

Big Bang, Big Data, Big Iron:

High Performance Computing for Cosmic Microwave Background Data Analysis

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A Brief History Of Cosmology

*Cosmologists are often in error,
but never in doubt.*

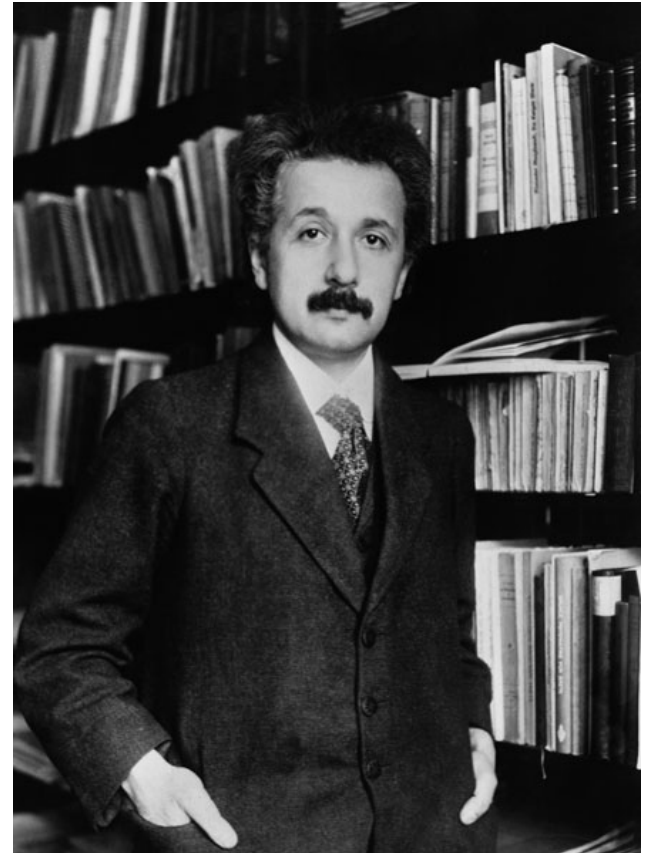
- Lev Landau

1916 – General Relativity

- General Relativity
 - Space tells matter how to move
 - Matter tells space how to bend

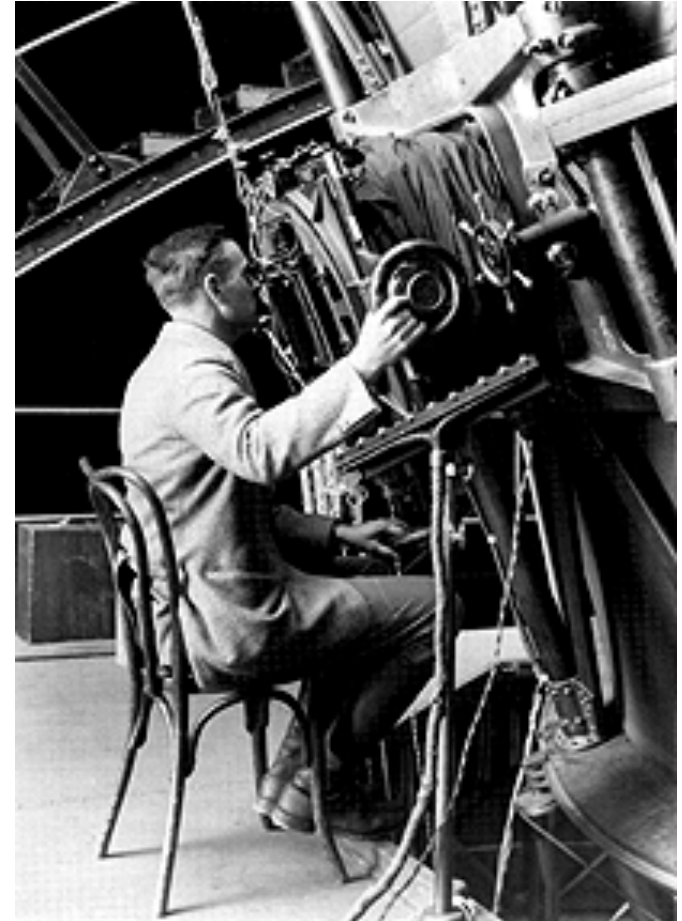
$$\underset{\text{Space}}{G_{\mu\nu}} = 8 \pi \underset{\text{Matter}}{G T_{\mu\nu}}$$

- But this implies that the Universe is dynamic and everyone *knows* it's static ...
- ... so Einstein adds a Cosmological Constant (even though the result is unstable equilibrium)



1929 – Expanding Universe

- Using the Mount Wilson 100-inch telescope Hubble measures nearby galaxies’
 - velocity (via their redshift)
 - distance (via their Cepheid variables)and finds velocity proportional to distance.
- Space is expanding!
- The Universe is dynamic after all.
- Einstein calls the Cosmological Constant “my biggest blunder”.

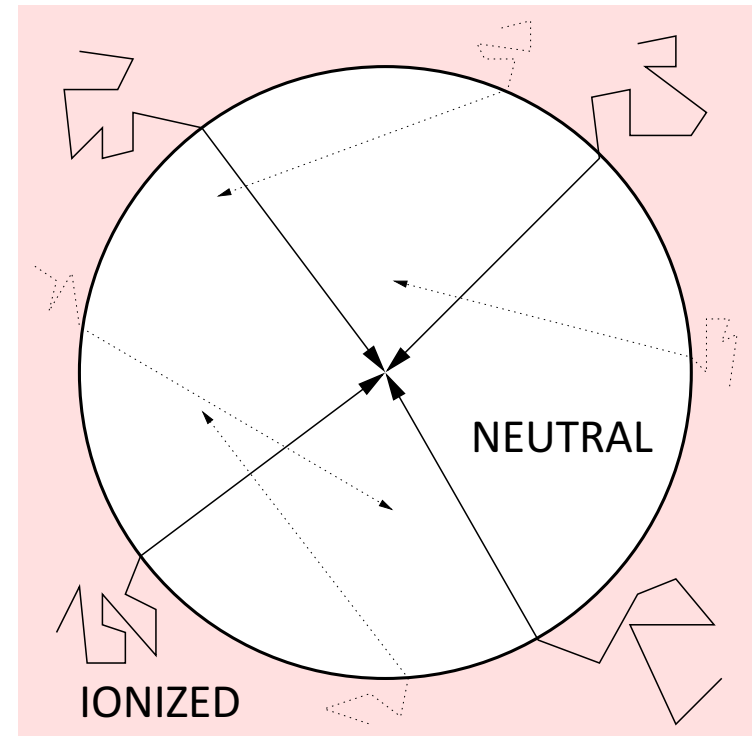


1930-60s – Steady State vs Big Bang

- What does an expanding Universe tells us about its origin and fate?
 - Steady State Theory:
 - new matter is generated to fill the space created by the expansion, and the Universe as a whole is unchanged and eternal (past & future).
 - Big Bang Theory:
 - the Universe (matter and energy; space and time) is created in a single explosive event, resulting in an expanding and hence cooling & rarifying Universe.

1948 – Cosmic Microwave Background

- In a Big Bang Universe the hot, expanding Universe eventually cools through the ionization temperature of hydrogen: $p^+ + e^- \Rightarrow H$.
- Without free electrons to scatter off, the photons free-stream to us.
- Alpher, Herman & Gamow predict a residual photon field at 5 – 50K
- COSMIC – filling all of space.
- MICROWAVE – redshifted by the expansion of the Universe from 3000K to 3K.
- BACKGROUND – primordial photons coming from “behind” all astrophysical sources.



1964 – First CMB Detection

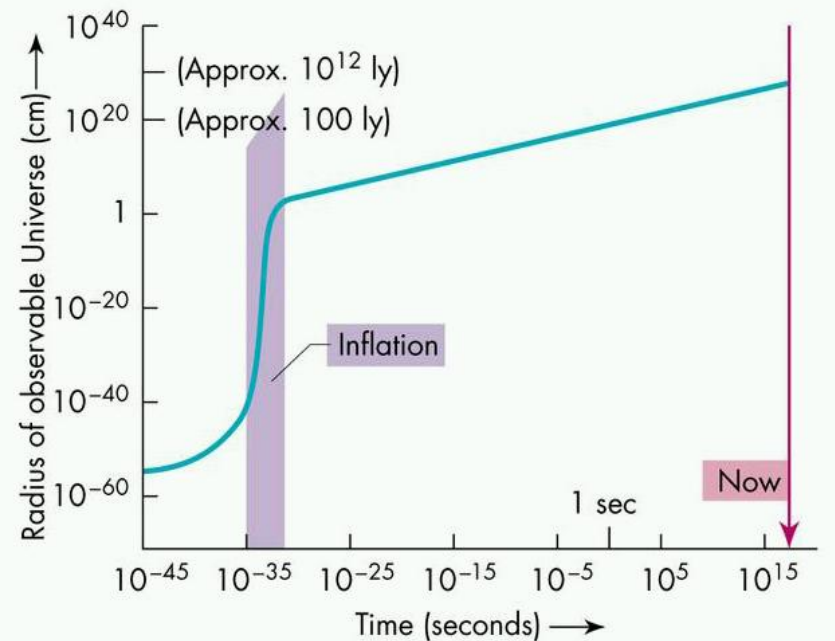
- Penzias & Wilson find a puzzling signal that is constant in time and direction.
- They determine it isn't a systematic – not terrestrial, instrumental, or due to a “white dielectric substance”.
- Dicke, Peebles, Roll & Wilkinson explain to them that they're seeing the Big Bang.
- Their accidental measurement kills the Steady State theory and wins them the 1978 Nobel Prize in physics.



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1980 – Inflation

- Increasingly detailed measurements of the CMB temperature show it to be uniform to better than 1 part in 100,000.
- At the time of last-scattering any points more than 1° apart on the sky today are out of causal contact, so how could they have exactly the same temperature? This is the horizon problem.
- Guth proposes a very early epoch of exponential expansion driven by the energy of the vacuum.
- This also solves the flatness & monopole problems.



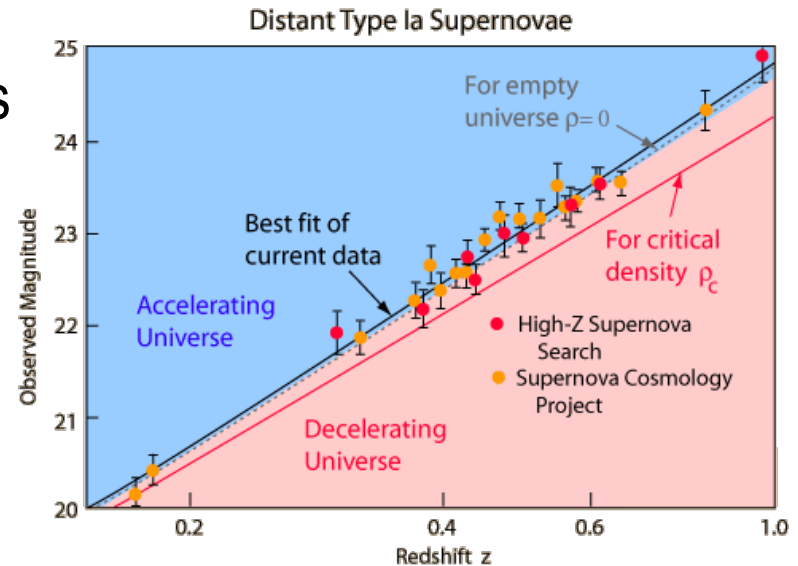
1992 – CMB Fluctuations

- For structure to exist in the Universe today there must have been seed density perturbations in the early Universe.
- Despite its apparent uniformity, the CMB must therefore carry the imprint of these fluctuations.
- After 20 years of searching, fluctuations in the CMB temperature were finally detected by the COBE satellite mission.
- COBE also confirmed that the CMB had a perfect black body spectrum, as a residue of the Big Bang would.
- Mather & Smoot share the 2006 Nobel Prize in physics.



1998 – The Accelerating Universe

- Both the dynamics and the geometry of the Universe were thought to depend solely on its overall density:
 - Critical ($\Omega=1$): expansion rate asymptotes to zero, flat Universe.
 - Subcritical ($\Omega<1$): eternal expansion, open Universe.
 - Supercritical ($\Omega>1$): expansion to contraction, closed Universe.
- Measurements of supernovae surprisingly showed the Universe is accelerating!
- Acceleration (maybe) driven by a Cosmological Constant!
- Perlmutter, Riess & Schmidt share 2011 Nobel Prize in physics.



2000 – The Concordance Cosmology

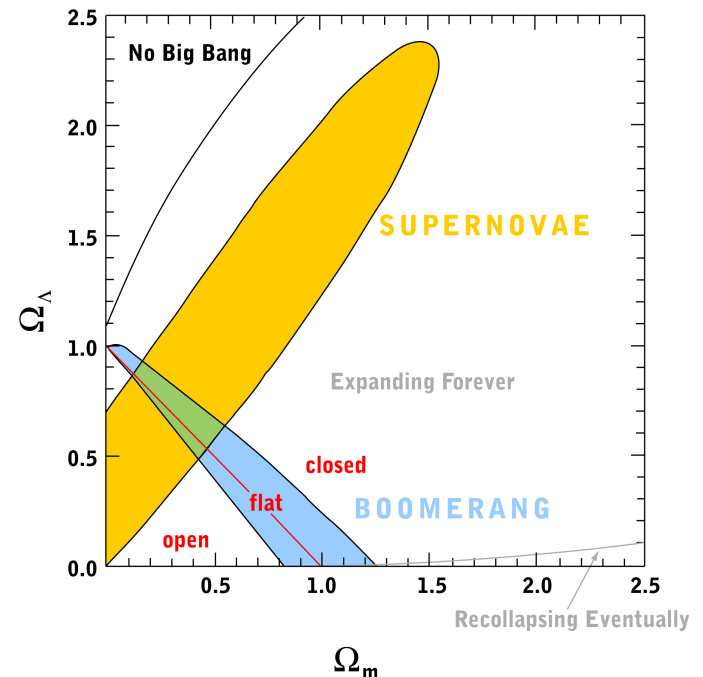
- The BOOMERanG & MAXIMA balloon experiments measure small-scale CMB fluctuations, demonstrating that the Universe is flat.
- CMB fluctuations encode cosmic geometry: $(\Omega_{\Lambda} + \Omega_m)$
- Type 1a supernovae encode cosmic dynamics: $(\Omega_{\Lambda} - \Omega_m)$
- Their combination breaks the degeneracy in each.

The Concordance Cosmology:

- 70% Dark Energy
- 25% Dark Matter
- 5% Baryons

=> 95% ignorance!

- What and why is the Dark Universe?

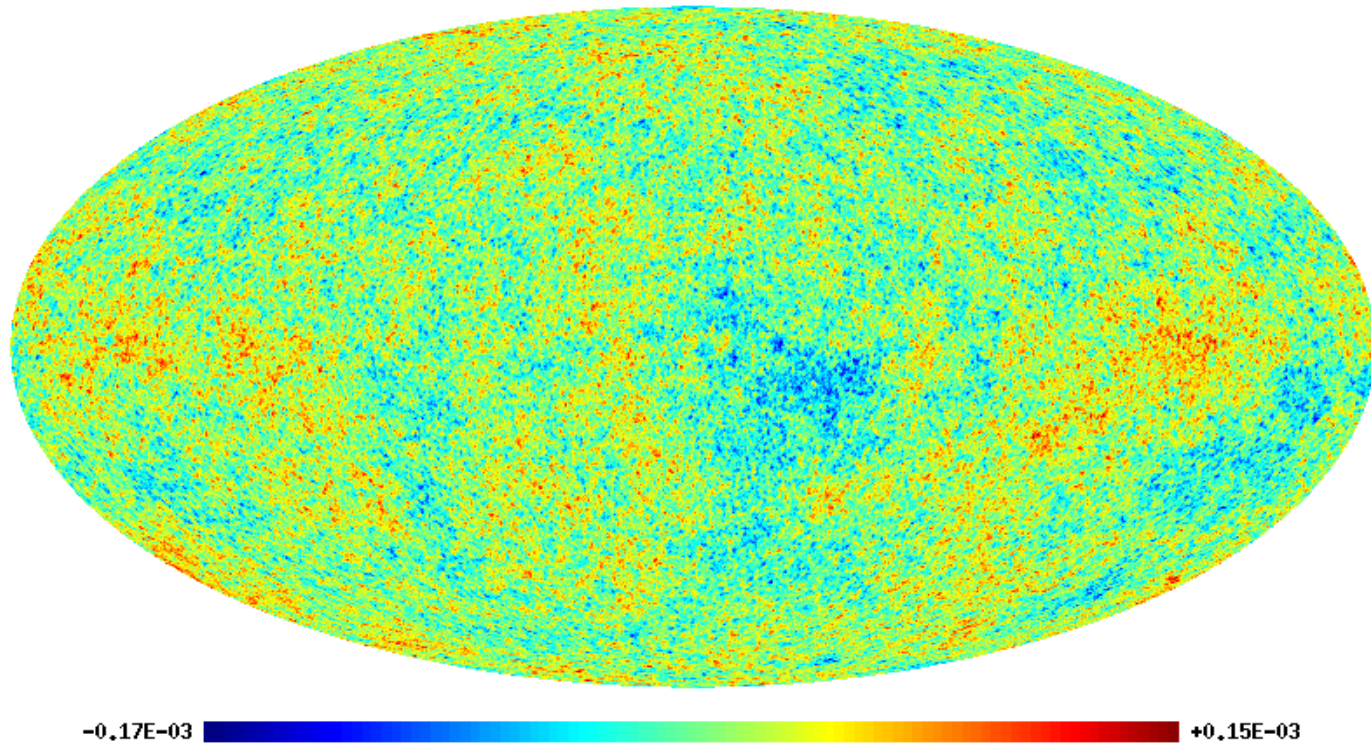


The Cosmic Microwave Background

CMB Science

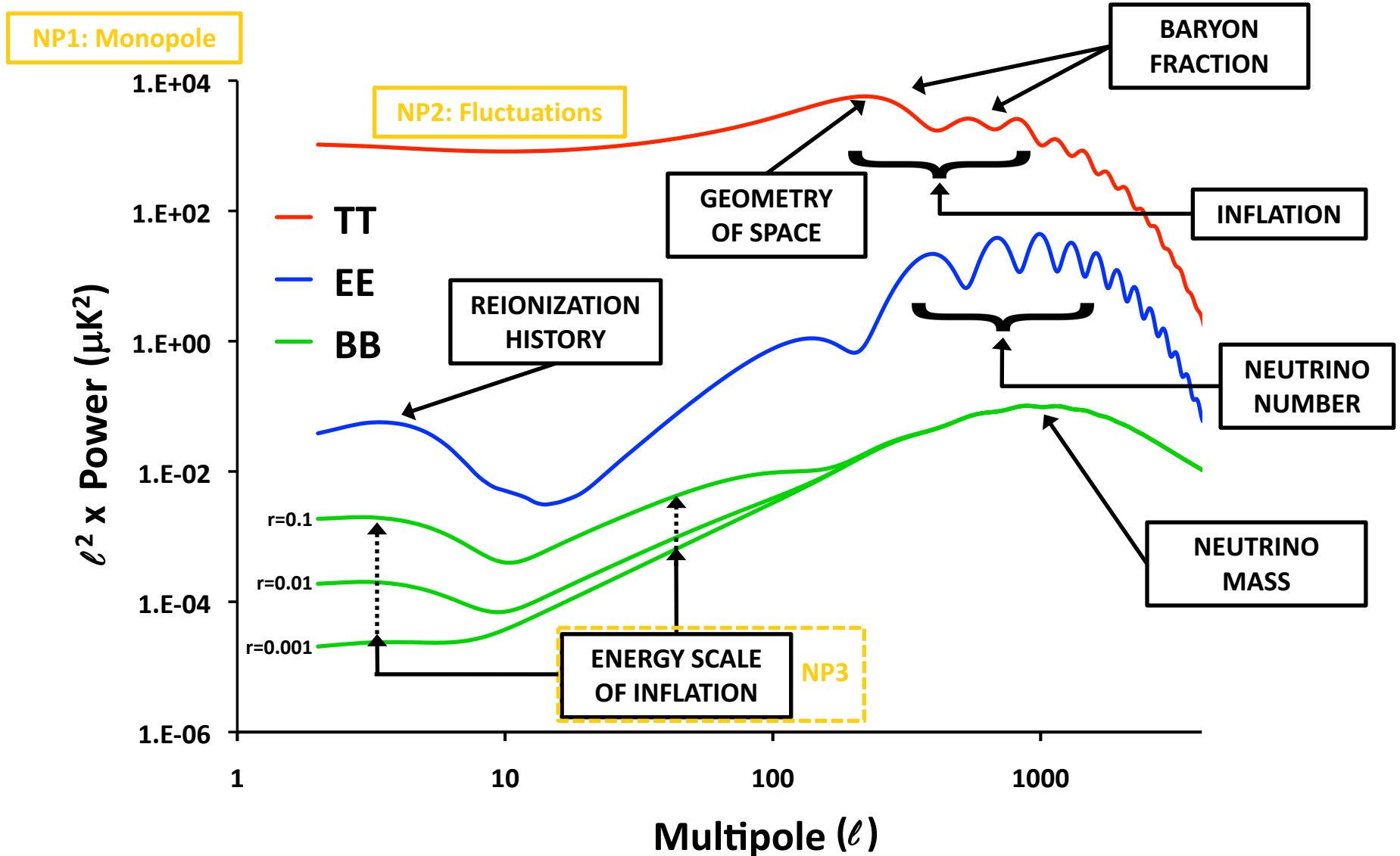
- Primordial photons experience the entire history of the Universe, and everything that happens leaves its trace.
- Primary anisotropies:
 - Generated before last-scattering, track physics of the early Universe
 - Fundamental parameters of cosmology
 - Quantum fluctuation generated density perturbations
 - Gravitational radiation from Inflation
- Secondary anisotropies:
 - Generated after last-scattering, track physics of the later Universe
 - Gravitational lensing by dark matter
 - Spectral shifting by hot ionized gas
 - Red/blue shifting by evolving potential wells

CMB Fluctuations



- Our map of the CMB sky is one particular realization – to compare it with theory we need a statistical characterization.

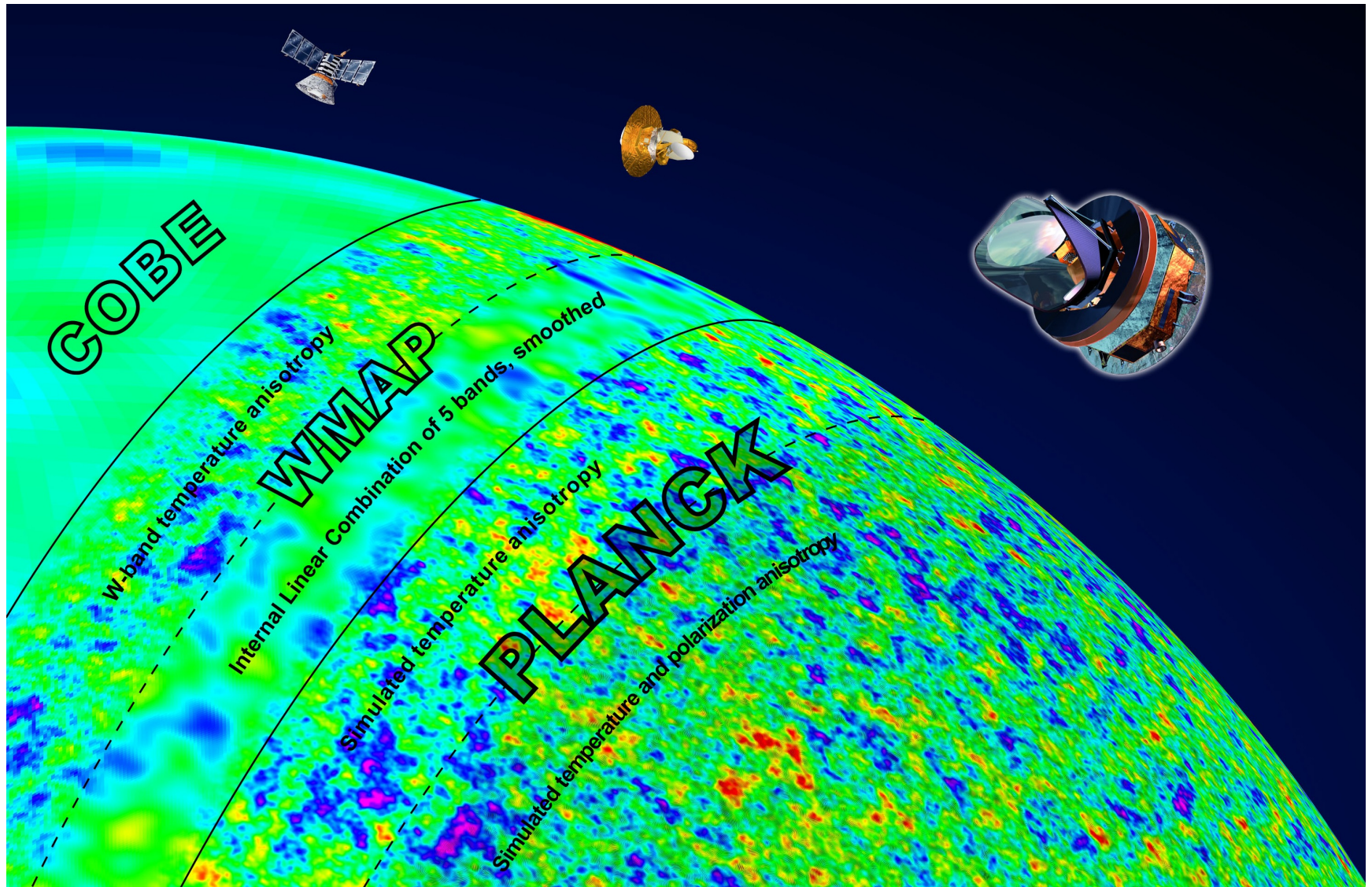
CMB Power Spectra



CMB Signals

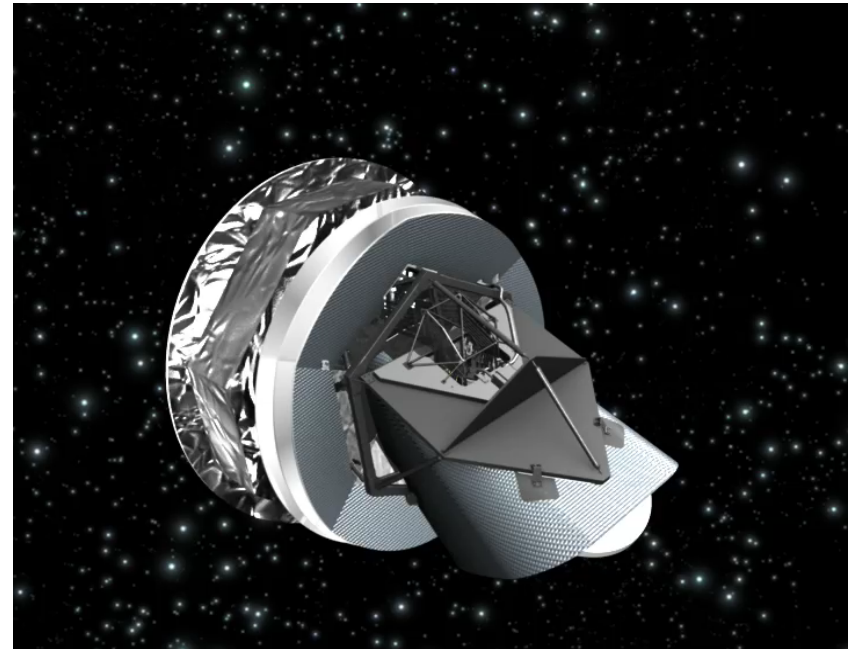
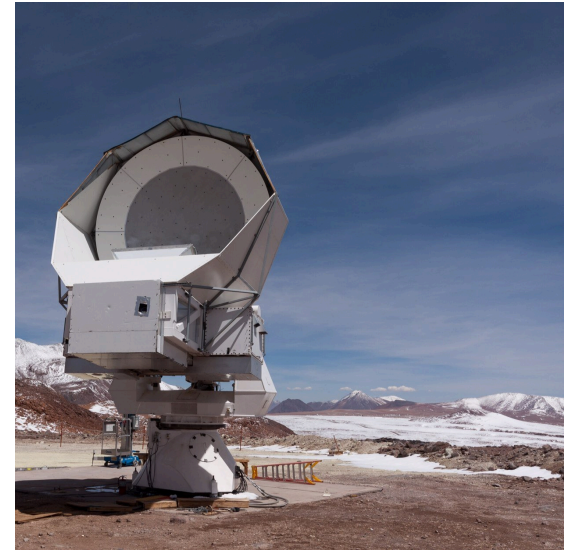
COMPONENT	AMPLITUDE (K)	ERA
TT : Monopole	1	1968 (Penzias & Wilson)
TT : Anisotropy	10^{-5}	1990 (COBE)
TT : Harmonic Peaks	10^{-6}	2000 (BOOMERanG, MAXIMA)
EE : Reionization	10^{-7}	2005 (DASI)
BB : Lensing	10^{-9}	2015 (SPT, POLARBEAR)
BB : Gravitational Waves	$< 10^{-9}$	2020+ (LiteBIRD, CMB-S4)

CMB Science Evolution



CMB Observations

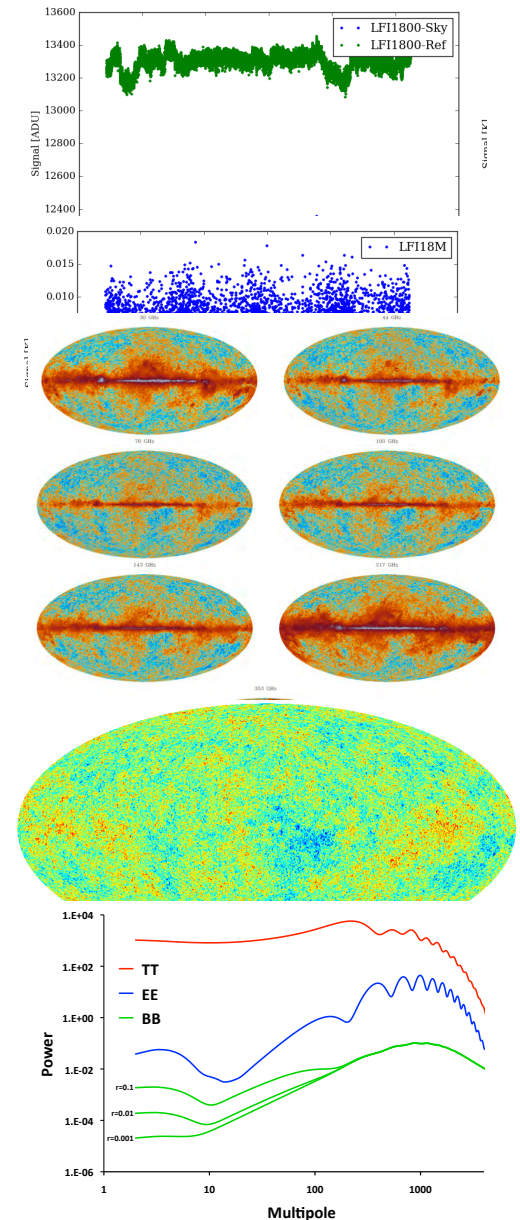
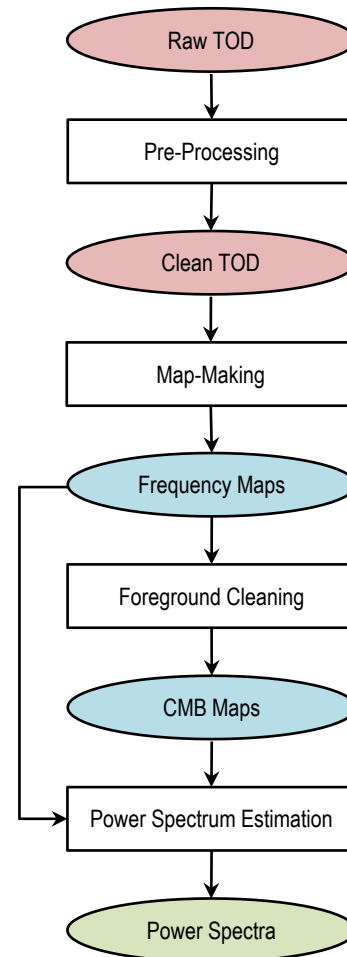
- Searching for micro- to nano-Kelvin fluctuations on a 3 Kelvin background.
- Need very many, very sensitive, very cold, detectors.
- Scan part of the sky from high dry ground or the stratosphere, or all of the sky from space.



Cosmic Microwave Background Data Analysis

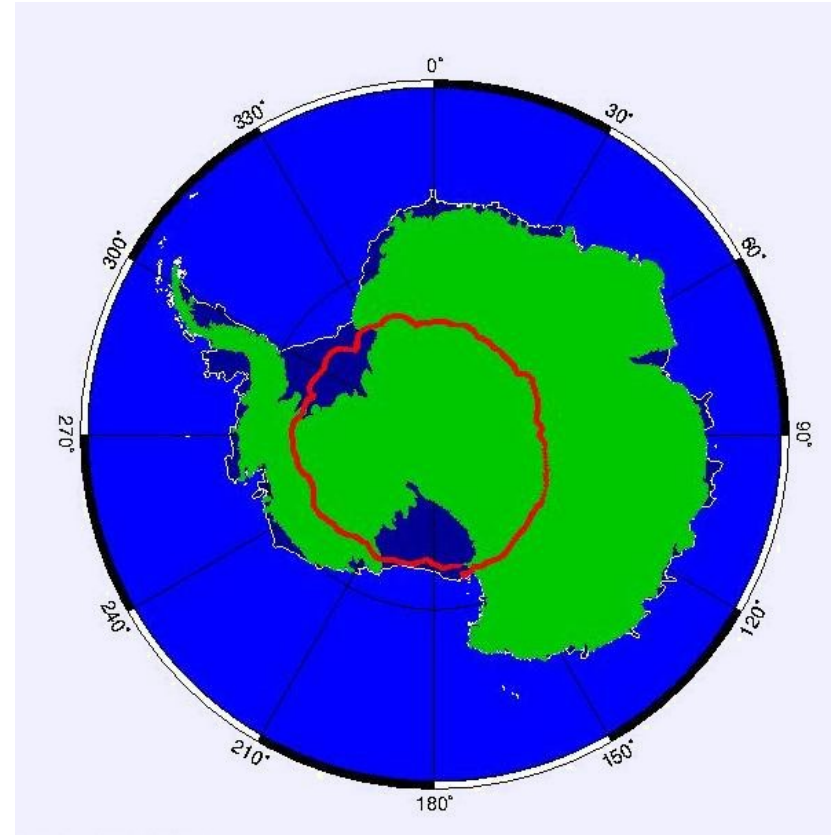
Data Reduction

- Sequence of S/N-increasing data compressions via domain transformations:
 - Time samples
 - Pixels
 - Multipoles
- Each domain exposes different systematics => iterative looping.
- Must propagate both data *and their covariance* for a sufficient statistic.



Case 1 – BOOMERanG (2000)

- Balloon-borne experiment flown from McMurdo Station.
- Spends 10 days at 35km float, circumnavigating Antarctica
- Gathers temperature data at 4 frequencies: 90 – 400GHz.



Exact CMB Analysis

- Model data as stationary Gaussian noise and sky-synchronous CMB

$$d_t = n_t + P_{tp} s_p$$

- Estimate the noise correlations from the (noise-dominated) data

$$N_{tt'}^{-1} = f(|t-t'|) \sim \text{invFFT}(1/\text{FFT}(d))$$

- *Analytically* maximize the likelihood of the map given the data and the noise covariance matrix N

$$m_p = (P^T N^{-1} P)^{-1} P^T N^{-1} d$$

- Construct the pixel domain noise covariance matrix

$$N_{pp'} = (P^T N^{-1} P)^{-1}$$

- *Iteratively* maximize the likelihood of the CMB spectra given the map and its covariance matrix $M = S + N$

$$L(c_l | m) = -\frac{1}{2} (m^T M^{-1} m + \text{Tr}[\log M])$$

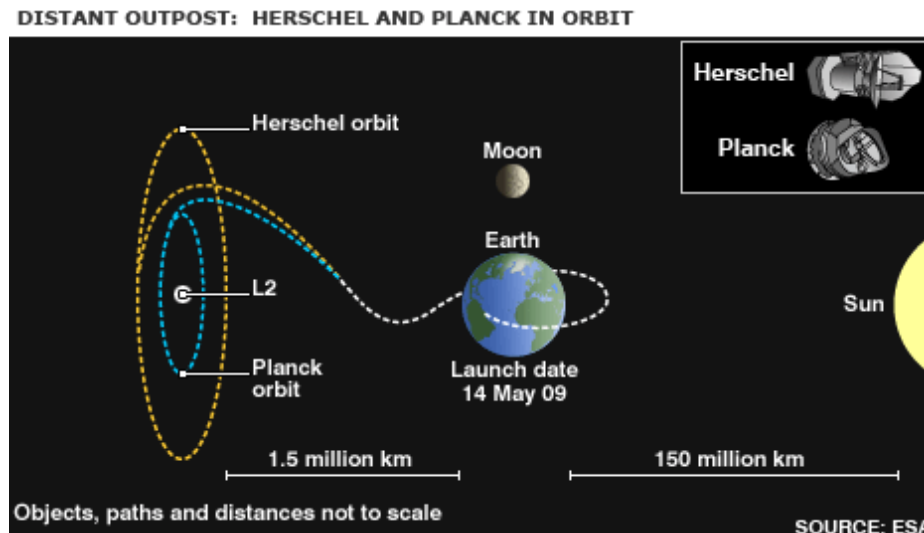
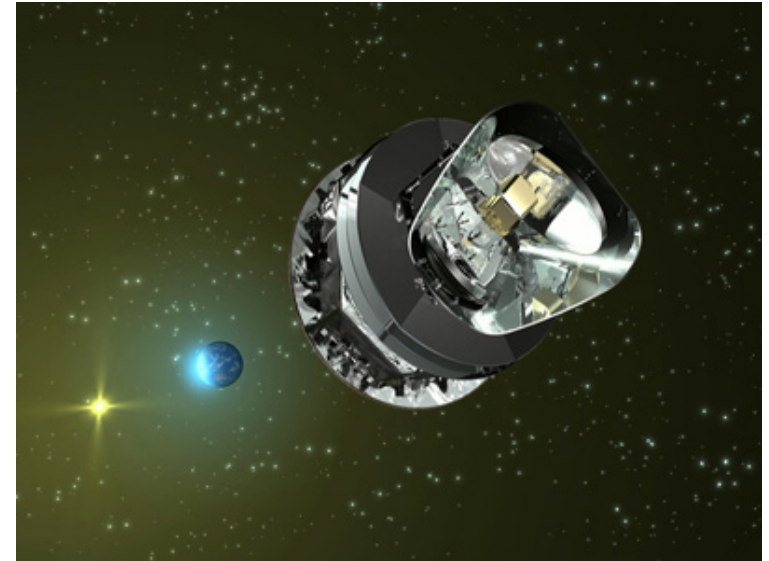
Algorithms & Implementation

- Dominated by dense pixel-domain matrix operations
 - Inversion in building N_{pp}
 - Multiplication in estimating c_l
- MADCAP CMB software built on ScaLAPACK tools, Level 3 BLAS
 - scales as $\mathcal{N}_p^3$
- Execution on NERSC's 600-core Cray T3E achieves ~90% theoretical peak performance.
- Spawns MADbench benchmarking tool, used in NERSC procurements.



Case 2 – Planck (2015)

- European Space Agency satellite mission, with NASA roles in detectors and data analysis.
- Spends 4 years at L2.
- Gathers temperature and polarization data at 9 frequencies: 30 – 857GHz



The Exact Analysis Challenge

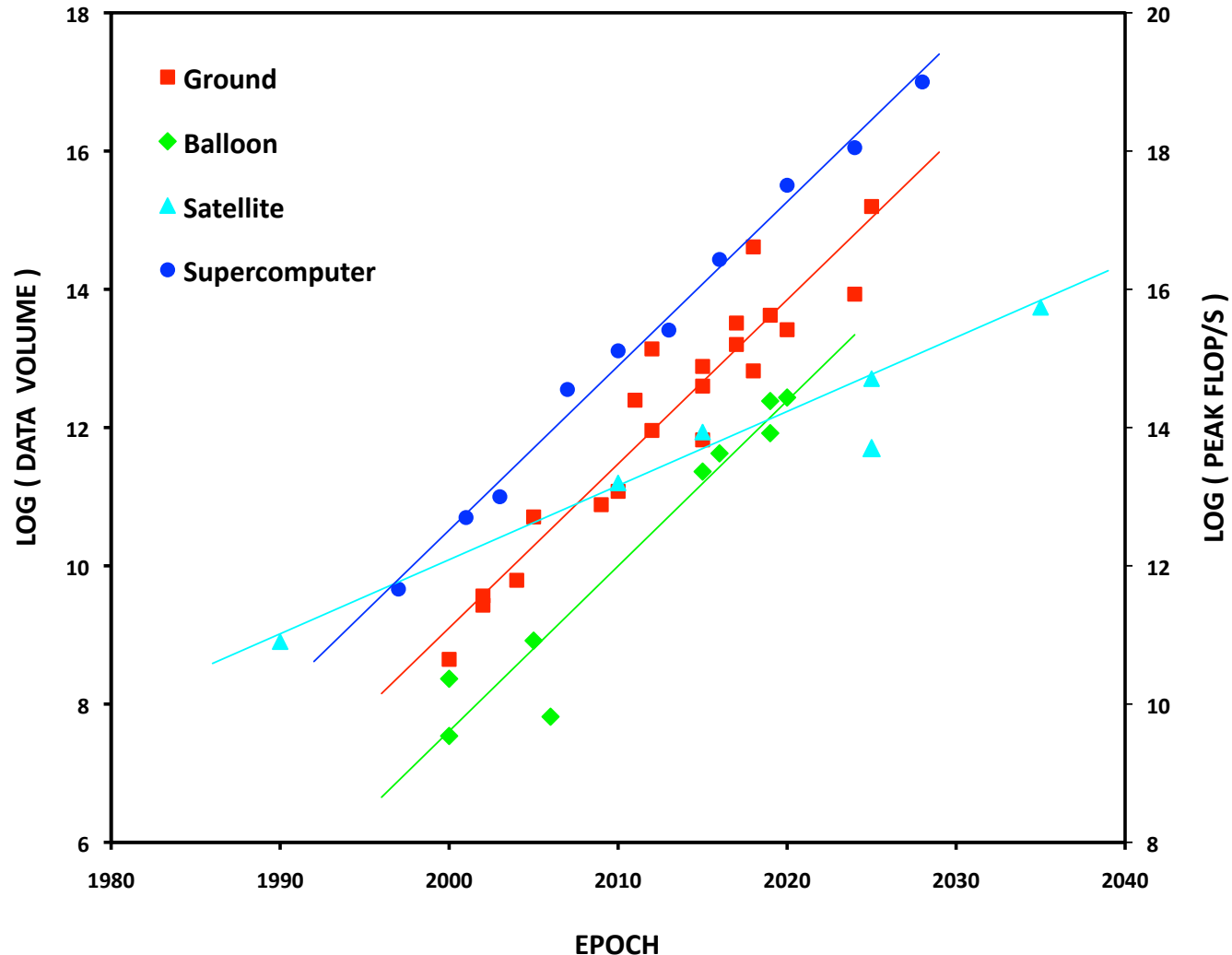
	BOOMERanG	Planck
Sky fraction	5%	100%
Resolution	20'	5'
Frequencies	1	9
Components	1	3
Pixels	$O(10^5)$	$O(10^9)$
Operations	$O(10^{15})$	$O(10^{27})$

- Science goals drive us to observe more sky, at higher resolution, at more frequencies, in temperature and polarization.
- Exact methods are no longer computationally tractable.

Approximate CMB Analysis

- Map-making
 - No explicit noise covariance calculation possible
 - Use PCG instead: $(P^T N^{-1} P) m = P^T N^{-1} d$
- Power-spectrum estimation
 - No explicit data covariance matrix available
 - Use pseudo-spectral methods instead:
 - Take spherical harmonic transform of map, simply ignoring inhomogeneous coverage of incomplete sky!
 - Use Monte Carlo methods to estimate uncertainties and remove bias.
- Dominant cost is simulating & mapping time-domain data for Monte Carlo realizations: $O(\mathcal{N}_{\text{mc}} \mathcal{N}_t)$

The Approximate Analysis Challenge



Ever fainter signals require ever larger data sets.

Simulation & Mapping: Algorithms

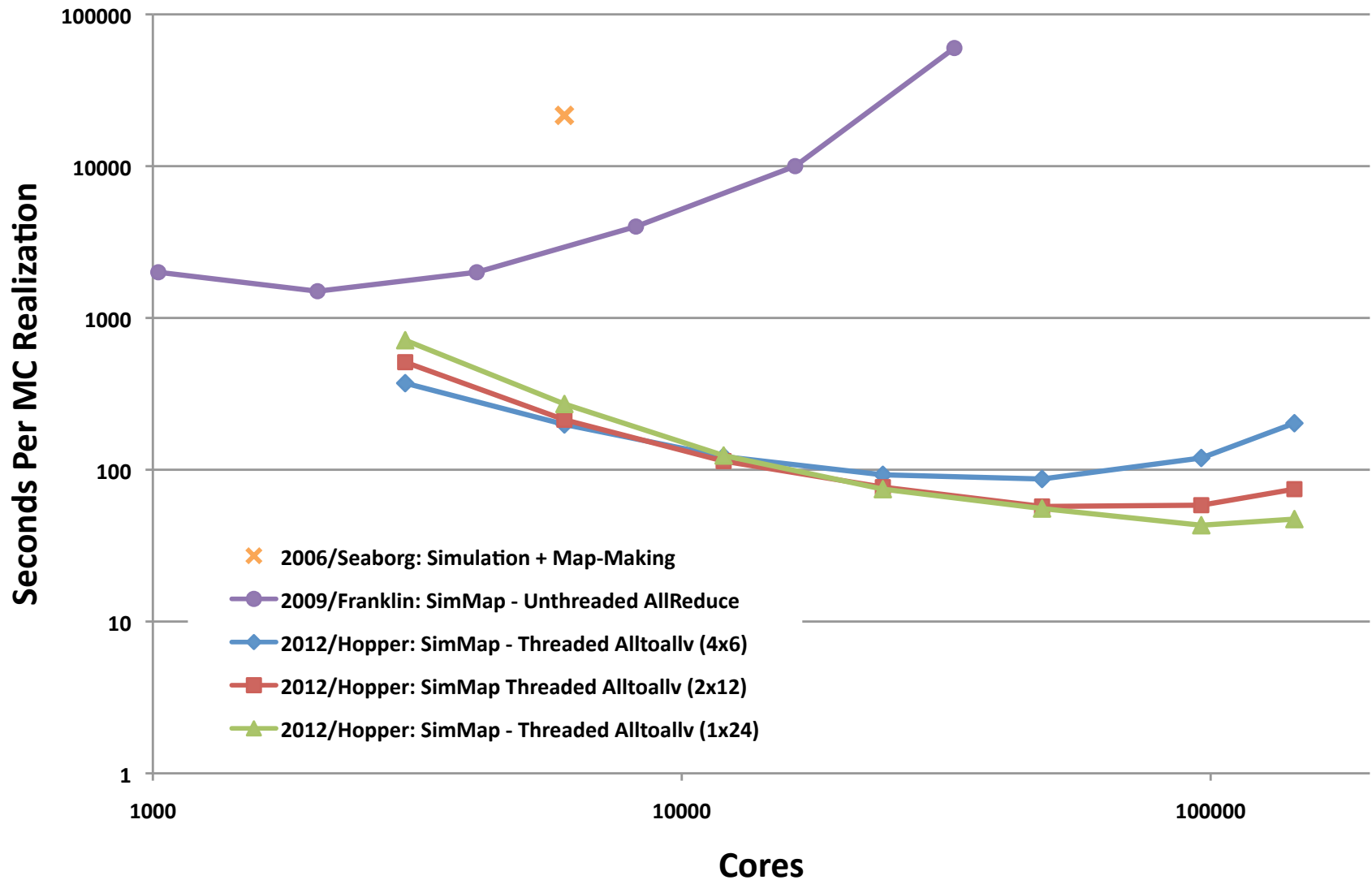
Given the instrument noise statistics & beams, a scanning strategy, and a sky:

- 1) SIMULATION: $d_t = n_t + s_t = n_t + P_{tp} s_p$
 - A realization of the piecewise stationary noise time-stream:
 - Pseudo-random number generation & FFT
 - A signal time-stream scanned & from the beam-convolved sky:
 - SHT
- 2) MAPPING: $(P^T N^{-1} P) d_p = P^T N^{-1} d_t$ (A x = b)
 - Build the RHS
 - FFT & sparse matrix-vector multiply
 - Solve for the map
 - PCG over FFT & sparse matrix-vector multiply

Simulation & Mapping: Implementation

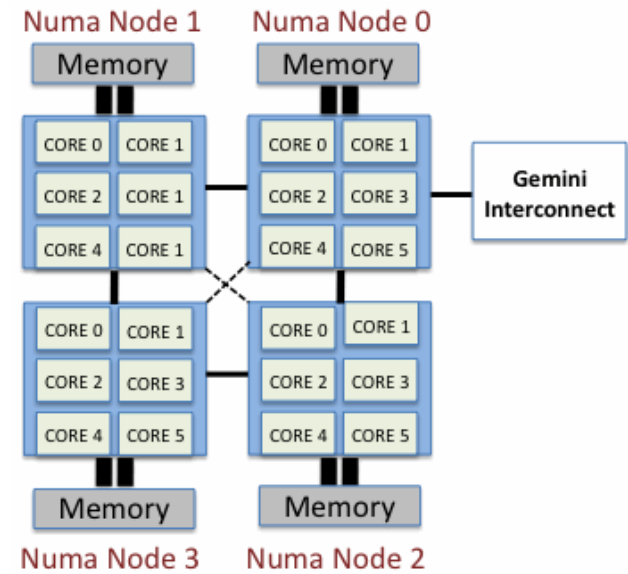
- Linear algorithms reduce calculation costs ...
... but I/O & communication costs become more significant
- Input/Output
 - On-the-fly simulation removes redundant write/read
 - Caching common data improves Monte Carlo efficiency
- Communication
 - Hybridization reduces number of MPI tasks
 - All-to-all removes redundant communication of zeros in Allreduce

Implementation/Architecture Evolution

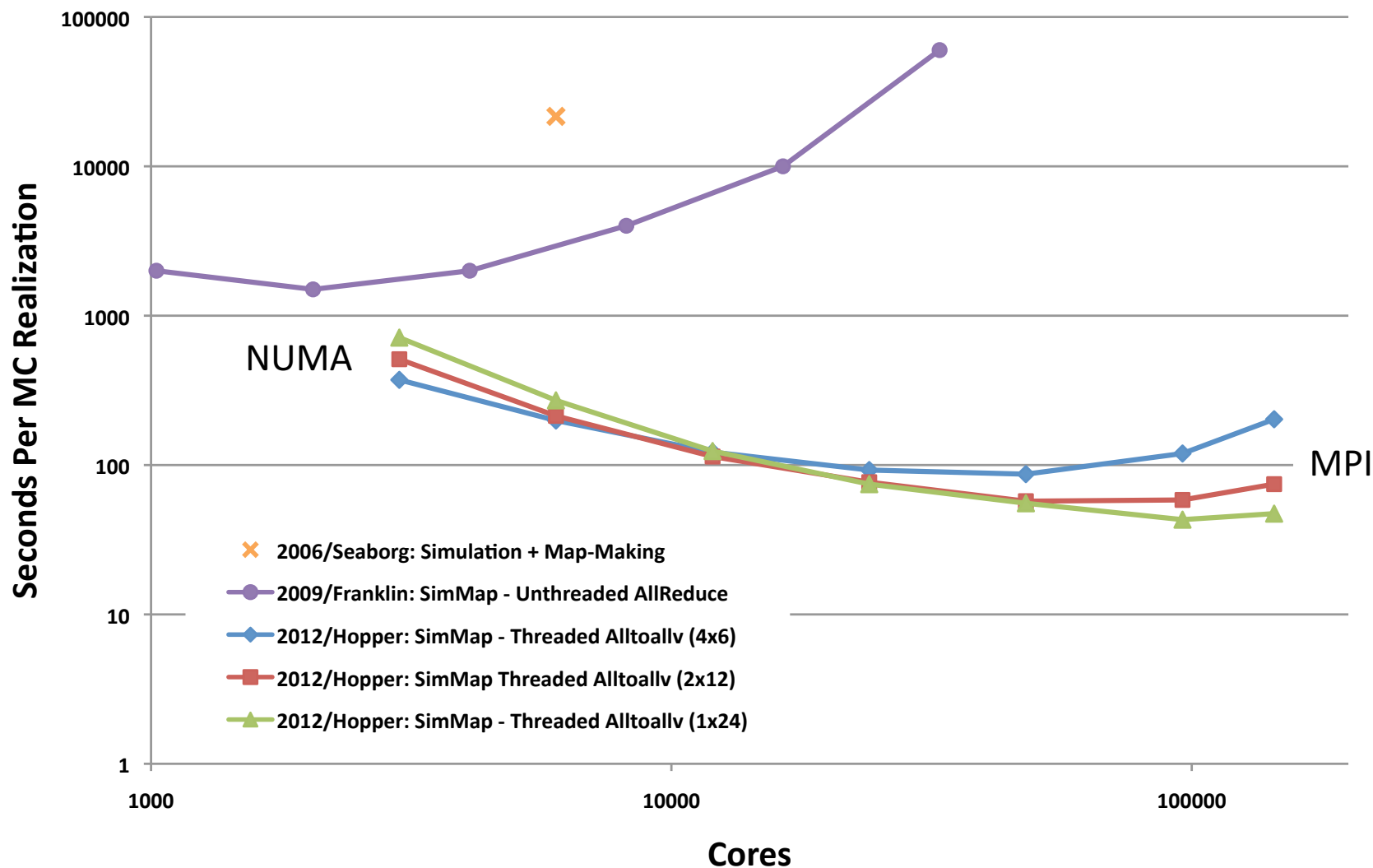


Architecture Evolution

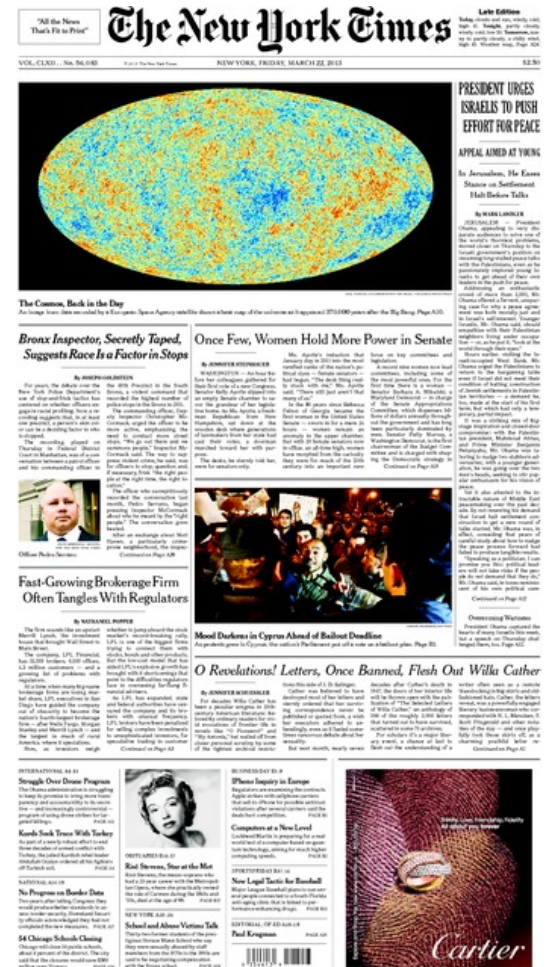
- Clock speed is no longer able to maintain Moore's Law.
- Many-core and GPU are two major approaches.
- Both of these will require
 - significant code development
 - performance experiments & auto-tuning
- Eg. NERSC's Cray XE6 system *Hopper*
 - 6384 nodes
 - 2 sockets per node
 - 2 NUMA nodes per socket
 - 6 cores per NUMA node
- What is the best way to run hybrid code on such a system?



Configuration With Concurrency

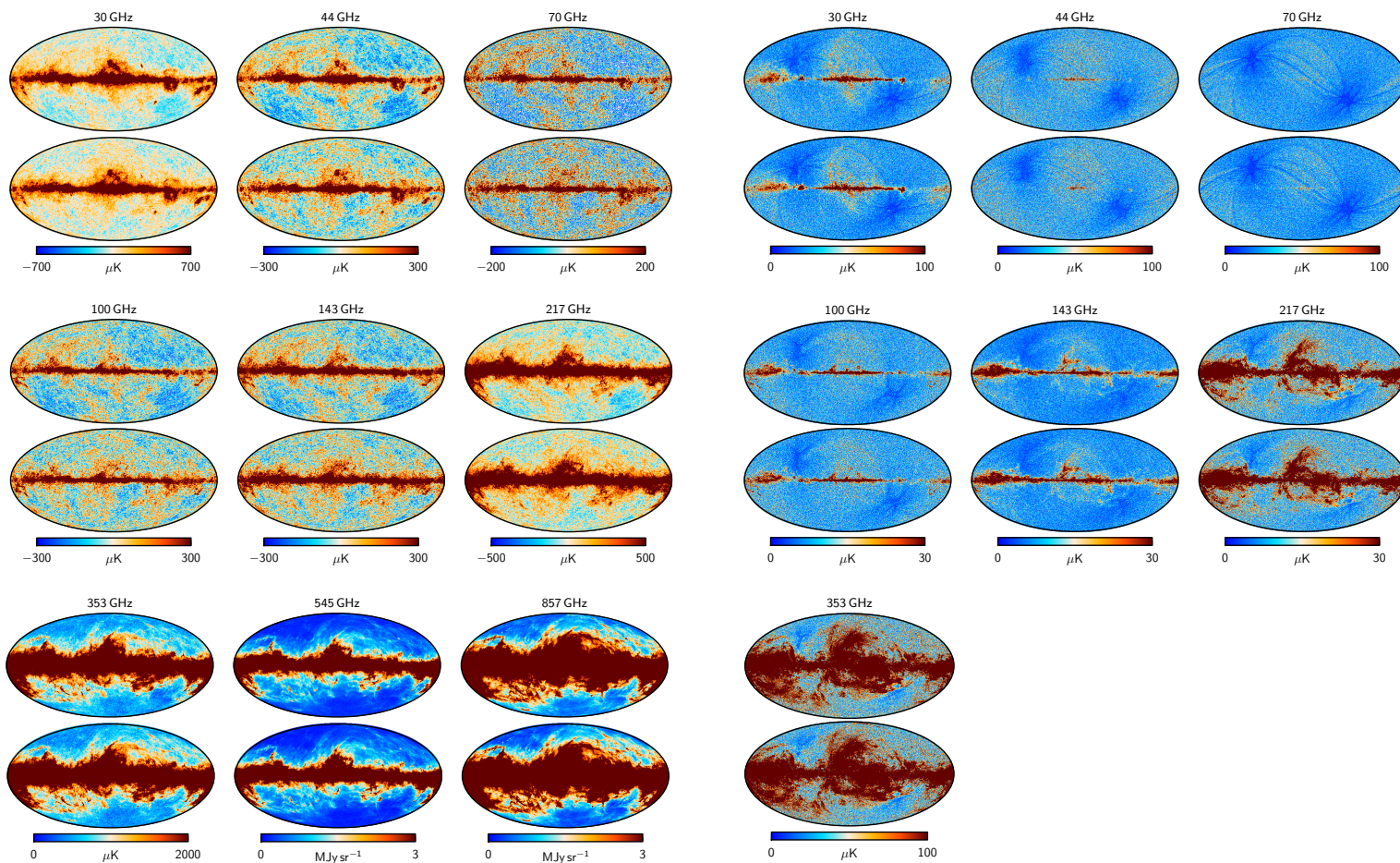


- Simulations including
 - CMB, foregrounds, detector noise
 - Detailed instrument model
- Fiducial realization for validation and verification of analysis algorithms and implementations.
- 10^3 Monte Carlo realizations for uncertainty quantification and de-biasing.
- Unanticipated multiplicity of maps
 - 1000 different data cuts per realization!
 - New challenge to on-the-fly simulation.



Results: Full Focal Plane 8 (2015)

- Fiducial realization in temperature and polarization

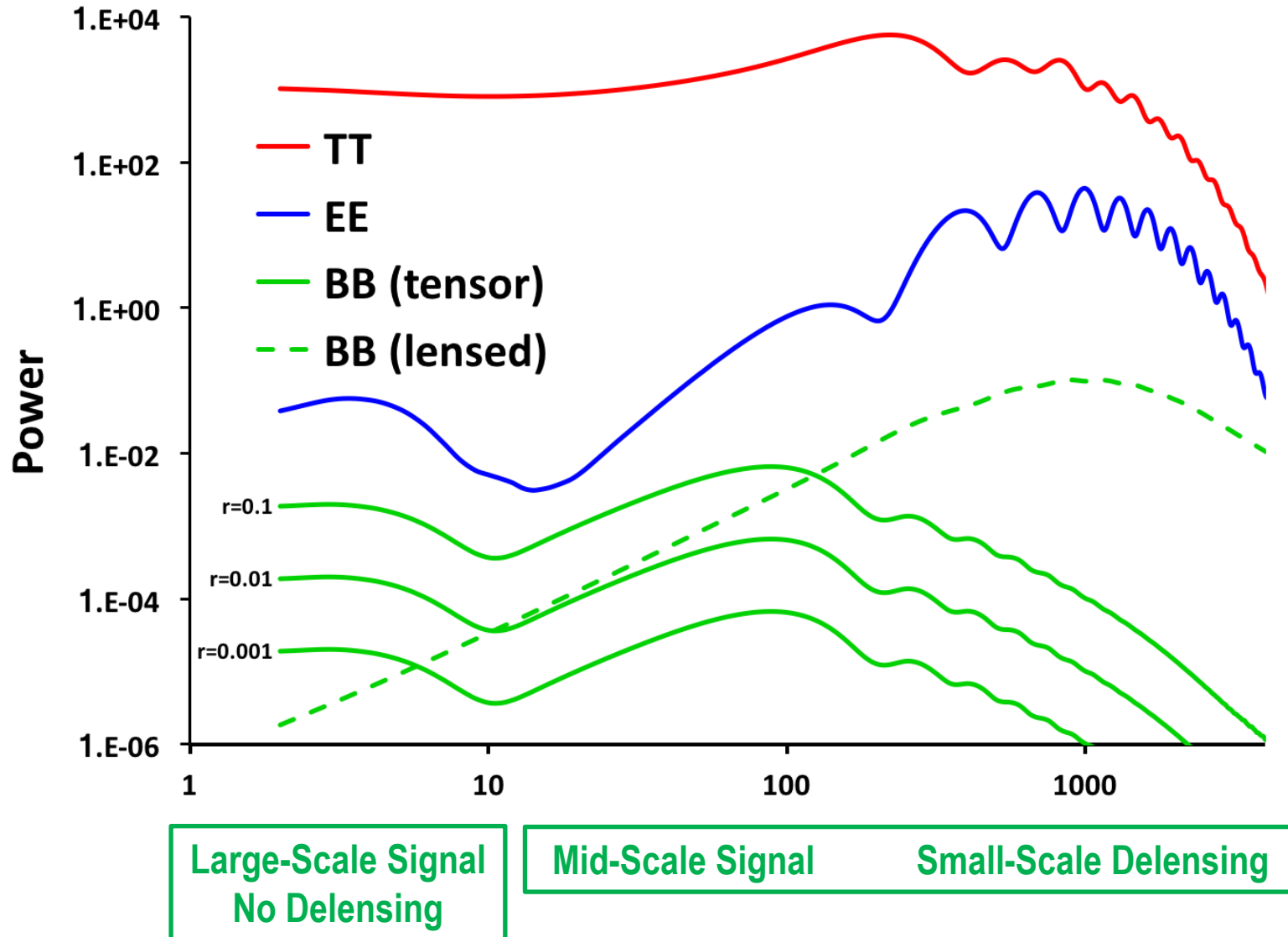


Results: Planck Full Focal Plane 8

- 10^4 Monte Carlo realizations reduced to 10^6 maps
 - multiple maps made per simulation



The Quest For B-Modes



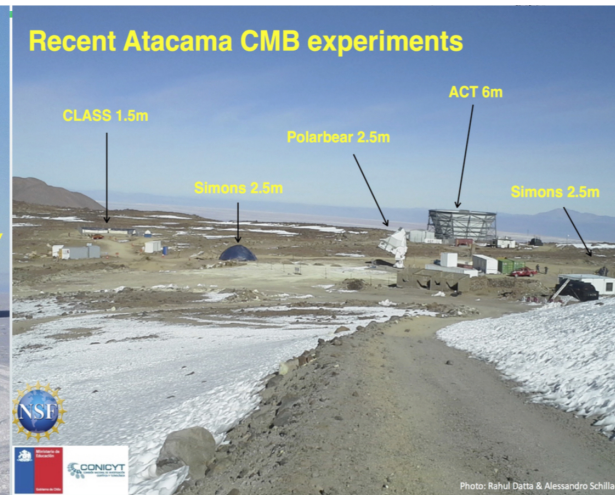
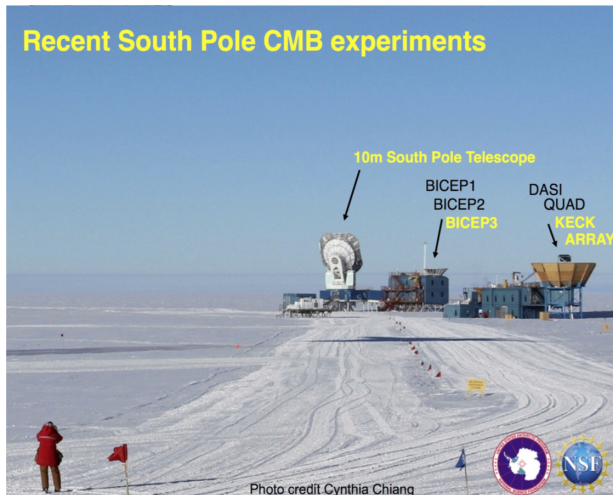
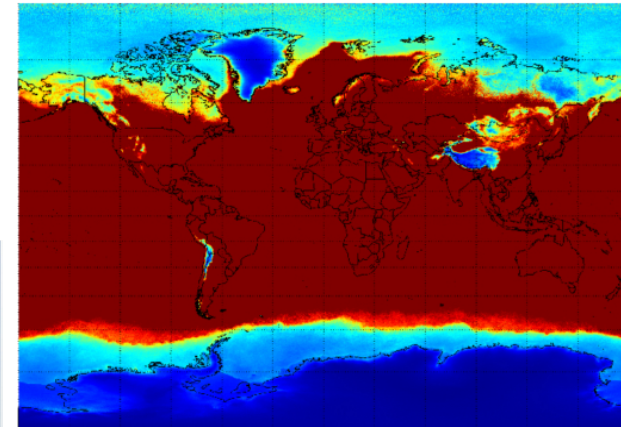
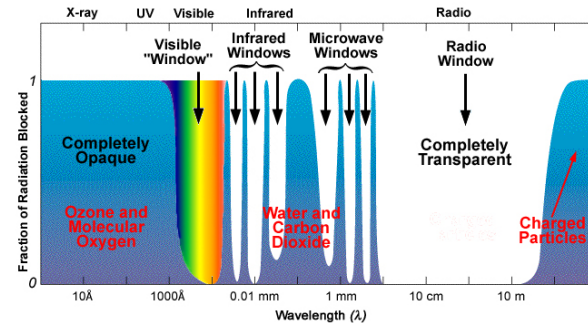
B-Mode Experiments By Cost

1. Mid-scale (recombination) bump only:
 - partial sky => ground-based
 - delensing => high resolution => large mirror
2. Large-scale (reionization) bump only:
 - full sky => space => satellite mission
 - low resolution => small mirror
3. Both bumps:
 - full sky + delensing => satellite mission + large mirror

In all cases, at enough frequencies to separate the CMB from the foregrounds!

Case 3: CMB-S4 (2025)

- Ultimate ground-based experiment from multiple high, dry, sites
- Plan: $O(500,000)$ detectors observing 70% of the sky for 5 years through 3 microwave atmospheric windows.

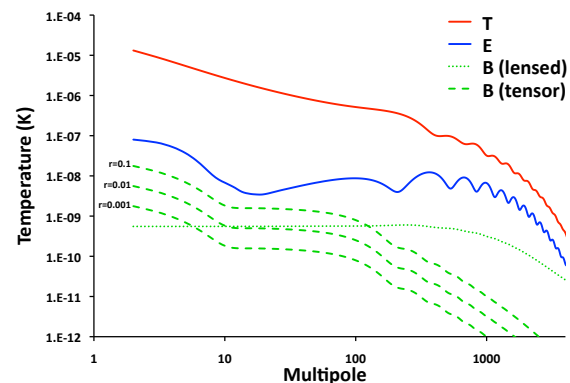


CMB-S4 Simulation Challenges

- More systematics sources

- Lower systematics threshold

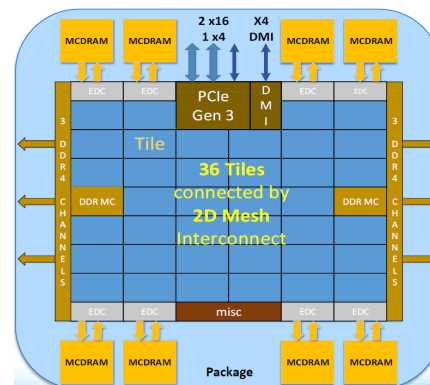
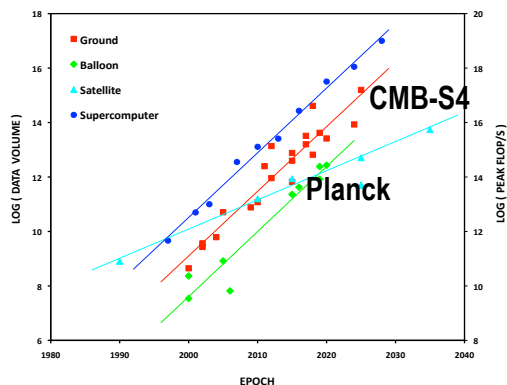
PRECISION



- Larger data volume

- Fewer watts per FLOP

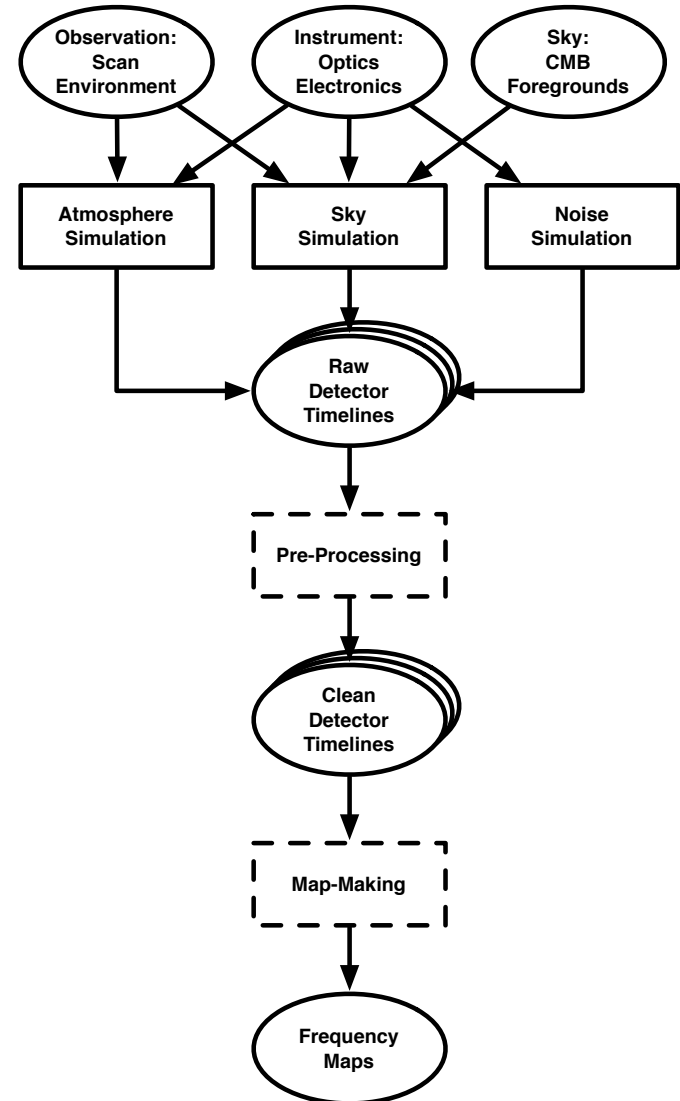
PERFORMANCE



Framework Development

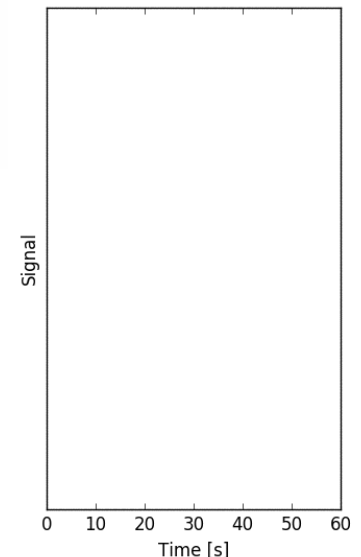
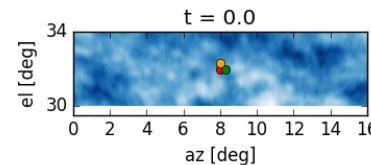
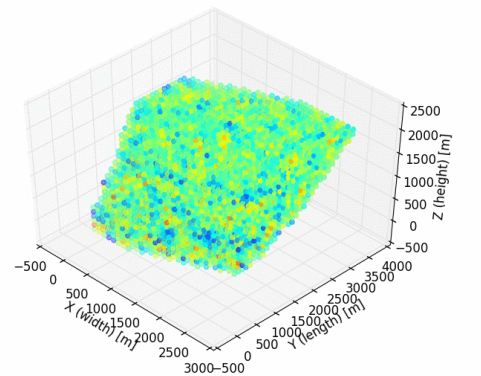
- Precise systematic mitigation implies as-yet unspecified algorithms for pre-processing and map-making.
- Huge time-ordered data volume implies massively-parallel, on-the-fly, simulation & reduction.
- Any framework must be:
 - a) Highly adaptable, strongly modular, readily useable, public.
 - b) Highly optimized, massively parallel, heavily threaded.

⇒ Python-wrapped MPI/OpenMP
hybrid C++ libraries on Github:
<http://github.com/hpc4cmb/toast>



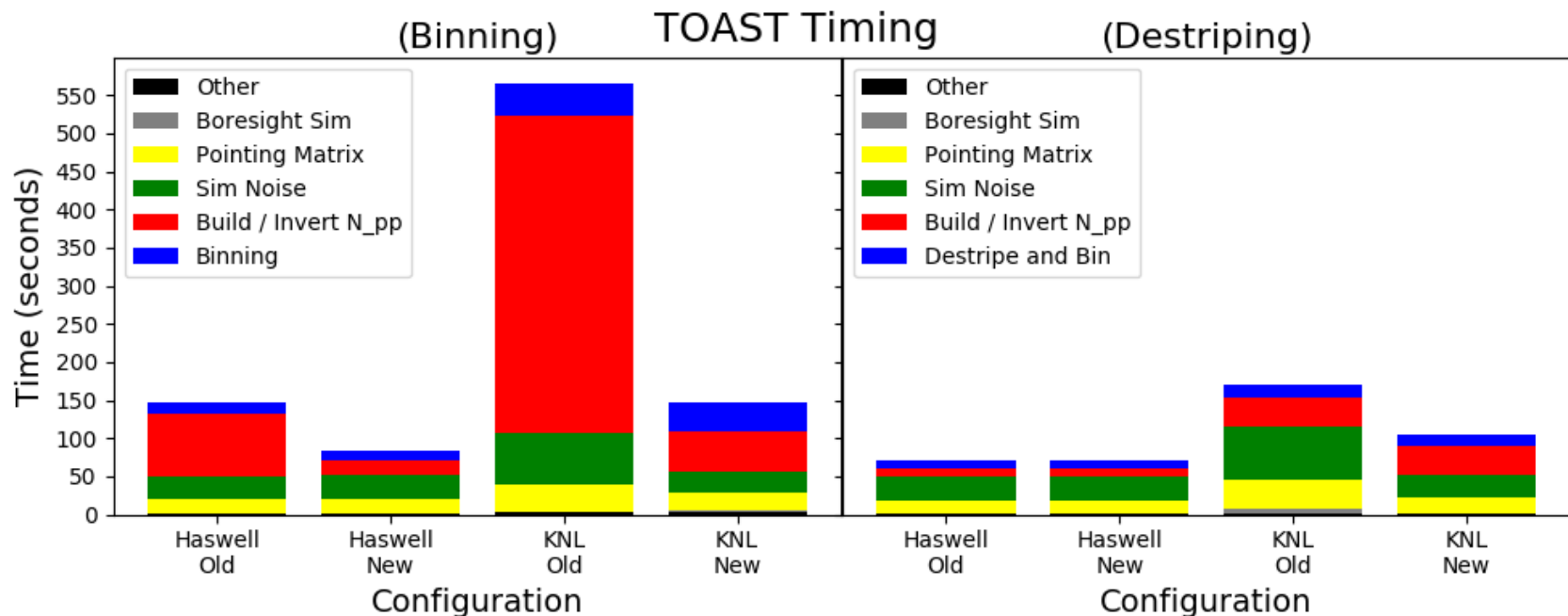
Atmosphere Simulation

- From the ground, atmosphere is a large, correlated, time-dependent contaminant.
- To reach CMB-S4 sensitivity we must validate and verify mitigation algorithms.
- 3-step algorithm:
 - Calculate bounding box based on scan & wind speed.
 - Generate atmosphere realization based on 2- & 3-D turbulent Kolmogorov spectra.
 - Perform line integral through box for each sample for each detector.



Xeon Phi Optimization

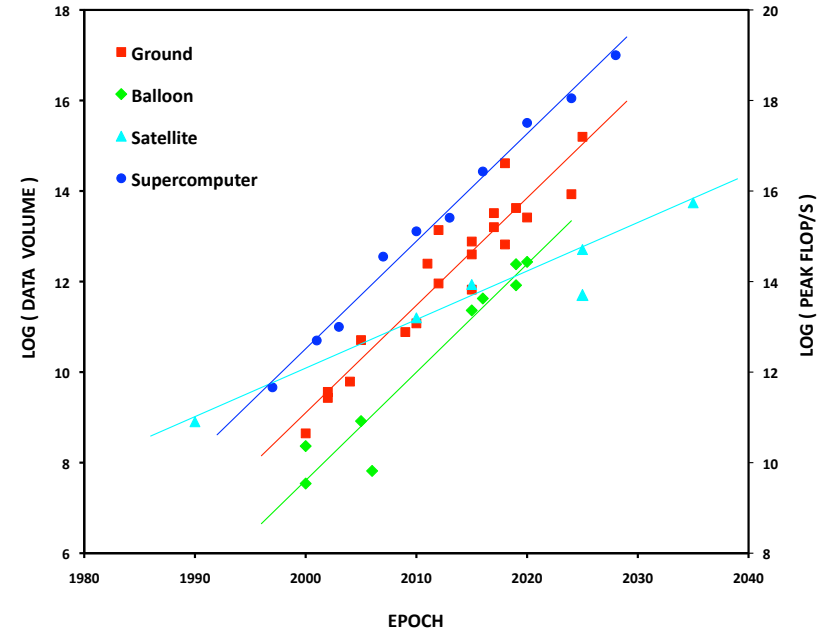
- 10x increase in thread-count from Edison to Cori-2
- Deeper, heterogeneous memory hierarchy
- Burst buffer



Case 4: LiteBIRD (2027)

PRO	CON
No atmosphere	Cost
Scanning strategy	Weight/size limits
Hardware quality	Inaccessibility

- We can now add computational tractability of a smaller data volume to the PRO column
 - More precise simulations
 - Larger MC realization sets
- Both clearly seen in Planck compared with Stage 2/3 expts.



Conclusions

- The Cosmic Microwave Background radiation provides a unique probe of the entire history of the Universe.
- Our quest for fainter and fainter signals requires
 - bigger and bigger data volumes, and
 - tighter and tighter control of systematics.
- Exponential data growth and increasingly complex analyses compels us to stay on the leading edge of high performance computing.
- Our analysis methods, algorithms and implementations necessarily evolve with both the data sets and HPC architectures.
- CMB-S4 and power-constrained HPC pose the most challenging data/architecture combination we have yet faced.