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Extreme Scaling and Performance Across Diverse Architectures

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HACC (Hardware/Hybrid Accelerated Cosmology Code) Framework

HACC (Hardware/Hybrid Accelerated Cosmology Code) Framework
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• Submit questions and comments via Twitter to @acmeducation – we’re reading them!

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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
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

\[
\frac{\partial f_i}{\partial t} + \dot{x} \frac{\partial f_i}{\partial x} - \nabla \phi \frac{\partial f_i}{\partial p} = 0, \quad p = a^2 \dot{x},
\]

\[
\nabla^2 \phi = 4\pi G a^2 (\rho(x, t) - \langle \rho_{\text{dm}}(t) \rangle) = 4\pi G a^2 \Omega_{\text{dm}} \delta_{\text{dm}} \rho_{\text{cr}},
\]

\[
\delta_{\text{dm}}(x, t) = \langle \rho_{\text{dm}} \rangle / \langle \rho_{\text{dm}} \rangle,
\]

\[
\rho_{\text{dm}}(x, t) = a^{-3} \sum_i m_i \int d^3 p f_i(x, \dot{x}, t).
\]

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

Can the Universe be run as a short computational ‘experiment’?
Architectural Challenges: The HACC Story

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

----

Power spectra ratios across different implementations *(GPU version as reference)*

![Power spectra ratios graph](image)
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**

- Newtonian Force
- Noisy CIC PM Force
- 6th-Order sinc-Gaussian spectrally filtered PM Force
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 $\sim 10,000 \times 100$); 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 $\sim$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

3.6 trillion particle benchmark*

HACC: Hybrid/Hardw are Accelerated Cosmology Code Framework

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

Habib et al. 2012

*largest ever run
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)
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

![Graph showing weak and strong scaling efficiencies with 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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