The missing mathematics of extreme scale simulation

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All talks speak from and into contexts

- **DOE and the world are at a crossroads with respect to the push towards extreme scale, which has proceeded steadily for three decades from mega- (1970s) to giga- (1988) to tera- (1998) to peta- (2008)**
  - **exa- is qualitatively different and will be much harder**
  - **FY 2012 authorization bills reserve a significant tranche, $126M, for exascale computation, but only $5M is new**
  - **base program scientists could feel threatened by a mandate that does not come with a new budget**
- **Base program represented at this meeting shows spectacular quality and creativity and must be protected from too disruptive a mandate**

A reminder from a wise one

Born 8 Dec 1865, Versailles

Died 17 Oct 1963, Paris

"Practical application is found by not looking for it, and one can say that the whole progress of civilization rests on that principle."

Jacques Salomon Hadamard

1896: proved the prime number theorem

1898: defined well-posedness (for boundary value problems)

Overlap of interests

- **Exascale's extremes change the game**
  - **mathematicians are back on the front line**
    - **without contributions in the form of new mathematics, the passage to the exascale will yield little fruit**
  - **mathematical scientists will find the computational power to do the things they want**
    - **room for creativity on many spine-tingling DOE challenges**
    - **mathematicians will participate in cross-disciplinary integration – "third paradigm" *and* "fourth paradigm"**
    - **remember that *exascale at the lab* means *petascale on the desk***
- **Let's mention some mathematical opportunities, after quickly reviewing the hardware challenges**

Game changers, in brief

- Reduced performance reliability of processor cores
- Reduced memory per core
- Reduced memory bandwidth per core
- Expensive (in time and energy) data motion
- Expensive (in time and energy) synchronization
- Proliferation of processor cores and SIMD units
- “Free flops” (if you don’t have to move the data)

Miracles "need not apply"

- **We should not expect to escape causal dependencies**
  - **if the input-to-output map of a problem description has all-to-all data dependencies, like an elliptic Green's function, we will have all-to-all communication**
- **But we should ask fundamental questions:**
  - **for the science of interest, do we need to evaluate the output everywhere?**
  - **is there another formulation that can produce the same scientific observables in less time and energy?**

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 will be limited by transmission

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

- **Hardware: many potentially exciting paths beyond today's CMOS silicon-based 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 main CDS&E workforce within the decade**

Prototype exascale hardware: a heterogeneous, distributed memory *GigaHz KiloCore MegaNode* system

Systems	2009	2018	Difference Today & 2018
System peak	**2 Pflop/s**	**1 Eflop/s**	**O(1000)**
Power	**6 MW**	**~20 MW**	**~3**
System memory	0.3 PB	32 - 64 PB [**.03 Bytes/Flop**]	O(100)
Node performance	125 GF	1,2 or 15TF	O(10) – O(100)
Node memory BW	25 GB/s	2 - 4TB/s [**.002 Bytes/Flop**]	O(100)
Node concurrency	12	O(1k) or 10k	O(100) – O(1000)
Total Node Interconnect BW	3.5 GB/s	200-400GB/s (1:4 or 1:8 from memory BW)	O(100)
System size (nodes)	18,700	O(100,000) or O(1M)	O(10) – O(100)
Total concurrency	225,000	O(billion) [O(10) to O(100) for latency hiding]	O(10,000)
Storage	15 PB	500-1000 PB (>10x system memory is min)	O(10) – O(100)
IO	0.2 TB	60 TB/s (how long to drain the machine)	O(100)
MTTI	days	O(1 day)	- O(10)

c/o P. Beckman, ANL

Some exascale themes (review)

- Clock rates cease to increase while arithmetic capacity increases dramatically w/concurrency
- Storage capacity diverges exponentially below arithmetic capacity
- Transmission capacity diverges exponentially below arithmetic capacity
- Mean time between hardware interrupts shortens
- Billions of dollars of scientific software hang in the balance until better algorithms arrive to span the architectural gap

Implications of operating on the edge

- **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 will have to be cycled off and on or clocks slowed and speeded based on compute schedules and based on cooling capacity**
  - **makes per node performance rate unreliable**

Implications of operating on the edge

- **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 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)**
- **It is already about 10^3 slower to to retrieve an operand from main DRAM memory than to perform an arithmetic operation – will get worse by a factor of ten**
  - **almost all operands must come from registers or upper cache**

Why push to extreme scale? (CSGF application essay question #3)

- Better resolve model's full, natural range of length or time scales
- Accommodate physical effects with greater fidelity
- Allow the model degrees of freedom in all relevant dimensions
- Better isolate artificial boundary conditions (e.g., in PDEs) or better approach realistic levels of dilution (e.g., in MD)
- Combine multiple complex models
- Solve an inverse problem, or perform data assimilation
- Perform optimization or control
- Quantify uncertainty
- Improve statistical estimates

"Third paradigm"

- Operate without models (machine learning)

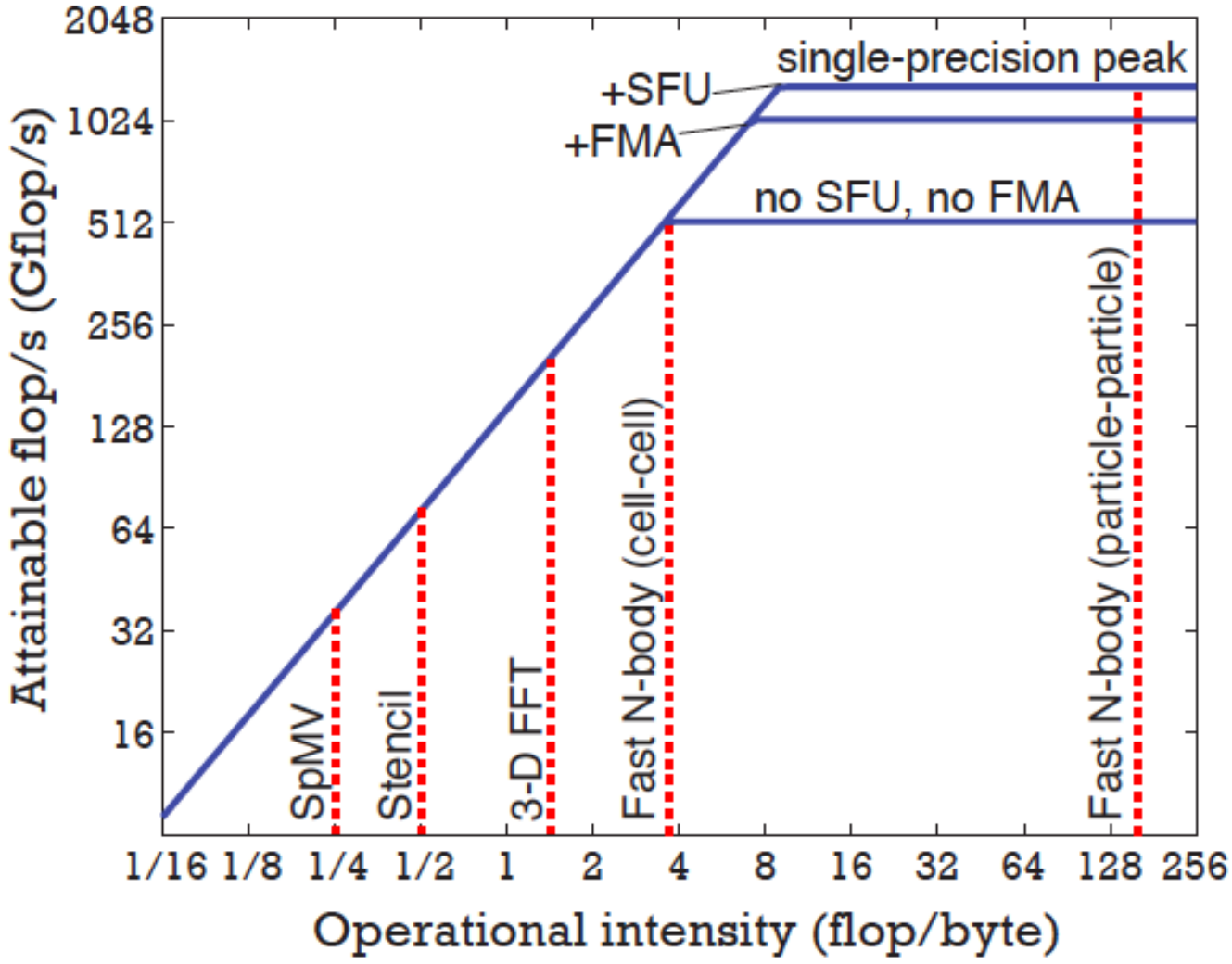
"Fourth paradigm"

"Missing" mathematics

- **New formulations with**
  - **greater arithmetic intensity (flops per bytes moved into and out of registers and upper cache)**
  - **reduced communication**
  - **reduced synchronization**
  - **assured accuracy with (adaptively) less floating-point precision**
- **Quantification of trades between limiting resources**
- ***Plus* all of the previously exciting analytical agendas that exascale is meant to exploit**

Arithmetic intensity example

Roofline model of FMM kernels on an NVIDIA C2050 GPU (Fermi). The 'SFU' label is used to indicate the use of special function units and 'FMA' indicates the use of fused multiply-add instructions. The order of multipole expansions was set to p = 15 .



How are most DOE workhorse codes implemented at the infra-petascale today?

- **Iterative methods based on data decomposition and message-passing**
  - **each individual processor works on a portion of the original problem and 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 SPMD/BSP/CSP**
  - **Single Program, Multiple Data**
  - **Bulk Synchronous Programming**
  - **Communicating Sequential Processes**

Estimating scalability

- **Given complexity estimates of the leading terms of:**
  - **the concurrent computation (per iteration phase)**
  - **the concurrent communication**
  - **the synchronization frequency**
- **And a model of the architecture including:**
  - **internode communication (network topology and protocol reflecting horizontal memory structure)**
  - **on-node computation (effective performance parameters including vertical memory structure)**
- **One can estimate optimal concurrency and optimal execution time**
  - **on per-iteration basis**
  - **simply differentiate time estimate in terms of problem size *N* and processor number *P* with respect to *P***

3D stencil computation weak scaling

(assume fast local network, tree-based global reductions)

- **Total wall-clock time per iteration (ignoring local comm.)**

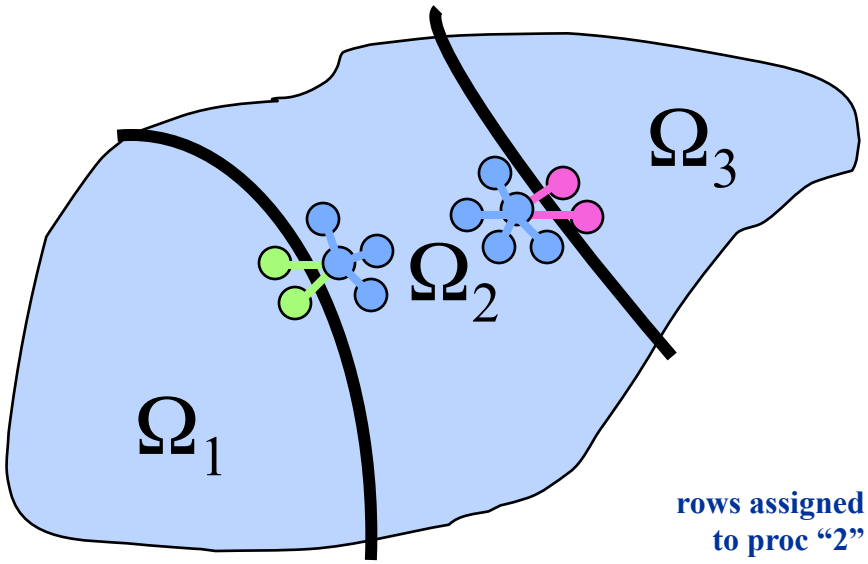
$$T(N,P) = A\frac{N}{P} + C\log P$$

- **For optimal P,** $\frac{\partial T}{\partial P} = 0$ **, or** $-A\frac{N}{P^2} + \frac{C}{P} = 0$

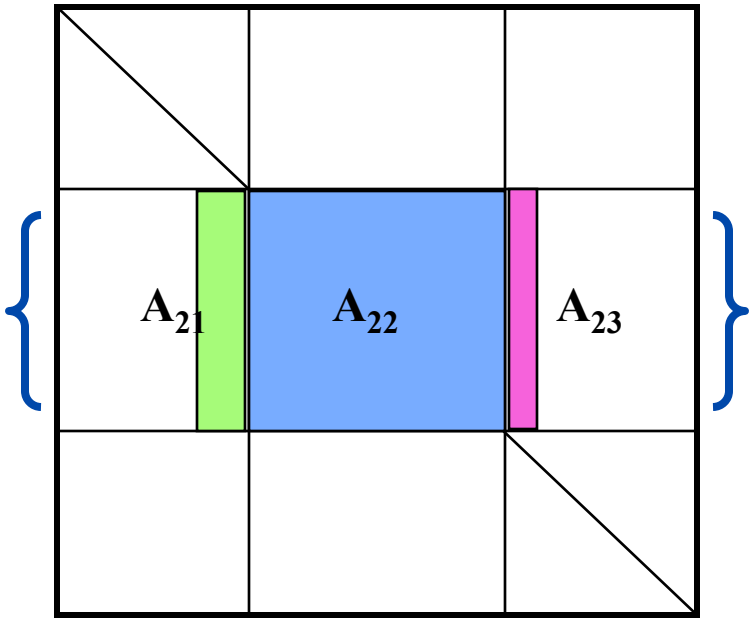
or $P_{opt} = \frac{A}{C}N$

- **P can grow linearly with N, and running time increases "only" logarithmically – as good as weak scaling can be!**
- **Problems: assumes perfect synchronization; and log of a billion may be "large"**

SPMD parallelism w/ domain decomposition: *an endangered species?*

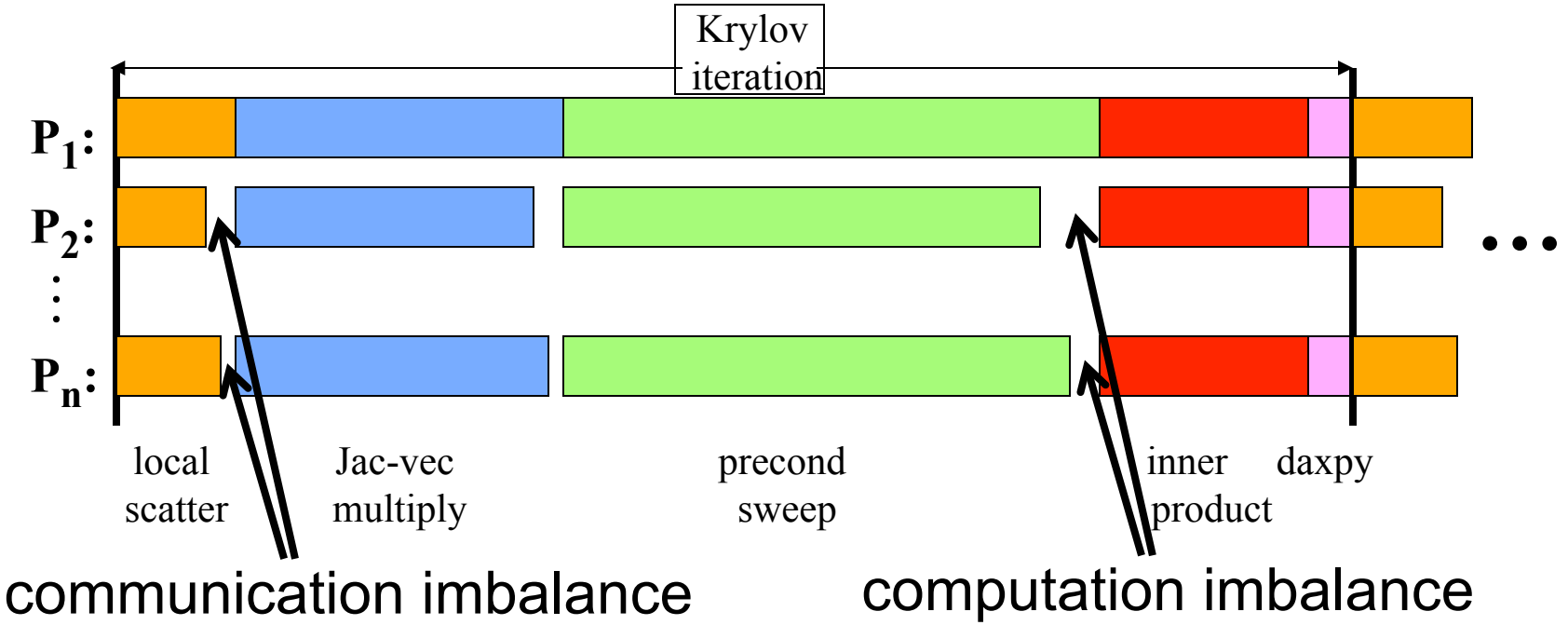


rows assigned to proc "2"



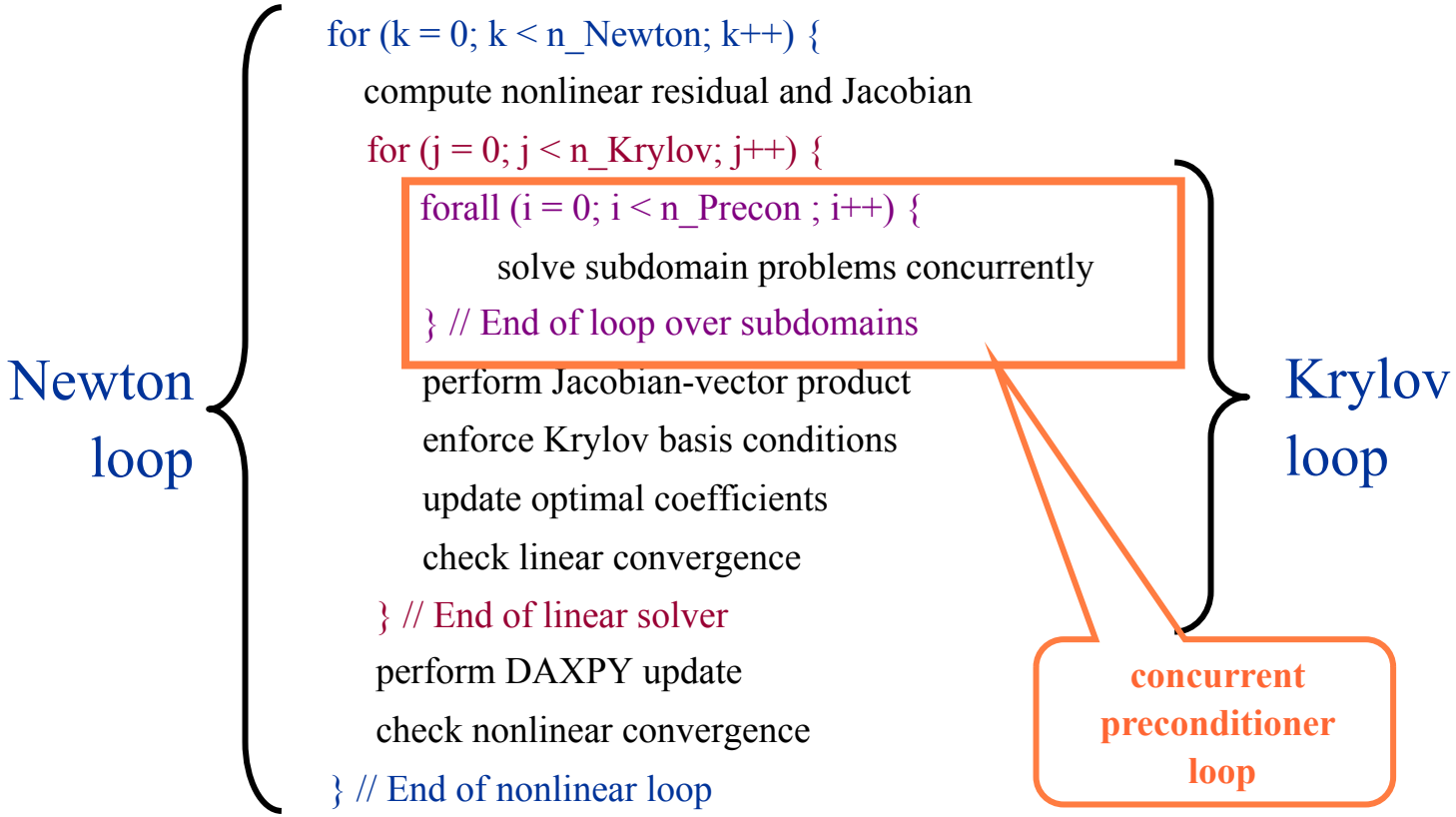
Partitioning of the grid induces block structure on the system matrix (Jacobian)

Workhorse innards: e.g., Krylov-Schwarz, a bulk synchronous implicit solver



Idle time due to load imbalance becomes a challenge at, say, one billion cores, when *one* processor can hold up *all* of the rest at a synchronization point

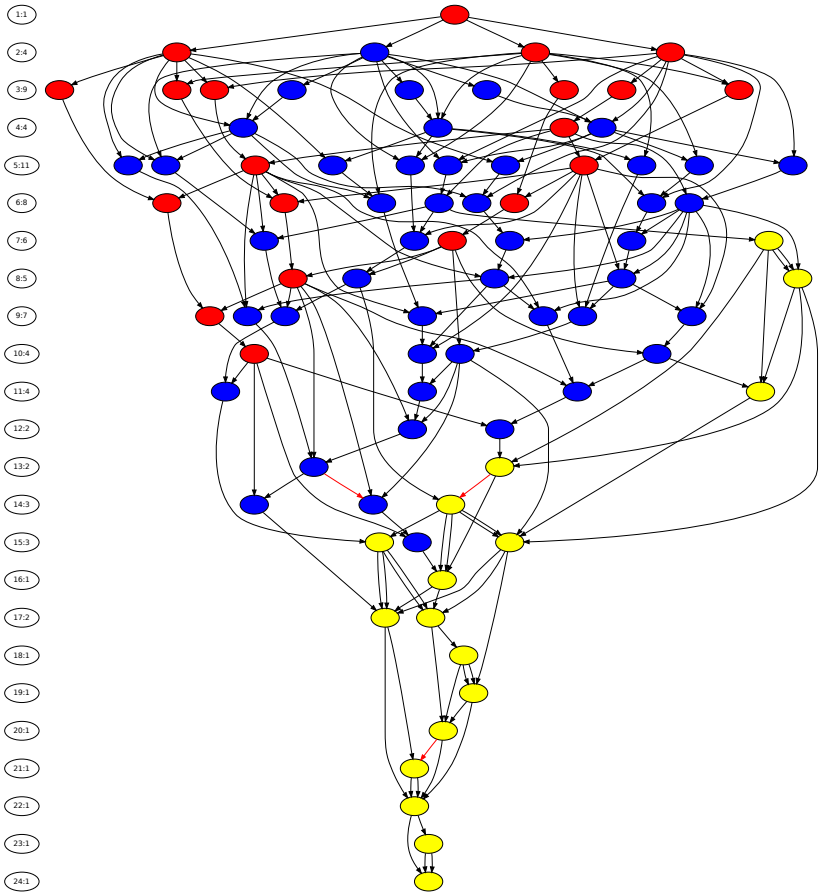
Our programming idiom is nested loops, e.g., Newton-Krylov-Schwarz



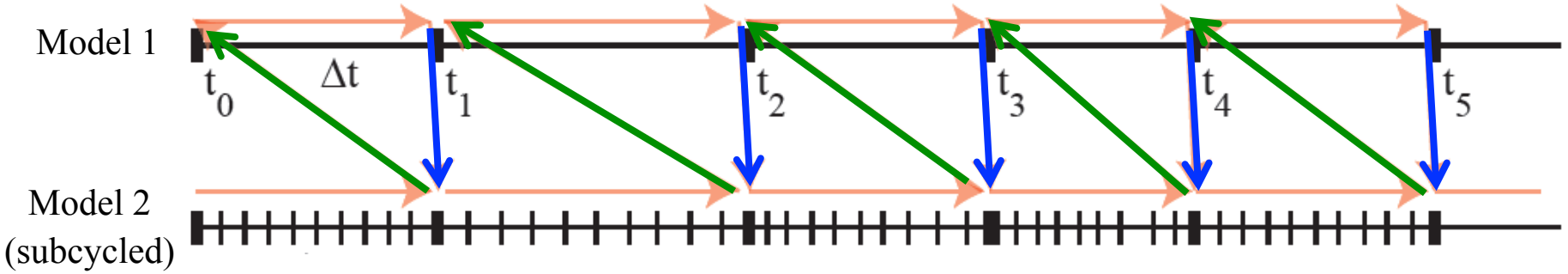
Outer loops (not shown): continuation, implicit timestepping, optimization

These loops, with their artifactual orderings, need to 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



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



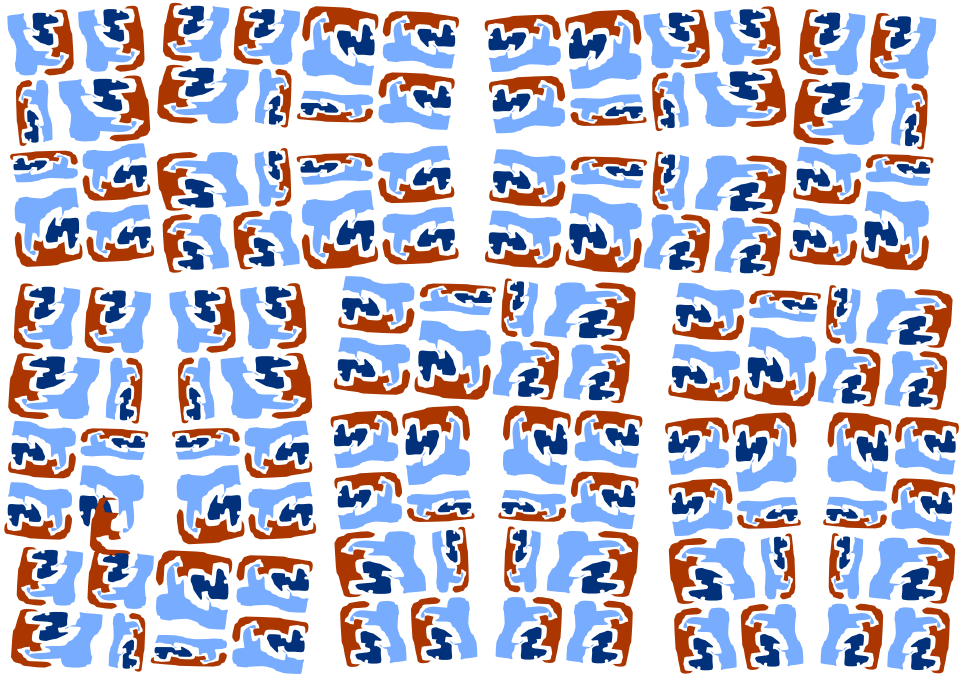
- **Many multiphysics codes operate like this, where the models may occupy the same domain in the bulk (e.g., reactive transport) or communicate at interfaces (e.g., ocean-atmosphere)***
- **The data transfer cost represented by the blue and green arrows may be much higher than the computation cost of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

*see forthcoming review paper from 2011 ICiS workshop

Many research frontiers 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

Bad news/good news (1)

- **One may have to control 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 under *Pax MPI*, already**
  - **but vertical replication into caches and registers was (until now with GPUs) 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 users into more arithmetically intensive formulations (e.g., fast multipole, lattice Boltzmann, rather than mainly PDEs)**
  - **tomorrow's optimal methods will (by definition) evolve to conserve what is expensive**

Bad news/good news (3)

- **Hardware nonuniformity may force abandonment of the Bulk Synchronous Programming (BSP) paradigm**
  - **it will be impossible for the user to control load balance sufficiently to make it work**
- **Hardware and algorithmic nonuniformity will be indistinguishable at the performance level**
  - **good solutions for the dynamically load balancing in systems space will apply to user space, freeing users**

Bad news/good news (4)

- **Default use of high precision may come to an end, as wasteful of storage and bandwidth**
  - **we will have to compute and communicate "deltas" between states rather than the full state quantities, as we did when double precision was expensive (e.g., iterative correction in linear algebra)**
  - **a combining network node will have to remember not just the last address, but also the last values, and send just the deltas**
- **Equidistributing errors properly while minimizing resource use will lead to innovative error analyses in numerical analysis**

For background, see the archives at *www.exascale.org*

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

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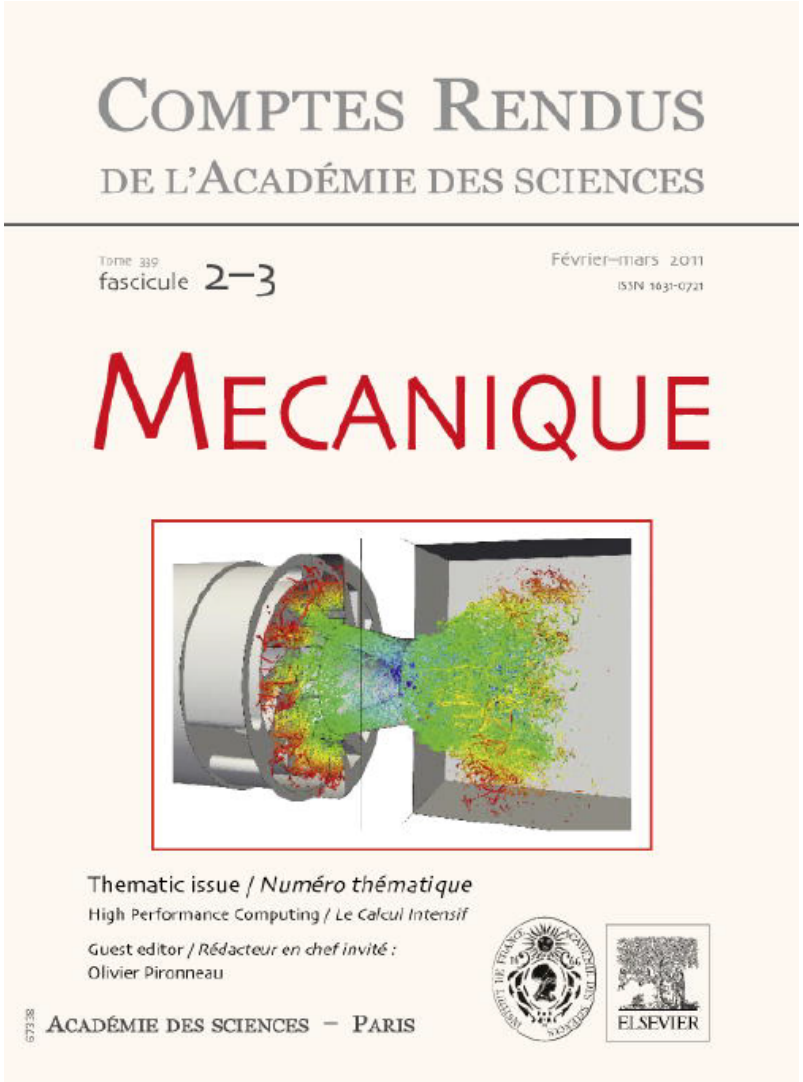
The International Exascale Software Roadmap,

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

See also a 2011 special issue of *Comptes Rendus*



Exaflop/s: The why and the how, D. E. Keyes, *Comptes Rendus de l'Academie des Sciences* **339**, 2011, 70—77.

Philosophy of an algorithmicist

- **Applications are *given* (as function of time)**
- **Architectures are *given* (as function of time)**
- **Algorithms and software *must be adapted or created* to bridge to hostile architectures for the sake of the complex applications**
  - **as important as ever today, with transformation of Moore's Law from speed-based to concurrency-based, due to power considerations**
  - **scalability still important, but new memory-bandwidth stresses arise when on-chip memories are shared**
  - **greatest challenge is lack of performance robustness of individual cores, which can spoil load balance**
- **Knowledge of algorithmic capabilities can usefully influence**
  - **the way applications are formulated**
  - **the way architectures are constructed**
- **Knowledge of application and architectural opportunities can usefully influence algorithmic development**

How will PDE computations adapt?

- Programming model will still be message-passing (due to large legacy code base), adapted to multicore 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)
- Noncritical parts will be made available for 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**
- **Steps in this direction**
  - **Asynchronous Dynamic Load Balancing (ADLB) [Lusk (Argonne), 2009]**
  - **Asynchronous Execution System [Steinmacher-Burrow (IBM), 2008]**

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**
  - **manufacturing, OS jitter, TLB/cache performance variations, network contention, dynamic power management, soft errors, 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 are similar when it comes to waiting at synchronization points**
- **Possible solutions for system nonuniformity will improve programmability, too**

Programming practice

- **Prior to possessing exascale hardware, users can prepare themselves by exploring new programming models**
  - **on manycore and heterogeneous nodes**
- **Attention to locality and reuse is valuable at all scales**
  - **will produce performance paybacks today *and* in the future**
  - **domains of coherence will be variable and hierarchical**
- **New algorithms and data structures can be explored under the assumption that flop/s are cheap and moving data is expensive**
- ***Independent tasks that have complementary resource requirements can be interleaved in time in independently allocated spaces***

Path for scaling up applications

- Weak scale applications up to distributed memory limits
  - proportional to number of nodes
- Strong scale applications beyond this
  - proportional to cores per node/memory unit
- Scale the workflow, itself
  - proportional to the number of instances (ensembles)
  - integrated end-to-end simulation
- Co-design process is staged, with any of these types of scaling valuable by themselves
- Big question: does the software for co-design factor? Or is all the inefficiency at the data copies at interfaces between the components after a while?

Algorithmic Priority Research Directions (1)

- **Advanced mathematical methods for scientific understanding in exascale simulations, including *in situ***
  - **uncertainty quantification, intrusive and nonintrusive**
  - **optimization, inverse problems, sensitivity**
  - **analysis and visualization**
  - **validation and verification**

Algorithmic Priority Research Directions (2)

- **Exascale algorithms that expose and exploit multiple levels of parallelism**
  - **communication-reducing algorithms**
  - **synchronism-reducing algorithms**
  - **fault resilient algorithms**
- **Algorithmic support for multiphysics, multiscale methods**
  - **relax the overspecified SPMD and BSP paradigms when joining multiple different codes**
  - **analyze stability of coupling**

Algorithmic Priority Research Directions (3)

- **Exascale algorithms for constructing and adapting discrete objects**
  - **these typically deal with unpredictable, dynamic structures and workloads and have few flops to hide**

Required software enabling technologies

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

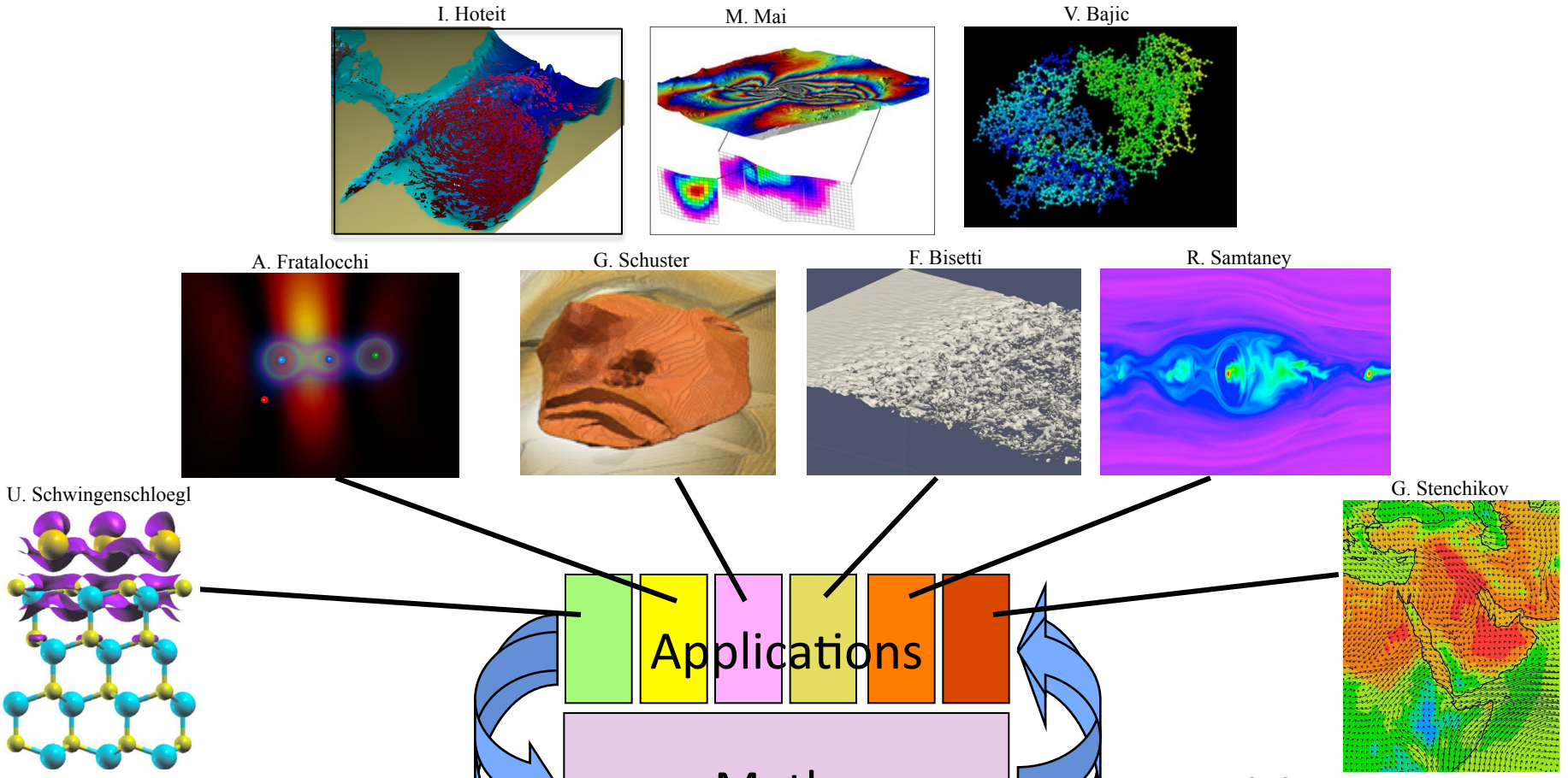
- Configuration systems
- Source-to-source translators
- Compilers
- Simulators
- Messaging systems
- Debuggers
- Profilers

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

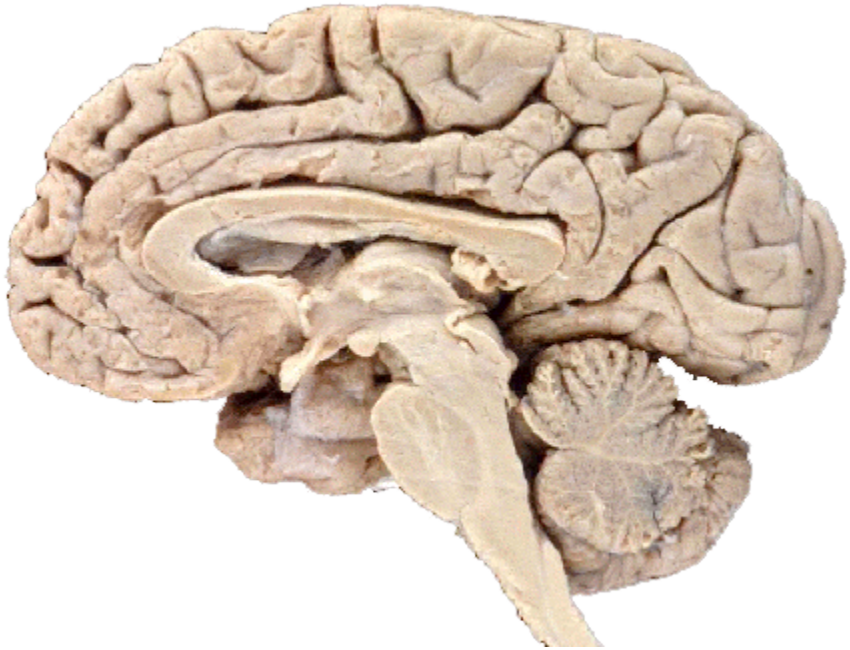
"SciDAC philosophy" of software investment



Kennedy's Challenge, 1962

"We choose to do [these] things, not because they are easy, but because they are hard, *because that goal will serve to organize and measure the best of our energies and skills*, because that challenge is one that we are willing to accept, one we are unwilling to postpone, and one which we intend to win..."

Acknowledgment: today's Peta-op/s machines



10^{12} neurons @ 1 KHz = 1 PetaOp/s

1.4 kilograms, 20 Watts