SciDAC-4: Inference and Machine Learning at Extreme Scales

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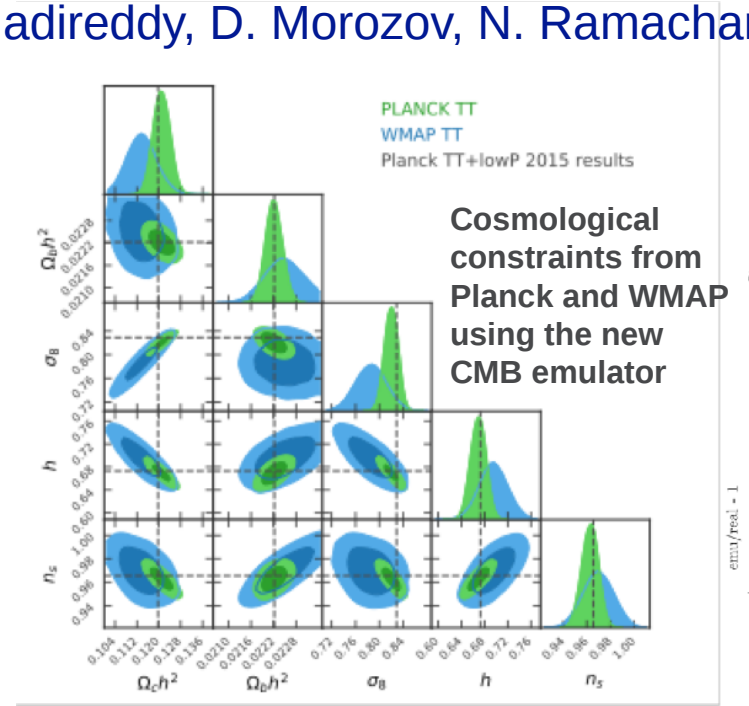
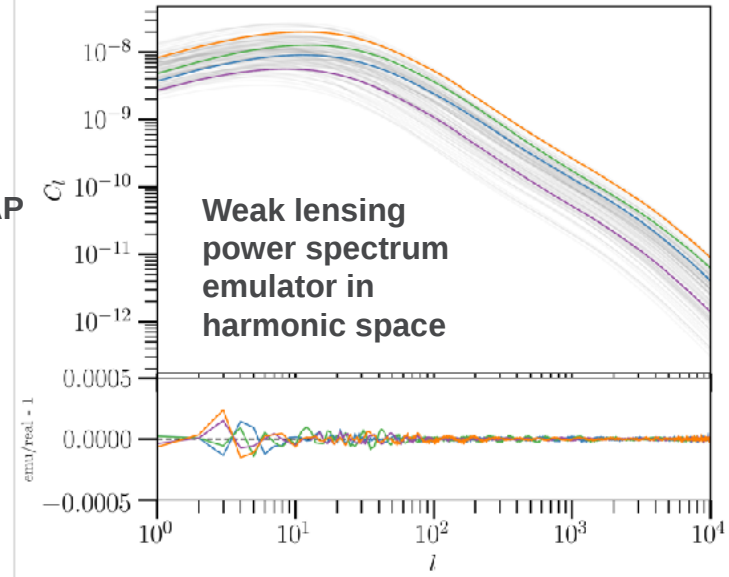
- **Opportunity:** Use of HPC resources for data-intensive statistical and machine learning (ML) methods for discovery science
- **Project Thrusts:** Melding HPC and observational datasets with ML/stats to solve scientific inference problems in Cosmic Frontier experiments — CMB-S4, DESI, LSST, SPT
- **Applications/Impact:** Cosmological parameter estimation, strong lens image classification/characterization, synthetic sky catalog generation, fast prediction of summary statistics, fast likelihood estimation, improved photo-z estimation





- **Examples — Cosmic Microwave Background and Weak Lensing**
  - Large training data sets using direct computation (CMB) or first-level emulation (lensing)
  - Dimensional reduction via unsupervised learning
  - High-dimensional non-parametric regression
  - Emulators yield **~1000** speed-up with 0.5% errors over the desired dynamic range, technique used by all future surveys

http://press3.mcs.anl.gov/cpac/projects/scidac/

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Unraveling the Cosmic Puzzle: HPC and ML Opportunities

- **Idea:** Use of HPC to generate high-fidelity, large data-volume, ***training sets*** for statistical and ML methods
- **Forward Modeling:** Use fast, ***high-accuracy forward models*** to attack a host of inverse problems with Bayesian methods
- **Uncertainty Quantification:** Error analysis and systematics modeling to develop a new set of ***robust analysis techniques***
- **Impact:** Methods developed by this team, especially the ***'emulation'*** concept are becoming the preferred approach for next-generation surveys

Cosmological scientific inference process showing forward modeling and systematic error exploration/control loop

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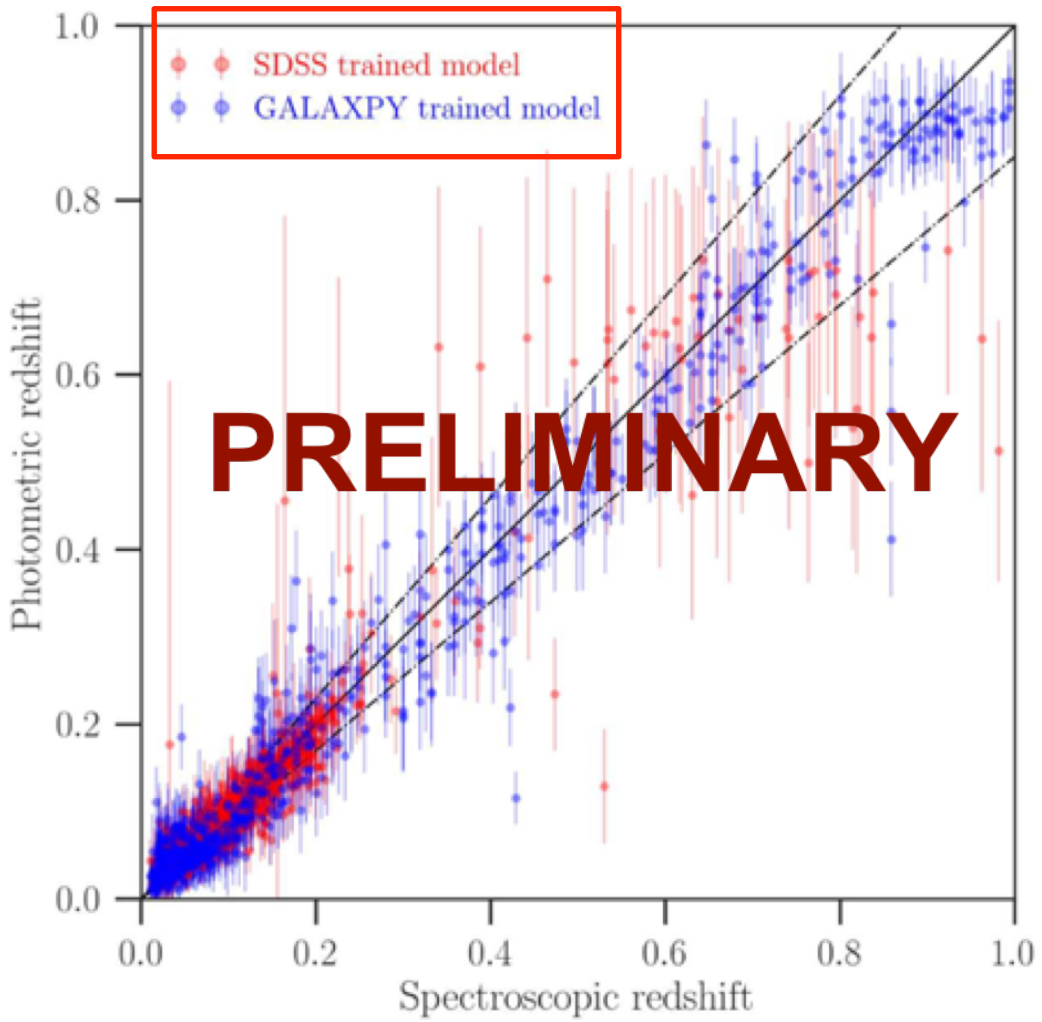
New Technique for Photometric Redshift Estimation



- **Redshift Estimation:** Next generation surveys will have billions of galaxies with image and “color” information (2-d); need to go from color information to the galaxy redshift (3-d) necessary for cosmology
- **Mixed Density Networks**: Method for mapping colors to redshifts, yields a p(z) for each object; degeneracies handled using Gaussian Mixtures
- **Improved Training Set:** Traditional use of ML has suffered from incomplete training sets for faint sources; we introduce GALAXPY, a detailed and robust generative model for emulating galaxy colors using Gaussian processes, fills data space not covered by observations
- **Tests on Real Data:** Clear reduction of outliers when using the GALAXPY training set versus using actual data

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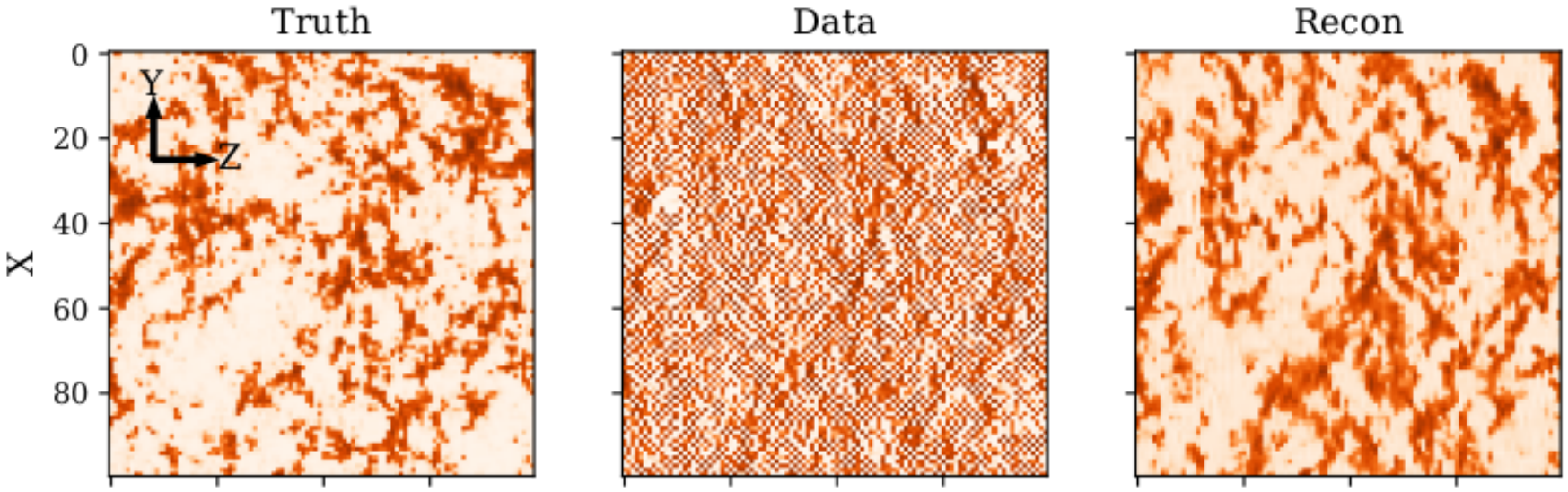
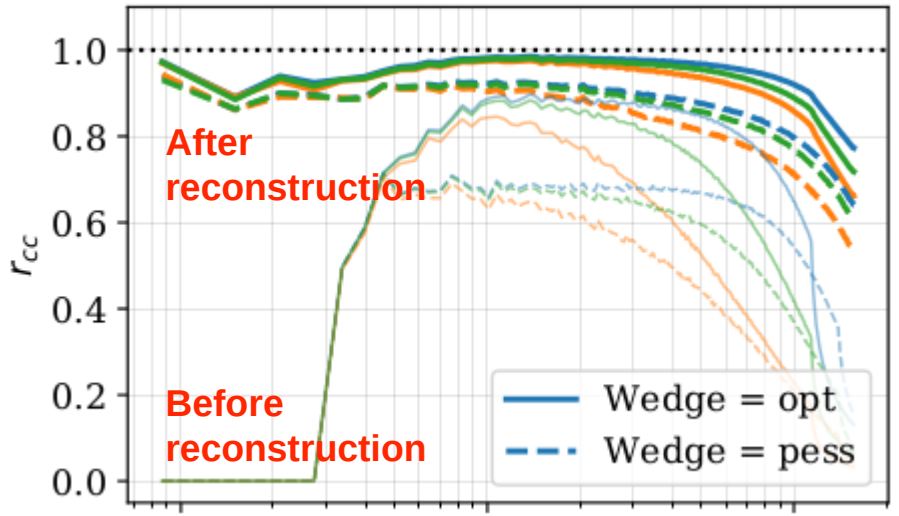
Information Recovery: The Case of 21cm Intensity Mapping



- **Problem:** Lose cosmologically important low-k modes in 21cm intensity mapping due to foreground filtering; can the information be recovered?

- **Nonlinear Flow:** Non-linear cosmological evolution moves low-k power to higher-k modes, less susceptible to filtering; suggests use of a ML-based reconstruction method
- **Results:** Use of ML/back-propagation methods enables solution for millions of parameters (works due to simple nature of bias and high redshift)
- **Impact:** The success of this technique will enable future 21cm experiments



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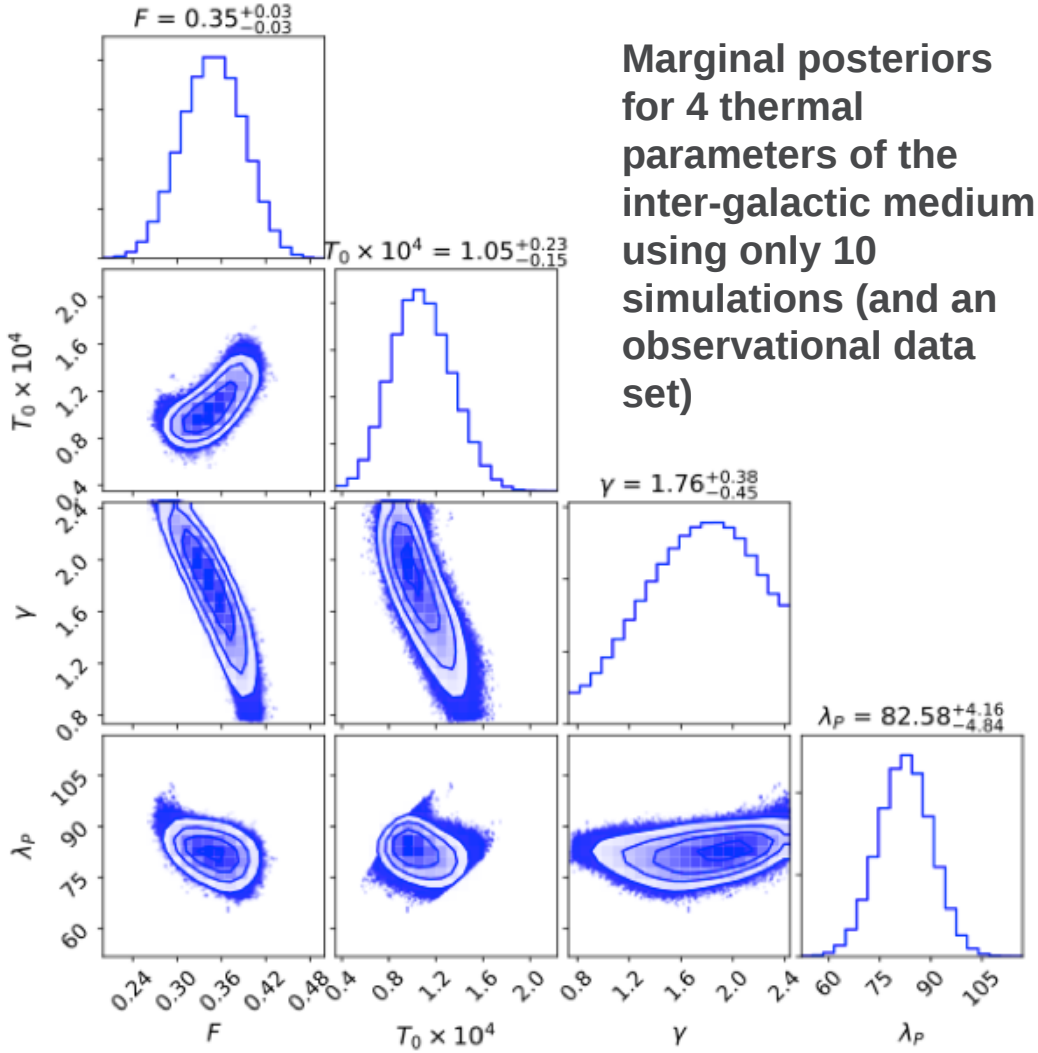
Inverse Problems with Expensive Simulations: Adaptive Exploration

- **Adaptive Exploration of Parameter Space:** HPC simulations can be very expensive; in some cases, they can be run beforehand to generate emulators, but not always — if observational data is available, efficient adaptive methods can be constructed
- **Methodology:** Used multi-output Gaussian Process emulators, adaptively constructed using Bayesian optimization
- **Science Case:** Used the Ly-alpha flux power spectrum observations to demonstrate power of new technique, demonstrating a significantly reduced number of simulations compared to non-adaptive methods



Marginal posteriors for 4 thermal parameters of the inter-galactic medium using only 10 simulations (and an observational data set)

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Solving Many Other Inference and ML Problems

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- **Deep Learning:** Lensing image classification and characterization; generative models for constructing sky maps at multiple wavebands; use of AI methods for domain translation (e.g., mapping hydrodynamic properties on gravity-only simulations)
- **Likelihood-Free Methods and Likelihood Emulation:** Next steps for full forward modeling based approaches
- **Cross-Connection with HEP-CCE (HEP Center for Computational Excellence):** Summer student program for work on HPC and data-intensive computing problems
- **Collaborations with Experiments:** Working with DESI, LSST, and SPT science working groups
- **SciDAC Institutes:** Strong connection with RAPIDS

Synthetic sky catalog for LSST — source for deep learning training data sets

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