\Omega \left\{ \begin{bmatrix} \vdots \\ u_i \\ \vdots \end{bmatrix} \right. = \overbrace{\begin{bmatrix} \ddots & & \\ & G_{ij} & \\ & & \ddots \end{bmatrix}}^{N_\Gamma} \begin{bmatrix} \vdots \\ \frac{\partial u_j}{\partial n} \\ \vdots \end{bmatrix} - \overbrace{\begin{bmatrix} \ddots & & \\ & \frac{\partial G_{ij}}{\partial n} & \\ & & \ddots \end{bmatrix}}^{N_\Gamma} \begin{bmatrix} \vdots \\ u_j \\ \vdots \end{bmatrix} + \overbrace{\begin{bmatrix} \ddots & & \\ & G_{ij} & \\ & & \ddots \end{bmatrix}}^{N_\Omega} \begin{bmatrix} \vdots \\ f_j \\ \vdots \end{bmatrix}$$

The preconditioner is reduced to a matvec, like the forward operator itself – the same philosophy of the sparse approximate inverse (SPAI), but cheaper.

***More concurrency, more intensity, less synchrony* than ILU, MG, DD, etc.**

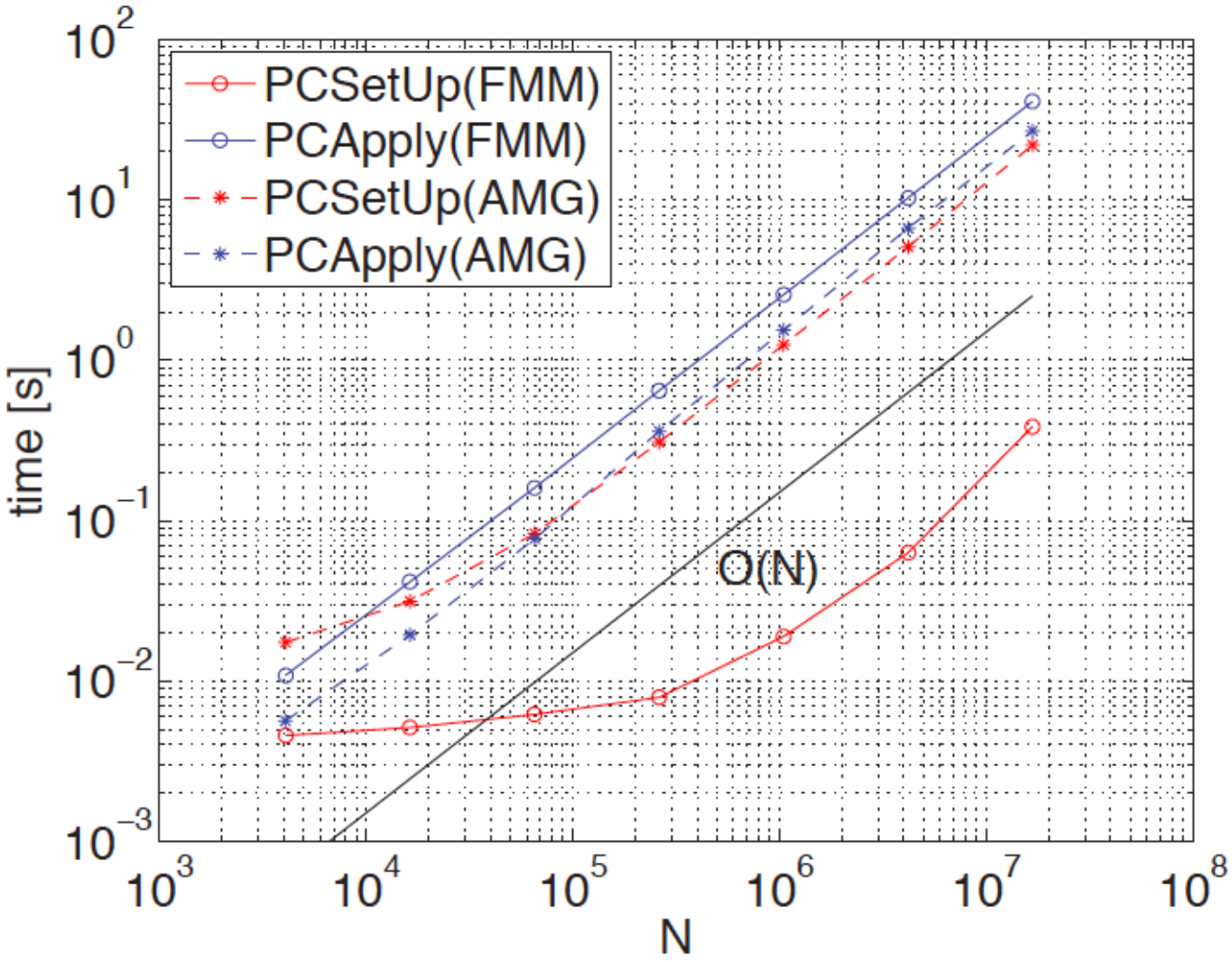
c/o H. Ibeid, KAUST, *et al.*

FMM/BEM preconditioning of FEM-discretized Poisson accelerated by CG



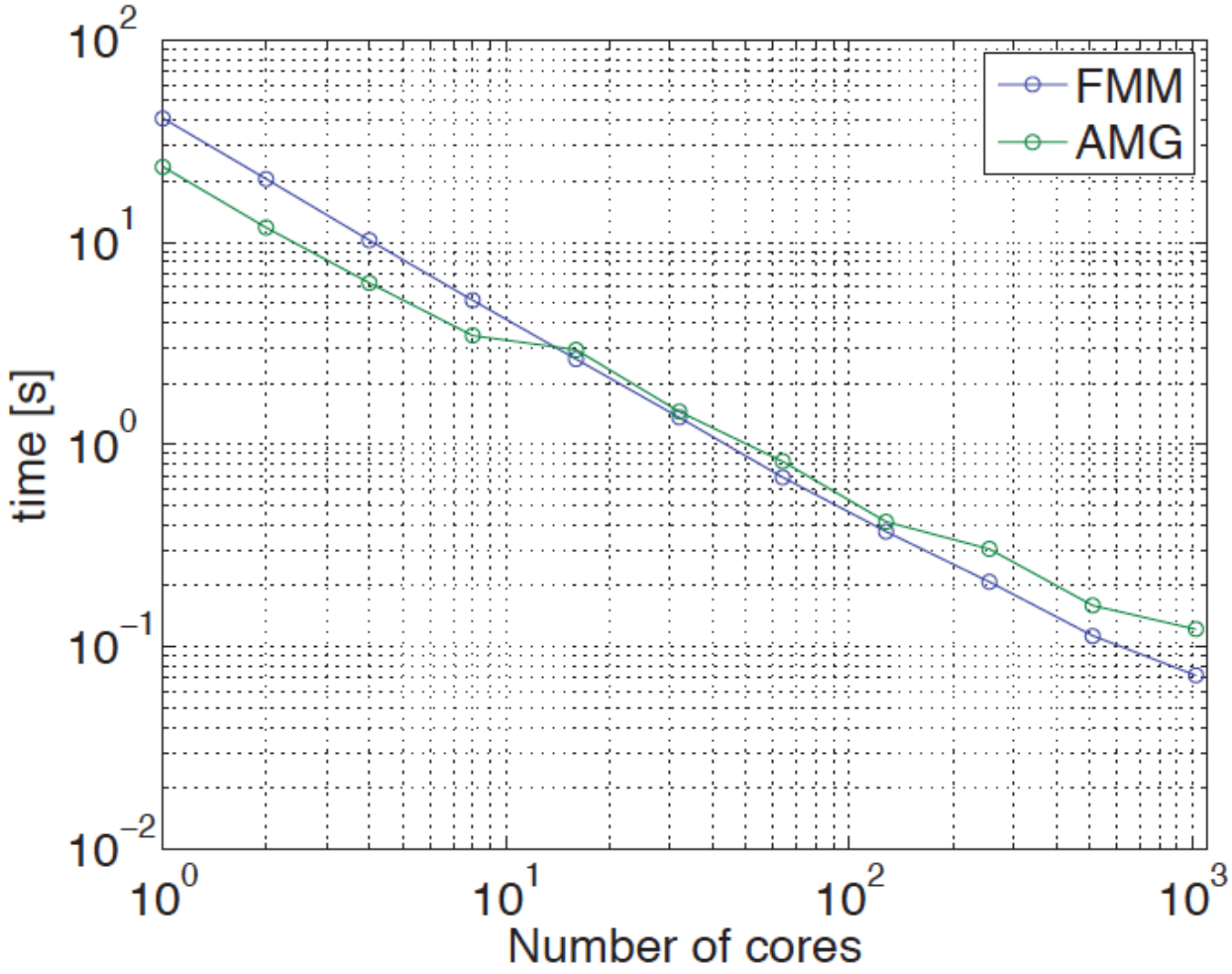
c/o R. Yokota, KAUST, *et al.*

FMM/BEM preconditioning of FEM-discretized Poisson



c/o R. Yokota, KAUST, *et al.*

FMM vs AMG preconditioning: strong scaling on Stampede*



*** FEM Poisson problem, Dirichlet BCs handled via BEM (cost included)**

c/o R. Yokota, KAUST, *et al.*

FMM as preconditioner

- Of course, when "trapped" inside a conventional preconditioned Krylov, FMM surrenders some potential benefits of relaxed synchrony because of the synchrony of the Krylov method
- Krylov methods need rework, generally, for any preconditioner
- Pipelined CG and GMRES are included now in PETSc and other Krylov libraries, proved practical

Algebraic Fast Multipole for variable coefficient equilibrium problems

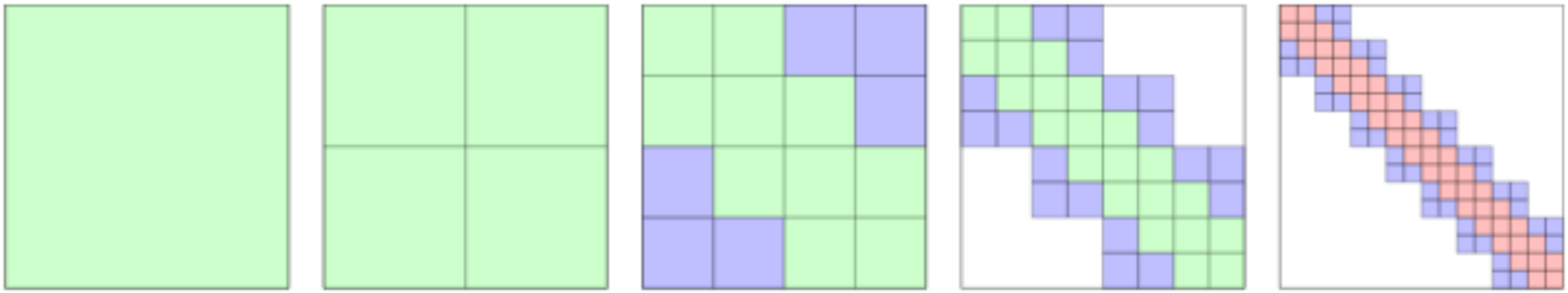
- All the benefits of Fast Multipole

plus

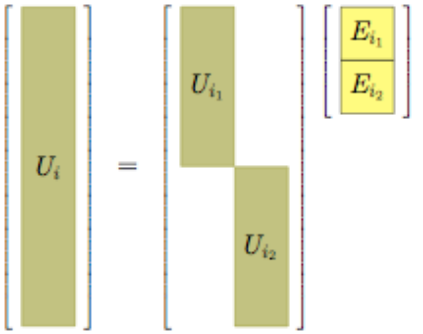
- Make Fast Multipole less fragile

Is there an algebraic FMM?

- Consider the H^2 hierarchical matrix method of Hackbusch, *et al.*



- Off diagonal blocks $A_{ij} \cong U_i S_{ij} V_j$ can have low rank, based on an "admissibility condition"
- Bases can be hierarchically nested
  - U_i for columns, V_j for rows



Reminder where low rank is found, e.g., 1D Laplacian

Full rank!

$$\mathbf{A} = 64 \times \begin{bmatrix} 2 & -1 & & & & & \\ -1 & 2 & -1 & & & & \\ & -1 & 2 & -1 & & & \\ & & -1 & 2 & -1 & & \\ & & & -1 & 2 & -1 & \\ & & & & -1 & 2 & -1 \\ & & & & & -1 & 2 \end{bmatrix}$$

Off diagonal blocks have low rank!

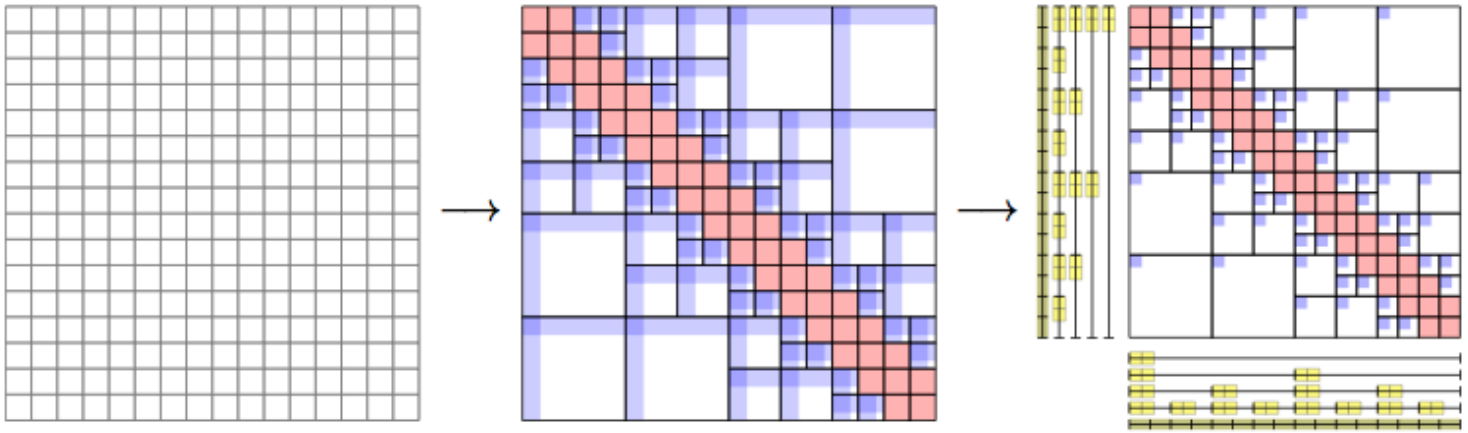
Full rank!

$$\mathbf{A}^{-1} = \frac{1}{512} \times \begin{bmatrix} 7 & 6 & 5 & 4 & 3 & 2 & 1 \\ 6 & 12 & 10 & 8 & 6 & 4 & 2 \\ 5 & 10 & 15 & 12 & 9 & 6 & 3 \\ 4 & 8 & 12 & 16 & 12 & 8 & 4 \\ 3 & 6 & 9 & 12 & 15 & 10 & 5 \\ 2 & 4 & 6 & 8 & 10 & 12 & 6 \\ 1 & 2 & 3 & 4 & 5 & 6 & 7 \end{bmatrix}$$

Off diagonal blocks have low rank!

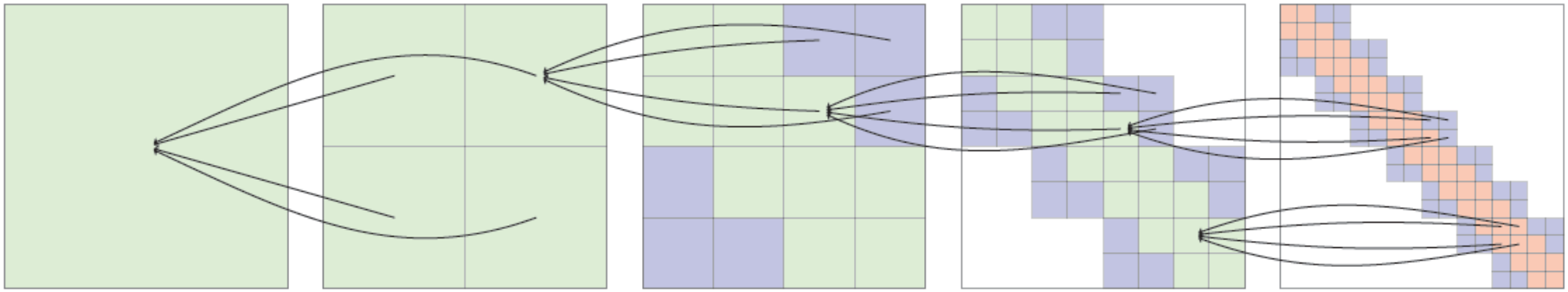
Is there an algebraic FMM?

- One needs to store the unreducible diagonal blocks, A_{ii}
- For the entire rest of the matrix, first the S_{ij} , the U_i and V_j at the finest level
- Then the E_{ij} (column basis conversion) and F_{ij} (row basis conversion) blocks at each level
- Two stage compression procedure: SVD each block, then convert to common bases



"Algebraic Fast Multipole" (AFM)

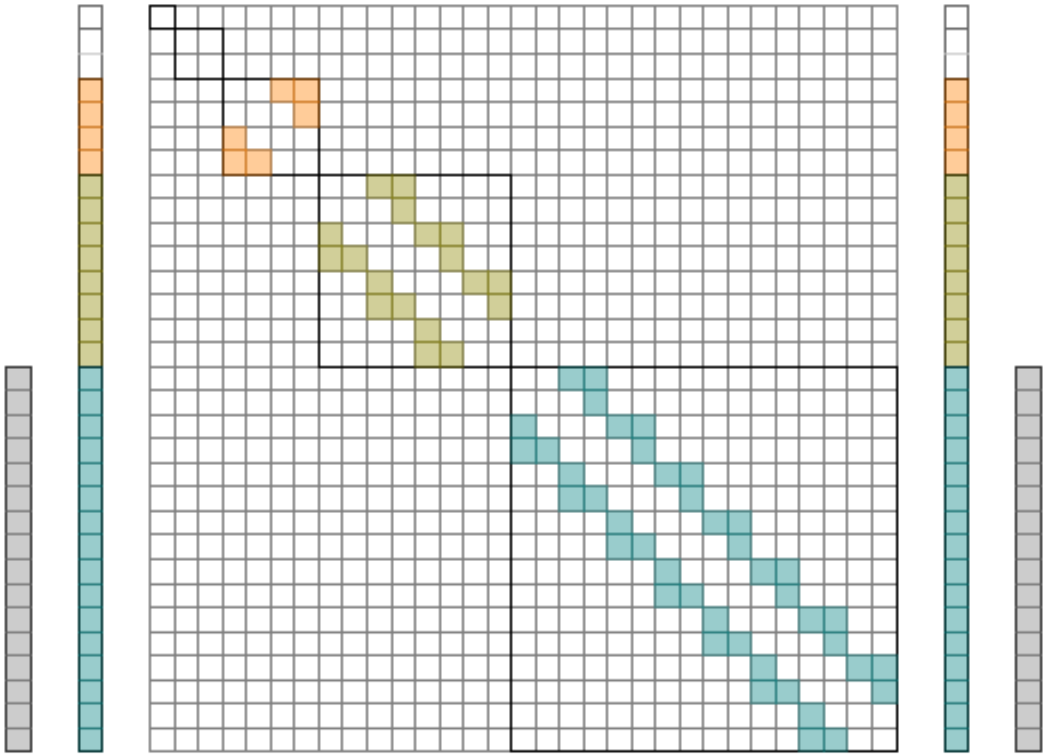
- **Can we cast general matrix operations (add, multiply, invert, etc.) in terms of the fast multipole recursive "tree-based" data structure?**



- **Yes, after compressing the matrix in H^2 form**
  - **presumes hierarchical low rank structure**
  - **may offer breakthrough in application performance**
  - **See *Supercomput. Front. Innov.* 1:62-83 (2014)**

Fast matrix-vector multiply, *y=Ax*

$$y = \left(\sum_{(i,j)\in D} A_{ij} \right) x + \left(\sum_{(i,j)\in L} U_i S_{ij} V_j^t \right) x = \underbrace{\sum_{(i,j)\in D} A_{ij} x_j}_{\text{Dense mat-vecs operations}} + \underbrace{\sum_{i\in I} U_i \underbrace{\sum_{(i,j)\in L} S_{ij} \underbrace{V_j^t x}_{\text{Upsweep}}}_{\text{Coupling phase}}}_{\text{Downsweep}}$$



Fast matrix-vector multiply, *y=Ax*

Table 5. Communication breakdown of hierarchical matrix-vector multiplication compared to FMM (cf. tab. 3).

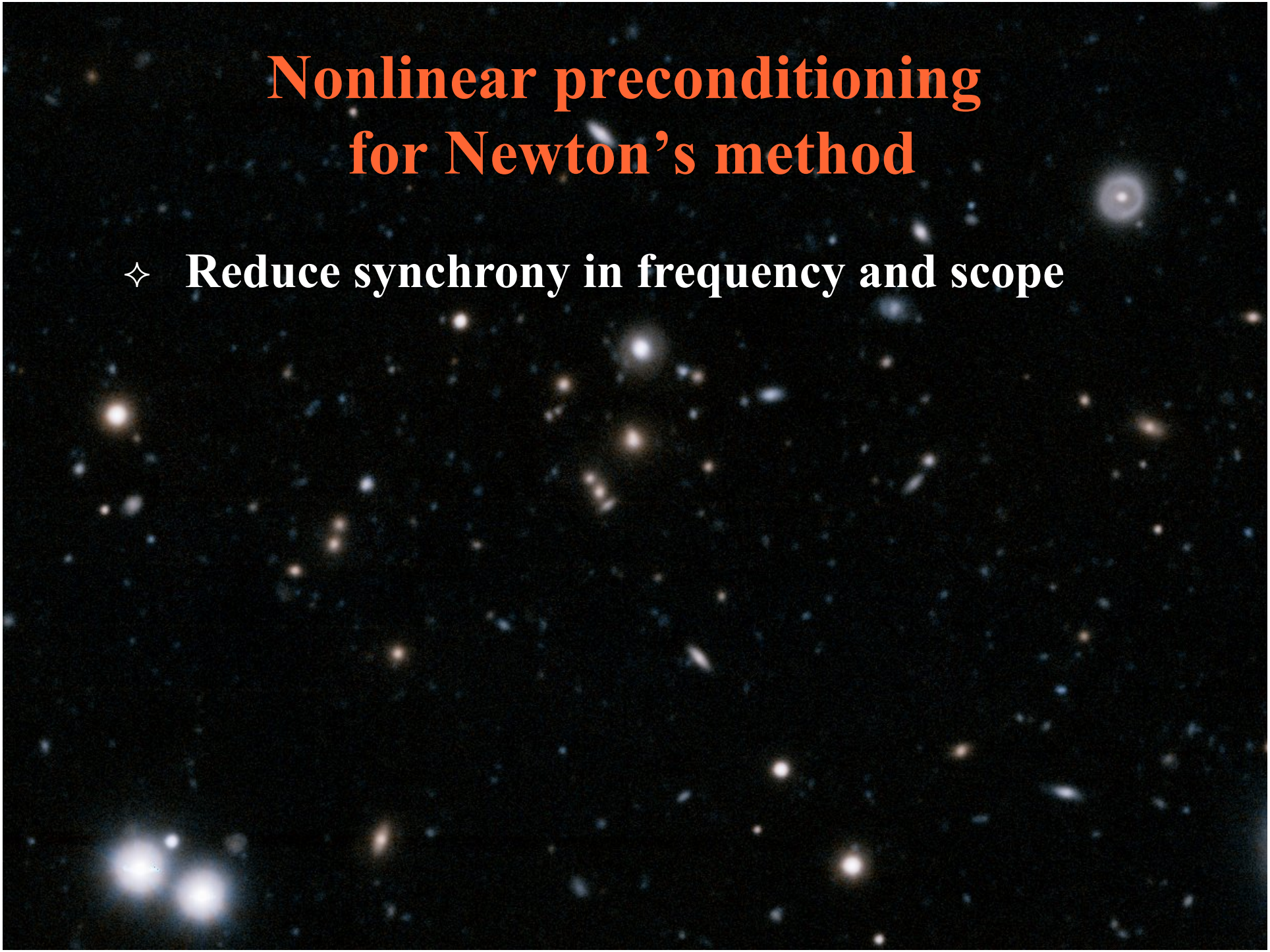
H-matrix operation	FMM operation	Processes	Blocks per level	Blocks per Process	Communication
Global $\sum S_{ij}\hat{x}_j$	Global M2L	$\sum_{i}^{\log P} \mathcal{O}(1)$	$\mathcal{O}(1)$	$\mathcal{O}(1)$	$\mathcal{O}(\log P)$
Global $\sum F_k^t \hat{x}_k$	Global M2M	$\sum_{i}^{\log P} \mathcal{O}(1)$	$\mathcal{O}(1)$	$\mathcal{O}(1)$	$\mathcal{O}(\log P)$
Local $\sum S_{ij}\hat{x}_j$	Local M2L	$\mathcal{O}(1)$	$\mathcal{O}(2^{(d-1)i})$	$\sum_{i}^{\log_{2^d}(N/P)} \mathcal{O}(2^{(d-1)i})$	$\mathcal{O}((N/P)^{\frac{d-1}{d}})$
Local $\sum A_{ij}x_j$	Local P2P	$\mathcal{O}(1)$	$\mathcal{O}(2^{(d-1)i})$	$\mathcal{O}(2^{(d-1)\log_{2^d}(N/P)})$	$\mathcal{O}((N/P)^{\frac{d-1}{d}})$

Optimal hierarchical algorithms

- **Some optimal hierarchical algorithms**
  - **Fast Fourier Transform (Cooley-Tukey, 1965)***
  - **Multigrid (Brandt, 1977)***
  - **Fast Multipole Method (Greengard-Rokhlin, 1985)**
  - **Sparse grids (Zenger, 1991)***
  - **$\mathcal{H}$-matrices (Hackbusch, 1999)**
  - **<your generation's method> – missing so far ☺**
- **What is the potential for reducing over-ordering and exposing concurrency with these flop-optimal methods?**

* References to popularizing paper, not earliest conception

Scalable Hierarchical Algorithms in Extreme Computing workshop, 4-6 May 2014



Nonlinear preconditioning for Newton's method

- Reduce synchrony in frequency and scope

Reduction of domain of synchronization in nonlinearly preconditioned Newton

- **Newton method for a global nonlinear system, $F(u)=0$,**
  - **computes a global distributed Jacobian matrix and synchronizes globally in both the Newton step and in solving the global linear system for the Newton**
- **Nonlinearly preconditioned Newton replaces this with a set of local problems on subsets of the global nonlinear system**
  - **each local problem has only local synchronization**
  - **each of the linear systems for local Newton updates has only *local* synchronization**
  - **there is still global synchronization in a number of steps, hopefully *many fewer* than required in the original Newton method**

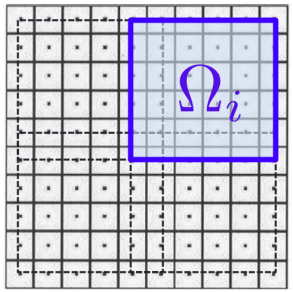
Implemented in PETSc, as "ASPIN"

Key idea

Finding the solution u^* by solving an equivalent nonlinear system

$$\mathcal{F}(u^*) = 0 \Leftrightarrow F(u^*) = 0$$

using Inexact Newton with Backtracking



How to construct the equivalent nonlinear system?

$$F_{\Omega_i}(u - T_{\Omega_i}(u)) = 0, \qquad i = 1, \ldots, N$$

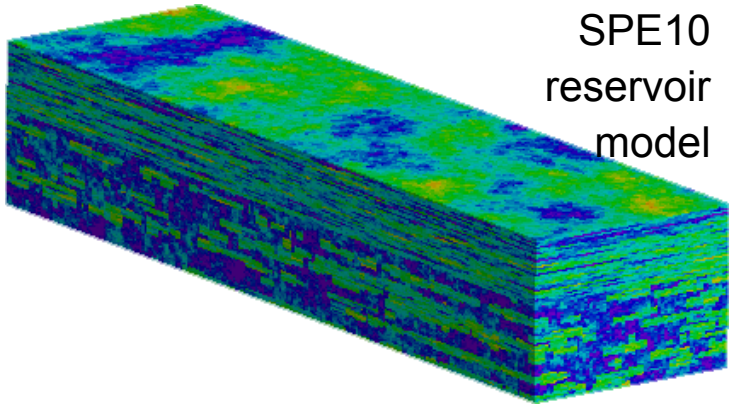
$$\mathcal{F}(u) = \sum_{i=1}^{N} T_{\Omega_i}(u) \qquad \bigcup_{i=1}^{N} \Omega_i = \Omega$$

Assumption

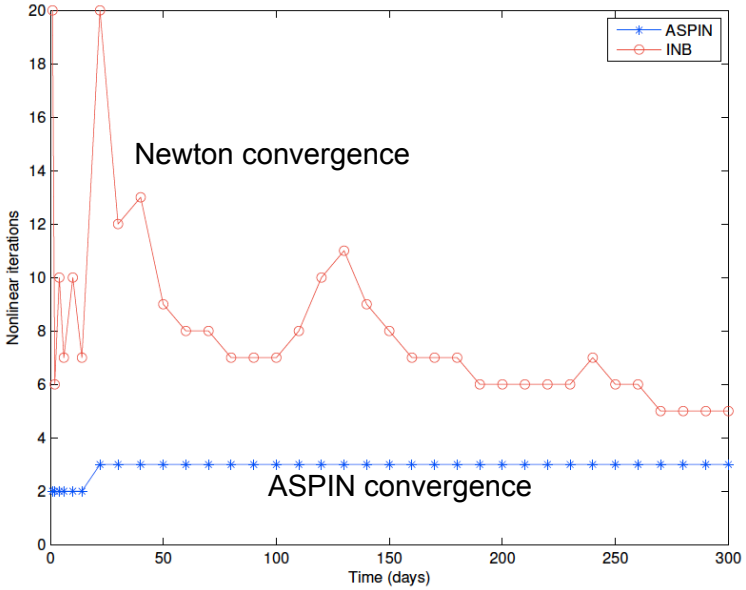
$F'(u)$ is continuous in a neighborhood D of the exact solution u^*, and the matrix $F'(u^*)$ is nonsingular.

Theorem

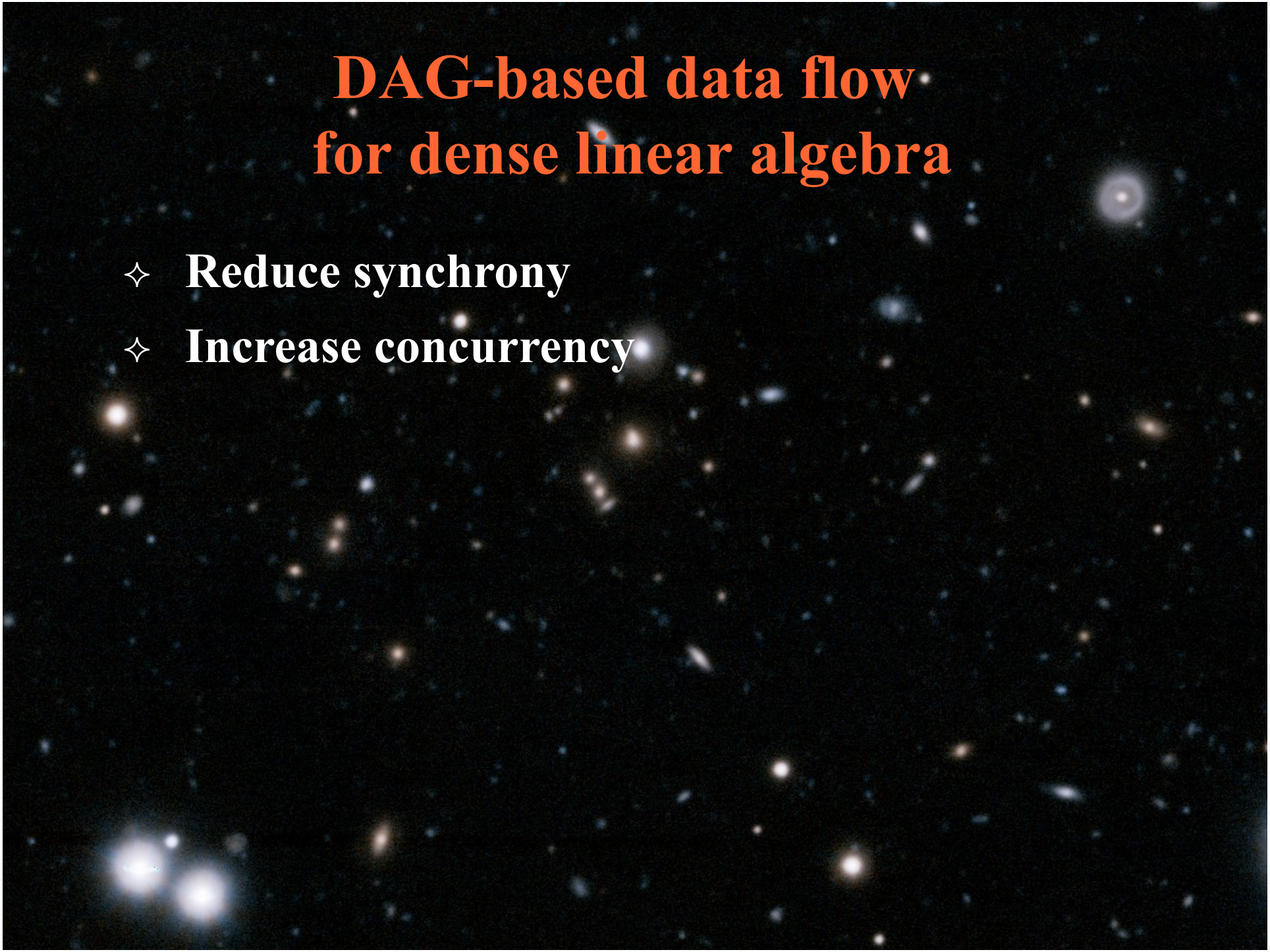
(Cai and Keyes, 2002). $F(u)$ and $\mathcal{F}(u)$ are equivalent in the sense that they have the same solution in a neighborhood of u^* in D.



SPE10 reservoir model



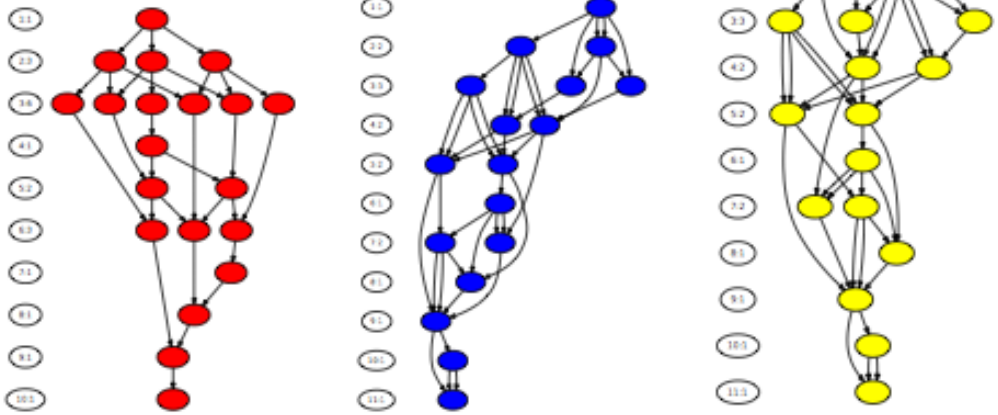
c/o L. Liu, KAUST


DAG-based data flow
for dense linear algebra
Reduce synchrony
Increase concurrency

Reducing over-ordering and synchronization through dataflow: e.g., generalized eigensolver

$$Ax = \lambda Bx$$

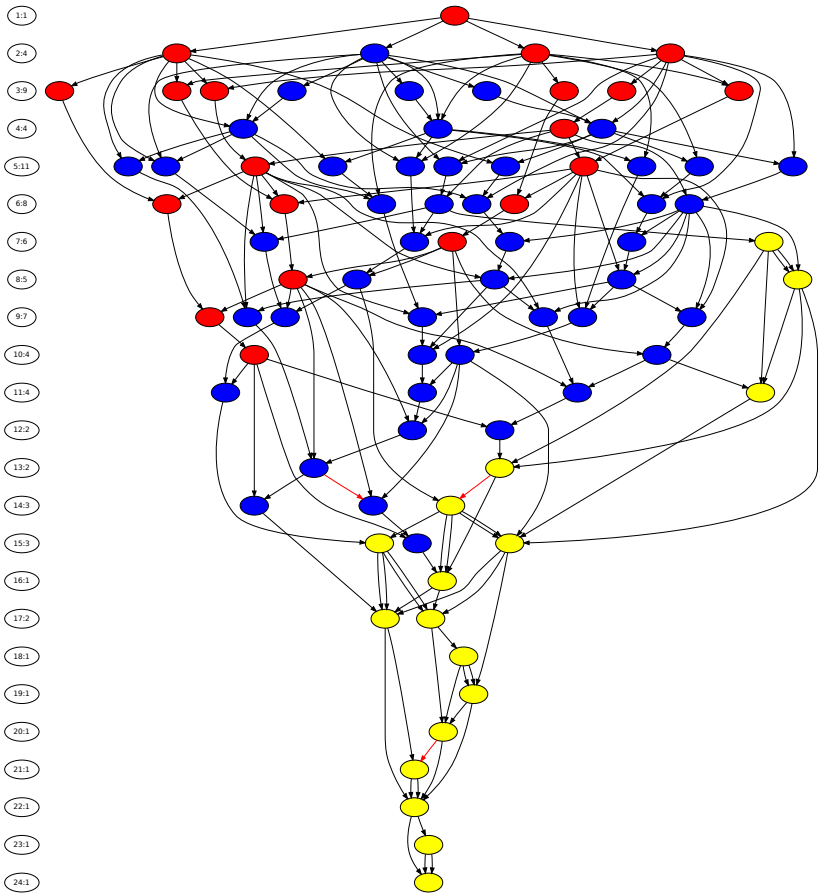
Operation	Explanation	LAPACK routine name
1. $B = L \times L^T$	Cholesky factorization	POTRF
2. $C = L^{-1} \times A \times L^{-T}$ or HEGST	application of triangular factors	SYGST
3. $T = Q^T \times C \times Q$	tridiagonal reduction	SYEVD or HEEVD
4. $Tx = \lambda x$	QR iteration	STERF



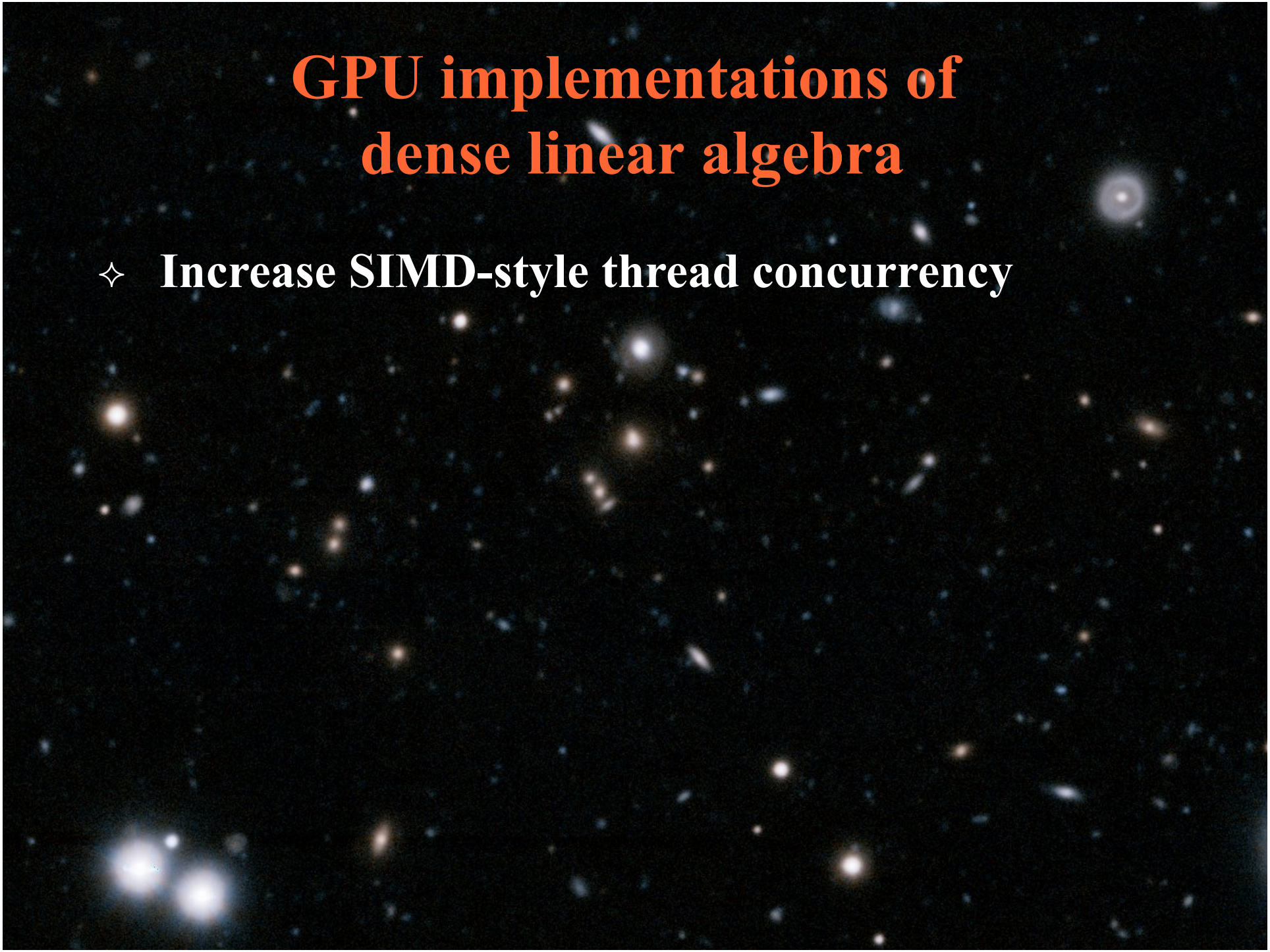
c/o H. Ltaief, KAUST

Loop nests and subroutine calls, with their over-orderings, can be replaced with DAGs

- Diagram shows a dataflow ordering of the steps of a 4×4 symmetric generalized eigensolver
- Nodes are tasks, color-coded by type, and edges are data dependencies
- Time is vertically downward
- Wide is good; short is good



c/o H. Ltaief, KAUST



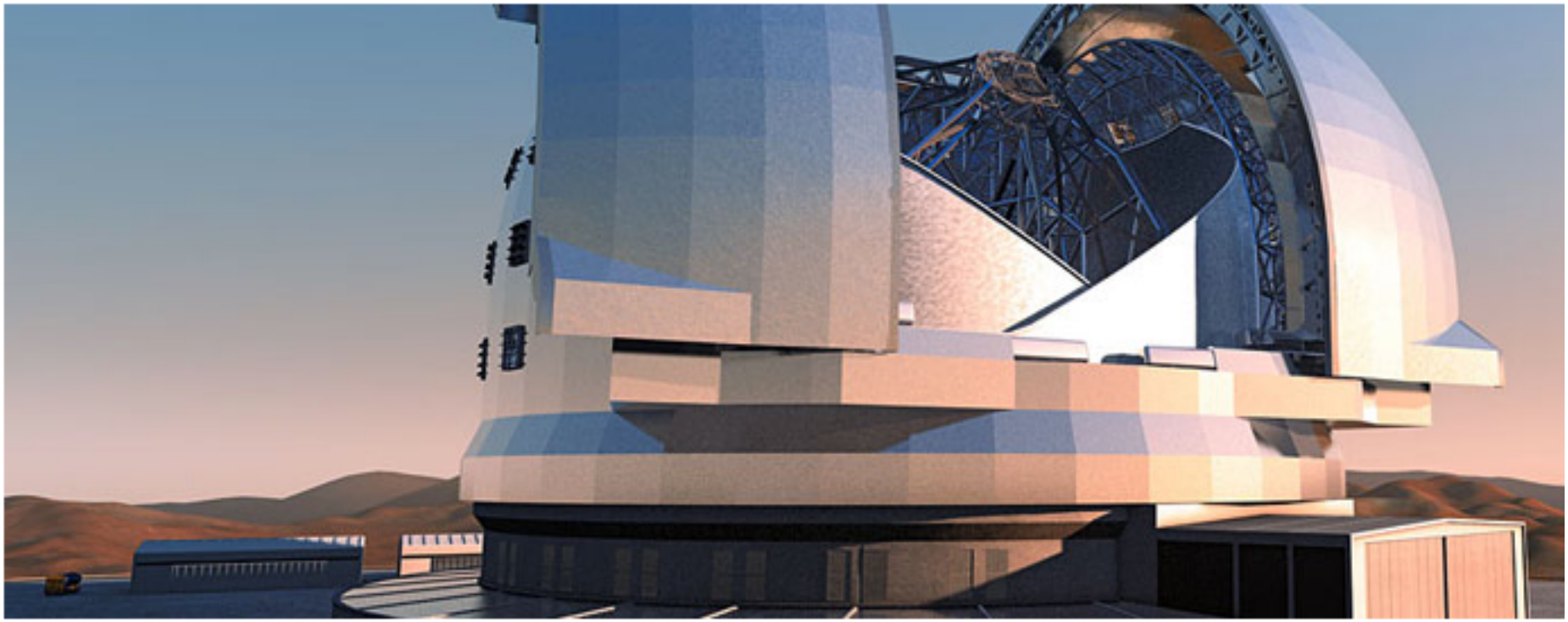
GPU implementations of dense linear algebra

- Increase SIMD-style thread concurrency

Applied in European telescope (ELT) (13X speedup - tech paper for SC'14)

The European Extremely Large Telescope

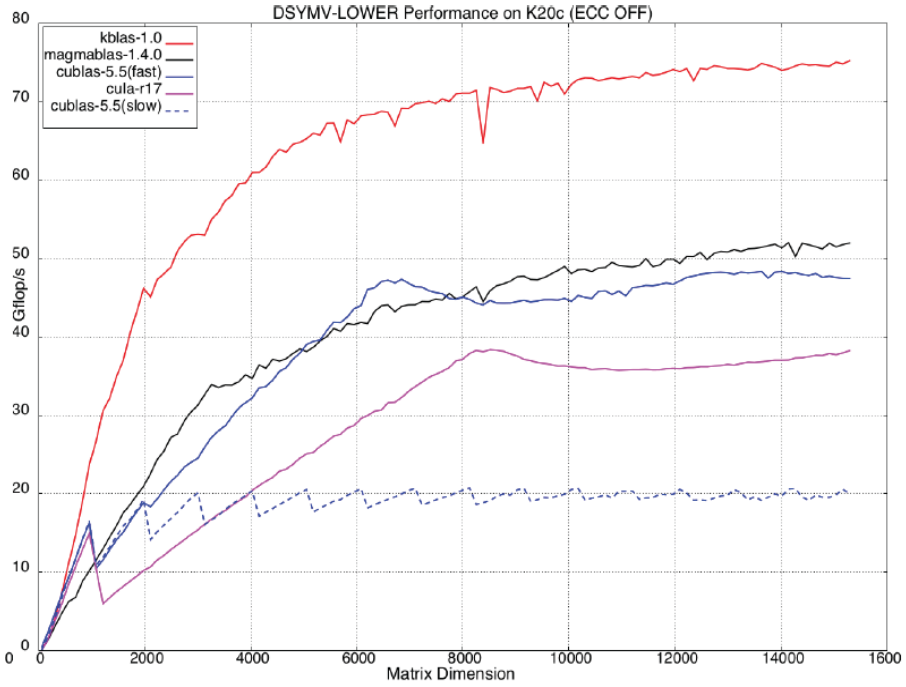
The world's biggest eye on the sky

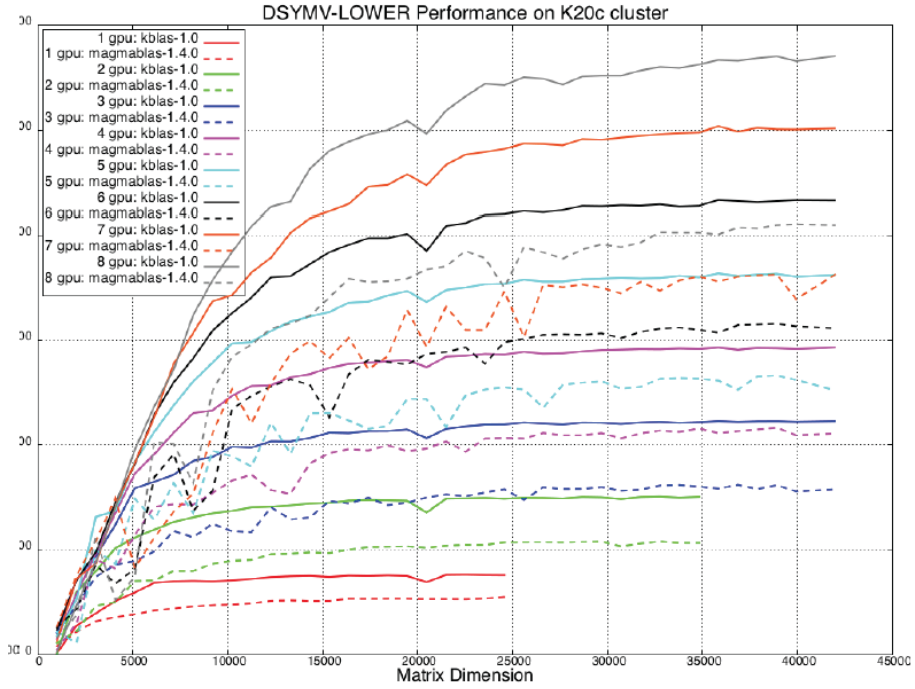


© ESO, https://www.eso.org/sci/facilities/develop/ao/ao_modes.html

c/o Ahmad Abdelfattah & Ali Charara, KAUST

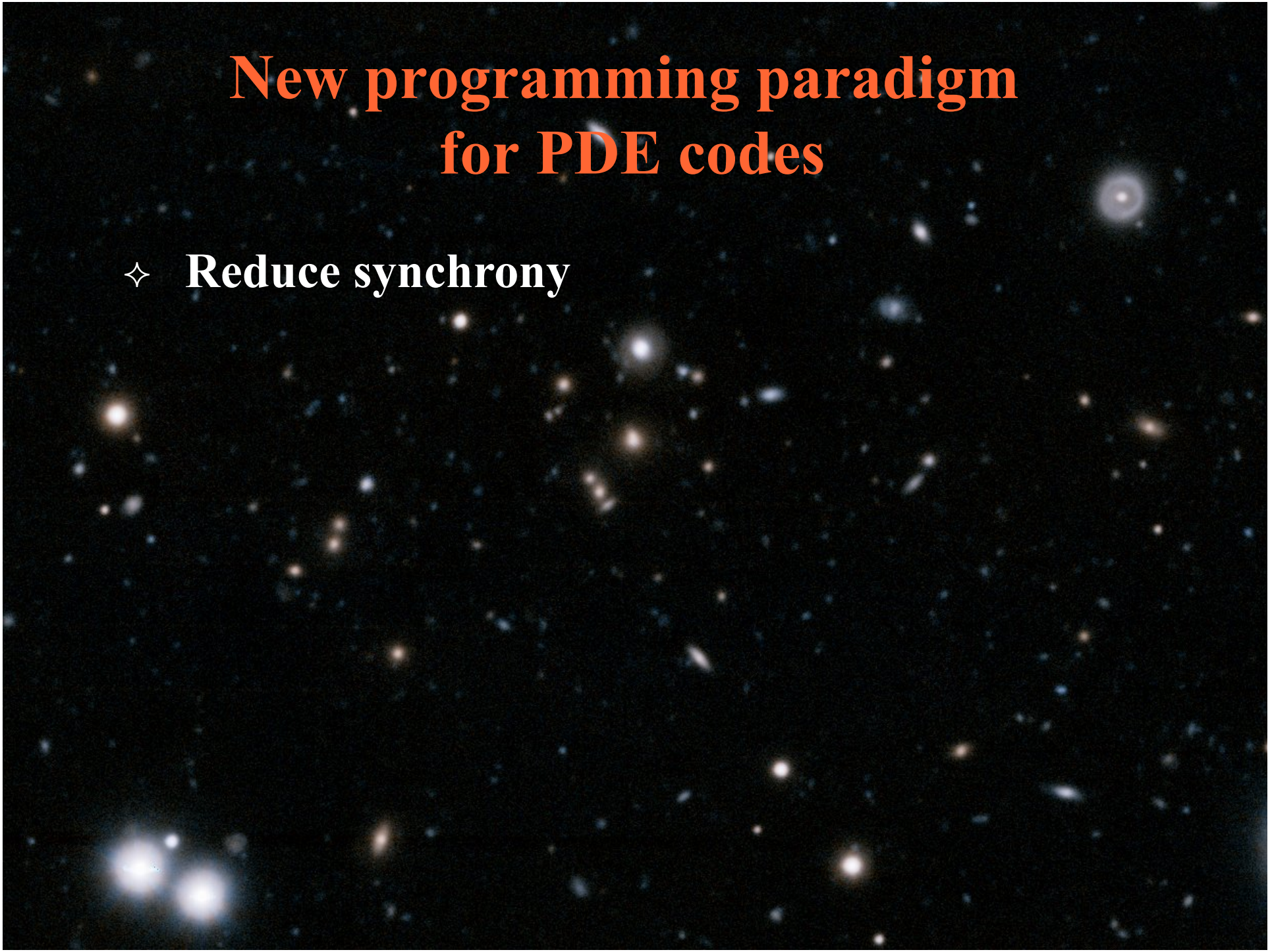
New linear algebra software, KAUST's GPU BLAS, now in NVIDIA's CUBLAS





- **Highly optimized GEMV/SYMV kernels**
- **NVIDIA has adopted for its CUBLAS 6.0 library**

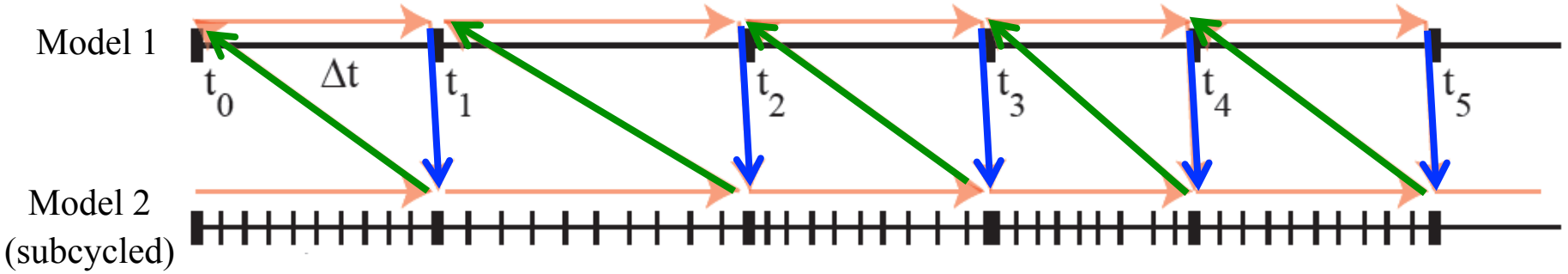
c/o Ahmad Abdelfattah, KAUST



New programming paradigm for PDE codes

- Reduce synchrony

Multiphysics w/ legacy codes: *an endangered species?*



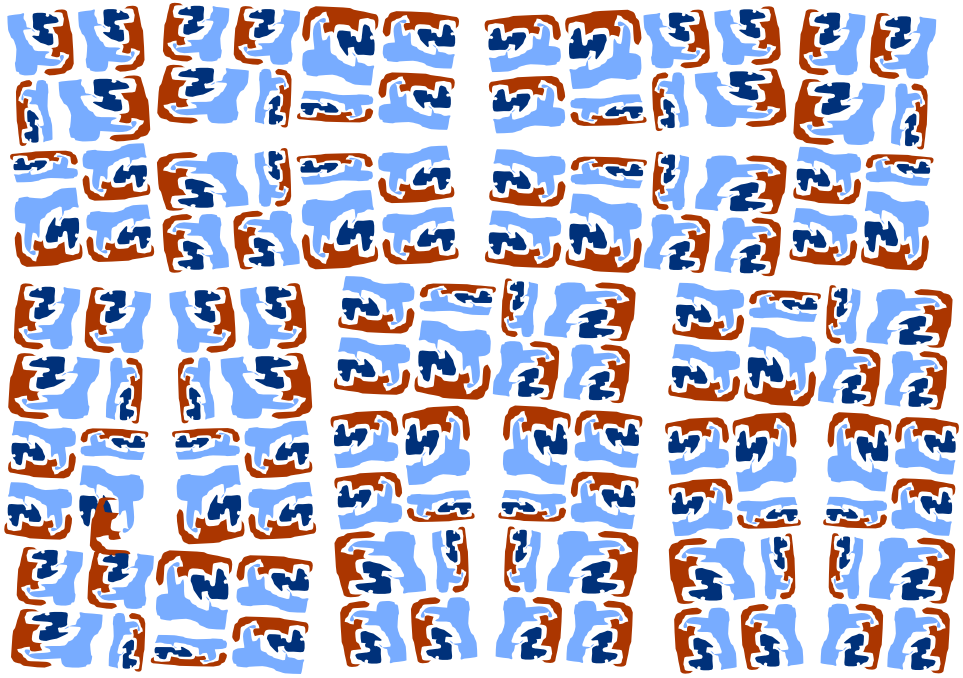
- **Many multiphysics codes operate like this, where the models may occupy the same domain in the bulk (e.g., reactive transport) or communicate at interfaces (e.g., ocean-atmosphere)***
- **The data transfer cost represented by the blue and green arrows may be much higher than the computation cost of the models, even apart from first-order operator splitting error and possible instability**

*see "Multiphysics simulations: challenges and opportunities" (IJHPCA)

Many codes have the algebraic and software structure of multiphysics

- **Exascale is motivated by these:**
  - **uncertainty quantification, inverse problems, optimization, immersive visualization and steering**
- **These may carry auxiliary data structures to/from which blackbox model data is passed and they act like just another "physics" to the hardware**
  - **pdfs, Lagrange multipliers, etc.**
- **Today's separately designed blackbox algorithms for these may not live well on exascale hardware: co-design may be required due to data motion**

Multiphysics layouts must invade blackboxes



- Each application must first be ported to extreme scale (distributed, hierarchical memory)
- Then applications may need to be interlaced at the data structure level to minimize copying and allow work stealing at synchronization points

THE INTERNATIONAL JOURNAL of HIGH PERFORMANCE COMPUTING APPLICATIONS

The International Journal of High Performance Computing Applications
27(1) 4–82

DOI: 10.1177/1094342012468181
hpc.sagepub.com
SAGE

Multiphysics simulations: Challenges and opportunities

David E Keyes[1,2], Lois C McInnes[3], Carol Woodward[4], William Gropp[5], Eric Myra[6], Michael Pernice[7], John Bell[8], Jed Brown[3], Alain Clo[1], Jeffrey Connors[4], Emil Constantinescu[3], Don Estep[9], Kate Evans[10], Charbel Farhat[11], Ammar Hakim[12], Glenn Hammond[13], Glen Hansen[14], Judith Hill[10], Tobin Isaac[15], Xiangmin Jiao[16], Kirk Jordan[17], Dinesh Kaushik[3], Efthimios Kaxiras[18], Alice Koniges[8], Kihwan Lee[19], Aaron Lott[4], Qiming Lu[20], John Magerlein[17], Reed Maxwell[21], Michael McCourt[22], Miriam Mehl[23], Roger Pawlowski[14], Amanda P Randles[18], Daniel Reynolds[24], Beatrice Rivière[25], Ulrich Rüde[26], Tim Scheibe[13], John Shadid[14], Brendan Sheehan[9], Mark Shephard[27], Andrew Siegel[3], Barry Smith[3], Xianzhu Tang[28], Cian Wilson[2] and Barbara Wohlmuth[23]

Abstract

We consider multiphysics applications from algorithmic and architectural perspectives, where "algorithmic" includes both mathematical analysis and computational complexity, and "architectural" includes both software and hardware environments. Many diverse multiphysics applications can be reduced, en route to their computational simulation, to a common algebraic coupling paradigm. Mathematical analysis of multiphysics coupling in this form is not always practical for realistic applications, but model problems representative of applications discussed herein can provide insight. A variety of software frameworks for multiphysics applications have been constructed and refined within disciplinary communities and executed on leading-edge computer systems. We examine several of these, expose some commonalities among them, and attempt to extrapolate best practices to future systems. From our study, we summarize challenges and forecast opportunities.

How will PDE computations adapt?

- Programming model will still be dominantly message-passing (due to large legacy code base), adapted to multicore or hybrid processors beneath a relaxed synchronization MPI-like interface
- Load-balanced blocks, scheduled today with nested loop structures will be separated into critical and non-critical parts
- Critical parts will be scheduled with directed acyclic graphs (DAGs) through dynamic languages or runtimes
  - e.g., ADLB, Charm++, Quark, StarPU, OmpSs, Parallex, Argo
- Noncritical parts will be made available for NUMA-aware work-stealing in economically sized chunks

Adaptation to asynchronous programming styles

- To take full advantage of such asynchronous algorithms, we need to develop greater expressiveness in scientific programming
  - create separate threads for logically separate tasks, whose priority is a function of algorithmic state, not unlike the way a time-sharing OS works
  - join priority threads in a directed acyclic graph (DAG), a task graph showing the flow of input dependencies; fill idleness with noncritical work or steal work

Evolution of Newton-Krylov-Schwarz: breaking the synchrony stronghold

- Can write code in styles that do not require artifactual synchronization
- Critical path of a nonlinear implicit PDE solve is essentially

  … lin_solve, bound_step, update; lin_solve, bound_step, update …
- However, we often insert into this path things that could be done less synchronously, because we have limited language expressiveness
  - Jacobian and preconditioner refresh
  - convergence testing
  - algorithmic parameter adaptation
  - I/O, compression
  - visualization, data mining

Sources of nonuniformity

- **System**
  - ***Already* important: manufacturing, OS jitter, TLB/cache performance variations, network contention,**
  - ***Newly* important: dynamic power management, more soft errors, more hard component failures, software-mediated resiliency, etc.**
- **Algorithmic**
  - **physics at gridcell/particle scale (e.g., table lookup, equation of state, external forcing), discretization adaptivity, solver adaptivity, precision adaptivity, etc.**
- **Effects of both types are similar when it comes to waiting at synchronization points**
- **Possible solutions for system nonuniformity will improve programmability, too**

Other galaxies

Other hopeful algorithmic directions

- **74 two-page whitepapers contributed by the international community to the Exascale Mathematics Working Group (EMWG) at**

  https://collab.mcs.anl.gov/display/examath/Submitted+Papers

- **20-21 August 2013 in Washington, DC**
  - **Randomized algorithms**
  - **On-the-fly data compression**
  - **Algorithmic-based fault tolerance**
  - **Adaptive precision algorithms**
  - **Concurrency from dimensions beyond space (time, phase space, stochastic parameters)**
  - **etc.**

Trends according to Pete Beckman, Argonne

Trending Up	Trending Down
Asynchrony, Latency Hiding	Block synchronous
Over Decomp & Load Balancing	Static partitioning per core
Massive Parallelism	Countable parallelism
Reduced RAM per Flop	Whole-socket shared memory
Software-managed memory	Simple NUMA
Expensive Data Movement	Expensive flops
Fault / Resilience Strategies	Pure checkpoint/restart
Low BW to Storage, in-situ analysis	Save all

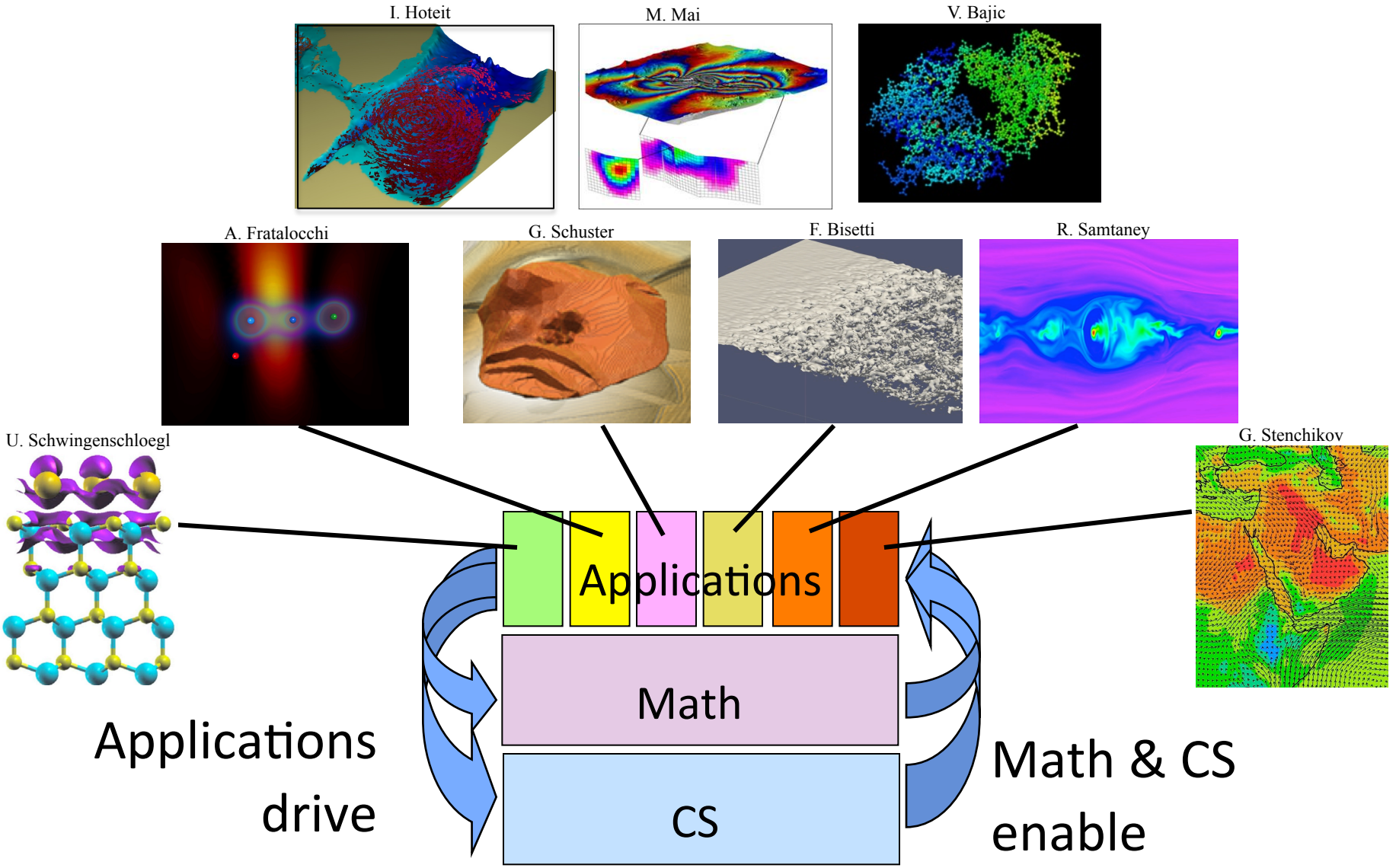
c/o P. Beckman, Intro to this meeting

More trends

Trending Up	Trending Down
User-controlled data replication	System-controlled data replication
User-controlled error handling	System-controlled error handling
Adaptive variable precision	Default high precision
Computing with "deltas"	Computing directly with QoI
High order discretizations	Low order discretizations
Exploitation of low rank	Default full rank

An algorithmic theme: defeat the curses of dimensionality and multiple scales with the blessings of continuity and low rank

"SciDAC philosophy" of software investment




Thank you
جامعة الملك عبدالله
للعلوم والتقنية
King Abdullah University of
Science and Technology
KAUST is recruiting! Your office here ☺
شكرا
david.keyes@kaust.edu.sa