Computing the Dark Universe

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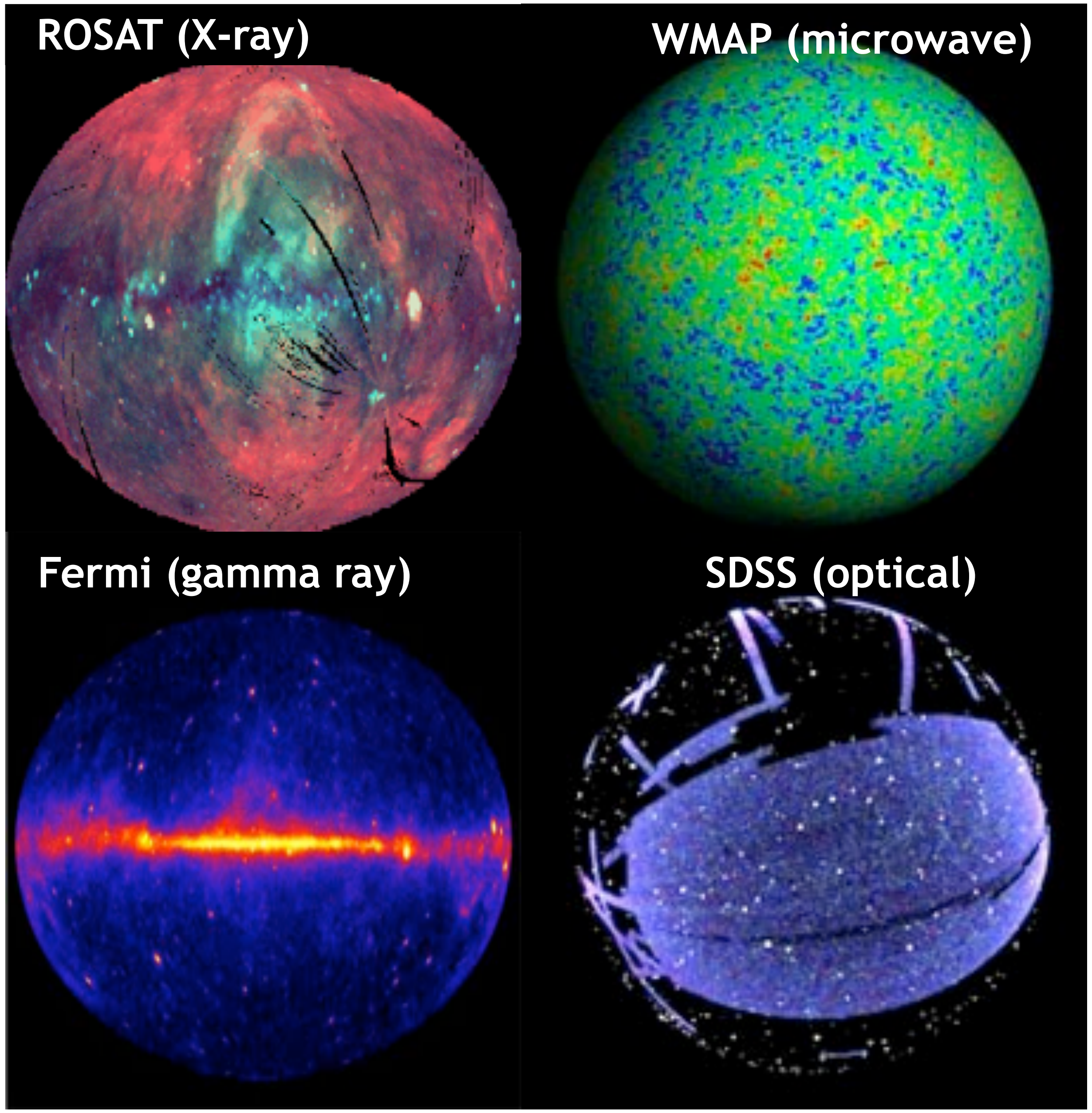
Modern Cosmology and Sky Maps

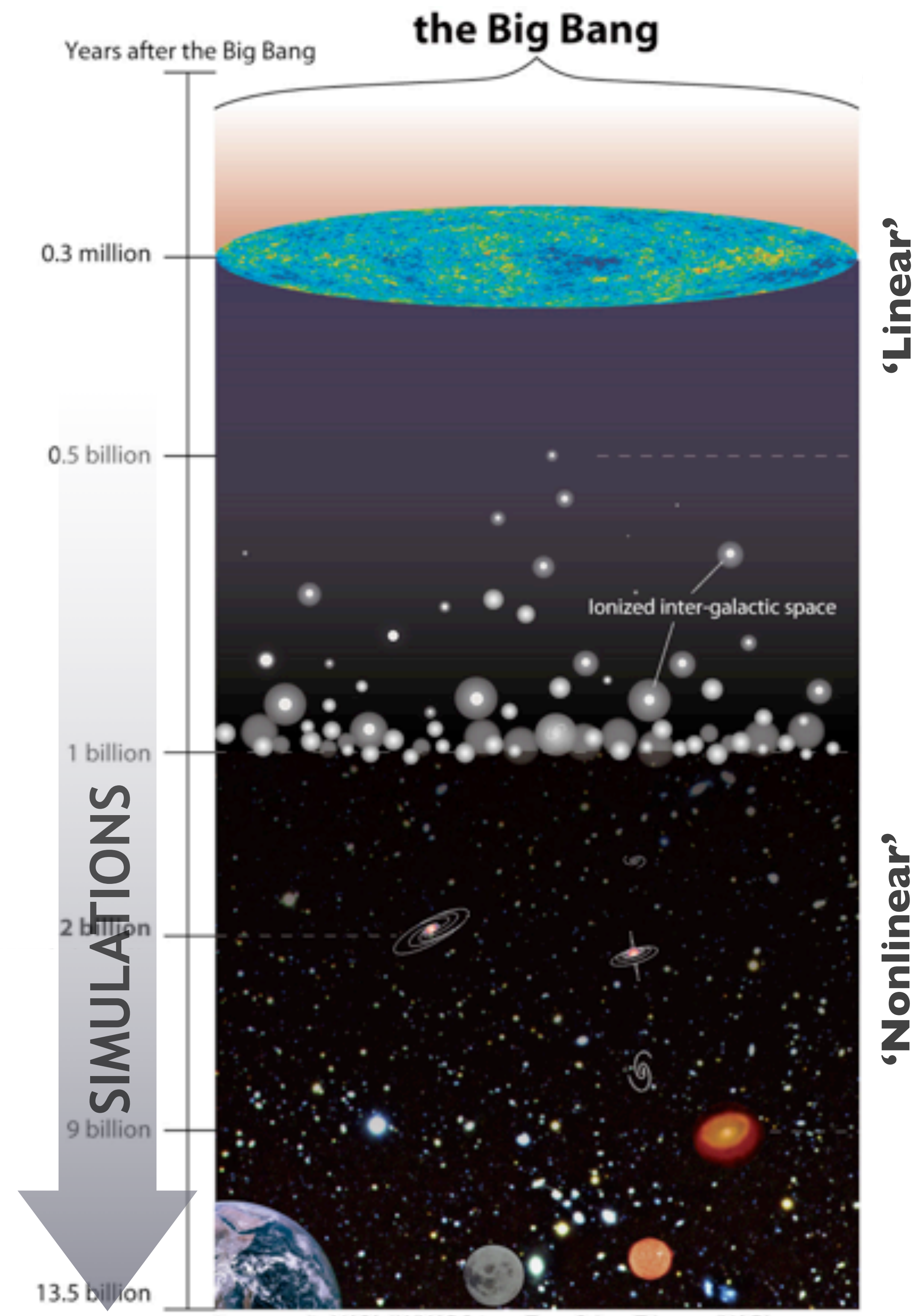
- Modern cosmology is the story of mapping the sky in multiple wavebands
- Maps cover measurements of objects (stars, galaxies) and fields (CMB temperature)
- Maps can be large (SDSS has~200 million galaxies, many billions for LSST)
- Statistical analysis of sky maps
- All precision cosmological analyses constitute a statistical inverse problem: from sky maps to scientific inference
- Therefore: No cosmology without (large-scale) computing



Explosion of information from sky maps: Precision Cosmology

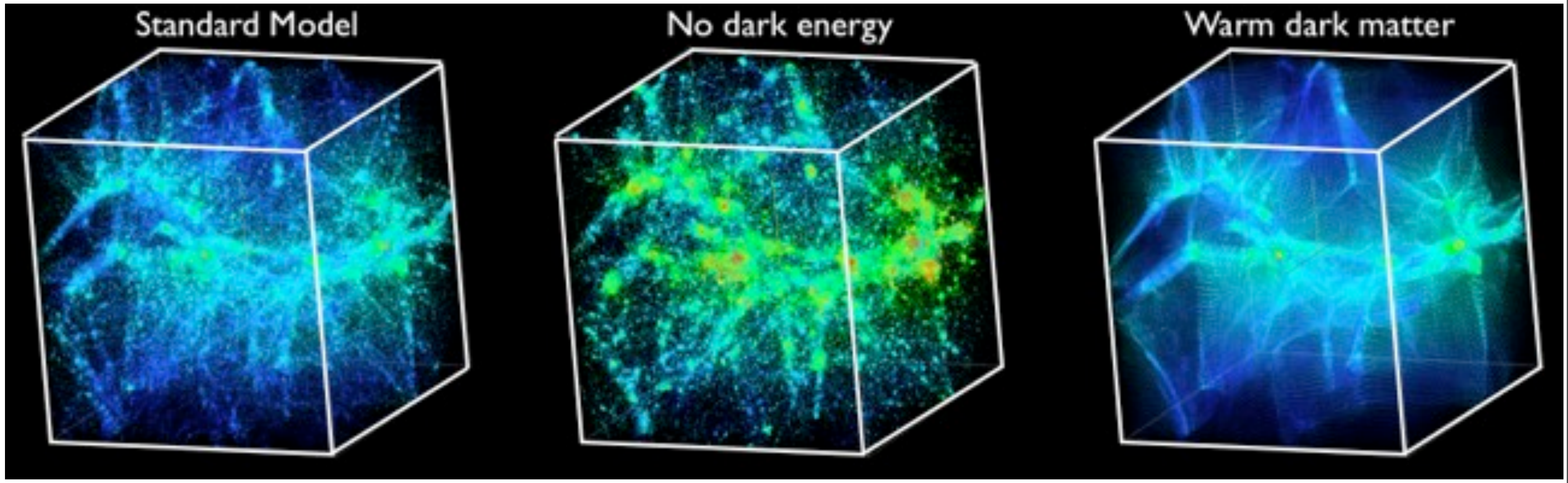
Structure Formation: The Basic Paradigm

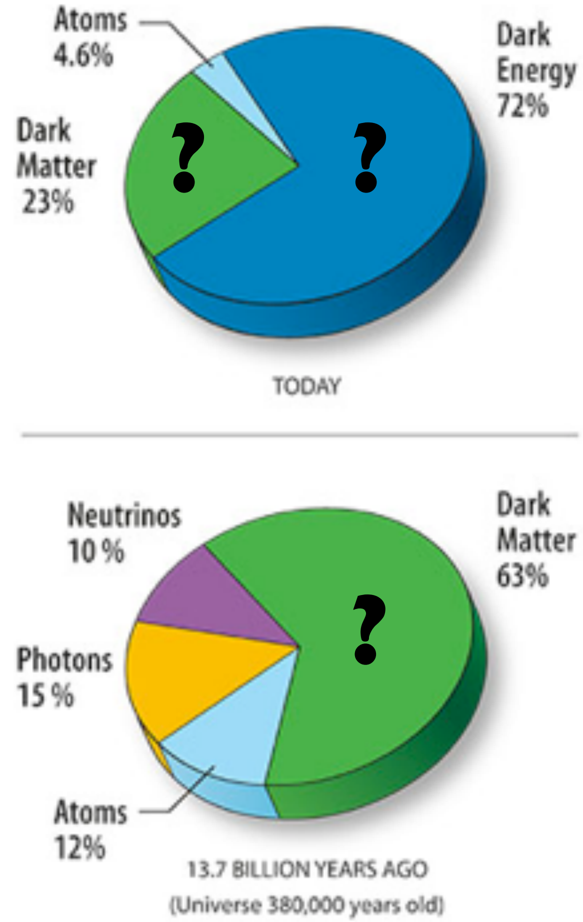
- **Solid understanding of structure formation; success underpins most cosmic discovery**
  - Initial conditions laid down by inflation
  - Initial perturbations amplified by gravitational instability in a dark matter-dominated Universe
  - Relevant theory is gravity, field theory, and atomic physics (‘first principles’)
- **Early Universe:** Linear perturbation theory very successful (CMB)
- **Latter half of the history of the Universe:** Nonlinear domain of structure formation, impossible to treat without large-scale computing



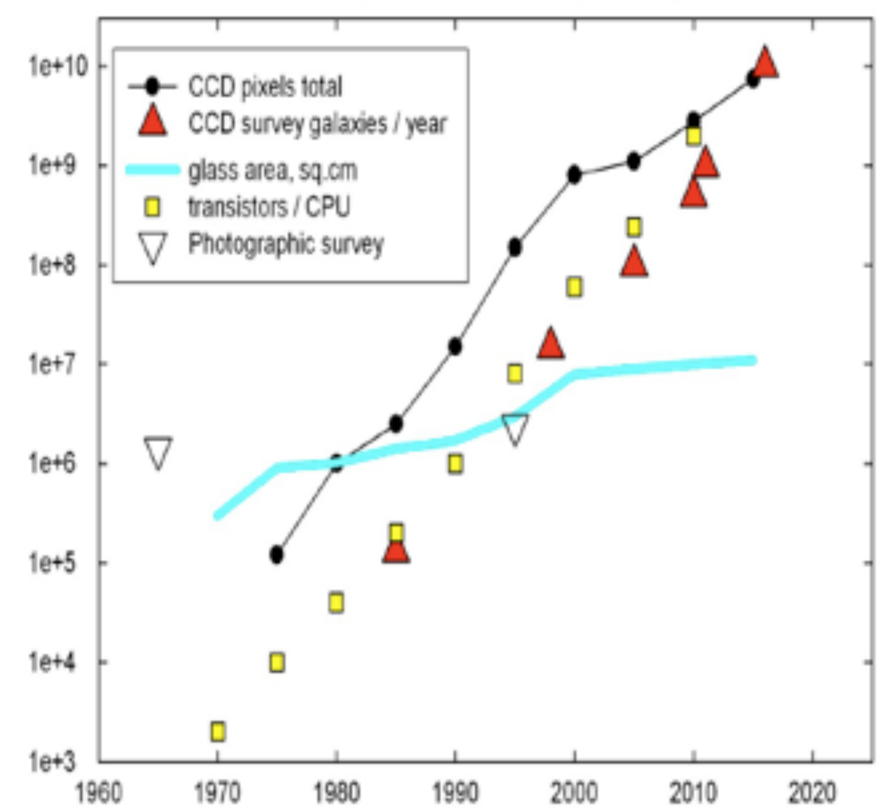
Precision Cosmology: “Inverting” the 3-D Sky

- **Cosmological Probes:** Measure geometry and presence/growth of structure
- **Examples:** Baryon acoustic oscillations (BAO), cluster counts, CMB, weak lensing, galaxy clustering, --
- **Standard Model:** Verified at the 5-10% level across multiple observations
- **Future Targets:** Aim to control survey measurements to the ~1% level, can theory and simulation keep up?





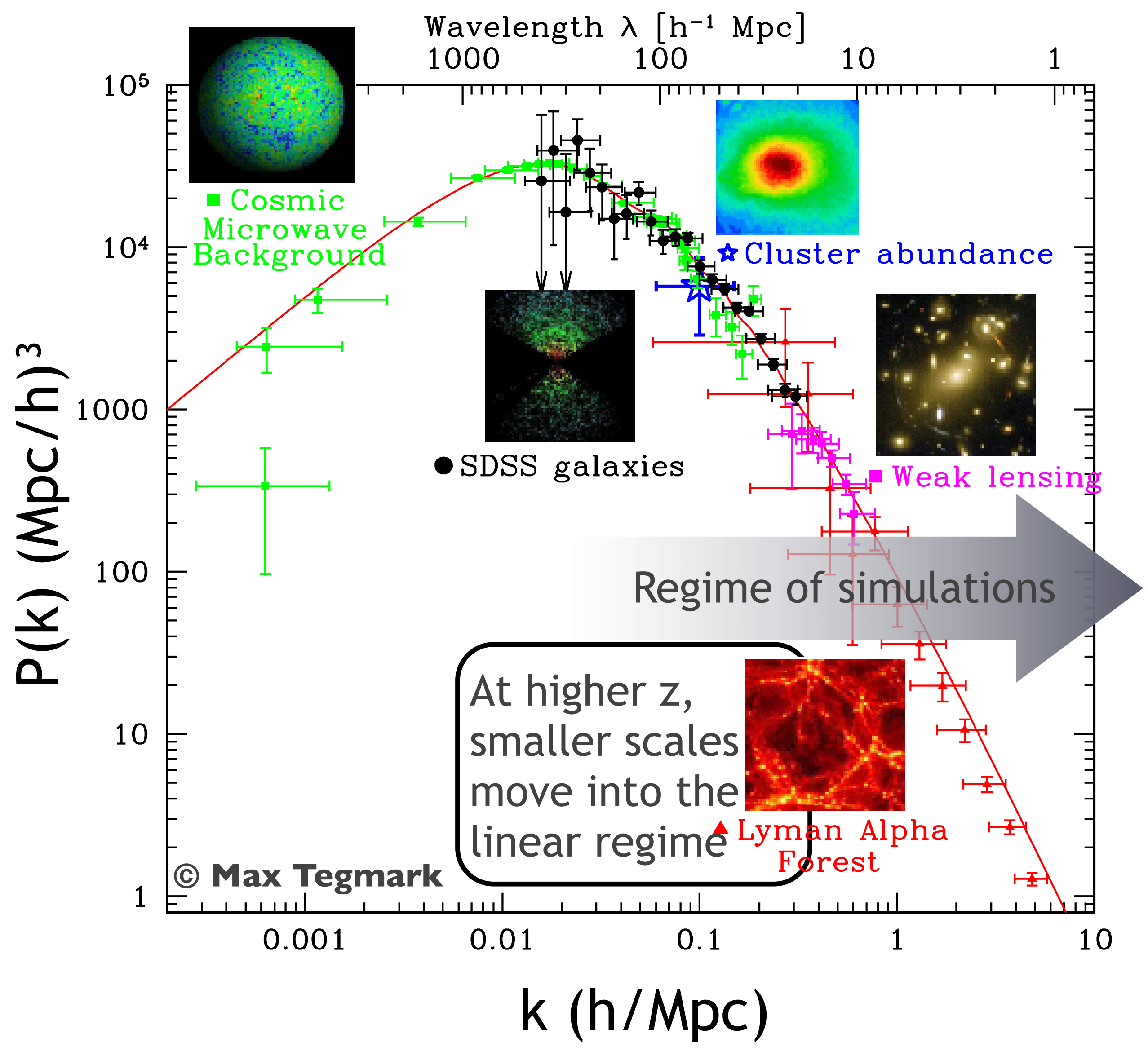
Cosmic content pie charts



Optical survey ‘Moore’s Law’

Measuring Large-Scale Structure

- **CMB probes large scales and early times, anchors paradigm (>10 Mpc)**
- **Neutral hydrogen seen by 21cm emission as tracer of structure (z>0.5)**
- **Lyα: Neutral hydrogen distribution seen as absorption features in spectra of distant objects (1-10 Mpc, 2<z<3)**
- **Lensing: Light deflection by density inhomogeneities (>~1 Mpc, 0<z~1)**
- **Galaxies are biased tracers of the density field (>1 Mpc, 0<z~2)**
- **Object abundance probes tails of density distribution, clusters most sensitive (~10 Mpc, 0<z~2)**

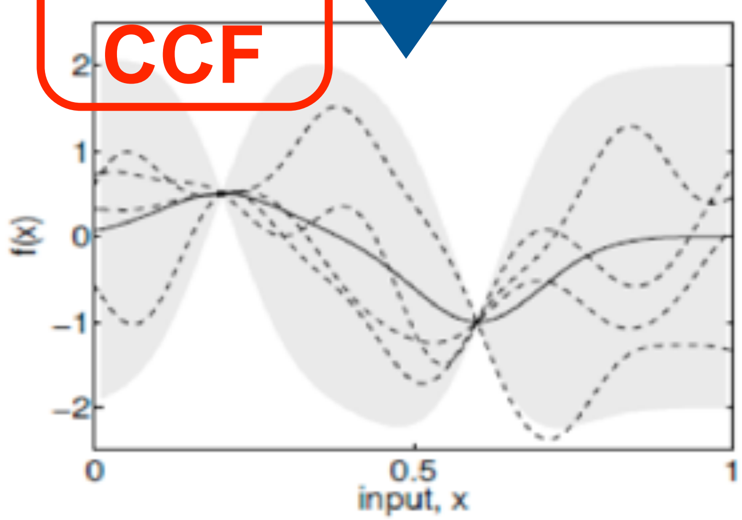


DARK ENERGY SURVEY

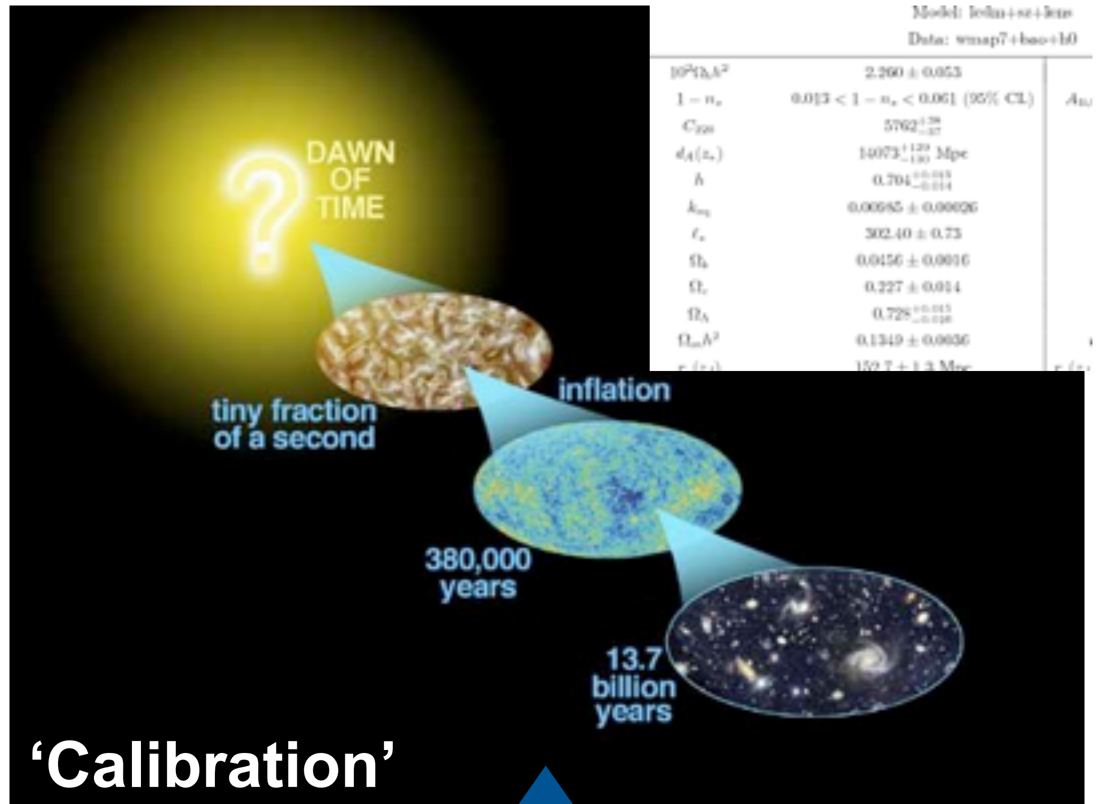
Precision Cosmology: Calibrating the Universe

Supercomputer Simulation Campaign

HACC + CCF

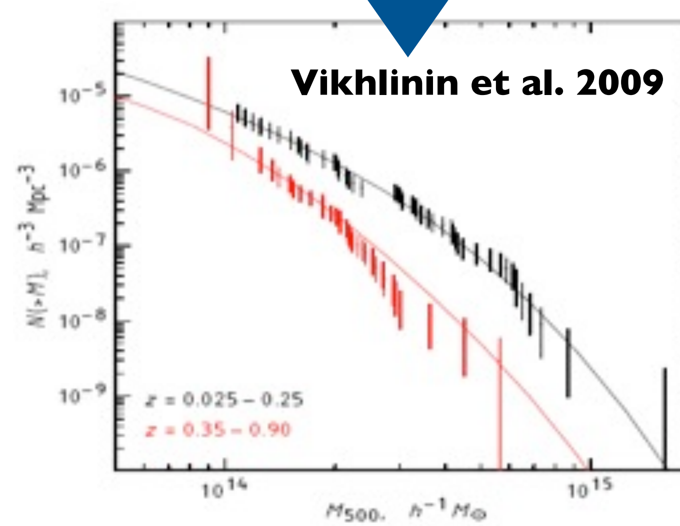


Emulator based on GP Model Interpolation in High-Dimensional Spaces



'Precision Oracle'

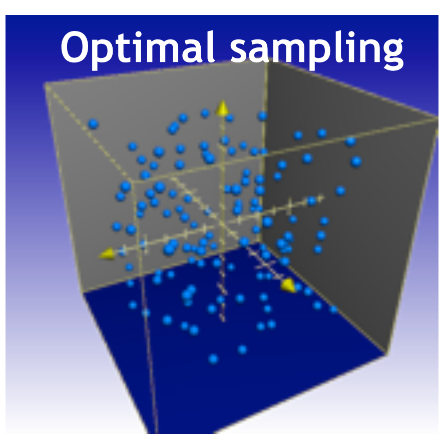
Mapping the Sky with Survey Instruments

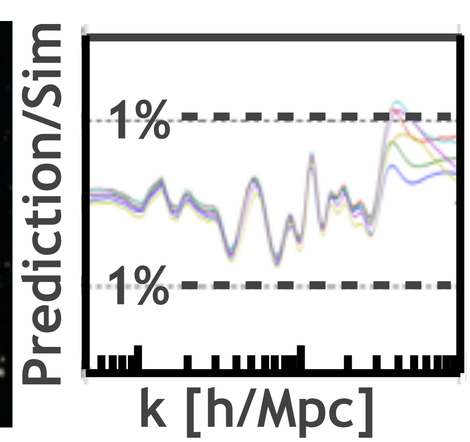


Observations: Statistical error bars will 'disappear' soon!

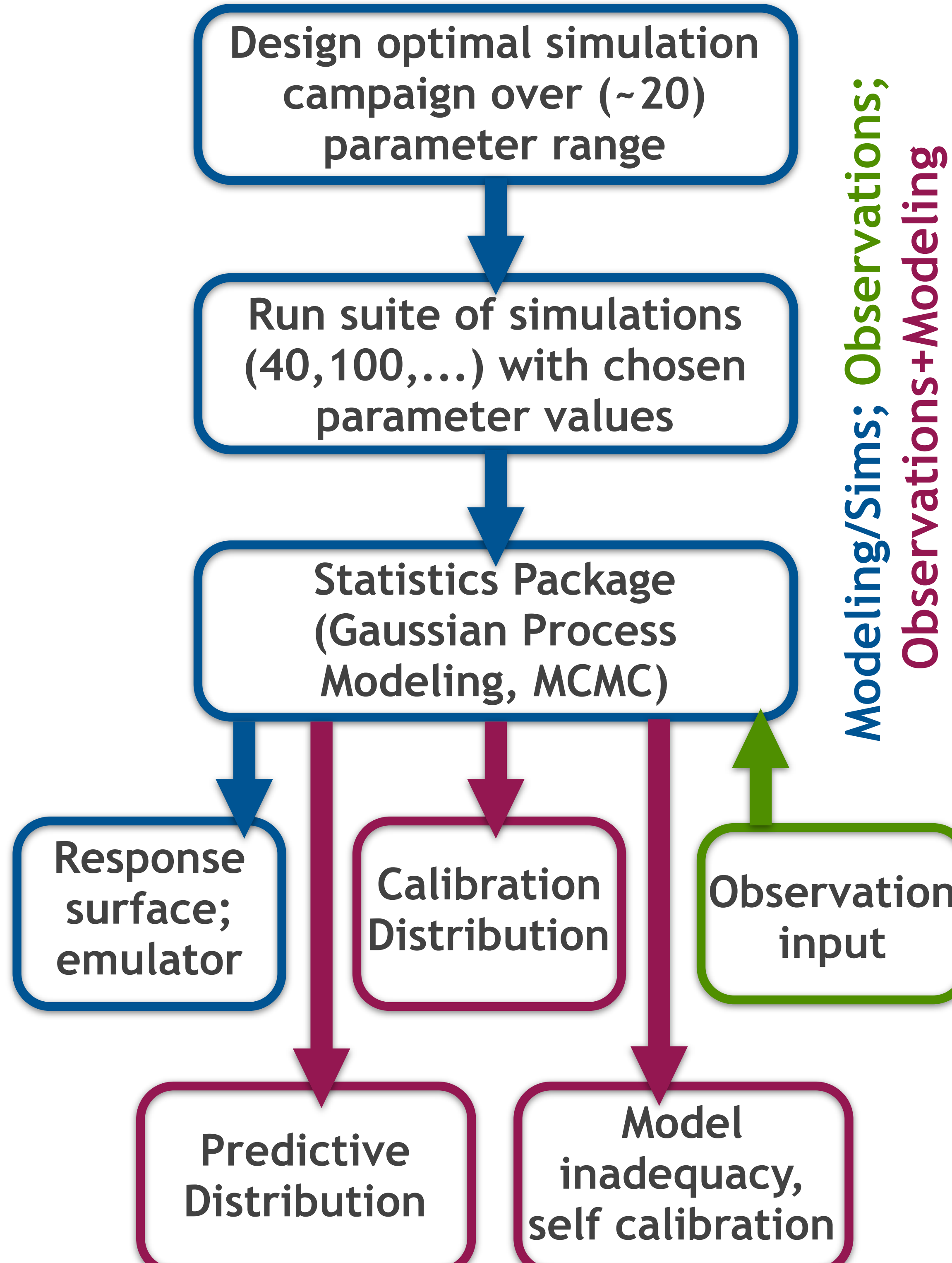
Cosmic Calibration: Solving the Inverse Problem

- **Challenge:** To extract cosmological constraints from observations in the nonlinear regime, need to run Markov Chain Monte Carlo; input: 10,000 - 100,000 different models
- **Brute Force:** Simulations, ~30 years on 2000 processor cluster ---
- **Current Strategy:** Fitting functions, e.g. for P(k), accurate at 10% level, not good enough!
- **Our Solution:** Precision emulators



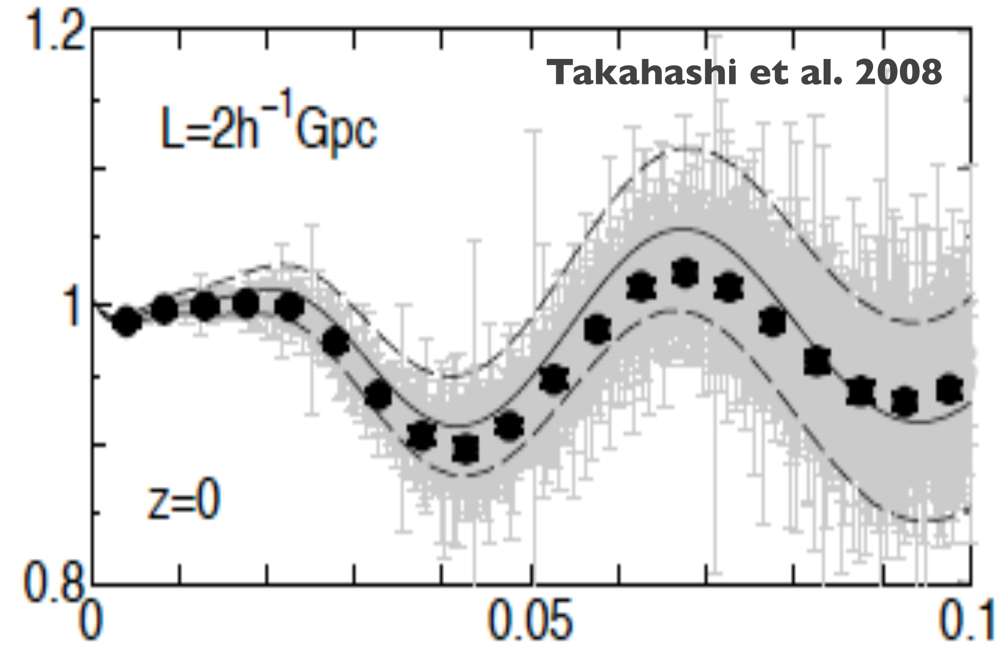


Heitmann et al. 2006, Habib et al. 2007

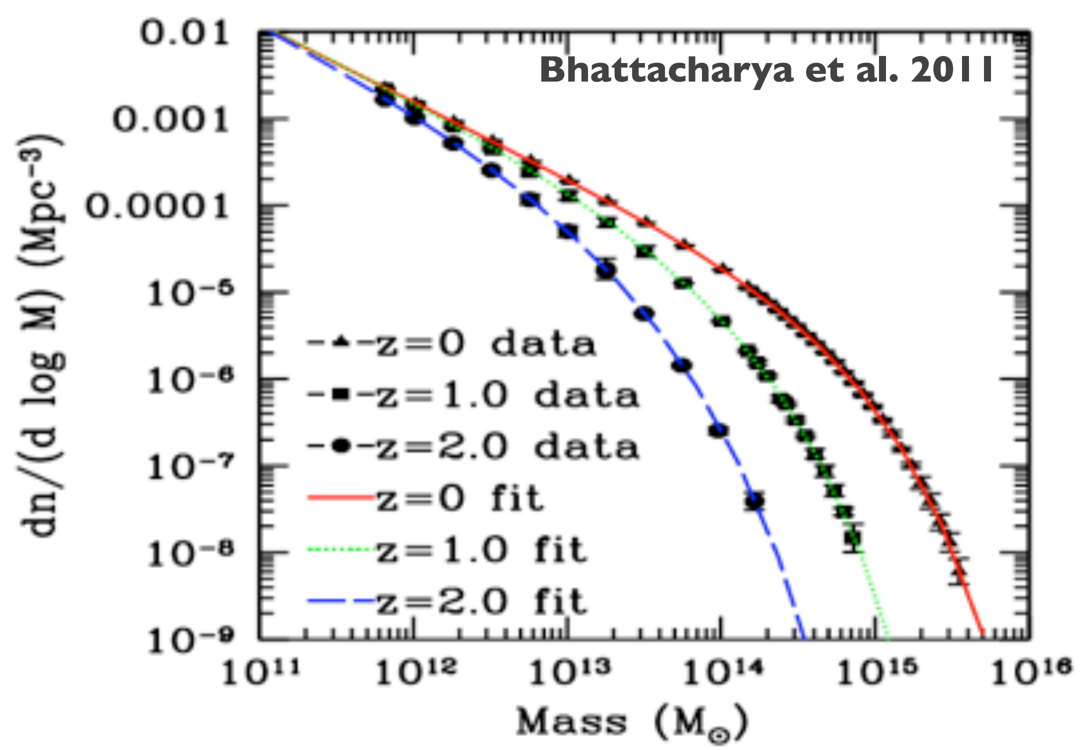


'Easy Problems' (Gravity-only) I

- **Baryon Acoustic Oscillations (BAO) from galaxy surveys (BOSS, DES, LSST)**
  - **Measurement:** Geometry at z<1
  - **Challenge:** Large volume N-body simulations to precisely determine BAO 'wiggles' in P(k) or peak in the correlation function

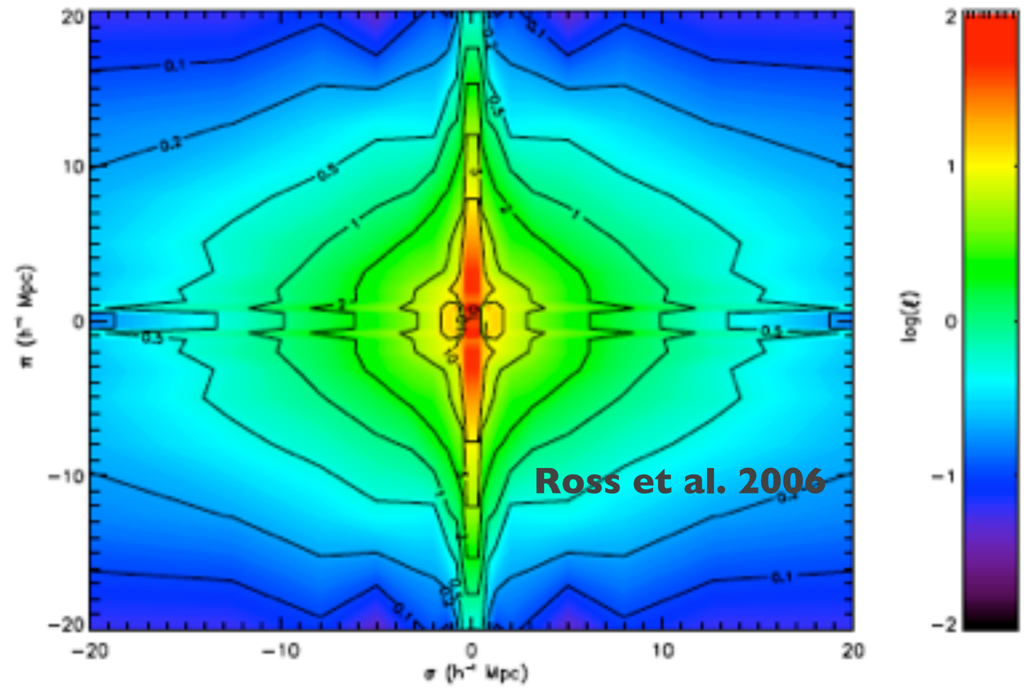


- **Cluster counts (DES, LSST)**
  - **Measurement:** Geometry and structure growth
  - **Challenge:** Large volume N-body (plus N-body/hydro to help characterize observable-mass relations)

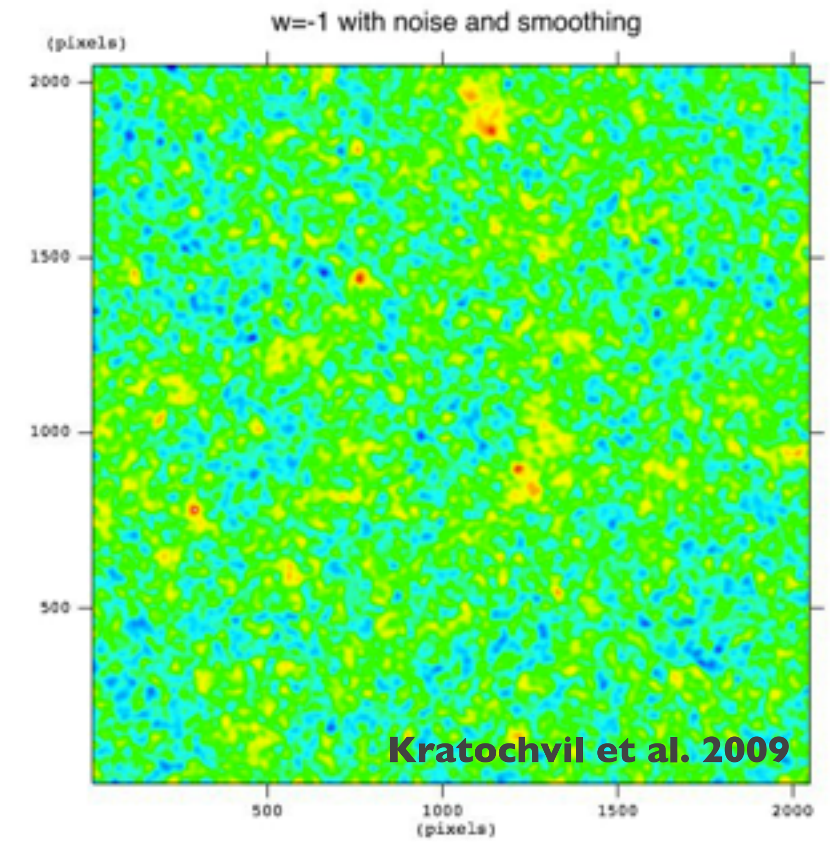


‘Easy Problems’ (Gravity-only) II

- **Redshift-space distortions (BOSS, DES, LSST)**
  - **Measurement:** Growth of structure, tests of modified gravity
  - **Challenge:** Large volume N-body simulations to determine and characterize/model galaxy velocities

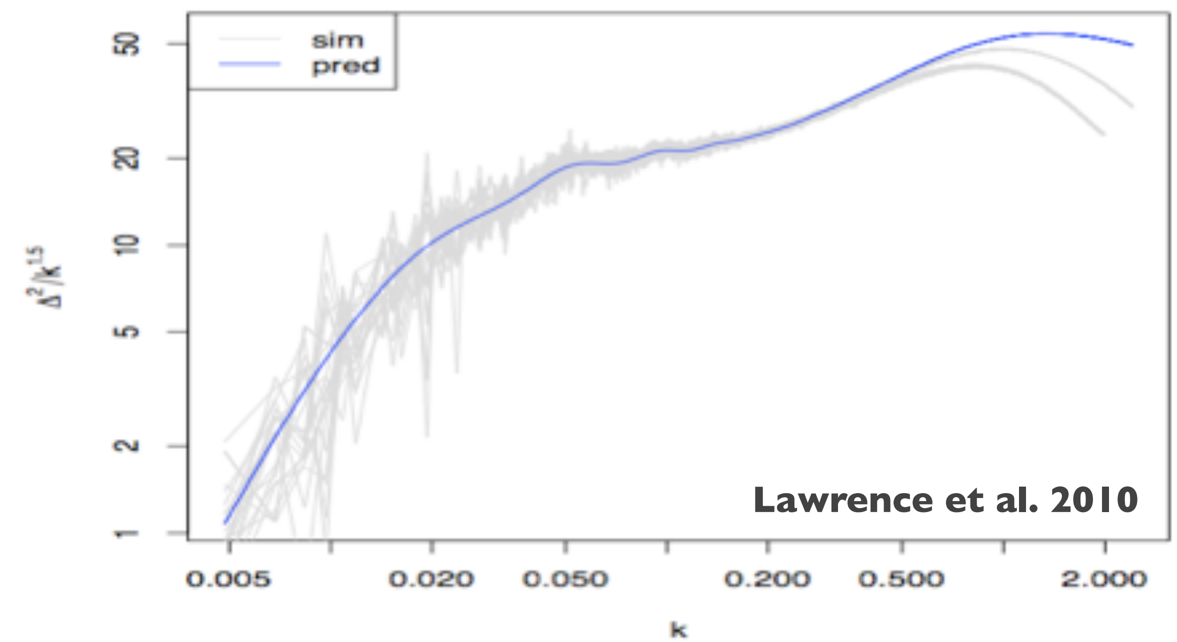


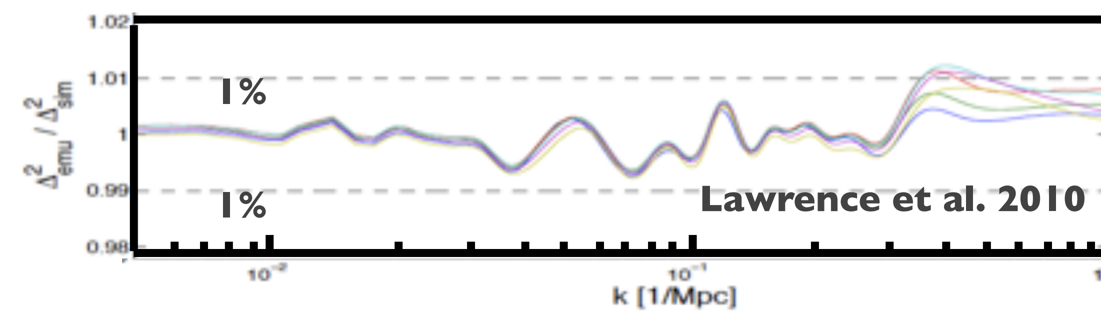
- **Weak lensing (DES, LSST)**
  - **Measurement:** Multiple uses -- geometry, growth, cluster mass
  - **Challenge:** Large volume N-body (plus N-body/hydro simulations to evaluate baryonic systematics)

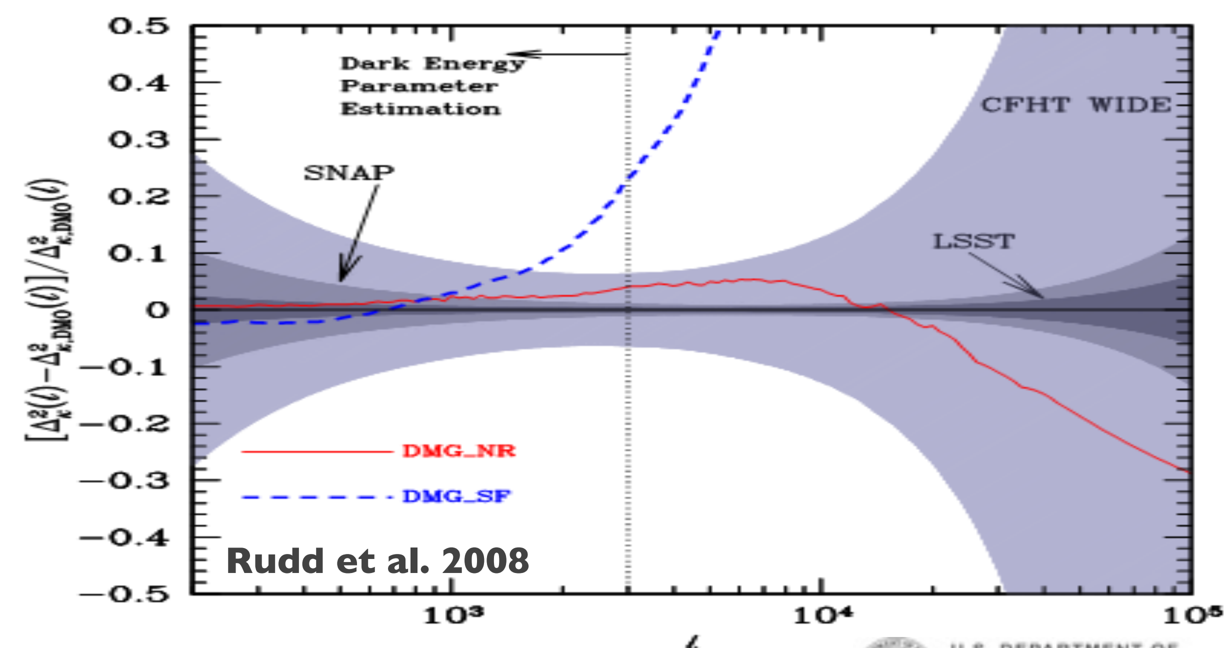


Added Note: Weak Lensing

- **Accuracy requirement:** P(k) calibration needed at ~1% level to k~10 h/Mpc (Huterer & Takada 2005) over a broad range of cosmologies
  - **Emulation:** ‘Coyote Universe’ suite of ~1000 simulations used to build predictors in the gravity-only case to ~1% absolute accuracy extending out to k~1 h/Mpc; covariance matrix requires another set of 1000’s of simulations
  - **Baryonic Effects:** Starting at scales of k~1 h/Mpc, baryonic effects become important (White 2004), posing a significant computational modeling challenge (add modeling component to N-body simulations)







Simulating the Universe

- Gravity dominates at large scales, key task: solve the Vlasov-Poisson equation (VPE)
- VPE is 6-D and cannot be solved as a PDE
- N-body methods; gravity has (i) no shielding but is (ii) naturally Lagrangian
- Are errors controllable?
- At smaller scales add gas physics, feedback, etc. (subgrid modeling inevitable)
- Calibrate simulations against observations

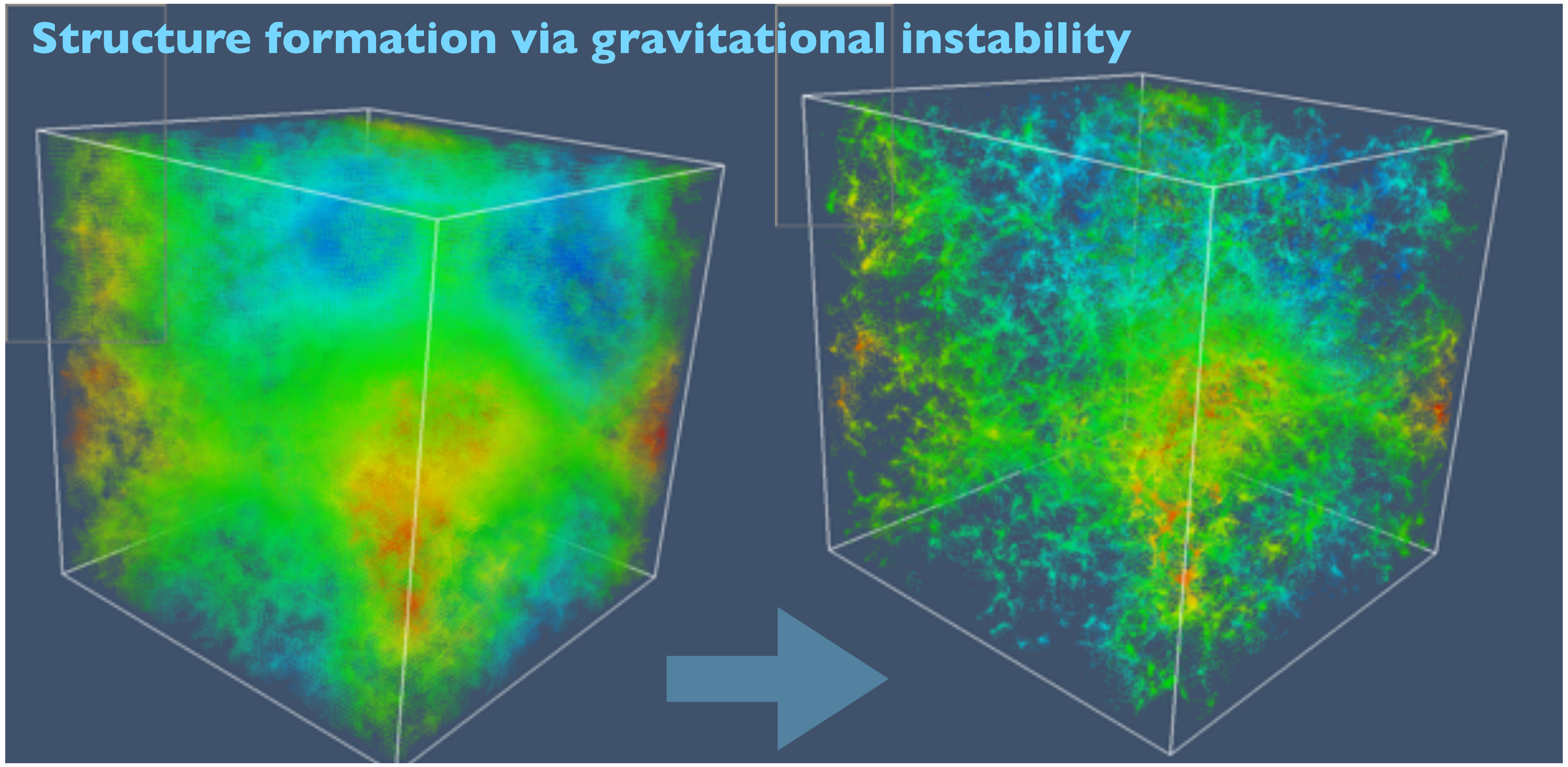
$$\frac{\partial f_i}{\partial t} + \dot{\mathbf{x}}\frac{\partial f_i}{\partial \mathbf{x}} - \nabla\phi\frac{\partial f_i}{\partial \mathbf{p}} = 0, \qquad \mathbf{p} = a^2\dot{\mathbf{x}},$$

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

$$\delta_{\rm dm}(\mathbf{x},t) = (\rho_{\rm dm} - \langle\rho_{\rm dm}\rangle)/\langle\rho_{\rm dm}\rangle),$$

$$\rho_{\rm dm}(\mathbf{x},t) = a^{-3}\sum_i m_i \int d^3\mathbf{p} f_i(\mathbf{x},\dot{\mathbf{x}},t).$$

Cosmological Vlasov-Poisson Equation: A 'wrong-sign' electrostatic plasma with time-dependent particle 'charge'



An Early Simulation

- Suite of 300 (and less) particle simulations
- Run on a CDC 3600, ~1Mflops, 32KB+ at LANL
- Is nine orders of magnitude improvement in both performance and memory good enough for precision cosmology?

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Structure of the Coma Cluster of Galaxies*

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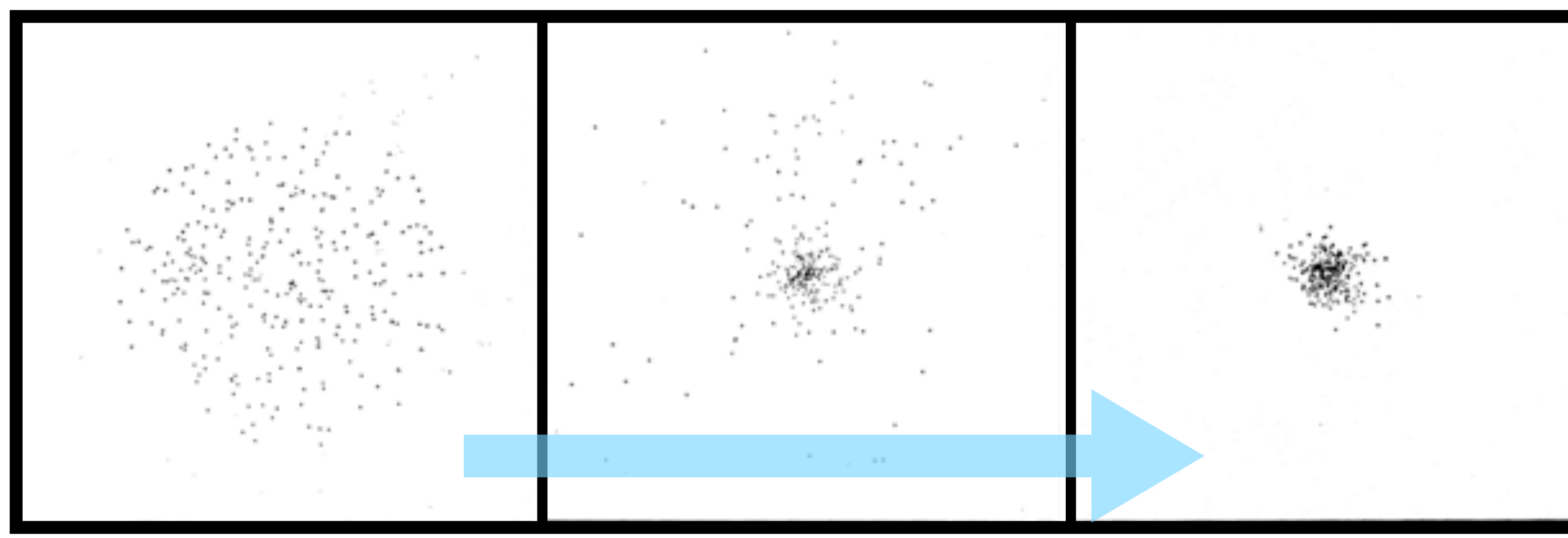
(Received 7 October 1969)

In some cosmologies, a cluster of galaxies is imagined to be a gravitationally bound system which, in analogy with the formation of the Galaxy, originated as a collapsing protocluster. It is shown that a numerical model based on this picture is consistent with the observed features of the Coma Cluster of galaxies. The cluster mass derived from this model agrees with previous values; however, an analysis of the observational uncertainty within the framework of the model shows that the derived mass could be consistent with the estimated total mass provided by the galaxies in the cluster.



"The Universe is far too complicated a structure to be studied deductively, starting from initial conditions and solving the equations of motion."

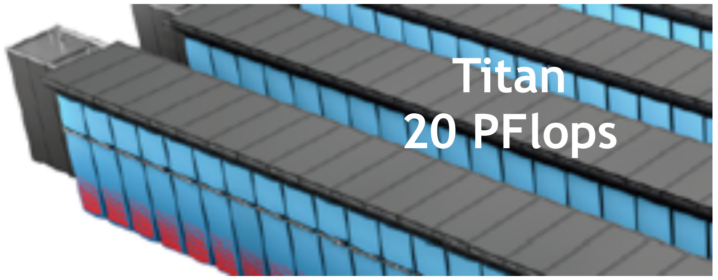
Robert Dicke (Jayne Lectures, 1969)

What's Needed: Simulating Surveys

- **Simulation Volume:** Large survey sizes impose simulation volumes ~ (**3** Gpc)^3, memory required **~100** TB **-- 1** PB
- **Number of Particles:** Mass resolutions depend on ultimate object to be resolved, number of particles can go to **~10^{12}**
- **Force Resolution:** ~kpc, yields a (global) spatial dynamic range of **10^6**
- **Hydrodynamics/Sub-Grid Models:** Phenomenological treatment of gas physics and feedback greatly adds to computational cost
- **Throughput:** Large numbers of simulations required (**100**'s **--1000**'s), development of analysis suites, and emulators; peta-exascale computing exploits
- **Data-Intensive-SuperComputing:** End-to-End simulations and observations must be brought together in a DISC environment (theory-observation feedback)

The Near Future --

- **Standard Approach:** Wait for supercomputers to get bigger, they have not gotten 'faster' since 2004; make sure codes weak scale (or hope Volker is doing this for you --)
  - **Problem:** Thus would work except for one BIG problem: billion-way concurrency requires way too much power! (~GW)
  - **Architecture Changes:** The end of Moore's Law has important ramifications ('pile of PCs' to 'pile of cell phones'?)
  - Proliferation of 'nodal' architectures (Cell/GPU/SOC, MIC, --)
  - Simpler cores, lower memory/core
  - Complex, heterogeneous nodes (e.g., including power management -- 'dark silicon')
  - Nasty memory and communication hierarchies
  - Programming environments unclear



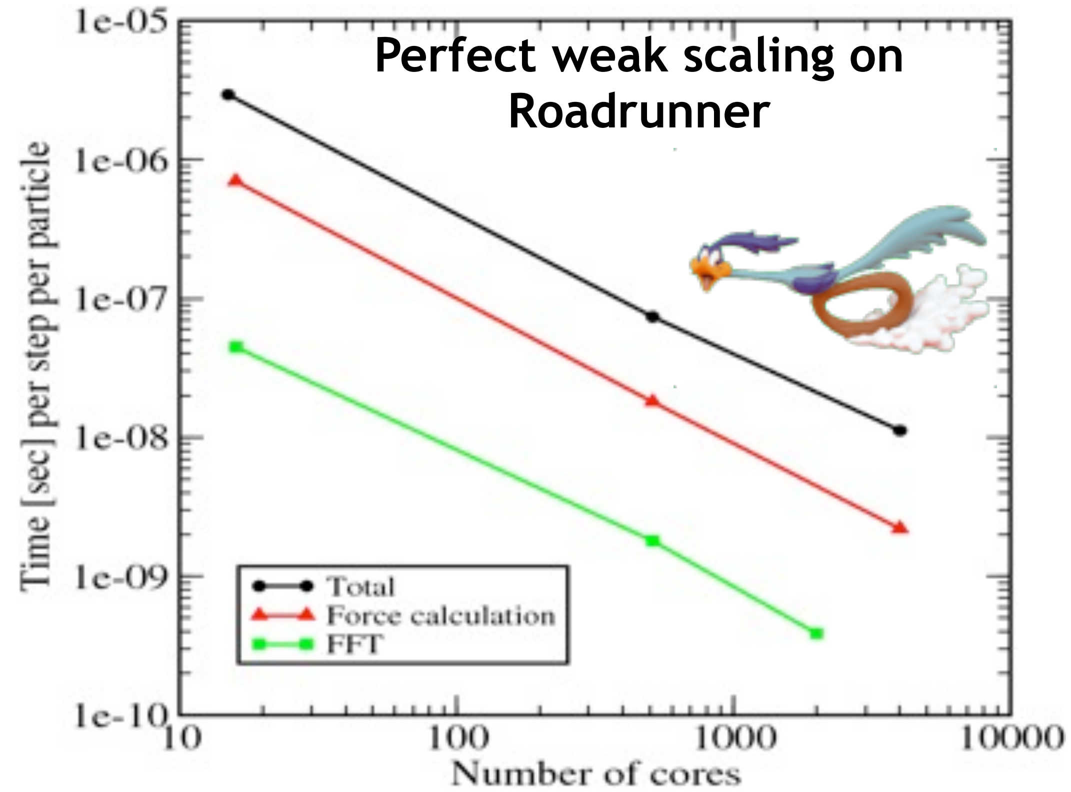
Defensive Design Approach

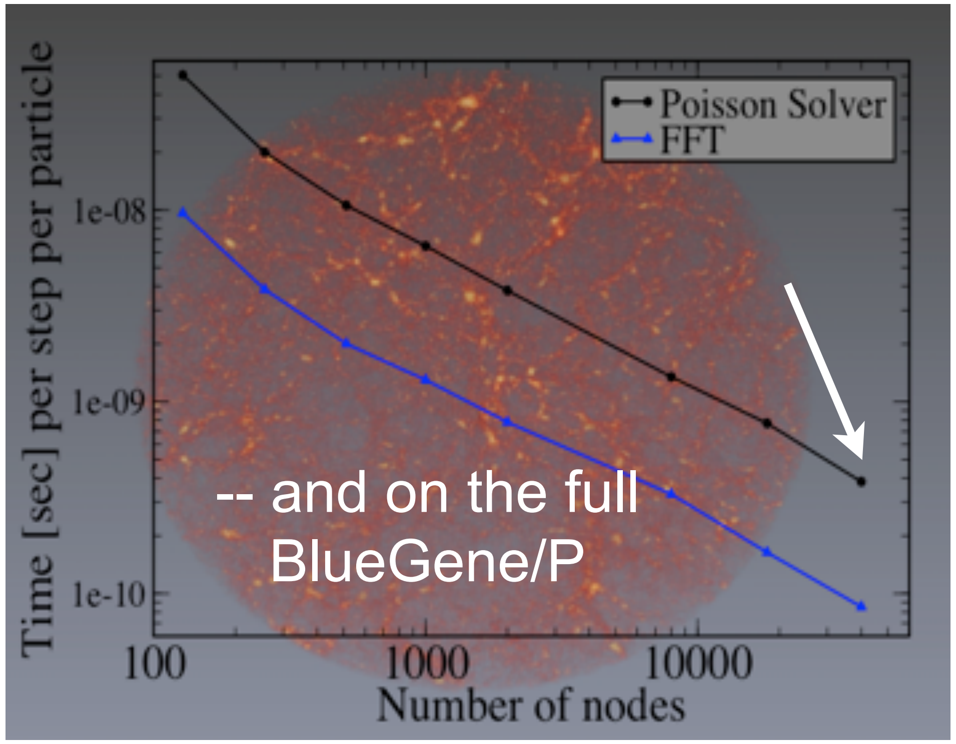
- **Architecture Assumption**
  - Supercomputers will have the following structure -- communication fabric connecting a large number of complex nodes (up to a million)
  - Analog of MPI (message-passing) will exist at the top level, i.e., require a universal, scalable communication layer -- seems reasonable!
  - Break algorithmic/programming task into two components: (i) program to the top level, (ii) program to the node
  - Node level code should be 'plug-in'
- **Physics/Algorithms**
  - **Essential Feature:** Gravity allows splitting of forces into long- and short-range components
  - **Grids and Particles:** Ability to use different representations of the density field allow for natural mapping across architectural layers

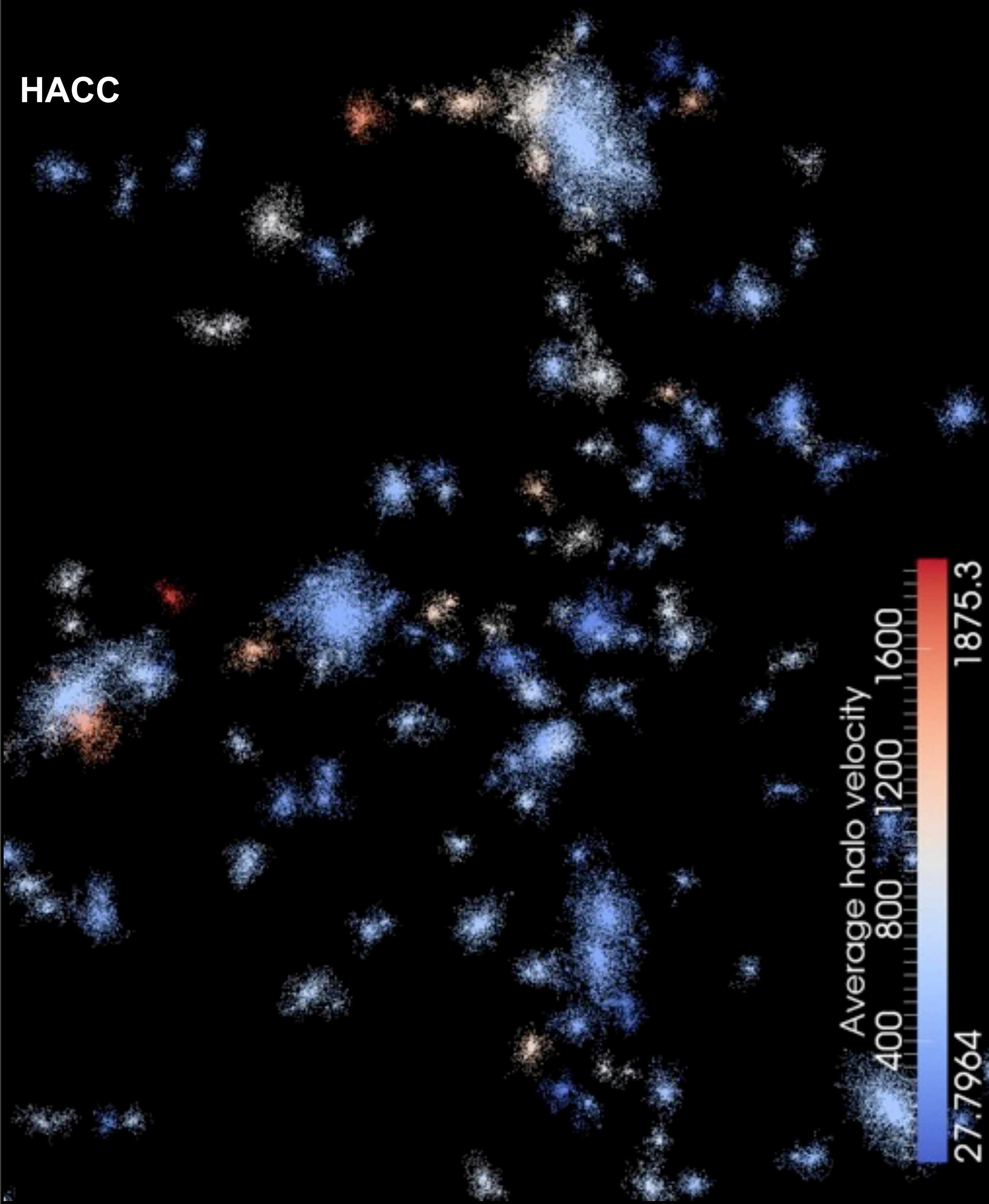
Hardware-Accelerated Cosmology Code (HACC) Framework

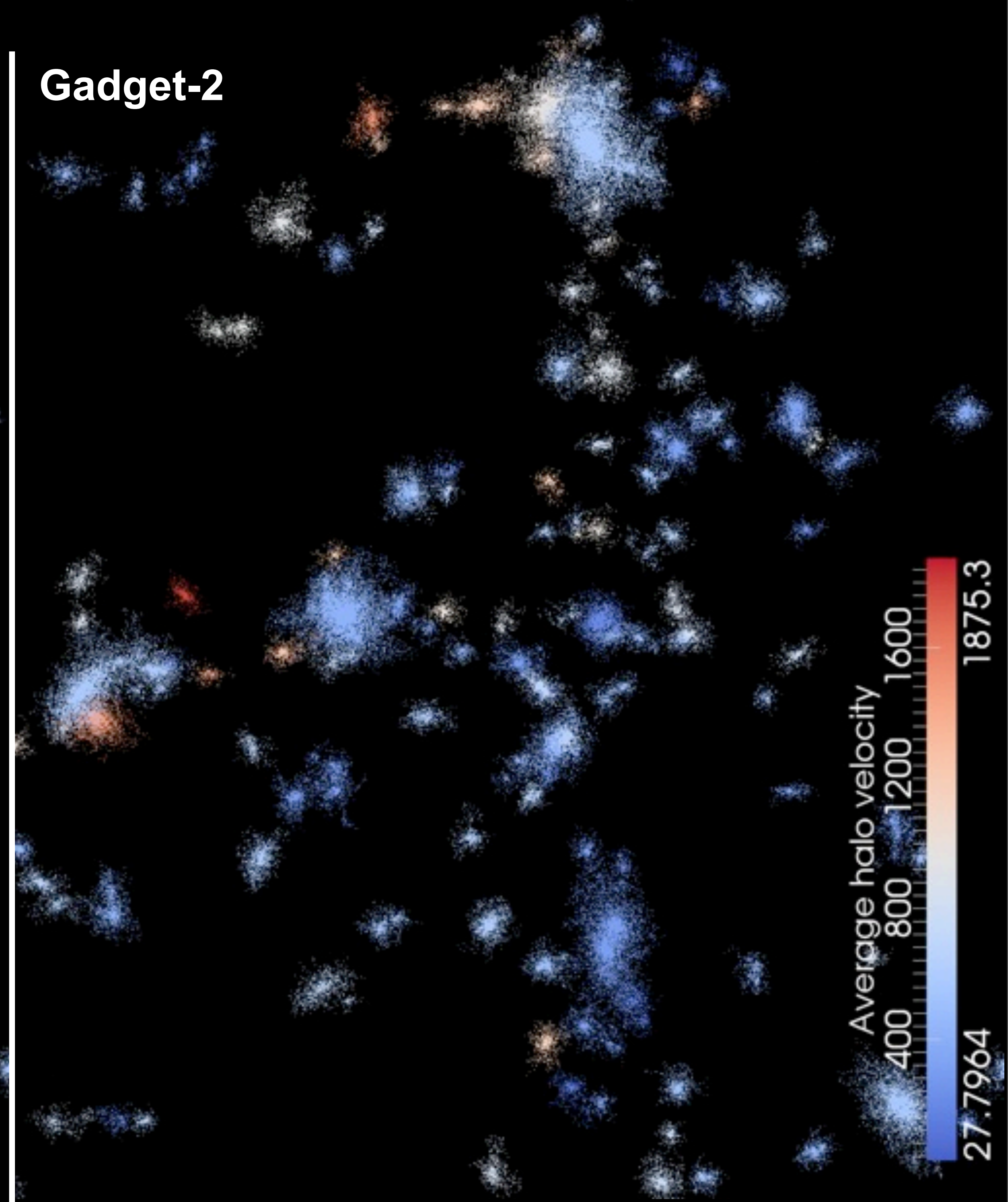
- **Code for the Future:** Follows defensive design principles: melds optimized performance, low memory footprint, embedded analysis, and scalability
- **Implementation:** Long/short-range force matching with spectral force-shaping (long-range=PM, short-range=PP, Tree; best to think of algorithm as TP3M)
- **Key Features:** Hybrid particle/grid design, particle overloading, spectral operators, mixed-precision, node-level 'plug-ins', target ~50% of peak Flops
- **Cross-Platform:** Designed for all current and future supercomputing platforms
- **Embedded Analysis:** High performance with low I/O and storage requirement

Habib et al. 2009, Pope et al. 2010

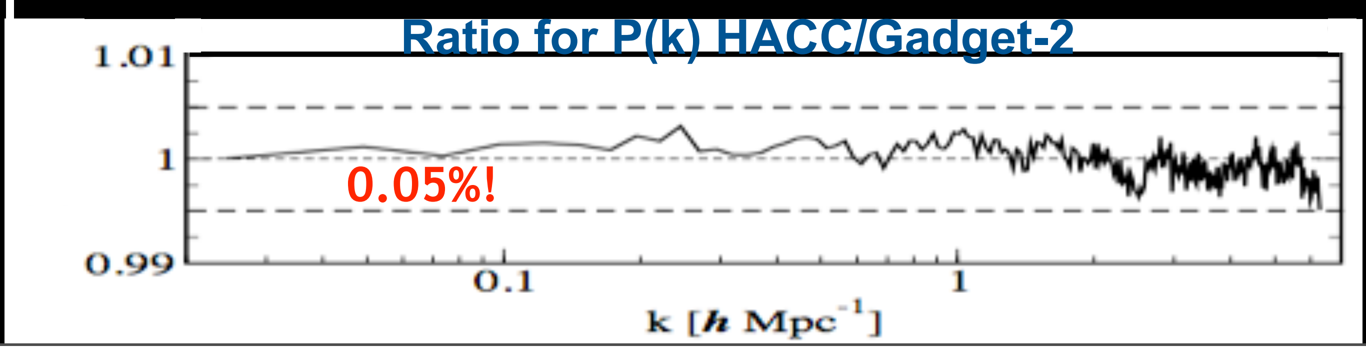








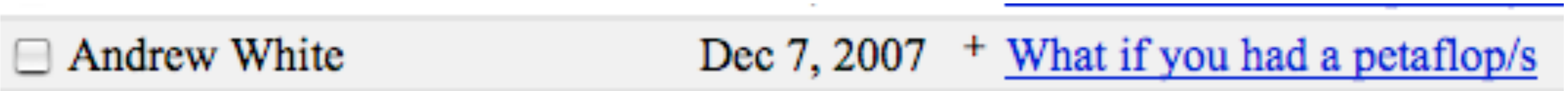
Snapshot from Code Comparison simulation, ~25 Mpc region; halos with > 200 particles, b=0.15
Differences in runs: P³M vs. TPM, force kernels, time stepper: MC³: a; Gadget-2: log(a)
Power spectra agree at sub-percent level



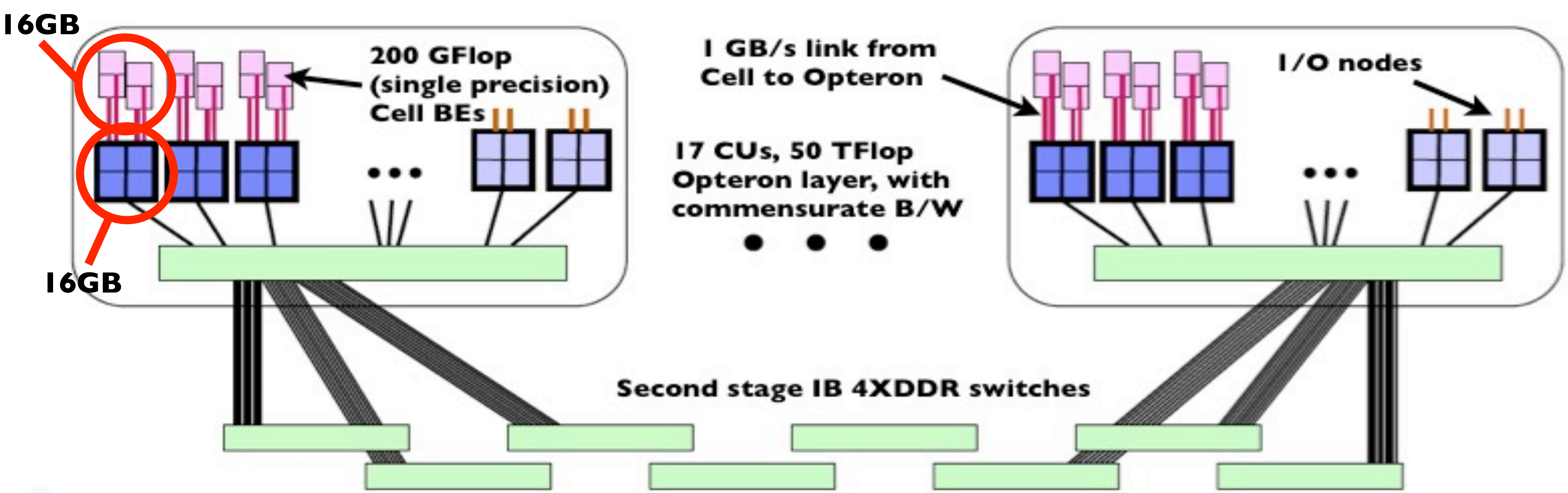
HACC Design Features

- **New Framework:** Not a port of an older code (too difficult)
- **Two-Layer Design:** Anticipates communication bottleneck between machine layers
- **Compute Sharing:** Compute complexity shifted to CPU+MPI layer (new algorithms), simple brute force computations assigned to accelerators, use mixed precision (CPU, double; accelerator, single)
- **Memory Trade-Off:** Small memory overhead used to reduce inter-layer communication and improve modularity
- **Cross-Platform:** Aimed at current and future supercomputing platforms using 'plug-in' short-range force modules optimized for a given nodal architecture (and using different algorithms)
- **In Situ Analysis:** Significant attention paid to 'on the fly' analysis methods to reduce I/O and storage; code design allows for essentially 'serial' methods to be trvially parallelized
- **Simplicity:** Relatively straightforward approach

HACC Beginnings: Roadrunner Universe Project

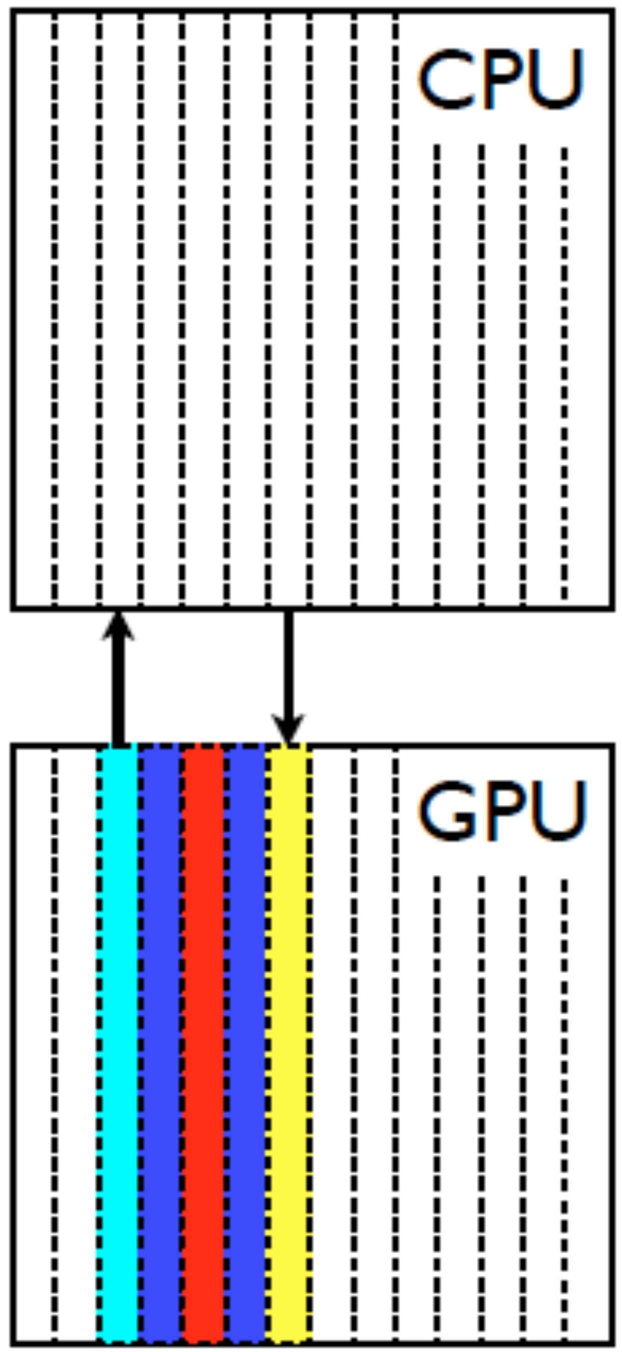


- Hybrid machine architecture, out of balance communication (50-100) and performance (20)
- Balanced memory (CPU=Cell)
- Multi-level programming paradigm
- Prototype for exascale code design problems
- Scalable approach extensible to all next-generation architectures (BG/Q, CPU/GPU, --)



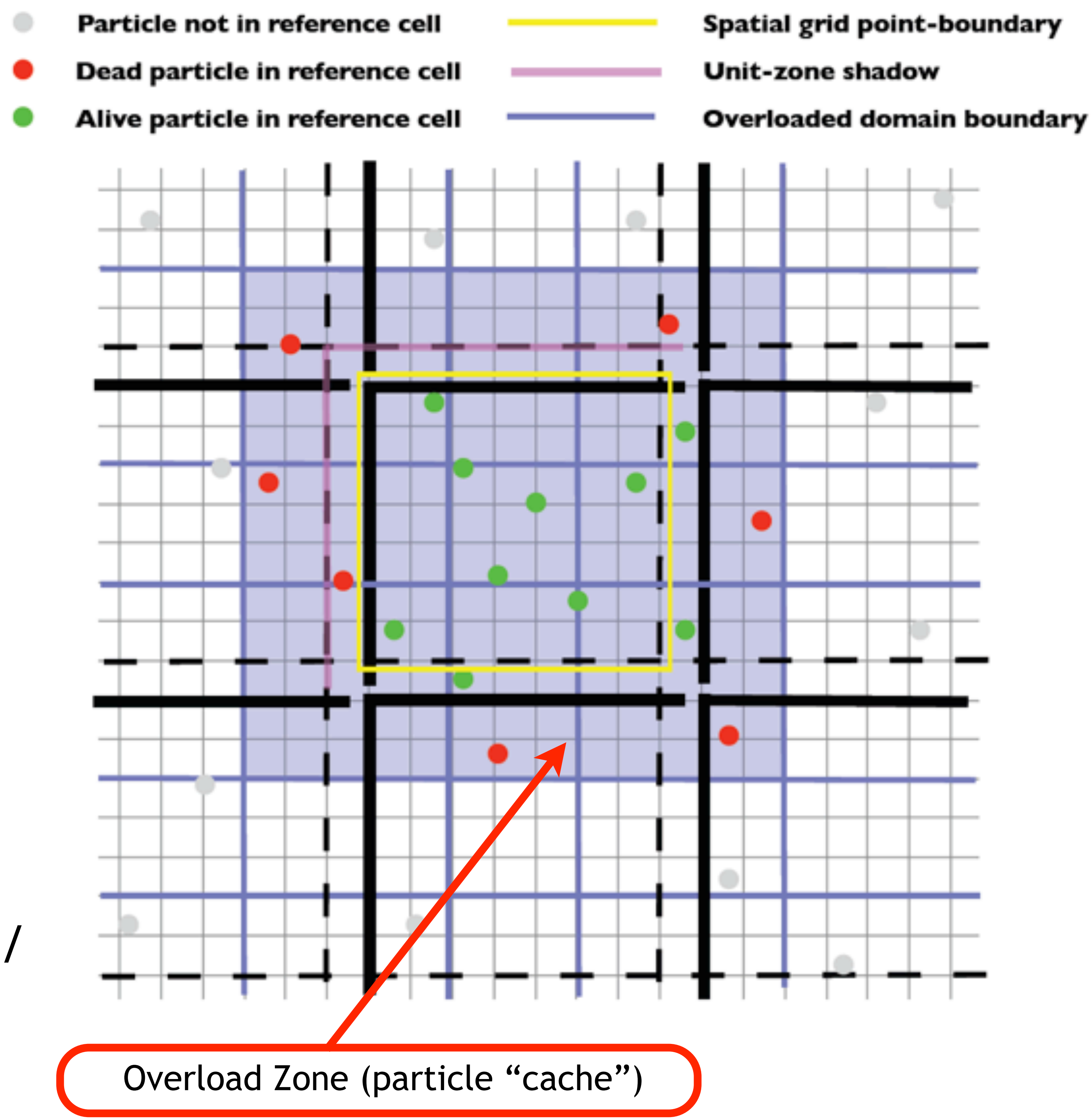
HACC Example 2: CPU+GPU

- CPU/GPU performance and communication out of balance, unbalanced memory (CPU/ main memory dominates)
- Multi-level programming (mitigate with OpenCL)
- Particles in CPU main memory, CPU does low flop/byte operations
- Stream slabs through GPU memory (pre-fetches, asynchronous result updates)
- Data-parallel kernel execution
- Many independent work units per slab -- many threads, efficient scheduling, good performance achieved (improves on Cell)
- Scalability of HACC is the same across all 'nodal' variants



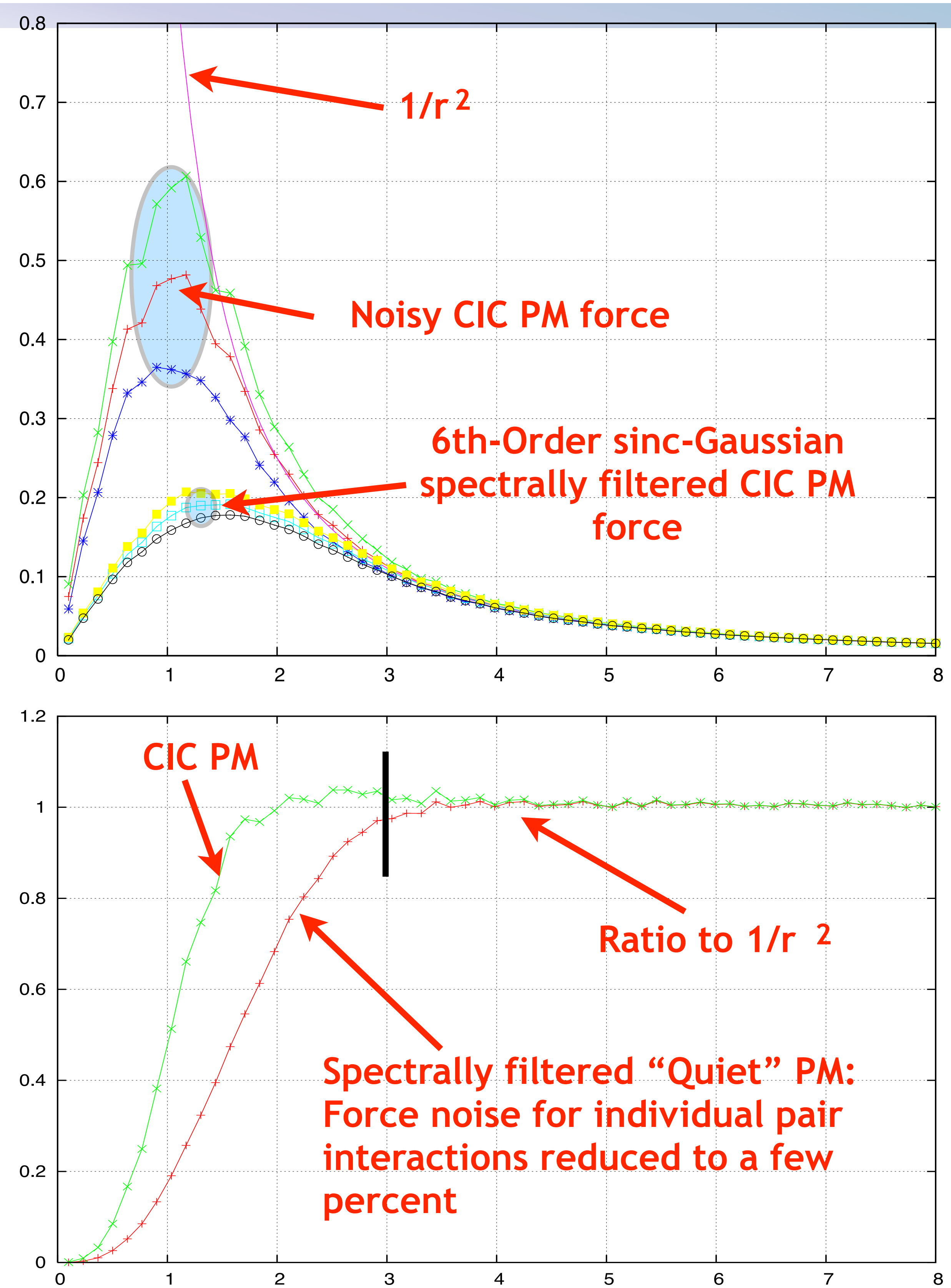
HACC Algorithmic Structure: Particle Overloading

- Solve compute imbalance: Split problem into long-range and short-range force updates
- Long-range handled by a grid-based Poisson solver
- Direct particle-particle short-range interactions
- Simplify and speed-up Cell computational tasks
- Reduce CPU/Cell traffic to avoid PCIE bottleneck: use simple CIC to couple particles to the grid, followed by spectral filtering on the grid
- Reduce inter-node particle communication: particle caching/ replication (ghost zone analog)
- ‘On the fly’ analysis and visualization to reduce I/O



HACC Algorithmic Structure: Filtering and Force-Splitting

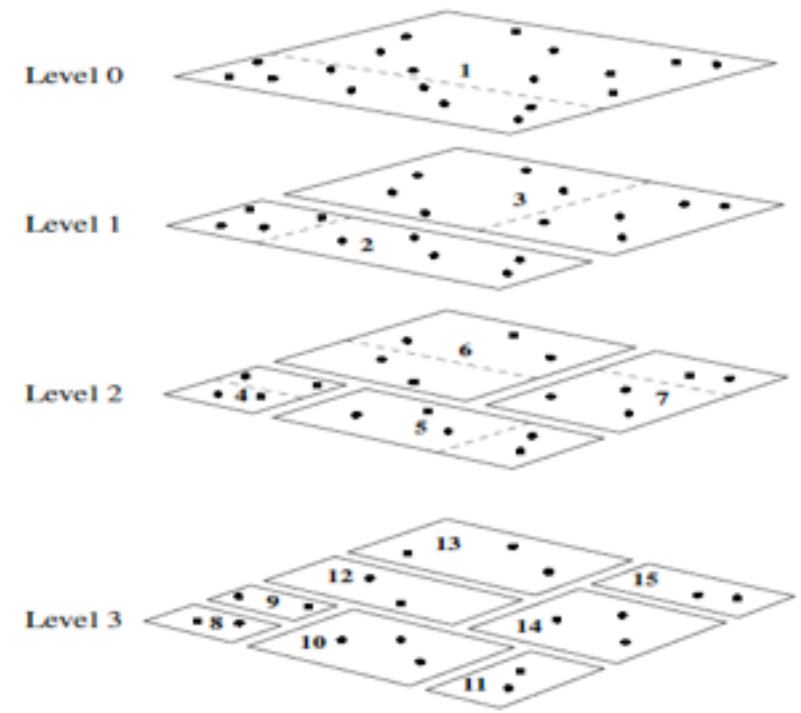
- Spectral smoothing of the CIC density field allows 6-th order Green function and 4th order super-Lanczos gradients for high-accuracy Poisson-solves
- Short-range force is fit to the numerical difference between Newtonian and long-range force (not conventional P^3M)
- Short-range force time-steps are sub-cycled within long-range force kicks via symplectic algorithm
- Short-range computations isolated as essentially ‘on-node’, replace or re-design for different architectures (e.g., BG/Q or GPU)



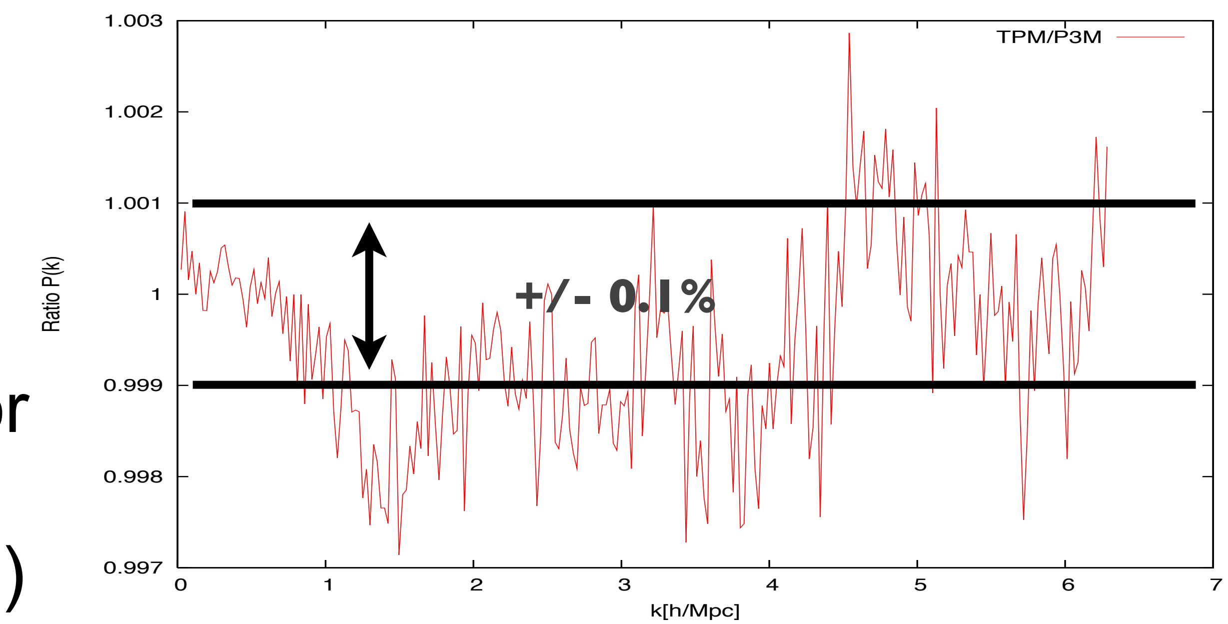
HACC Algorithmic Structure: The Local Force Computation

- Depending on the node architecture, switch between P3M and Tree algorithms (use both oct-tree and center-of-mass RCB tree, pseudo-particle method used to go beyond monopole order)
- Multiple algorithms/methods useful to check accuracy (very good agreement between our individual tree and chaining-mesh P3M implementations)
- By tuning number of particles in leaf nodes and error control criteria, can optimize for computational efficiency
- Can achieve 50% of peak on BG/Q (but painful, involves assembly)
- P3M is more straightforward -- waiting for Titan to fire up (try out later in 2012 on Jaguar upgrade, moving to Titan in 2013)

Gafton and Rosswog 2011



RCB Tree Hierarchy



HACC Force Algorithm Test: TPM vs. P3M

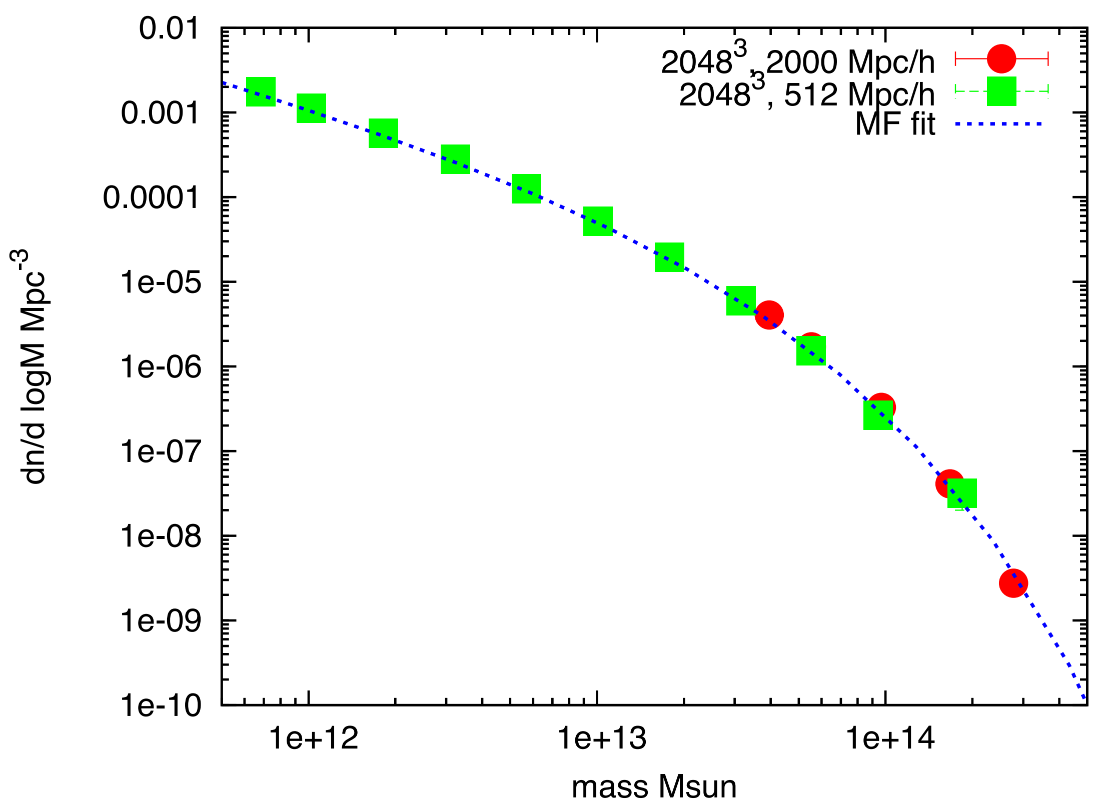
HACC Application: The c(M) Relation for Clusters

Bhattacharya, Habib, Heitmann, and Vikhlinin 2011

- **The DM Halo:** NFW halos are shape-fixed and chacterized by two things (i) the mass, and (ii) the concentration parameter
- **The c(M) Relation:** Concentration and mass are connected, how well do we (i) know this, and (ii) can measure it observationally?
- **Simulation Status:** Substantial scatter in current results (including non-intuitive relationships)
- **Observational Status:** Somewhat confusing (WL results not convergent), X-ray has its issues, SL+WL getting better, galaxy kinematics --

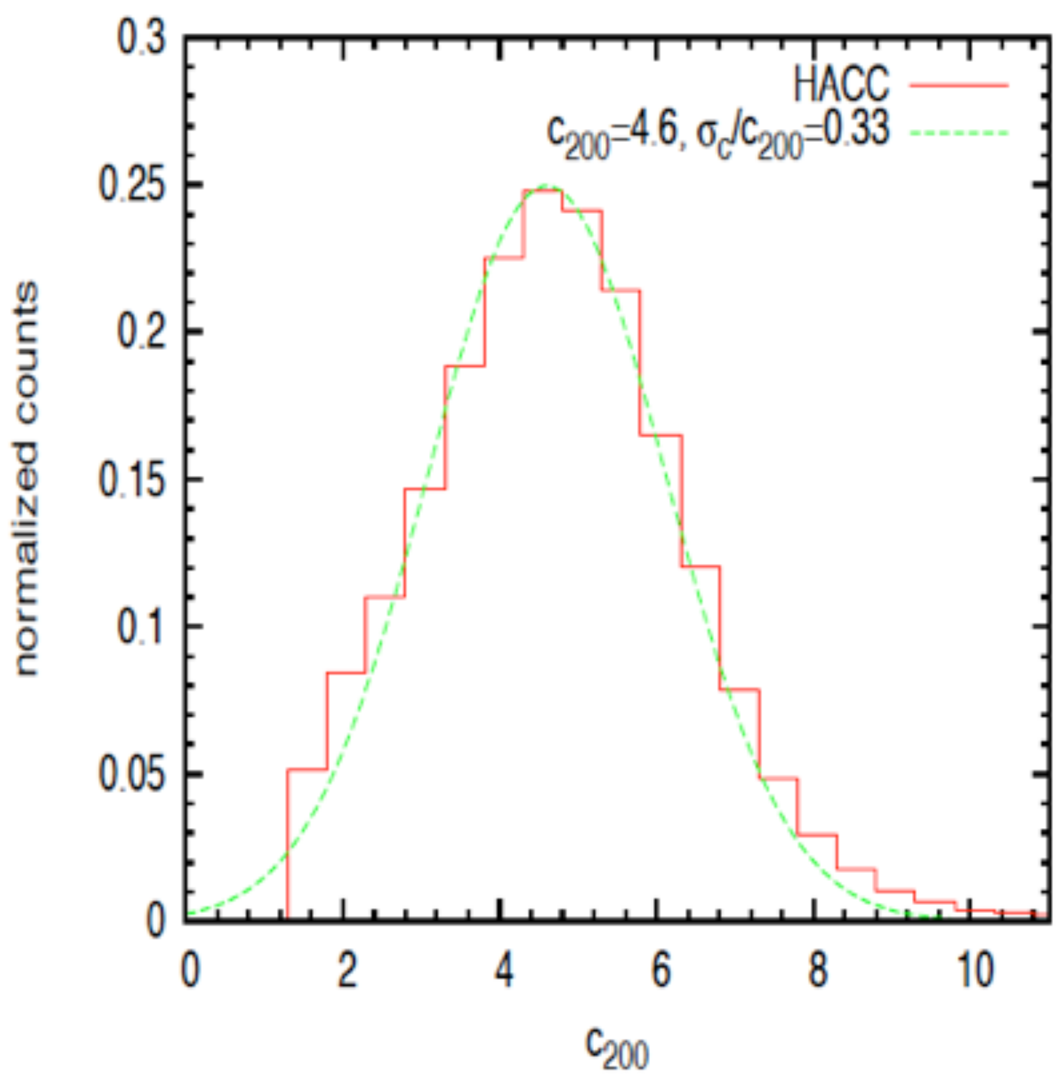
$$\rho(r) = \frac{\delta\rho_{\rm crit}}{(r/r_s)(1+r/r_s)^2}$$

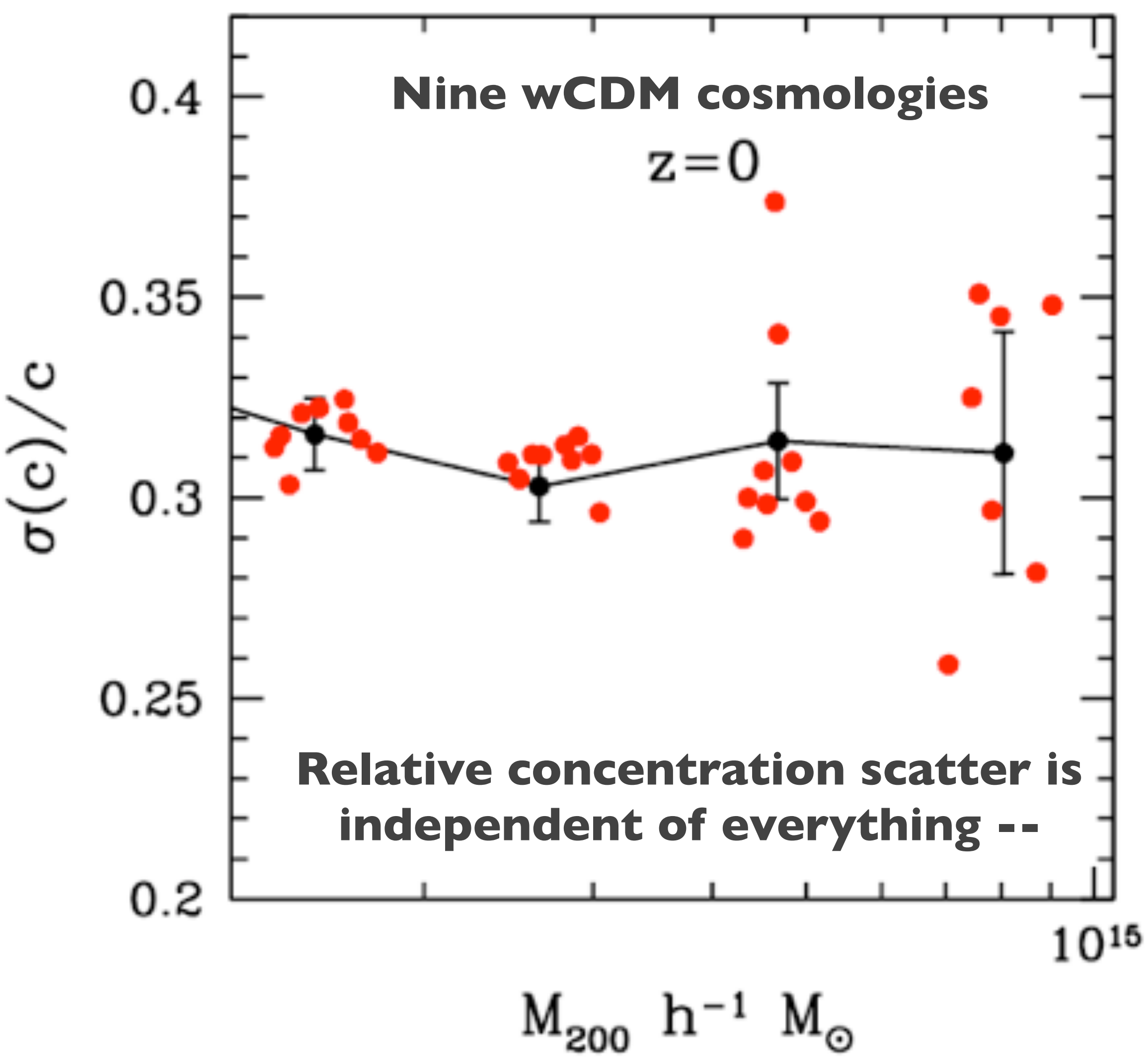
$$c_\Delta = r_\Delta / r_s$$



The Mass Function: Two 8-billion Particle Runs

The c(M) Relation from Simulations

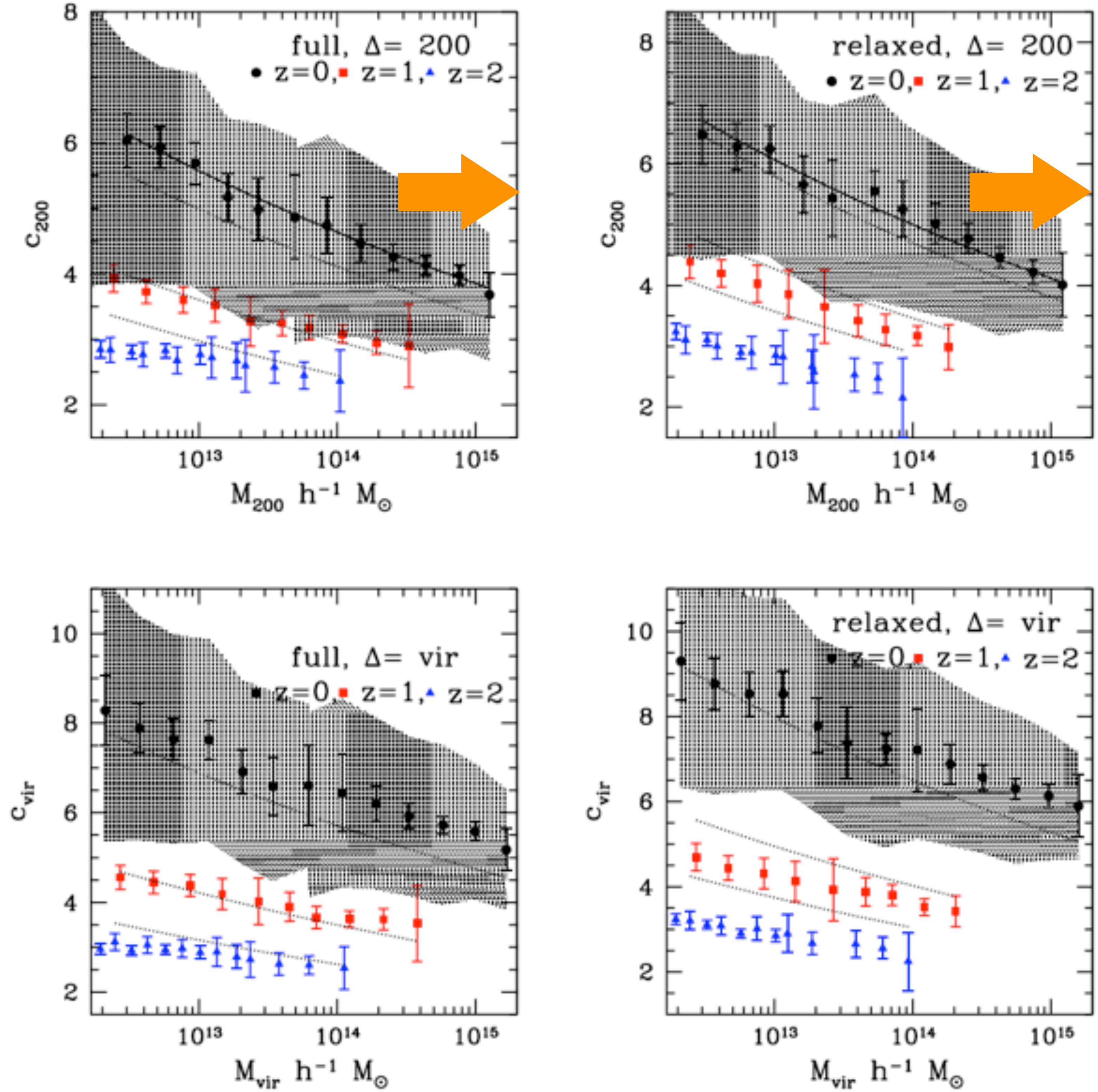




- **Cosmologies Studied:** One 'WMAP5' model studied in detail and a large number of wCDM cosmologies (37) from previous simulations
- **The c(M) Relation:** The c(M) distribution is Gaussian with a **universal** relative variance $\sigma_c = 0.33c$

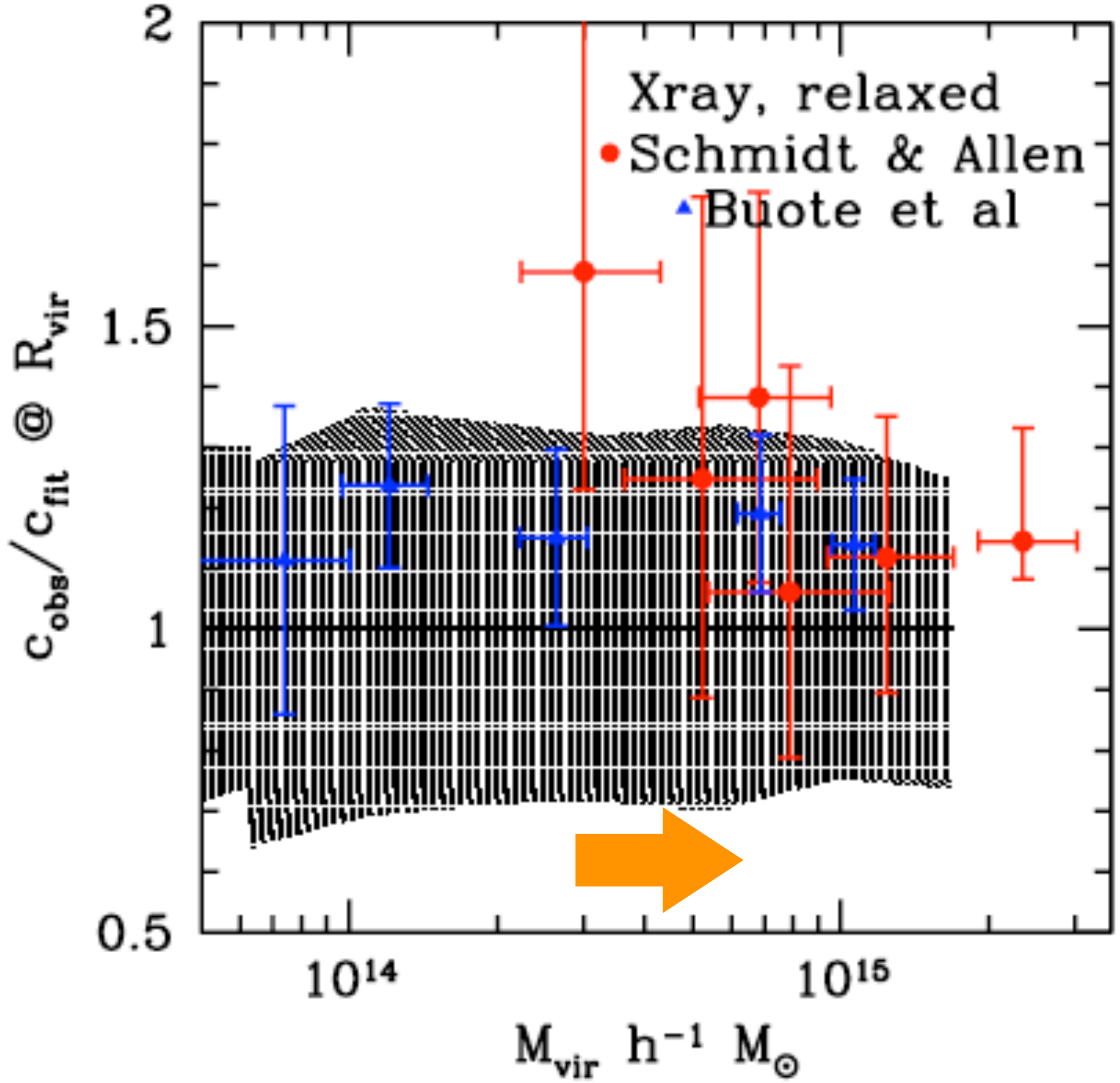
The c(M) Relation as a Function of Redshift

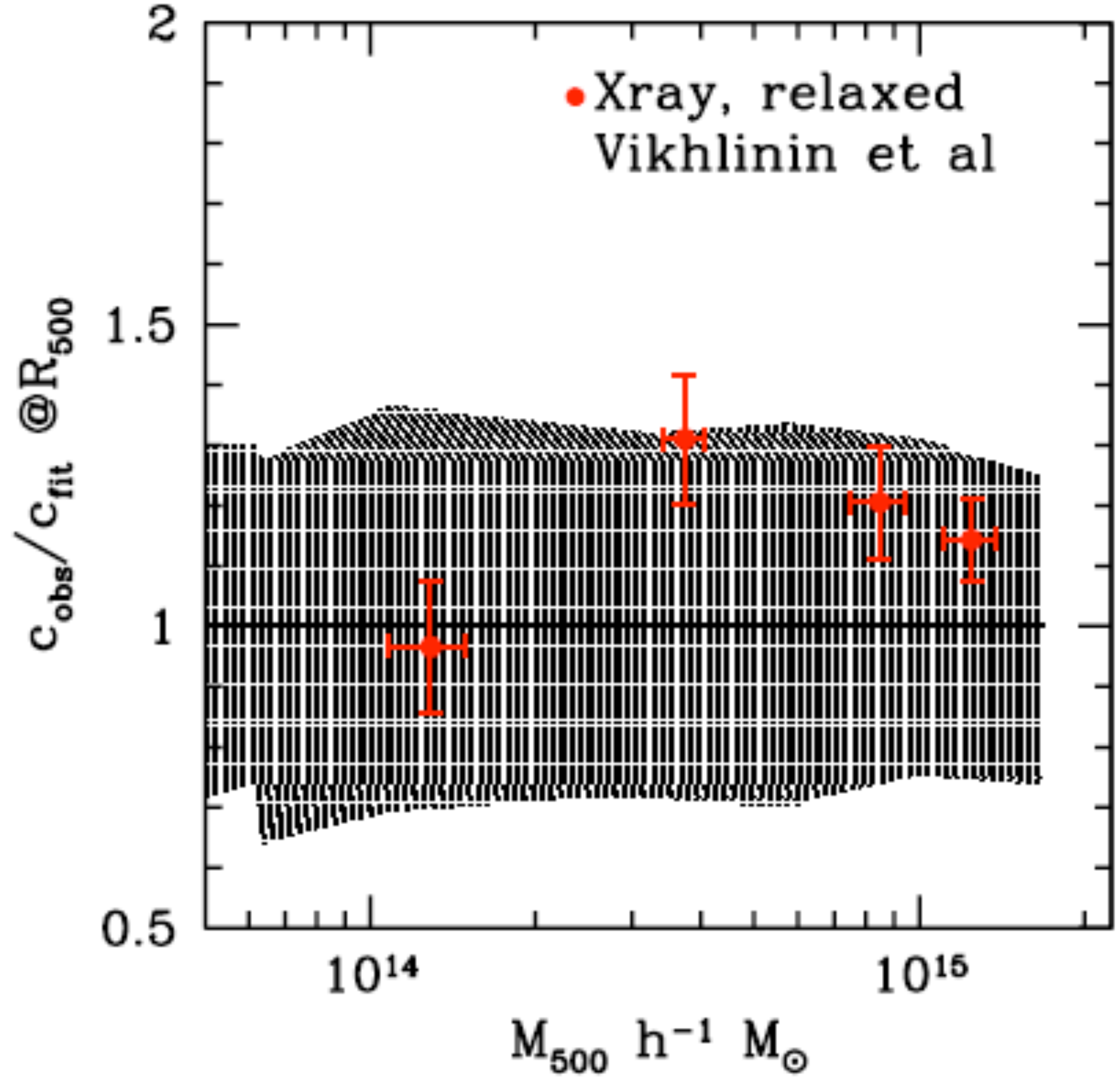
- **c(M) Evolution:** The c(M) relation has a well-defined evolution with redshift, the relation is lower and flatter at high z
- **Relaxed vs. Unrelaxed:** Not a major difference -- over the range of cluster masses, the mean concentration varies from 5 to 4 (relaxed) and from 4.3 to 3.8 (unrelaxed) with a large scatter (of order unity)
- **Simulation Agreement:** Disagree with Bolshoi and Multi-Dark, agree (more or less) with others



c(M) relation as a function of redshift

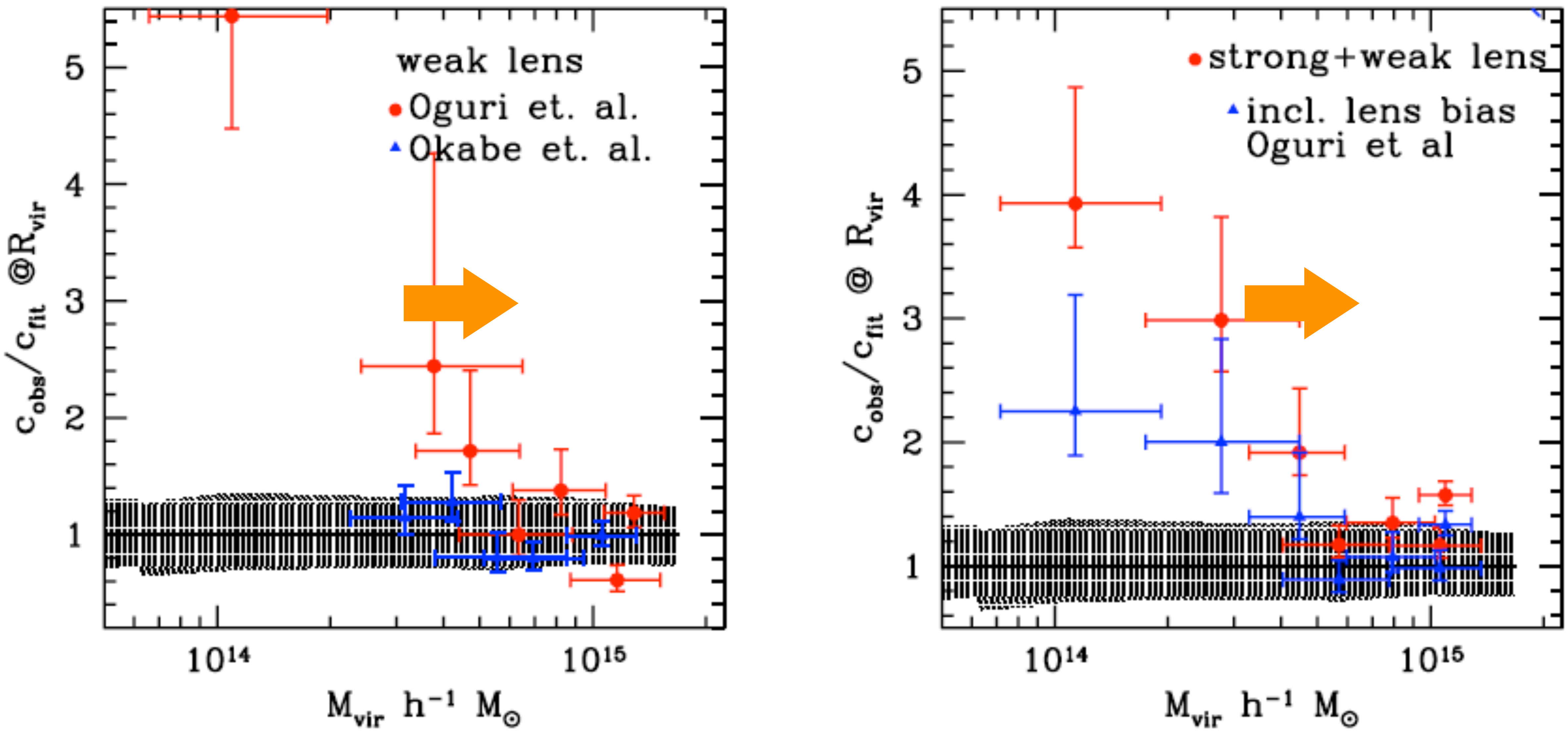
The c(M) Relation: Theory vs. Observations (X-Ray)





- **X-Ray Observations:** Reasonably good agreement with observations (each bin is roughly 5 objects). Systematic errors in observations need to be better characterized.

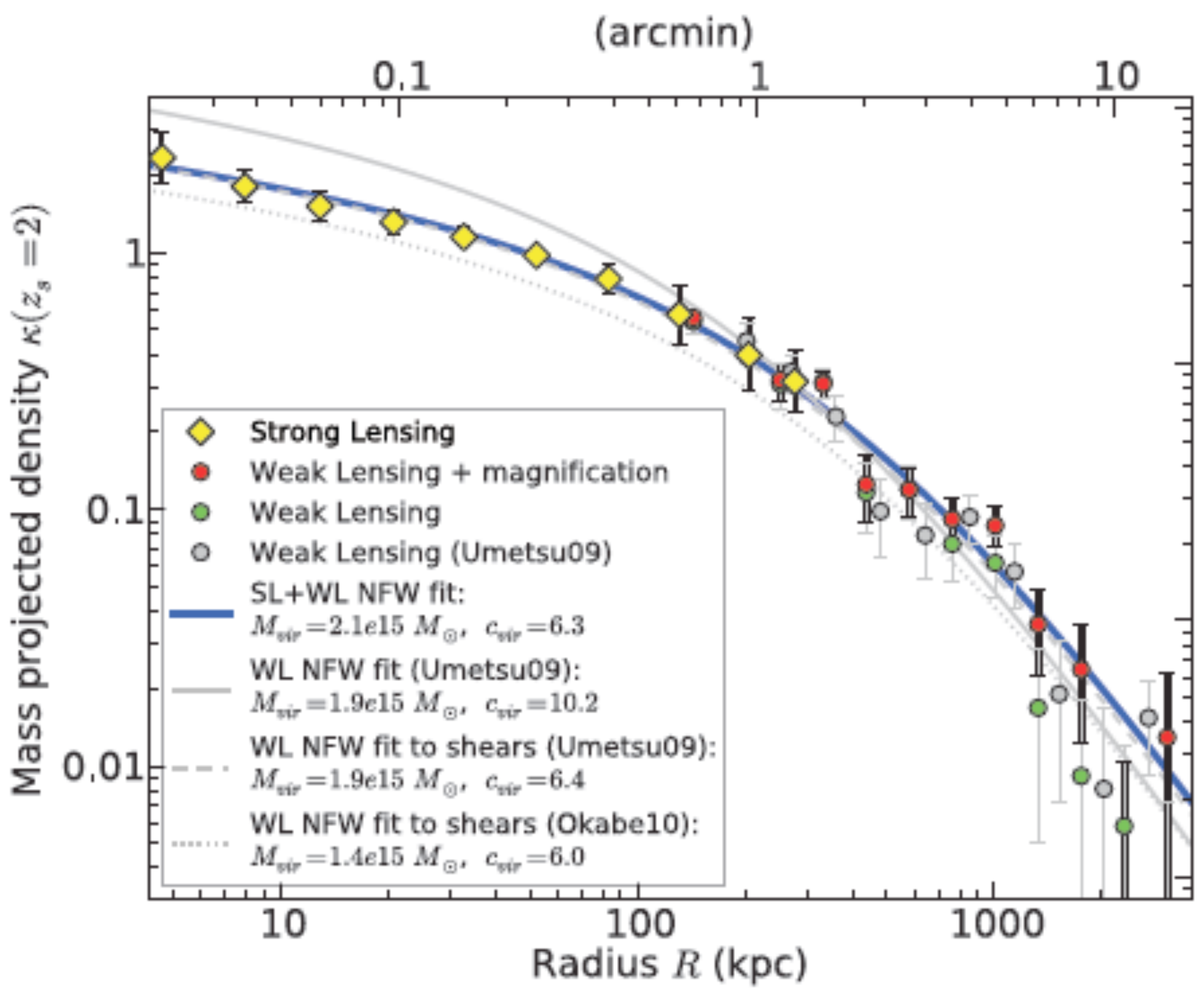
The c(M) Relation: Theory vs. Observations (Lensing)

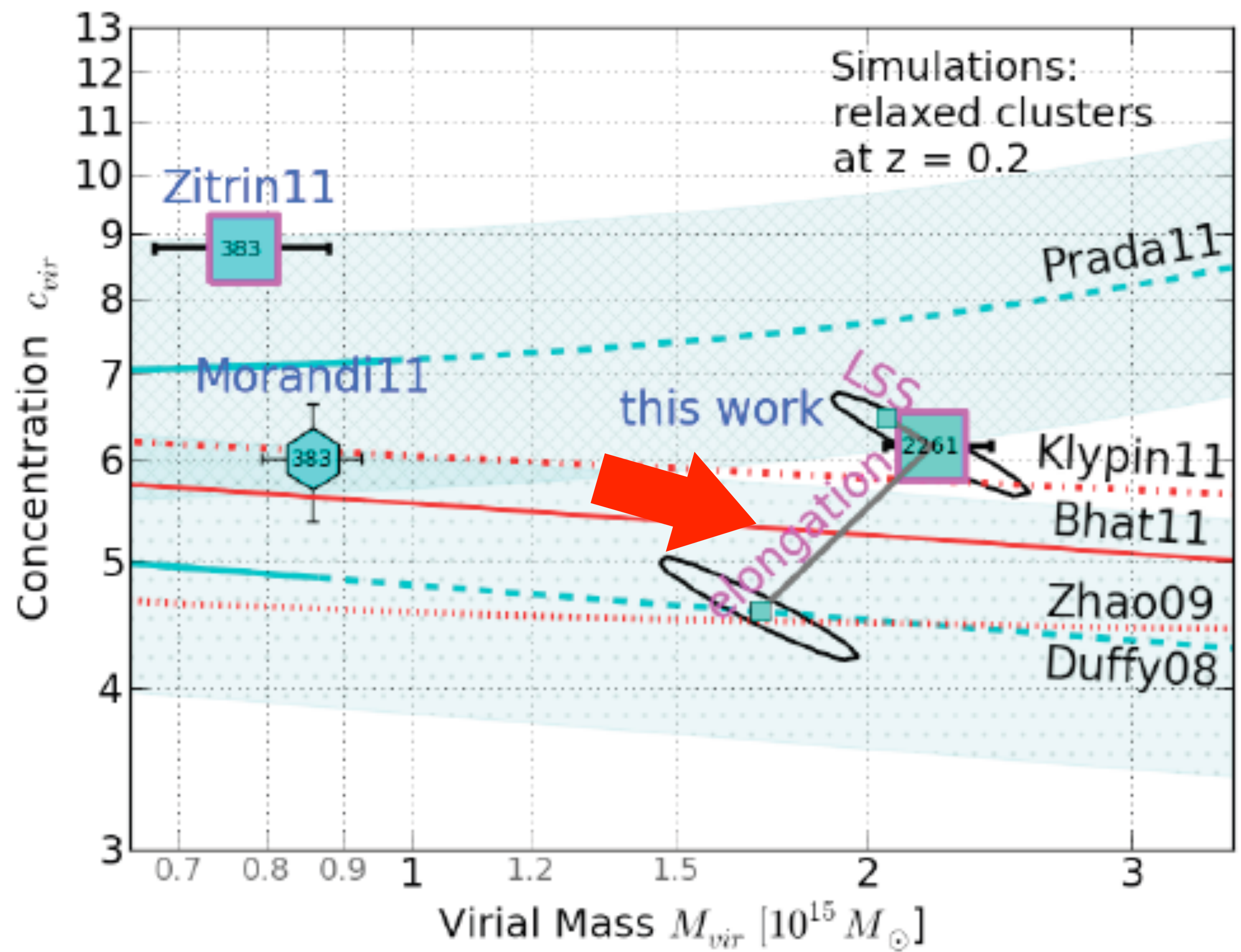


- **Weak + Strong Lensing Surveys:** Good/reasonable agreement with observations (each bin is roughly 5 objects) where selection systematics are understood.

The c(M) Relation: No Clash with CLASH!

Coe et al 2011





- **Cluster Lensing and Supernova Survey with Hubble (CLASH):** Good agreement for Abell 2261 (z=0.225)

Summary

- N-body future appears to be fine although not painless
- Much needs to be done in terms of analysis (in situ/real-time/post-simulation)
- Many interesting science projects to do --
- Looking for collaborations (as always!)

ANL Cosmic Frontier Theory Group & Collaborators

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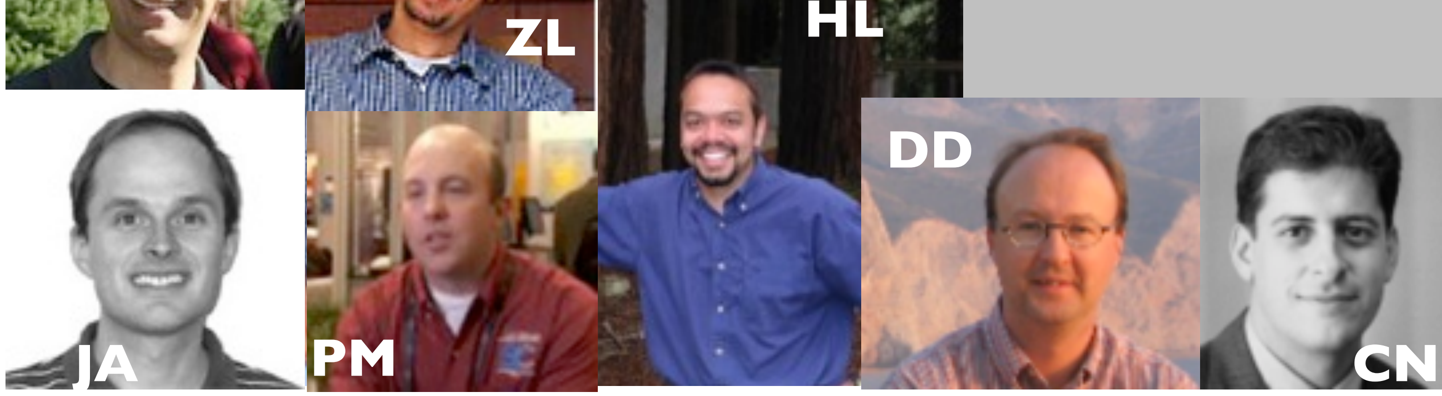

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