"Housekeeping"

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Extreme Scaling and Performance Across Diverse Architectures

HACC (Hardware/Hybrid Accelerated Cosmology Code) Framework

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Los Alamos National Laboratory

Zarija Lukic
Lawrence Berkeley National Laboratory

Justin Luitjens
NVIDIA

George Zagaris
Kitware

ASCR
HEP

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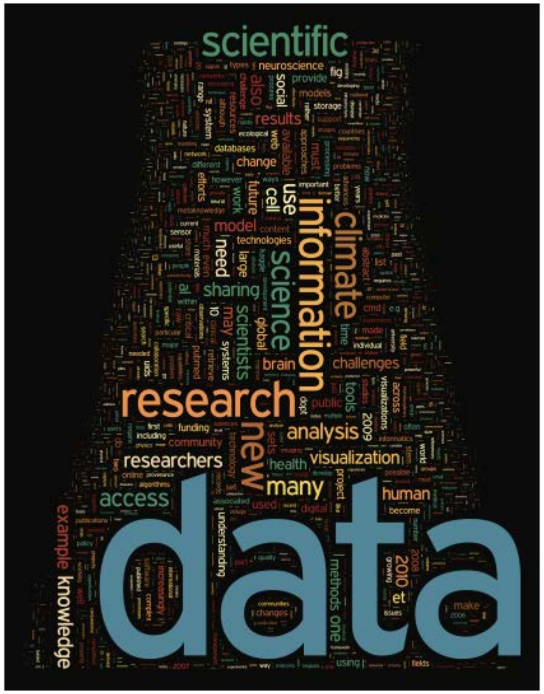
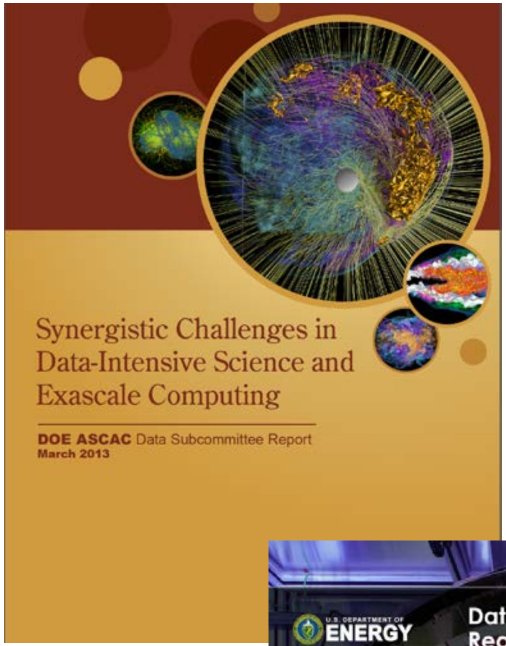
Computing Needs for Science

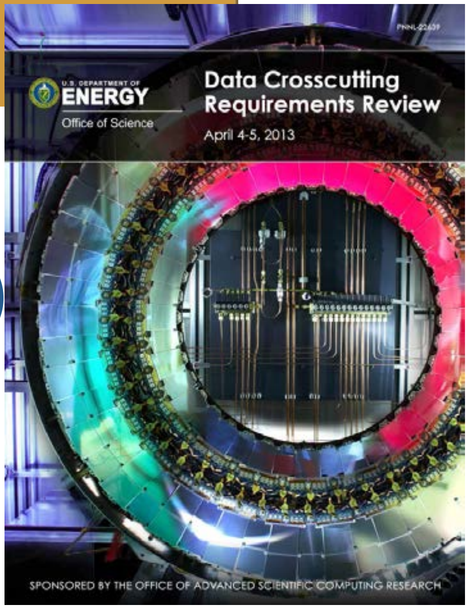
- **Many Communities use Large-Scale Computational Resources**
  - Biology
  - Synchrotron Light Sources
  - Climate/Earth Sciences
  - High Energy Physics
  - Materials Modeling
- **Message: Overall scientific computing use case is driven by traditional supercomputing as well as by data-intensive applications**
- **Optimization of overall balance of compute + I/O + storage + networking**
- **Should think of performance within this global context**



Different Flavors of Computing

- **High Performance Computing ('PDEs')**
  - Parallel systems with a fast network
  - Designed to run tightly coupled jobs
  - High performance parallel file system
  - Batch processing
- **Data-Intensive Computing ('Analytics')**
  - Parallel systems with balanced I/O
  - Designed for data analytics
  - System level storage model
  - Interactive processing
- **High Throughput Computing ('Events'/'Workflows')**
  - Distributed systems with 'slow' networks
  - Designed to run loosely coupled jobs
  - System level/Distributed data model
  - Batch processing



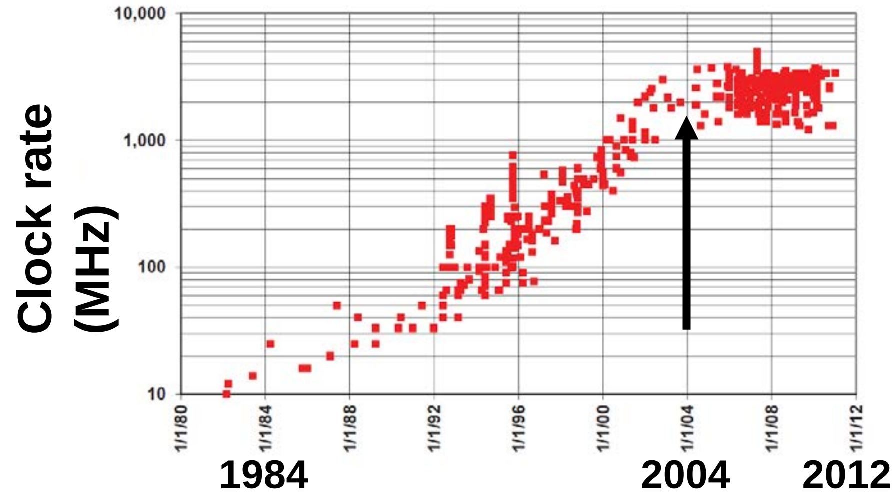


Motivating HPC: The Computational Ecosystem

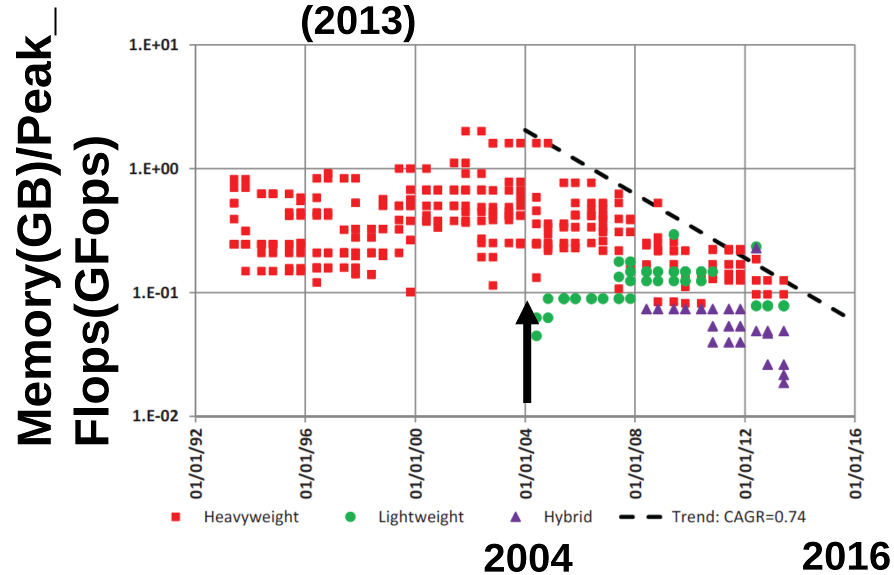
- Motivations for large HPC campaigns:
    1) Quantitative predictions for complex, nonlinear systems
    2) Discover/Expose physical mechanisms
    3) System-scale simulations (‘impossible experiments’)
    4) Large-Scale inverse problems and optimization
- Driven by a wide variety of data sources, computational cosmology must address ALL of the above
- Role of scalability/performance:
    1) Very large simulations necessary, but not just a matter of running a few large simulations
    2) High throughput essential (short wall clock times)
    3) Optimal design of simulation campaigns (parameter scans)
    4) Large-scale data-intensive applications

Supercomputing: Hardware Evolution

- **Power is the main constraint**
  - 30X performance gain by 2020
  - ~10-20MW per large system
  - power/socket roughly const.
- **Only way out: more cores**
  - Several design choices
  - None good from scientist's perspective
- **Micro-architecture gains sacrificed**
  - Accelerate specific tasks
  - Restrict memory access structure (SIMD/SIMT)
- **Machine balance sacrifice**
  - Memory/Flops; comm BW/Flops — all go in the wrong direction
  - (Low-level) code must be refactored



Kogge and Resnick (2013)



Supercomputing: Systems View

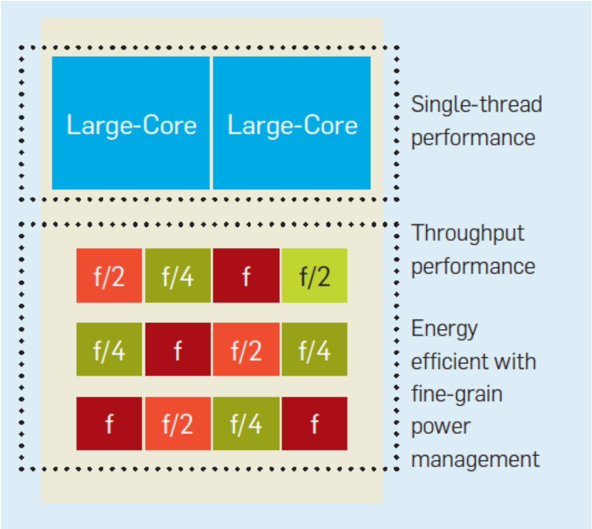
- **HPC is not what it used to be!**
  - HPC systems were meant to be balanced under certain metrics — nominal scores of unity (1990's desiderata)
  - These metrics now range from ~0.1 to ~0.001 on the same system currently and will get worse (out of balance systems)
  - RAM is expensive: memory bytes will not scale like compute flops, era of weak scaling (fixed relative problem size) has ended
- **Challenges**
  - Strong scaling regime (fixed absolute problem size) is much harder than weak scaling (since metric really is 'performance' and not 'scaling')
  - Machine models are complicated (multiple hierarchies of compute/memory/network)
  - Codes must add more physics to use the available compute, adding more complexity
  - Portability across architecture choices must be addressed (programming models, algorithmic choices, trade-offs, etc.)

Supercomputing Challenges: Sociological View

- **Codes and Teams**
  - Most codes are written and maintained by small teams working near the limits of their capability (no free cycles)
  - Community codes, by definition, are associated with large inertia (not easy to change standards, untangle lower-level pieces of code from higher-level organization, find the people required that have the expertise, etc.)
  - Lack of consistent programming model for “scale-up”
  - In some fields at least, something like a “crisis” is approaching (or so people say)
- **What to do?**
  - We will get beyond this (the vector to MPP transition was worse)
  - Transition needs to be staged (not enough manpower to entirely rewrite code base)
  - Prediction: There will be no ready made solutions
  - Realization — “You have got to do it for yourself”

Co-Design vs. Code Design

- **HPC Myths**
  - The magic compiler
  - The magic programming model/language
  - Special-purpose hardware
  - Co-Design (not now anyway, but maybe in the future —)
- **Dealing with Today's Reality**
  - Code teams must understand all levels of the system architecture, but do not be enslaved by it (software cycles are long)!
  - Must have a good idea of the 'boundary conditions' (what may be available, what is doable, etc.)
  - 'Code Ports' is ultimately a false notion
  - Start thinking out of the box — domain scientists and computer scientists and engineers must work together



Future heterogeneous manycore system, Borkar and Chien (2011)

Large Scale Structure: Vlasov-Poisson Equation

$$\frac{\partial f_i}{\partial t} + \dot{\mathbf{x}}\frac{\partial f_i}{\partial \mathbf{x}} - \nabla\phi\frac{\partial f_i}{\partial \mathbf{p}} = 0, \qquad \mathbf{p} = a^2\dot{\mathbf{x}},$$

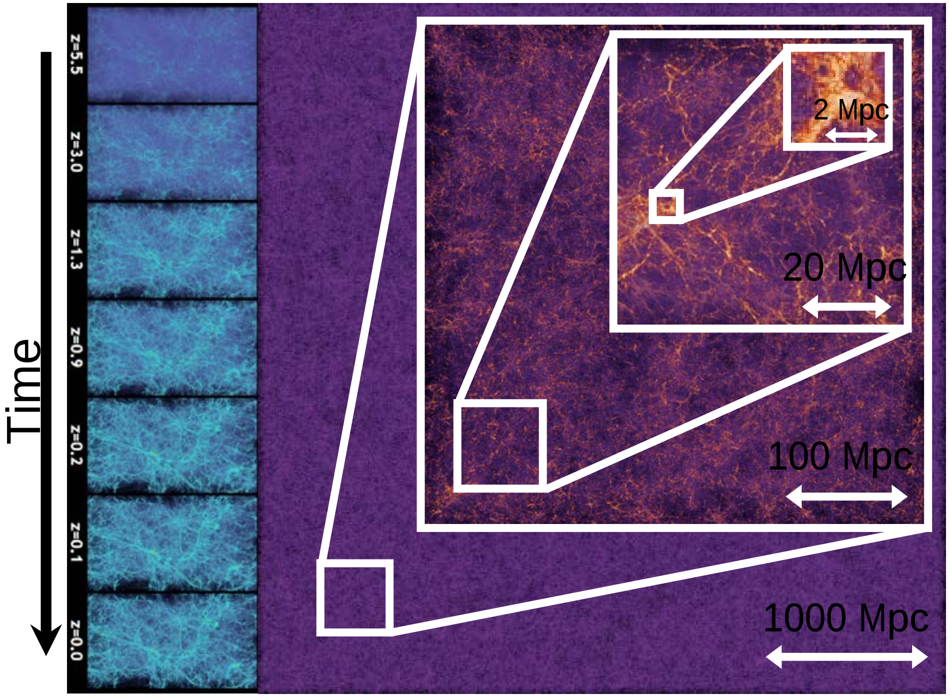
$$\begin{aligned}
\nabla^2\phi &= 4\pi G a^2(\rho(\mathbf{x},t) - \langle\rho_{\rm dm}(t)\rangle) = 4\pi G a^2\Omega_{\rm dm}\delta_{\rm dm}\rho_{\rm cr},\\
\delta_{\rm dm}(\mathbf{x},t) &= (\rho_{\rm dm} - \langle\rho_{\rm dm}\rangle)/\langle\rho_{\rm dm}\rangle),\\
\rho_{\rm dm}(\mathbf{x},t) &= a^{-3}\sum_i m_i \int d^3\mathbf{p}\, f_i(\mathbf{x},\dot{\mathbf{x}},t).
\end{aligned}$$

Cosmological Vlasov-Poisson Equation

- Properties of the Cosmological Vlasov-Poisson Equation:
  - 6-D PDE with long-range interactions, no shielding, all scales matter; models gravity-only, collisionless evolution
  - Jeans instability drives structure formation at all scales from smooth Gaussian random field initial conditions
  - Extreme dynamic range in space and mass (in many applications, million to one in both space and density, ‘everywhere’)

Large Scale Structure Simulation Requirements

- Force and Mass Resolution:
  - Galaxy halos ~100kpc, hence force resolution has to be ~kpc; with Gpc box-sizes, a dynamic range of a million to one
  - Ratio of largest object mass to lightest is ~10000:1
- Physics:
  - Gravity dominates at scales greater than ~Mpc
  - Small scales: galaxy modeling, semi-analytic methods to incorporate gas physics/feedback/star formation
- Computing 'Boundary Conditions':
  - Total memory in the PB+ class
  - Performance in the 10 PFlops+ class
  - Wall-clock of ~days/week, in situ analysis



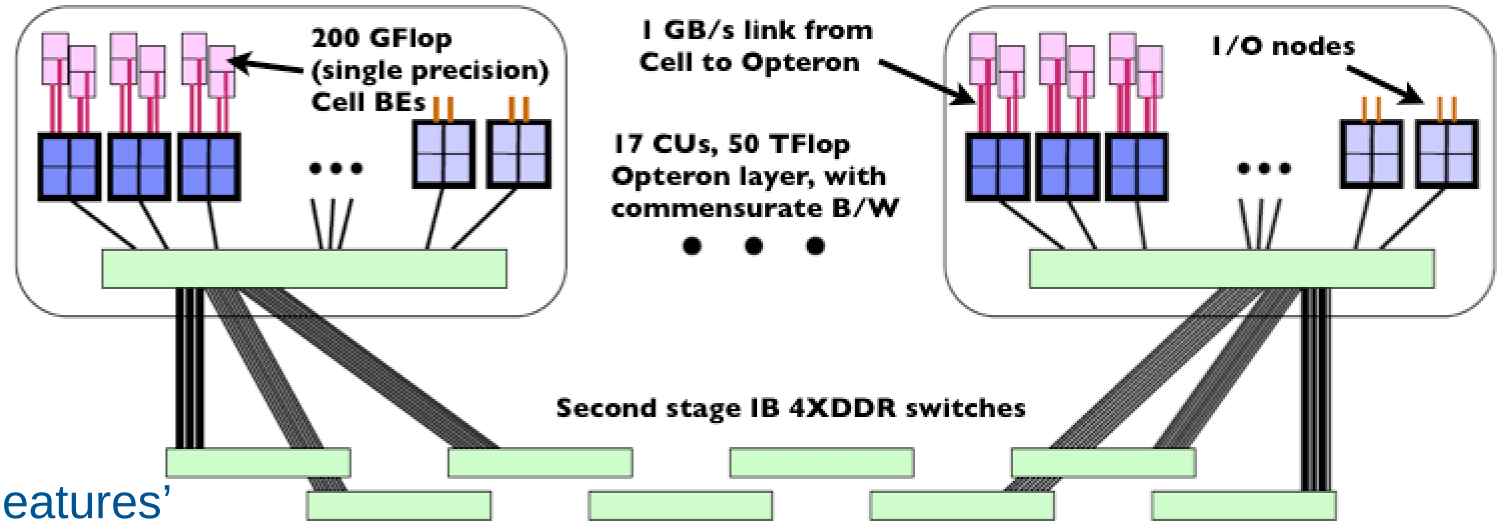
Gravitational Jeans Instability

Can the Universe be run as a short computational 'experiment'?

Architectural Challenges: The HACC Story

Andrew White Dec 7, 2007 + What if you had a petaflop/s

Roadrunner: Prototype for modern accelerated architectures, first to break the PFlops barrier



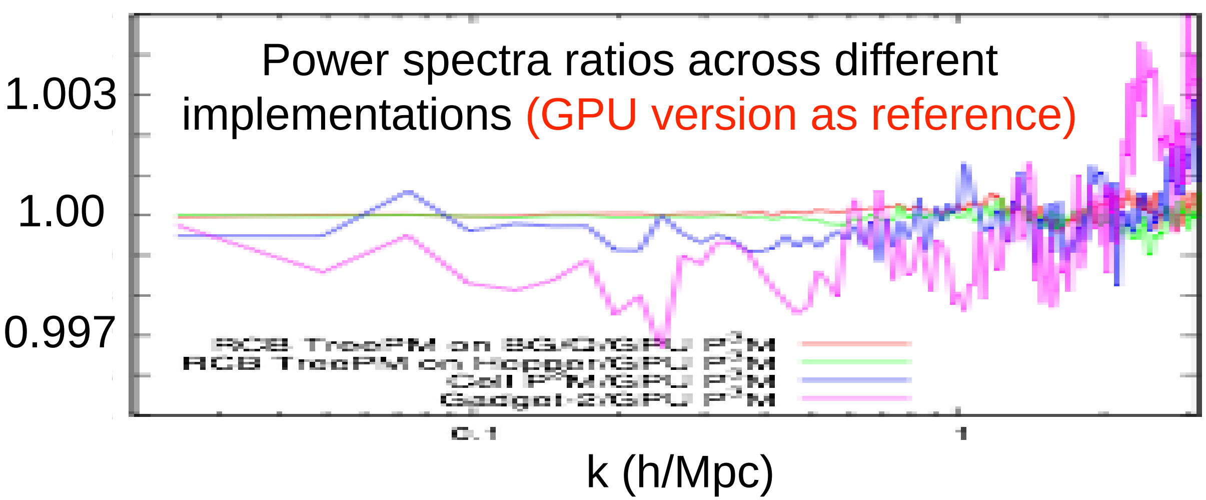
Architectural 'Features'

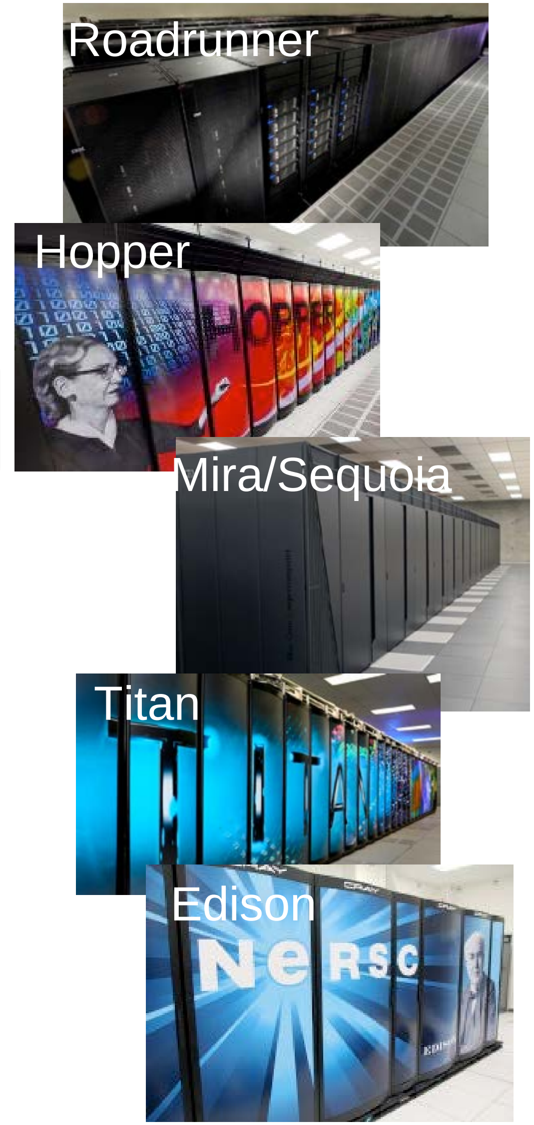
- Complex heterogeneous nodes
- Simpler cores, lower memory/core, no real cache
- Skewed compute/communication balance
- Programming models?
- I/O? File systems?
- Effect on code longevity

HACC team meets Roadrunner

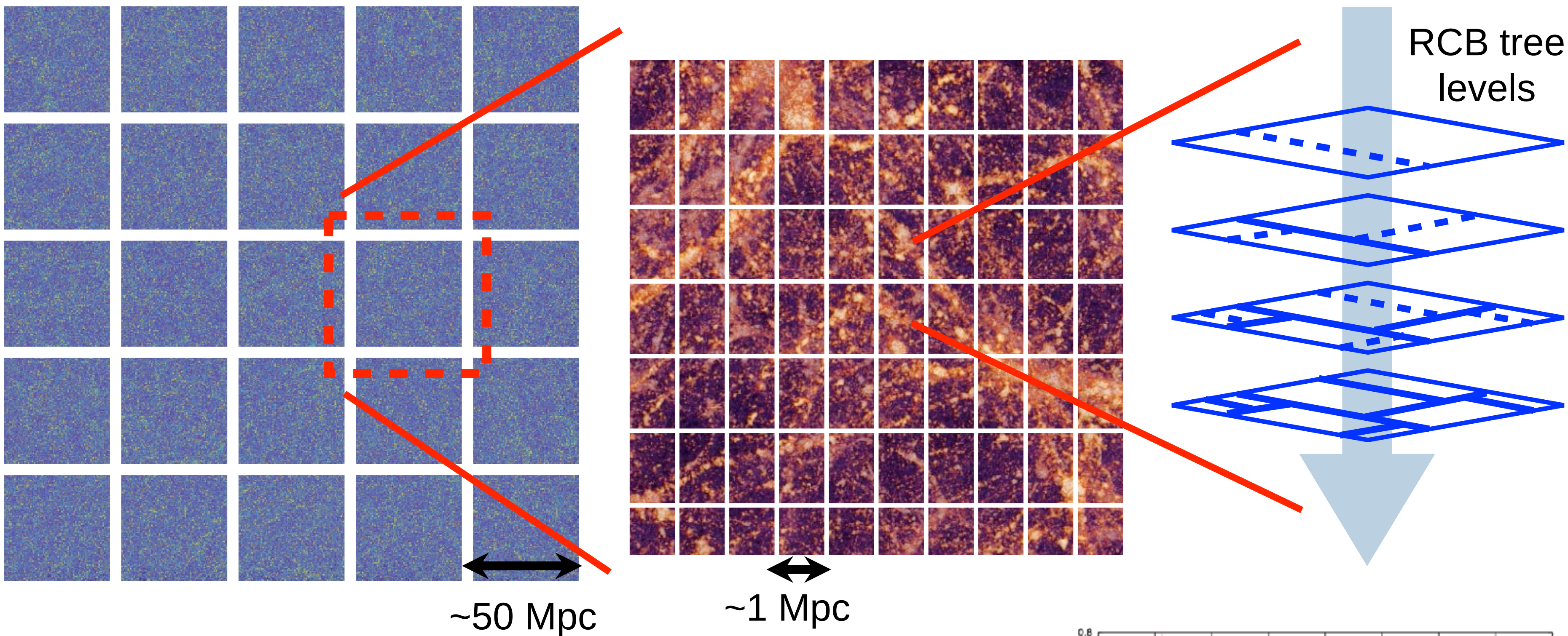
Combating Architectural Diversity with HACC

- Architecture-independent performance/scalability: 'Universal' top layer + 'plug in' node-level components; minimize data structure complexity and data motion
- Programming model: 'C++/MPI + X' where X = OpenMP, Cell SDK, OpenCL, CUDA, --
- Algorithm Co-Design: Multiple algorithm options, stresses accuracy, low memory overhead, no external libraries in simulation path
- Analysis tools: Major analysis framework, tools deployed in stand-alone and in situ modes





HACC Structure: Universal vs. Local Layers

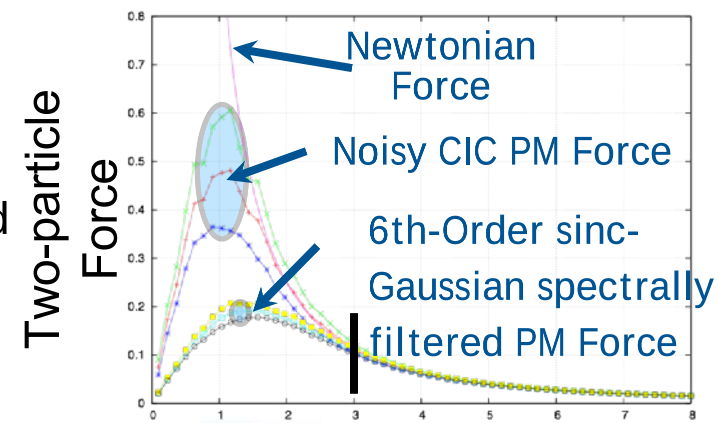


HACC Top Layer:
3-D domain decomposition with particle replication at boundaries ('overloading') for Spectral PM algorithm (long-range force)

Host-side: Scaling controlled by FFT

HACC 'Nodal' Layer:
Short-range solvers employing combination of flexible chaining mesh and RCB tree-based force evaluations

Performance controlled by short-range solver



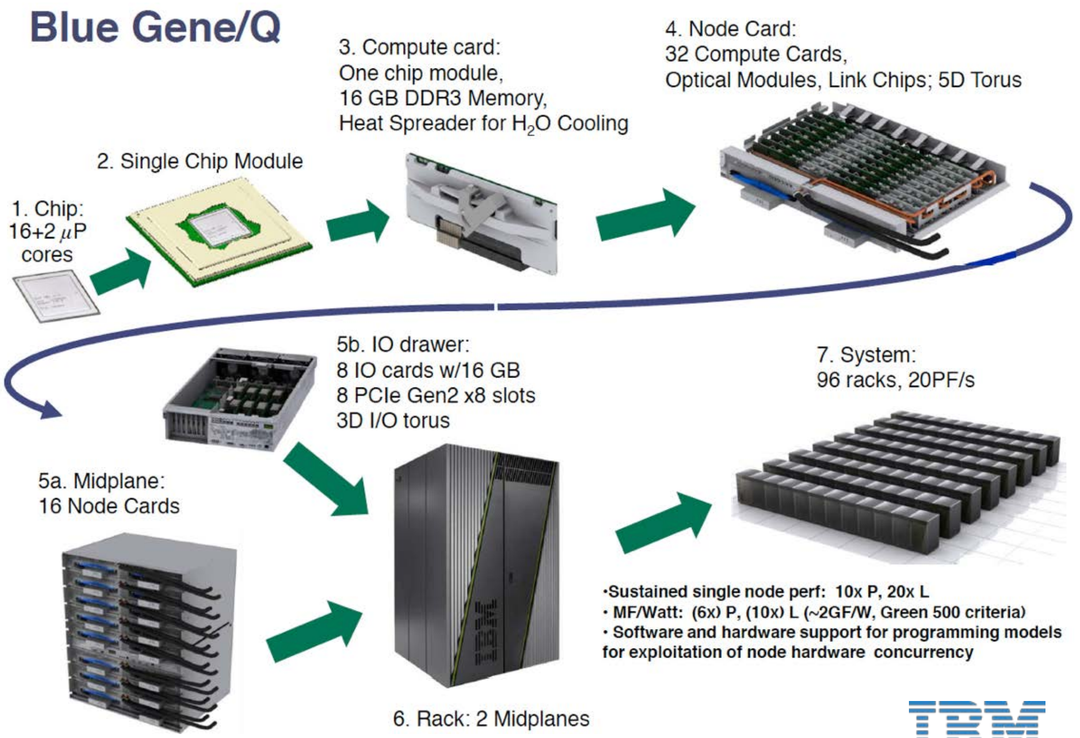
HACC: Algorithmic Features and Options

- Fully Spectral Particle-Mesh Solver: 6th-order Green function, 4th-order Super-Lanczos derivatives, high-order spectral filtering, high-accuracy polynomial for short-range forces
- Custom Parallel FFT: Pencil-decomposed, high-performance FFT (up to 15K^3)
- Particle Overloading: Particle replication at 'node' boundaries to reduce/delay communication (intermittent refreshes), important for accelerated systems
- Flexible Chaining Mesh: Used to optimize tree and P3M methods
- Optimal Splitting of Gravitational Forces: Spectral Particle-Mesh melded with direct and RCB ('fat leaf') tree force solvers (PPTPM), short hand-over scale (dynamic range splitting ~ 10,000 X 100); pseudo-particle method for multipole expansions
- Mixed Precision: Optimize memory and performance (GPU-friendly!)
- Optimized Force Kernels: High performance without assembly
- Adaptive Symplectic Time-Stepping: Symplectic sub-cycling of short-range force timesteps; adaptivity from automatic density estimate via RCB tree
- Custom Parallel I/O: Topology aware parallel I/O with lossless compression (factor of 2); 1.5 trillion particle checkpoint in 4 minutes at ~160GB/sec on Mira

HACC on the IBM Blue Gene/Q

HACC BG/Q Experience

- System: BQC chip — 16 cores, 205GFlops, 16GB RAM, 32MB L2, 400GB/s crossbar; 5-D torus network at 40GB/s
- Programming Models: Two-tiered programming model (MPI+OpenMP) very successful, use of vector intrinsics (QPX) essential
- I/O: Custom I/O implementation (one file per I/O node, disjoint data region/process) gives ~2/3 of peak performance under production conditions
- Job Mix: Range of job sizes running on Mira, from 2 to 32 racks

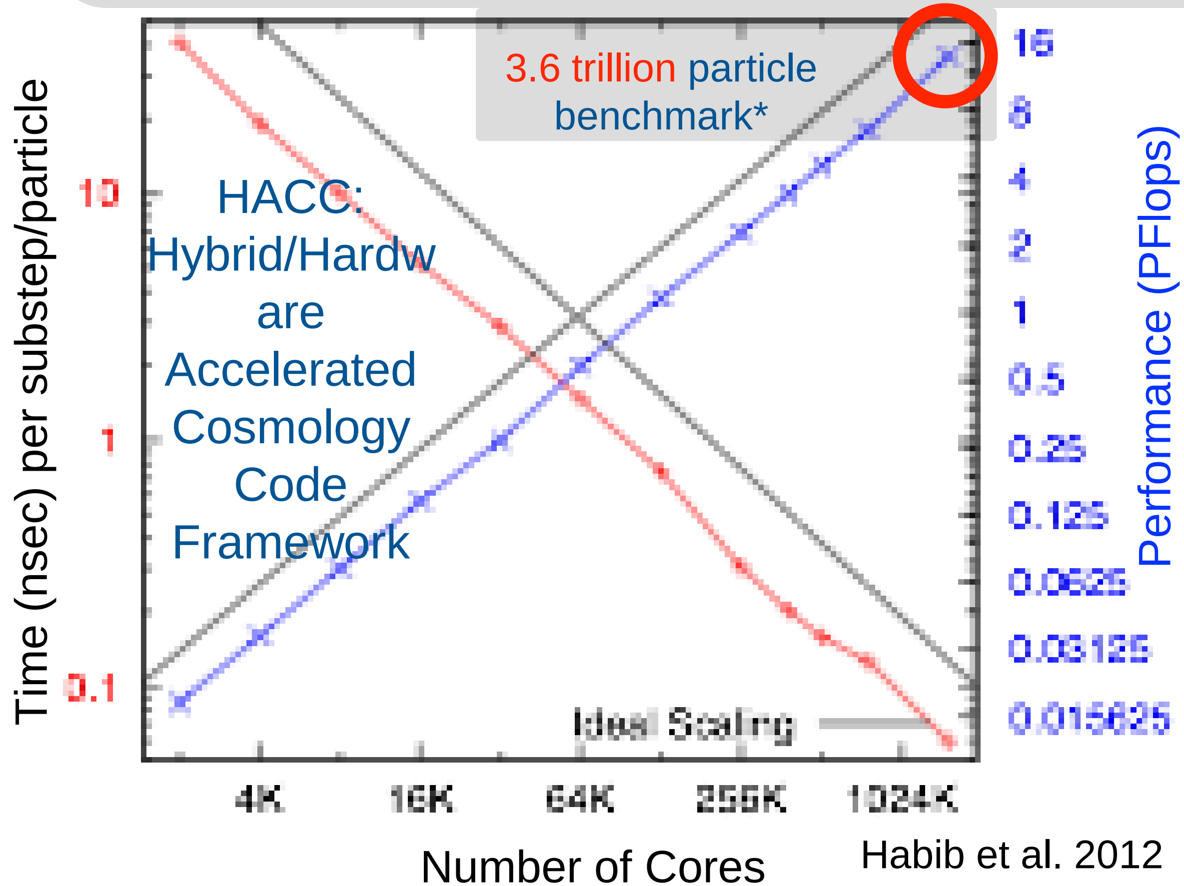


HACC on the BG/Q

HACC BG/Q Version

- Algorithms: FFT-based SPM; PP+RCB Tree
- Data Locality: Rank level via ‘overloading’, at tree-level use the RCB grouping to organize particle memory buffers
- Build/Walk Minimization: Reduce tree depth using rank-local trees, shortest hand-over scale, bigger p-p component
- Force Kernel: Use polynomial representation (no look-ups); vectorize kernel evaluation; hide instruction latency

13.94 PFlops, 69.2% peak, 90% parallel efficiency on 1,572,864 cores/MPI ranks, 6.3M-way concurrency



Habib et al. 2012

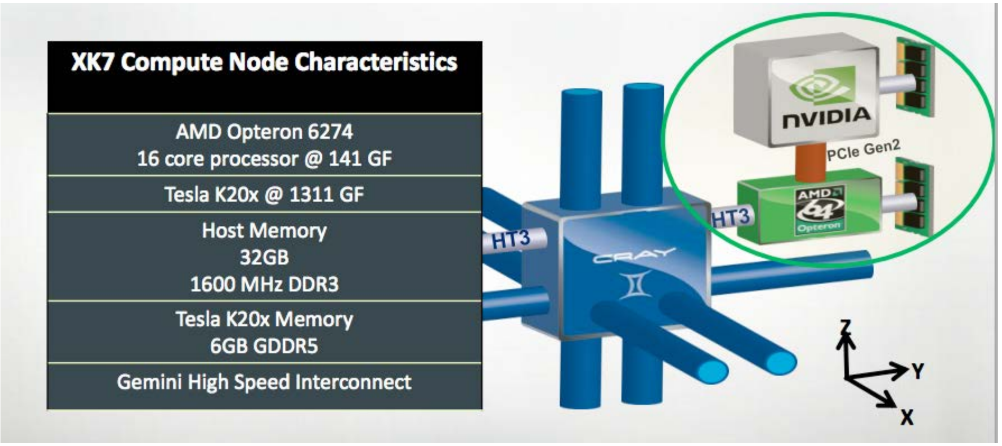
*largest ever run

HACC weak scaling on the IBM BG/Q (MPI/OpenMP)

Accelerated Systems: HACC on Titan (Cray XK7)

Imbalances and Bottlenecks

- Memory is primarily host-side (32 GB vs. 6 GB) (against Roadrunner's 16 GB vs. 16 GB), important thing to think about (in case of HACC, the 'grid/particle' balance)
- PCIe is a key bottleneck; overall interconnect B/W does not match Flops (not even close)
- There's no point in 'sharing' work between the CPU and the GPU, performance gains will be minimal — GPU must dominate
- The only reason to write a code for such a system is if you can truly exploit its power (2 X CPU is a waste of effort!)



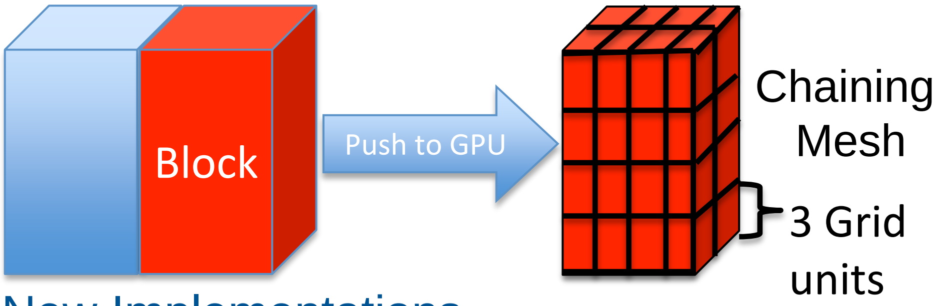
Strategies for Success

- It's (still) all about understanding and controlling data motion
- Rethink your code and even approach to the problem
- Isolate hotspots, and design for portability around them (modular programming)
- Pragmas will never be the full answer (with maybe an exception or two)

HACC on Titan: GPU Implementation (Schematic)

P3M Implementation (OpenCL):

- Spatial data pushed to GPU in large blocks, data is sub-partitioned into chaining mesh cubes
- Compute forces between particles in a cube and neighboring cubes
- Natural parallelism and simplicity leads to high performance
- Typical push size ~2GB; large push size ensures computation time exceeds memory transfer latency by a large factor
- More MPI tasks/node preferred over threaded single MPI tasks (better host code performance)

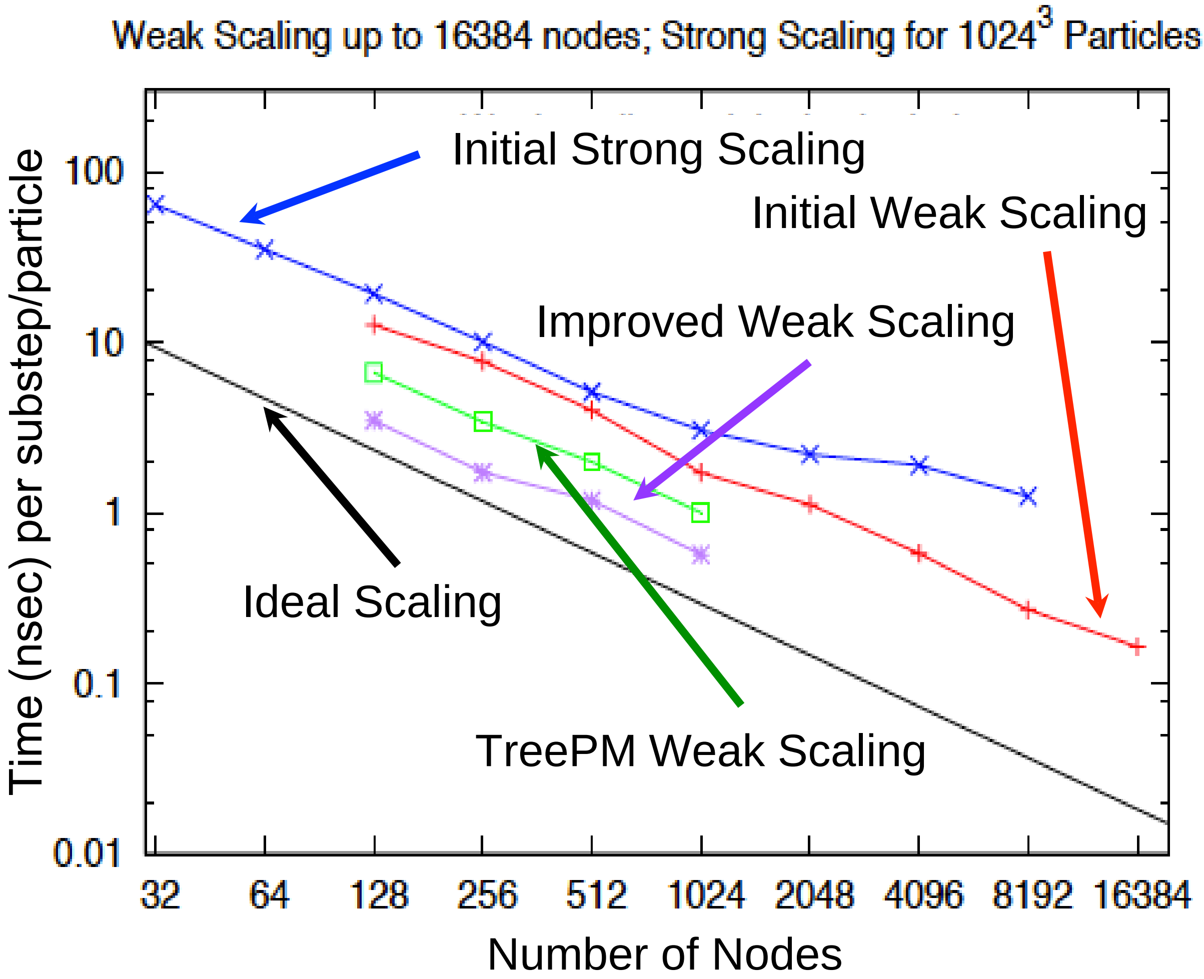


New Implementations (OpenCL and CUDA):

- P3M with data pushed only once per long time-step, completely eliminating memory transfer latencies (orders of magnitude less); uses ‘soft boundary’ chaining mesh, rather than rebuilding every sub-cycle
- TreePM analog of BG/Q code written in CUDA, also produces high performance

HACC on Titan: GPU Implementation Performance

- P3M kernel runs at 1.6TFlops/node at 40.3% of peak (73% of algorithmic peak)
- TreePM kernel was run on 77% of Titan at 20.54 PFlops at almost identical performance on the card
- Because of less overhead, P3M code is (currently) faster by factor of two in time to solution



99.2% Parallel Efficiency

Summary

Basic Ideas:

- Thoughtful design of flexible code infrastructure; minimize number of computational ‘hot spots’, explore multiple algorithmic ideas — exploit domain science expertise
- Because machines are so out of balance, focusing only on the lowest-level compute-intensive kernels can be a mistake (‘code ports’)
- One possible solution is an overarching universal layer with architecture-dependent, plug-in modules (with implications for productivity)
- Understand data motion issues in depth — minimize data motion, always look to hide communication latency with computation
- Be able to change on fast timescales (HACC needs no external libraries in the main simulation code — helps to get on new machines early)
- As science outputs become more complex, data analysis becomes a very significant fraction of available computational time — optimize performance with this in mind

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