Present and Future Computing Requirements for Computational Cosmology

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Cosmic Frontier Computing Collaboration

Computational Cosmology SciDAC-3 Project

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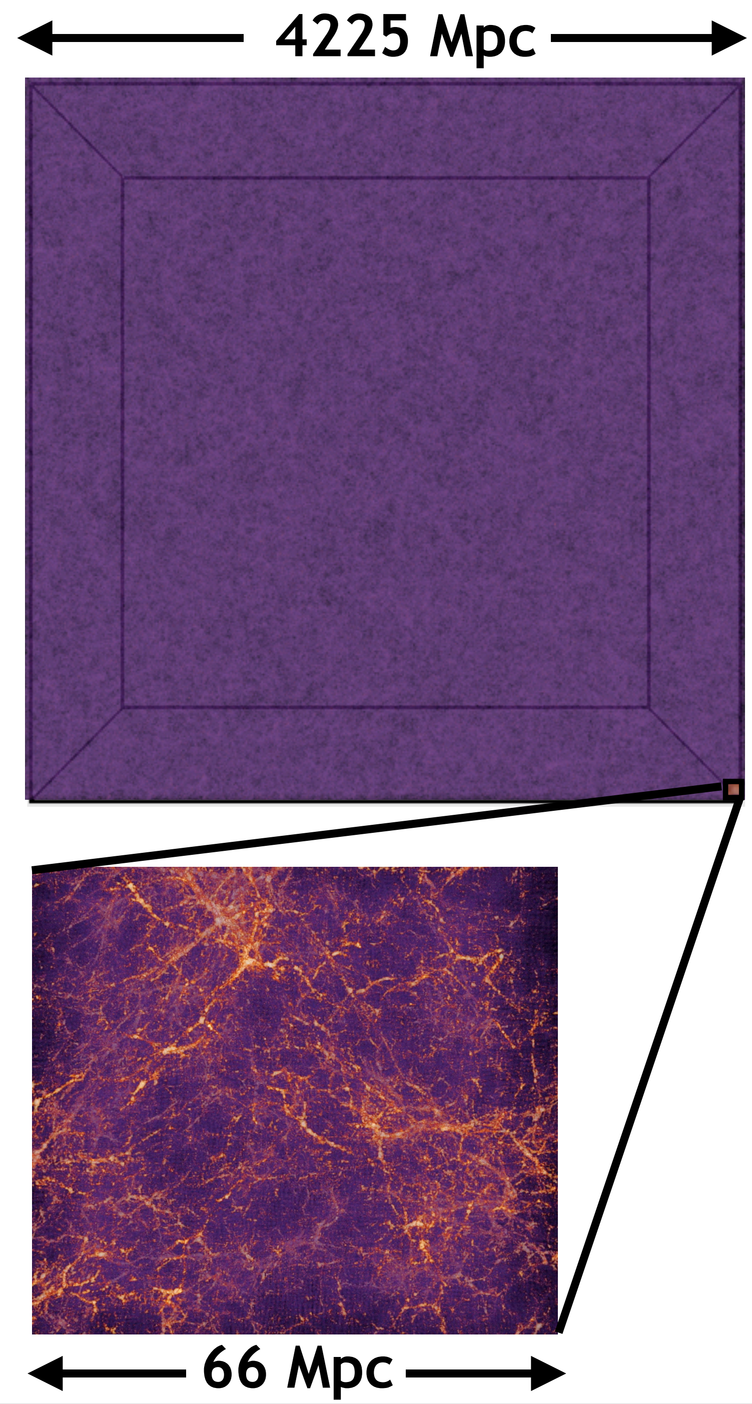
Large Scale Production Computing and Storage Requirements for High Energy Physics Research

A DOE Technical Program Review

November 27-28, 2012

Project Description

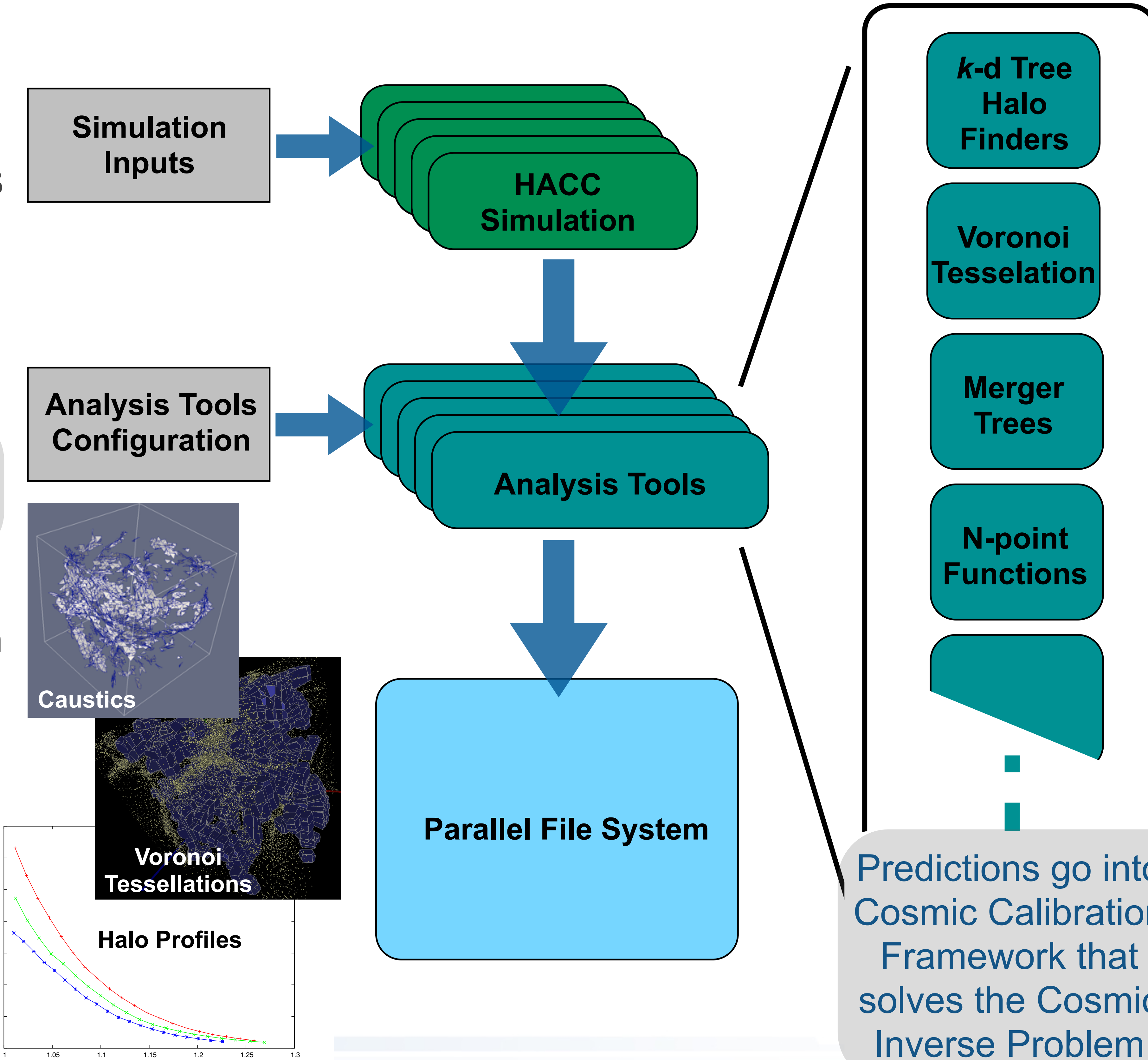
- **Project Science (will continue through and beyond 2017):**
  - **Large-scale structure simulations**
  - **Multi-physics simulations at smaller scales**
  - **Cosmic probes, mock catalogs**
  - **Fast prediction for forward models, uncertainty quantification**
  - **Support HEP Cosmic Frontier -- BOSS, DES, SPT, BigBOSS/DESpec, LSST projects**
  - **Large data analytics; in situ and post-processing**
- **Where Do We Expect to be in 2017:**
  - **Large-scale structure simulations in the 30+ trillion particle class**
  - **Sophisticated particle-based and AMR hydro simulations for galaxy formation at increased volumes**
  - **Very high degree of realism and fidelity in ‘mock skys’ for systematics control**
  - **Precision ‘emulators’ at the <1% error range**
  - **Extensive use of large-scale data analytics with 10+ PB**

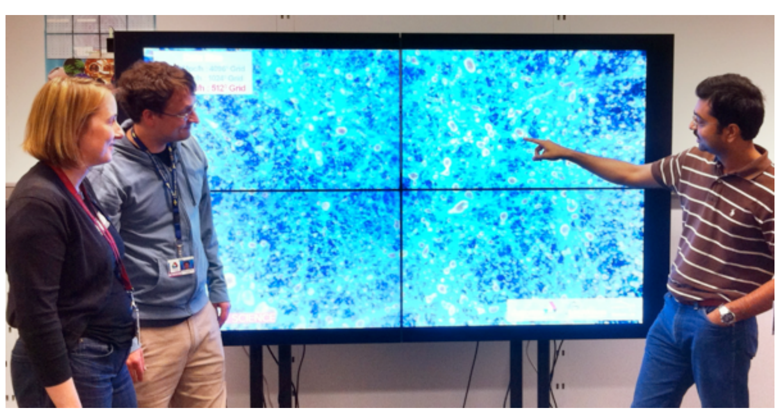


1.1 trillion particle HACC science run at z = 3 on Mira illustrating the dynamic range of a large, high-resolution, cosmological N-body simulation

HACC Example: *Fast* In Situ Analysis

- **Data Reduction:** A trillion particle simulation with 100 analysis steps has a storage requirement of ~4 PB -- in situ analysis reduces it to ~200 TB
- **I/O Chokepoints:** Large data analyses difficult because I/O time > analysis time, plus scheduling overhead
- **Fast Algorithms:** Analysis time is only a fraction of a full simulation timestep
- **Ease of Workflow:** Large analyses difficult to manage in post-processing





Predictions go into Cosmic Calibration Framework that solves the Cosmic Inverse Problem

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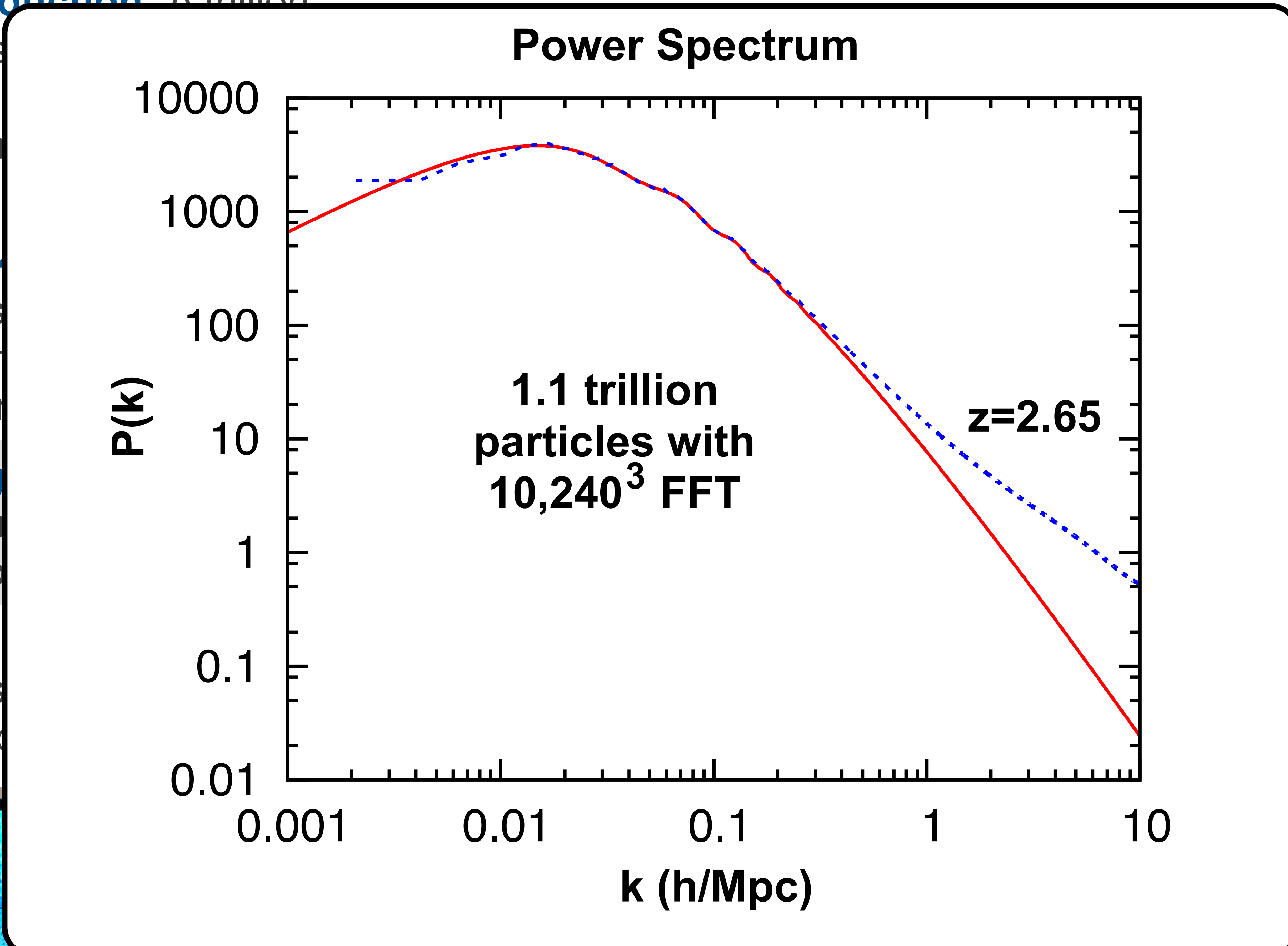

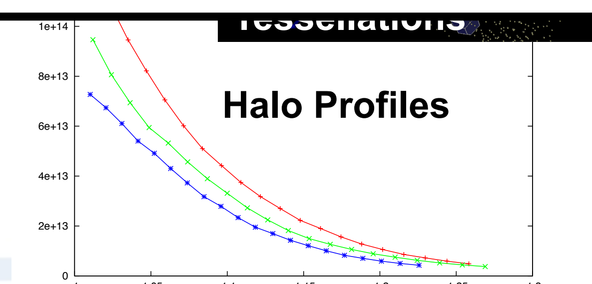

***k*-d Tree Halo Finders**

Voronoi Tesselation

Merger Trees

N-point Functions

Predictions go into Cosmic Calibration Framework that solves the Cosmic Inverse Problem

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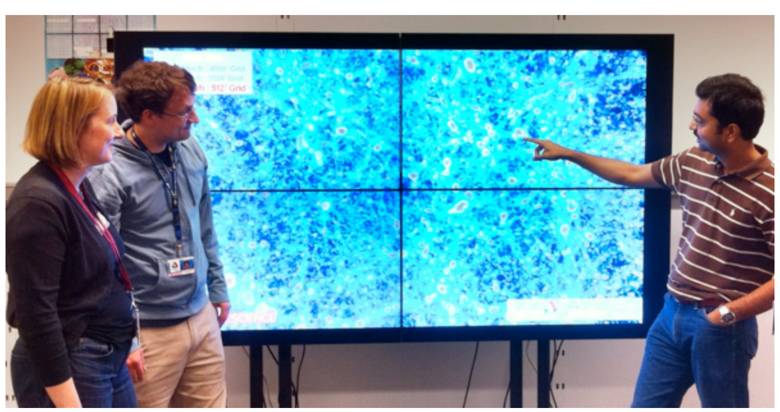
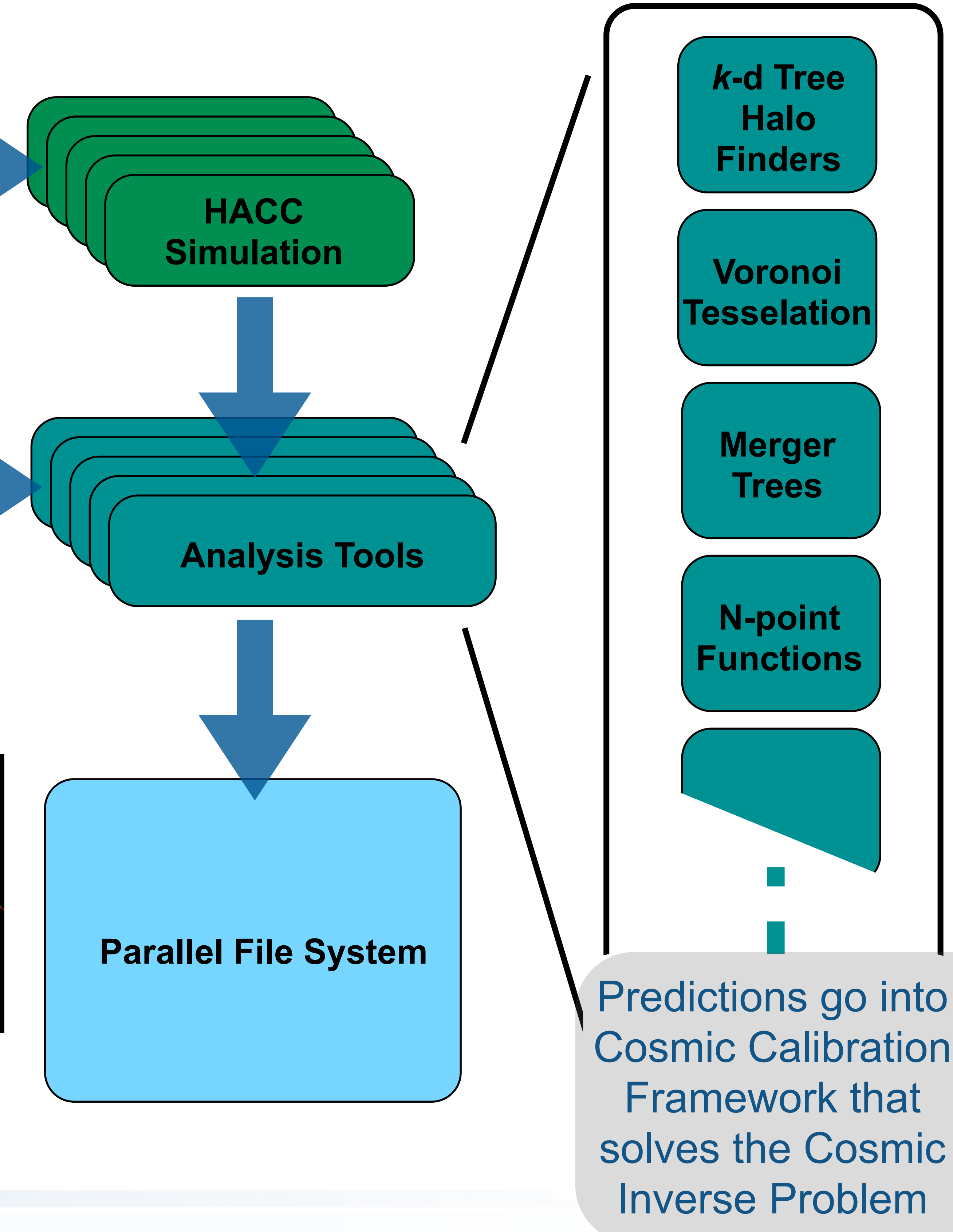
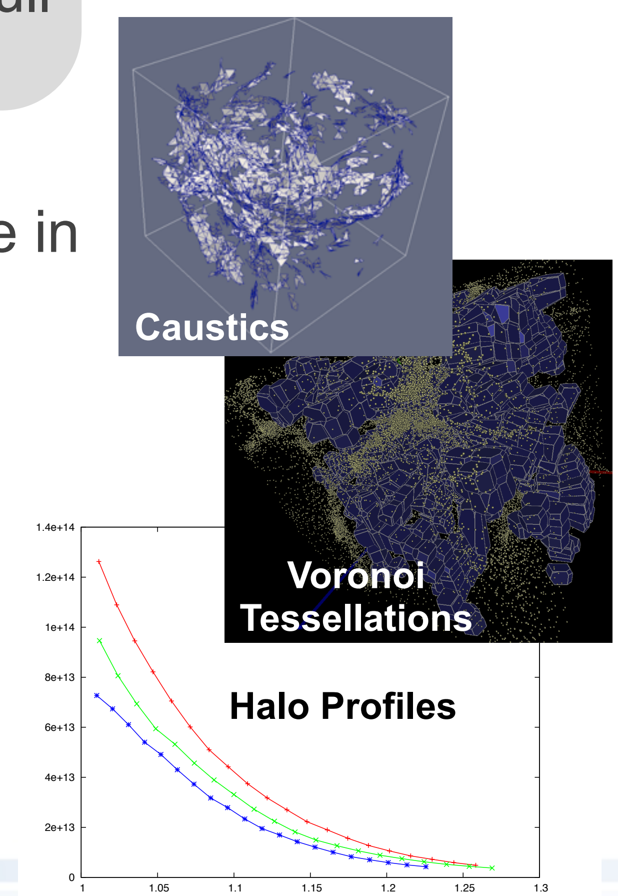
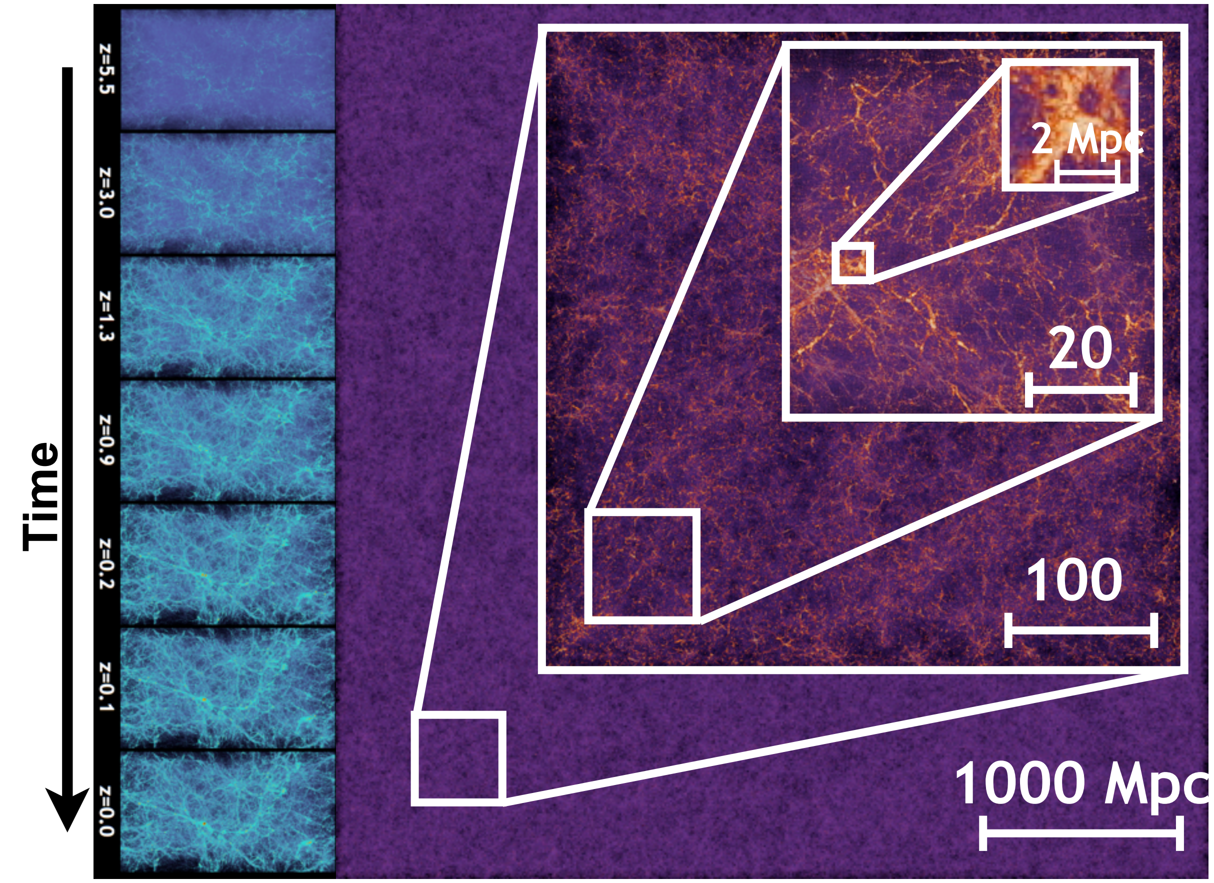






Computational Cosmology: Not One Problem, But Many!

- **Structure Formation:**
  - Initial conditions -- non-Gaussian, multi-scale, baryons, GR effects in large boxes, etc.
  - Gravity-only simulations (N-body) require dynamic ranges of > million-to-one
  - Gasdynamics simulations at smaller scales
- **Physics:**
  - Gravity dominates at scales greater than ~Mpc
  - At small scales: galaxy distribution modeling, sub-grid models, full hydro too difficult
- **Algorithms:**
  - N-Body: Melds of direct particle-particle, tree, and particle-mesh algorithms (including AMR)
  - Hydro: AMR, SPH, and variations
- **Computational Challenges/Scaling Limitations:**
  - Complex data structures
  - Large memory/core requirements
  - Inherent limitations on Flops/Bytes ratio
  - Analytics (in situ or post-processing)



Gravitational Jeans Instablity

- **Changes in Approach:**
  - Code algorithmic structure (e.g., HACC for N-body simulations)
  - Revamped data structures
  - New algorithms with higher Flops/Bytes ratio
  - However, not everything will change (long duration software cycles, especially for community codes)

Primary Codes

- **N-Body:**
  - Solvers: Poisson solver for the PM component; direct particle-particle, tree, and multipole methods for the short-range solvers
  - Gadget -- TreePM, public domain, primarily written by Volker Springel, currently scales to 1000's of MPI ranks, available in MPI and MPI/OpenMP versions (can be run to hundreds of billions of particles)
  - HACC (Hardware/Hybrid Accelerated Cosmology Codes) Framework -- PPTreePM, primary development team at Argonne, supports a number of programming models (MPI, MPI/OpenMP, MPI/OpenCL, MPI/Cell_SDK, --), arbitrarily scalable (~exascale design point), has been run on > 1.5M cores/MPI ranks at 14 PFlops with 3.6 trillion particles; typical runs in the tens of billions to multi-trillions of particles (memory bound)
- **AMR Hydro:**
  - Solvers: Poisson solvers on an AMR mesh (relaxation/Multigrid); Euler solvers on AMR meshes, various rad. transfer algorithms, local methods for feedback, cooling, star formation, etc.
  - ART -- cell-structured (refinement trees) AMR code for gravity + gasdynamics + feedback + --, primary development at Fermilab and UChicago, currently scales to ~10K cores (work is underway to improve this); can run up to billions of particles with 2000^3 AMR meshes
  - Gadget -- Adds SPH hydro to TreePM solver
  - Nyx -- new block-structured (nested hierarchy of rectangular grids) AMR code for gravity + gasdynamics + rad. transfer + feedback + --, based on BoxLib framework, primary development at LBNL, supports MPI and MPI/OpenMP; weak scaling verified to 200K processors, currently capability extends to running up to tens of billions of particles with 4000^3 AMR meshes

Current HPC Usage

- **Facilities and Machines:**
  - Facilities -- ALCF, NERSC, OLCF, NSF Centers
  - Architectures -- IBM BG/P and BG/Q, Cray XT, IBM iDataPlex, Cray XK7, Cray XE6, various Linux clusters, CPU/GPU clusters
- **Usage:**
  - Total computational hours per year (2012, est.) -- ~75M core-hours (50M@ALCF, 20M@NERSC, 5M at other places, will use more as new systems come on line)
  - Number of cores in a typical production run -- thousands to hundreds of thousands
  - Wall clock for a single production run -- ~days to two weeks
  - Minimum memory required per core -- depends on the code, 1 GB to 4 GB
  - Data read and written per run -- ranges from ~1 TB to 100's of TB
  - Size of checkpoint files -- ranges from tens of GB to ~100 TB
  - Amount of data moved in/out of NERSC -- 10's to 100's of TB
  - On-line file storage requirement -- 300 TB currently (on data-intensive computing project at NERSC, have ~50 TB in place, more coming!)
  - Off-line archival storage requirement -- in general, not thrilled with HPSS (example bottleneck 1)
  - Example bottleneck 2: Would like faster I/O to the Global File System from Hopper

HPC Requirements for 2017(!)

- **Compute "hours" needed:**
  - In 2013, our "project" has somewhere in the realm of 200M core-hours, historically science needs are inexhaustible -- especially since in our case we have to chase down a large number of science issues -- no doubt there will be surprises
  - Extrapolating from the 2012/2013 experience and knowing that the present installed supercomputing base at major centers will be more or less stable (within a factor of a few) until the next major jump (~2015/16?), by 2017, we could be looking at multi-billion to 10-billion core-hours (in "Hopper" units)
- **Usage patterns for 2017:**
  - Parallel concurrency changes are only to be expected; next-generation architectures such as the Intel Xeon Phi are already one order of magnitude shy of memory provisioning at fixed performance compared even to a BG/Q, so average concurrency for memory-bound codes (typical of cosmology) will likely increase by factors in the 10's to 100 (or people will just give up)
  - Run times in terms of wall clock will never be longer than ~month; beyond this, doing science becomes hopeless; number of runs per year will go up as simulations become ever more important to extracting science from observations, perhaps a factor of 10 or more than current practice
  - Data read/written will likely depend on (i) simulation sizes, (ii) extent of in situ analysis and compression, (iii) external factors such as I/O bandwidth, size/stability of filesystems -- is likely to go up by a factor of 10-100
  - Minimum memory requirements -- globally, one expects something in the low 10's of PB, which would, at 100 million-way concurrency, translate to ~100 MB/"core"; this is fine for HACC but not so much for AMR codes, may need (equivalent of) ~GB/"core"
  - On-line file storage requirement -- 10's of PB, but in "active" storage (off-line, hopeless)

Strategies for New Architectures

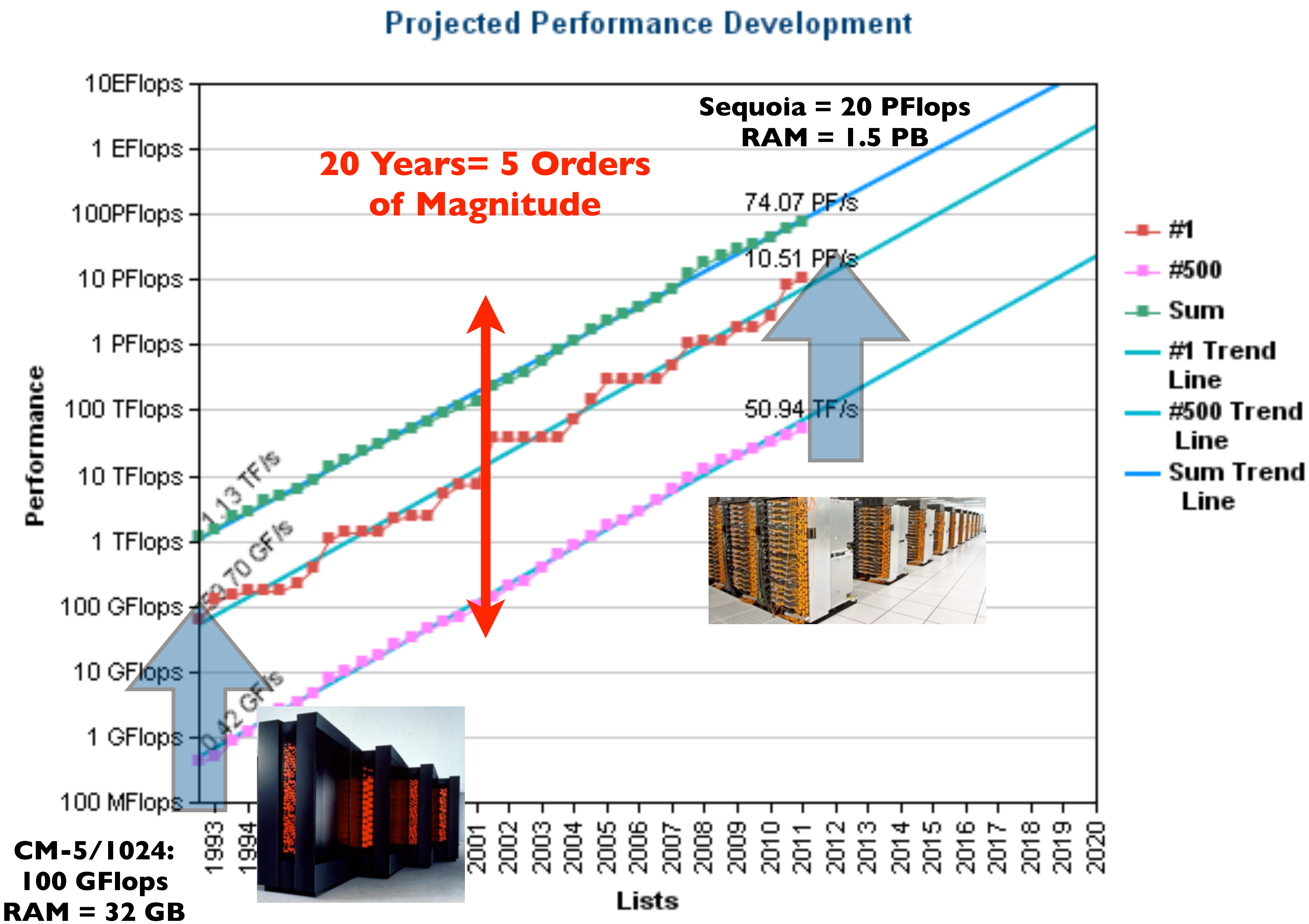
- **N-Body:**
  - Ready now: HACC runs on CPU/GPU, SoC, CPU/MIC already, based on a multi-algorithmic design targeted to future architectures (see arXiv:1211.4864 [cs.CE]), we don't expect major changes to the framework to get ready for 2017
- **AMR Codes:**
  - For AMR codes this is likely to be a research project which will not be done by 2017
  - Send computation-heavy pieces to accelerator (atomic physics, radiative transfer)
  - For many-core systems, the small memory/core and cost of nonlocal memory access within and across nodes will be a major problem -- needs to be addressed
  - Possible intermediate solution to get something to run and be more portable -- use of directives (pragmas) as in OpenACC, good place for NERSC to provide expertise, collect early science project teams
  - DSLs unlikely to be available by 2017 in production form
- **Data Analytics:**
  - A major challenge will be to rewrite a large set of analysis routines for new architectures, especially if there is an ecology of different architectures
  - We are highly competent-people-limited! Help in this area would be very useful --

Summary I

- **New Science:**
  - First, not so much new science as much as planned science -- improvements in NERSC services will be required for supporting the science of ongoing and next-generation cosmological surveys (BOSS, DES, BigBOSS/DESpec, LSST)
  - Second, our project has already planned future work based on expected improvements in computational capabilities at NERSC and other centers
  - Key science results relate to dark energy, dark matter properties, early Universe physics, neutrino mass constraints, and perhaps, new surprises --
- **Recommendations:**
  - Hard to tell what will be the “conservative option” in 2017 for NERSC to follow, there may not be one! (as there wasn’t in the mid-90’s)
  - Most important -- work to to keep the NERSC userbase informed of coming changes well in advance; perhaps availability of early prototype systems, help with code “ports”
  - Data analytics and supercomputing are likely to be intertwined by 2017, NERSC may want to be one of the leaders in this
  - Maintain continuous interaction with applications teams, many of us know what we are doing ;-)

Summary II

- **Expanded Resources:**
  - A factor of 30 is significant, but far from outrageous (in terms of a 3D problem size it's only a factor of ~3); some science cases will be unaffected by this increase, just as they have not been affected by many orders of magnitude in the past --
  - Some science cases will no doubt be affected -- we will be!



- **How?**
  - Need to expand significantly in the "supercomputing meets big data" direction
  - A "data analysis cloud" or equivalent, with dynamically allocatable resources would be a very useful complement to the supercomputer
  - Help codes with complex data structures and low Flops/ Bytes figure out strategies for next generation architectures
  - Key issue will be dealing with a number of programming models unless one clear winner emerges (highly unlikey?) -- help userbase with this