Cosmic Calibration -- Or How I Learned to Stop Worrying and Love Supercomputers

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Thanks to many collaborators!
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 (temperature)
- Maps can be large (Sloan Digital Sky Survey has ~200 million galaxies, many billions for planned surveys)
- 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
Outline

• What have we learned so far from these observations?
  ▶ Content of the Universe
  ▶ Evolution of the Universe

• How do we extract this knowledge from the data?
  ▶ Focus here on optical surveys and simulations

• **Precision Cosmology:** Where do we want to go next and how do we get there?

• Simulating cosmological surveys with **HACC (Hardware/Hybrid Accelerated Cosmology Code):** An N-body code designed for extreme scaling

• **Cosmic Calibration:** Building efficient prediction tools from expensive simulations
The Content of the Universe: It’s dark!

- **Dark Energy:** Multiple observations show that the expansion of the Universe is accelerating (first in 1998, Nobel prize 2011)
- **Questions:** What is it? Why is it important now? Being totally ignorant, currently our main task is to characterize it better and exclude some of the possible explanations
- Independent of what we find, we will learn new, fundamental physics, this is not just the hunt for a couple numbers!
- **Dark Matter:** Observations show that ~27% of the matter in the Universe is “dark”, i.e. does not emit or absorb light
- So far: indirect detection, aims: characterize nature of dark matter and detect the actual dark matter particle
- ~95% of the Universe is “dark” -- we do not understand the nature and origin of dark energy and dark matter.
Structure Formation: The Basic Paradigm

- Solid understanding of structure formation; success underpins most cosmic discovery
  - Initial conditions determined by primordial fluctuations
  - 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
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- 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
• Simulate the formation of the large scale structure of the Universe via dark matter tracer particles
• Take dark energy into account in the expansion history
• Measure the high-density peaks (dark matter halos) in the mass distribution
• “Light traces mass” to first approximation, therefore populate the halos with galaxies, number of galaxies depends on mass of halo (constraints from observations)
• Galaxy population prescription (hopefully) independent of cosmological model
Precision Cosmology: “Inverting” the 3-D Sky

- **Standard Model of Cosmology:** Verified at the 5-10% level across multiple observations, describes make-up and evolution of the Universe

- **Next generation observatories:** aim to push the current boundaries by orders of magnitude

- Scales that are resolved by future surveys become smaller and smaller, demanding (i) ever larger simulations with increased mass and force resolution; (ii) more detailed physics

- **Next frontier:** Nonlinear regime of structure formation

- **Future Targets:** Aim to control survey measurements to the ~1% level, *can theory and simulation keep up?*
Why do we need higher accuracy measurements?
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It's the f...... Universe, guys! It deserves at least two decimal places!

Douglas Scott, UBC at the Santa Fe Cosmology Workshop in 2005
Why do we need higher accuracy measurements?

- Convincing argument! In addition:
- Fundamental physics questions await answers:
  - Modified gravity or dark energy?
    - Measure growth of structure and expansion history of the Universe
  - If dark energy: Cosmological constant or dynamical origin?
  - If modified gravity: How do structures form?

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Why do we need higher accuracy in our predictions?

- Example in this talk: matter power spectrum
- Question: how badly will our constraints on dark energy be biased if we do not reach the same accuracy in our modeling as we might have in our data?
- Generate mock data set with the expected 1% error
- Analyze data with current method using HaloFit to model the matter power spectrum
  - HaloFit (Smith et al. 2003): semi-analytic fit for the power spectrum, based on modeling approach and tuned to simulations, accurate at the 5-10% level

\[
\Delta^2(k) = \frac{k^3 P(k)}{2\pi^2}; \quad P(k) = \langle \delta^2(k) \rangle
\]
The Matter Power Spectrum

2-point correlation function:
\[ \xi(x) = \int \frac{d^3 \bar{y}}{V} \delta(\bar{y} - \bar{x}) \delta(\bar{y}) = \int \frac{d^3 \bar{k}}{(2\pi)^3} |\delta_k|^2 e^{i\bar{k} \cdot \bar{x}} \]

- 2-point correlation function: excess probability of finding an object pair separated by a distance \( r_{12} \) compared to that of a random distribution
- \( P(k) \): power spectrum, Fourier transform of correlation function

\[ \Delta^2(k) = \frac{k^3 P(k)}{2\pi^2} \]
- Power spectrum very sensitive to physics of interest: amount and properties of dark matter, dark energy, neutrino mass, ...
- Many different probes for measuring \( P(k) \)

Length scale of interest:
- 1 parsec (pc) = 3.26 light years \( \approx 3 \cdot 10^{13} \) km, separation of stars in a galaxies
- Mpc = 10^6 pc: separation of bright galaxies
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![Graph showing expected measurements and simulation results with HaloFit comparison. The graph highlights a 5-10% error in the non-linear regime.](image)
Analysis of the “True data”

- Generate mock data from high-resolution simulation
- Use Halofit for analysis; remember, halofit ~5-10% inaccurate on scales of interest
- Parameters are up to 20% wrong! (We checked that with more accurate predictions the answer is correct)
- Only solution: precision simulations
- Analysis takes at least 10,000 input power spectra for MCMC, each simulation takes ~20,000 CPU hours
- With a 2000 node cluster running 24/7, our analysis will take ~30 years, hmmm...

![Diagram showing analysis results and input values](image-url)
What do we need --

• **Very accurate predictions** for the cosmological measurements of interest (power spectra/correlation functions, mass functions, galaxy power spectra ... **[YOUR FAVORITE STATISTICS HERE]**
  - For gravity-only and galaxies in post-processing: **HACC** (Hardware/Hybrid Accelerated Cosmology Code, coming next)
  - For full treatment of baryonic effects: another talk at another time ...

• **Very fast predictions** for your favorite statistics
  - While HACC is fast, we need something much faster, sub-seconds preferably!
  - **Cosmic Calibration Framework**: Prediction tools build from a small but very accurate number of simulations (last part of the talk)
HACC’s Task: Computing the Universe

- Gravity dominates at large scales, key task: solve the Vlasov-Poison equation (VPE)
- VPE is 6-D and cannot be solved as PDE, therefore N-body methods
- Particles are tracers of the dark matter in the Universe, mass typically at least $\sim 10^{9} M_\odot$
- At smaller scales, add gas physics, feedback etc., sub-grid modeling inevitable

\[ \frac{\partial f_i}{\partial t} + \dot{x} \frac{\partial f_i}{\partial x} - \nabla \phi \frac{\partial f_i}{\partial p} = 0, \quad p = a^2 \dot{x}, \]
\[ \nabla^2 \phi = 4\pi G a^2 (\rho(x, t) - \langle \rho_{dm}(t) \rangle) = 4\pi G a^2 \Omega_{dm} \delta_{dm} \rho_{cr}, \]
\[ \delta_{dm}(x, t) = (\rho_{dm} - \langle \rho_{dm} \rangle) / \langle \rho_{dm} \rangle, \]
\[ \rho_{dm}(x, t) = a^{-3} \sum_i m_i \int d^3 p f_i(x, \dot{x}, t). \]

“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)
Computing the Universe: Simulating Surveys

- **Simulation Volume:** Large survey sizes impose simulation volumes \(\sim (4 \, \text{Gpc})^3\), memory required \(\sim 100 \, \text{TB} - 1 \, \text{PB}\)

- **Number of Particles:** Mass resolution depends on ultimate object to be resolved, \(\sim 10^8 M_\odot - 10^{10} M_\odot\), \(N\sim 10^{11} - 10^{12}\)

- **Force Resolution:** \(\sim\text{kpc}\), yields a (global) spatial dynamic range of \(10^6\)

- **Throughput:** Large numbers of simulations required (100’s --1000’s), development of analysis suites, and emulators; peta-exascale computing exploits

- **Computationally very challenging!** HACC is aimed to meet these requirements
The HACC Story Begins ...

• ... with an email: Los Alamos National Lab offers the opportunity to run open science projects on the fastest supercomputer in the world for the first six months of the machine’s existence: **Roadrunner**

• **Roadrunner**: First machine to achieve Petaflop performance via Cell-acceleration, CPU/Cell hybrid architecture (more details later) (equivalent to ~200,000 laptops)

• The Challenges:
  • The machine has a “crazy” architecture, requiring major code re-designs and rewrites (we ended up writing a brand new code)
  • Roadrunner probably one of a kind, code-design needs to be flexible and portable to other future architectures

• Cosmologists are poor -- so we took on the challenge!

• Outcome: **MC³** (Mesh-based Cosmology Code on the Cell) which later morphed into HACC, N-body code to simulate large-scale structure formation in the Universe
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The Story Continues … and makes it into “Die Süddeutsche”

Newspaper I read every morning

“He is the fastest calculator in the world:”

Er ist der schnellste Rechner der Welt; der amerikanische Supercomputer "Roadrunner" hat die Petaflop-Grenze geknackt. Sein Job: die Simulation von Atombombenexplosionen.


Supercomputer mit Vorbildfunktion

“leads by example”


Technologisch dürfte Roadrunner Vorbildwirkung haben. "Es zeichnet sich ab, dass Hybrid-Technologie auf jeden Fall Zukunft haben“ meint Lippert. Damit sind Systeme gemeint, die klassische CPUs mit Beschleunigern wie beispielsweise den Cell-Chips oder Grafikprozessoren kombinieren.

“technology of the future”
So we started thinking --

Crazy architectures.... how can we use them?

The future -- exascale -- hybrid machines -- MIC, GPU, Cell, multicore...

(from S. Furlanetto)
The Roadrunner Architecture

- **Opterons** have little compute (5% of total compute) but half the memory and balanced communication, for N-body codes, memory is limiting factor, so want to make best use of CPU layer

- **Cells** dominate the compute but communication is poor, 50-100 times out of balance (also true for CPU/GPU hybrid systems)

- **Multi-layer programming model:** C/C++/MPI (Message Passing Interface) for Opterons, C/Cell-intrinsics for Cells
Design Challenges and Solutions for MC³ CHANGE

- **Challenges (summarized from last slide):**
  - Opterons have half of the machine’s memory, balanced communication, but not much compute, standard programming paradigm, C/C++/MPI
  - Cells have other half of machine’s memory, slow communication, lots of compute (95% of machine’s compute power), new language required

- **Design desiderata:**
  - Distribute memory requirements on both parts of the machine
  - Give the Cell lots of (communication limited) work to do, make sure that Cell part is easy to code and later on easy to replace by different programming paradigm

- **Our Solution:** P³M algorithm (long range - short range split)
  - Particle Mesh (PM) solver for long-range force, FFT based, grid lives on the Opterons, all coarse-grained parallelism here, base grid is maximized
  - Direct Particle-Particle solver for short range force, particles live on the Cells, lots of compute, simple data structure, easy to implement, can be replaced by tree for different architecture
  - Overloading trick to minimize communication needs, only simple grid information flows between Cells and Opterons; enables node level short-range force plug-ins
**MC³ Performance**

- **Perfect weak-scaling** of P³M code
- Perfect weak-scaling of long range solver on full Roadrunner

**Weak scaling:** problem size grows while core count increases

**Strong scaling:** problem size fixed while core count increases

Cell computation gives an improvement of two orders of magnitude over the Opterons for the short-range force.
Snapshot from Code Comparison simulation, ~25 Mpc region; halos with > 200 particles, b=0.15
Differences in runs: $P^3M$ vs. TPM, force kernels, time stepper: $MC^3$: $a$; Gadget-2: $\log(a)$
Power spectra agree at sub-percent level

Ratio for $P(k)_{HACC}/Gadget-2$

0.05%!
The Story continues, MC³ becomes HACC: CPU+GPU

• **Proof of concept for easy portability:** replace Cell part by GPU implementation
• Paul Sathre (CS undergraduate at the time) in summer 2010 successfully ports code within weeks (with guidance from Adrian Pope)
• **New challenges:**
  • CPU/GPU performance and communication out of balance AND unbalanced memory (CPU/main memory dominates)
  • New programming language on GPU, OpenCL
• **With the arrival of Titan in 2013 (GPU accelerated supercomputer at Oak Ridge National Lab):**
  • Nick Frontiere completely rewrote and optimized HACC-P3M version for GPUs
  • NVIDIA’s Justin Luitjens and Argonne’s Vitali Morozov wrote TreePM version

**Weak and Strong Scaling Results**

S. Habib et al. 2013: SuperComputing13, Gordon Bell Finalist (decision: Nov. 21)

“The Gordon Bell Award recognizes outstanding achievement in high-performance computing applications.”

• Achieved 20.54 Pflops peak performance evolving 1.23 trillion particles in test run on ~75% of machine (full machine currently not available)
• Why is this important? Qualify for more computing time!
Another Challenge: Multi-core systems, BG/Q

- Proof of concept for “easy” portability II: IBM Blue Gene (BG) systems
  - BG/Q Mira at Argonne: 10 PFlops, arrived in 2012, 750,000 cores, 16GB per node
  - BG/Q Sequoia at Livermore: twice as large

- New challenges:
  - BG/Q systems have many cores but no accelerators
  - Slab-decomposed FFT does not scale well on very large number of cores

- Solutions:
  - Particle-particle interaction now replaced by tree, OpenMP node parallel
  - Pencil decomposed FFT
  - Adaptive time stepping

- Achieved 13.94PFlops on Sequoia, 90% parallel efficiency on 1,572,864 cores
- 3.6 trillion particle benchmark run
Mira Science: The Outer Rim Simulation

32 Racks of Mira, 262,144 cores, 1.1 trillion particles

Output from 1 core
Some HACC Science Results --

- Mass resolution of Millennium simulation and Outer Rim run very similar (~ $10^9 M_\odot$ particle mass), but volume different by a factor of 216 (Outer Rim volume = Millennium XXL)
- Exceptional statistics at high resolution enable many science projects
Some HACC Science Results --

- Investigate different physical effects on e.g. the matter power spectrum at high accuracy
- Here: 2100 Mpc simulations with ~32.8 billion particles, $10^{10} M_\odot$ particle mass to study massive neutrinos as well as time varying dark energy EOS
- Develop “higher order” perturbation theory approach

A. Upadhye et al. 2013
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A. Upadhye et al. 2013
Some HACC Science Results --

Lyman-alpha Forest

Roadrunner view (halos) of the Universe at z=2 from a 64 billion particle run (9 runs on one weekend)

M. White et al. 2010
• HACC works great! But still cannot generate simulations in seconds ...
• Challenge: To extract cosmological constraints from observations in nonlinear regime, need to run Marko Chain Monte Carlo code; input: 10,000 - 100,000 different models
• Current strategy: Fitting functions for e.g. P(k), accurate at 10% level, as we saw this is not good enough!
• Our alternative: Emulators, fast prediction schemes built from a manageable set of simulations
• Example here: Power spectrum emulator
  • Step 1: Show simulations have required accuracy (Heitmann et al. 2005, 2008, 2010)
  • Step 2: Determine minimum number of simulations needed and develop sophisticated interpolation scheme that provides the power spectrum for any cosmology within a given parameter space prior (Heitmann et al. 2006, 2009; Habib et al. 2007)
  • Step 3: Carry out simulation and build final emulator (Lawrence et al. 2010, Heitmann et al. 2013)
Cosmic Calibration Framework

• Step 1: Design simulation campaign, rule of thumb: \( O(10) \) models for each parameter
• Step 2: Carry out simulation campaign and extract quantity of interest, in our case, power spectrum
• Step 3: Choose suitable interpolation scheme to interpolate between models, here Gaussian Processes
• Step 4: Build emulator
• Step 5: Use emulator to analyze data, determine model inadequacy, refine simulation and modeling strategy...
• “Simulation design”: For a given set of parameters to be varied and a fixed number of runs, at what settings should the simulations be performed?

• Example: Five cosmological parameters, tens of high-resolution runs are affordable

• First idea: Grid
  ▸ Space filling but poor projection properties

• Second idea: Random sampling
  ▸ Good projection properties but poor space coverage

• Our approach: Orthogonal-array Latin hypercubes (OA-LH) design
  ▸ Stratified random sampling approach
  ▸ Good projection properties AND space filling

The Simulation Design for wCDM Cosmologies

Priors:

$0.020 \leq \omega_b \leq 0.025$

$0.11 \leq \omega_m \leq 0.15$

$0.85 \leq n_s \leq 1.05$

$-1.3 \leq w \leq -0.7$

$0.6 \leq \sigma_8 \leq 0.9$

Priors are informed by current cosmological constraints, the tighter the priors, the easier to build a prediction tool. Restriction in number of parameters also helps!
The Interpolation Scheme: Gaussian Processes + PCA

- After simulation design specification: Build non-parametric interpolation scheme
- Gaussian Process (GP): fits in function space
- GP involves matrix inversion in conditioning step ("curse of dimensionality")
- Data compression: Express power spectra in terms of principal component (PC) basis (can use other basis too)
- GP over over PC coefficients
Cosmic Emulator in Action

- Instantaneous ‘oracle’ for nonlinear power spectrum, reduces compute time from weeks to negligible, accurate at 1% out to $k \sim 1$/Mpc for wCDM cosmologies
- Enables direct MCMC with results from full simulations

Heitmann et al. 2009, 2010
Lawrence et al. 2010
Heitmann et al. 2013
The Cosmic Emu(lator)

- Prediction tool for matter power spectrum has been constructed
- Accuracy within specified priors between $z=0$ and $z=1$ out to $k=1 \, h/\text{Mpc}$ at the 1% level achieved
- Emulator has been publicly released, C code
- Extension: Include $h$ as sixth parameter, out to $k=10 \, h/\text{Mpc}$ and $z=4$
  - Nested simulations to cover large $k$-range
  - Approach degrades accuracy to ~3%

Emulator performance: Comparison of prediction and simulation output for a model not used to build emulator at 6 redshifts.
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Emulating the Galaxy Power Spectrum

- Idea: find halos in the simulation, depending on their mass, populate them with galaxies
- Above mass threshold: each halo hosts central galaxy; the heavier the halo, the more satellites
- 5 parameter model, parameters adjusted by comparison to observations, different classes of galaxies = different models

\[ N_{\text{cen}}(M) = \frac{1}{2} \text{erfc} \left( \frac{\ln(M_{\text{cut}}/M)}{\sqrt{2} \sigma} \right) \]

\[ N_{\text{sat}}(M) = \left( \frac{M - \kappa M_{\text{cut}}}{M_1} \right)^\alpha \]

Zheng et al. 2008

Brighter galaxies

Dimmer galaxies

Data from SDSS-3 (CMASS sample) shot noise subtracted

Measurement from Anderson et al. 2012

CMASS HOD from White et al. 2011

Best fit HOD, \( M_{\text{cut}} = 13.13 \)

Kwan et al. 2013
The Next Step: The Mira Universe

- Extend parameter space to include varying $w(z)$ and massive neutrinos
- Build “nested designs”: enable to build emulator from first set of 25 models, improve with additional 27 models, final precision with 99 models overall
- Various emulators for $P(k)$, mass function, c-M relation, derived quantities...
- LCDM done, finalizing set-up based on this run

![Graph showing emulator accuracy and LCDM simulation results]
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Parameters

$0.12 \leq \omega_m \leq 0.155$

$0.0215 \leq \omega_b \leq 0.0235$

$0.7 \leq \sigma_8 \leq 0.9$

$0.55 \leq h \leq 0.85$

$0.85 \leq n_s \leq 1.05$

$-1.3 \leq w_0 \leq -0.7$

$-1.5 \leq w_a \leq 1.15$

$0.0 \leq \omega_\nu \leq 0.01$. 

[Graphs and diagrams showing $P(k)$ and emulator performance]
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Summary and Outlook

- Precision cosmology needs high accuracy predictions! Can we avoid being theory limited?
- HACC is a large scale computational tool to address this challenge
- Cosmic Calibration Framework allows us to build fast prediction tools for ongoing and future surveys
- Largest ever high-resolution run, *The Outer Rim Simulation*, currently running, analysis ongoing
  - Many hurdles had to be overcome to make this happen, including memory management, I/O, adaptive time stepper, and analysis tools
  - Exciting science extracted, e.g. strong lensing predictions
- *The Mira Universe* will lead to an unprecedented set of simulations, spanning 8 cosmological parameters, including different dark energy models and neutrinos
- In this talk: Focus on power spectrum science but many more science results have already been extracted from HACC simulations