Inference and Machine Learning at Extreme Scales

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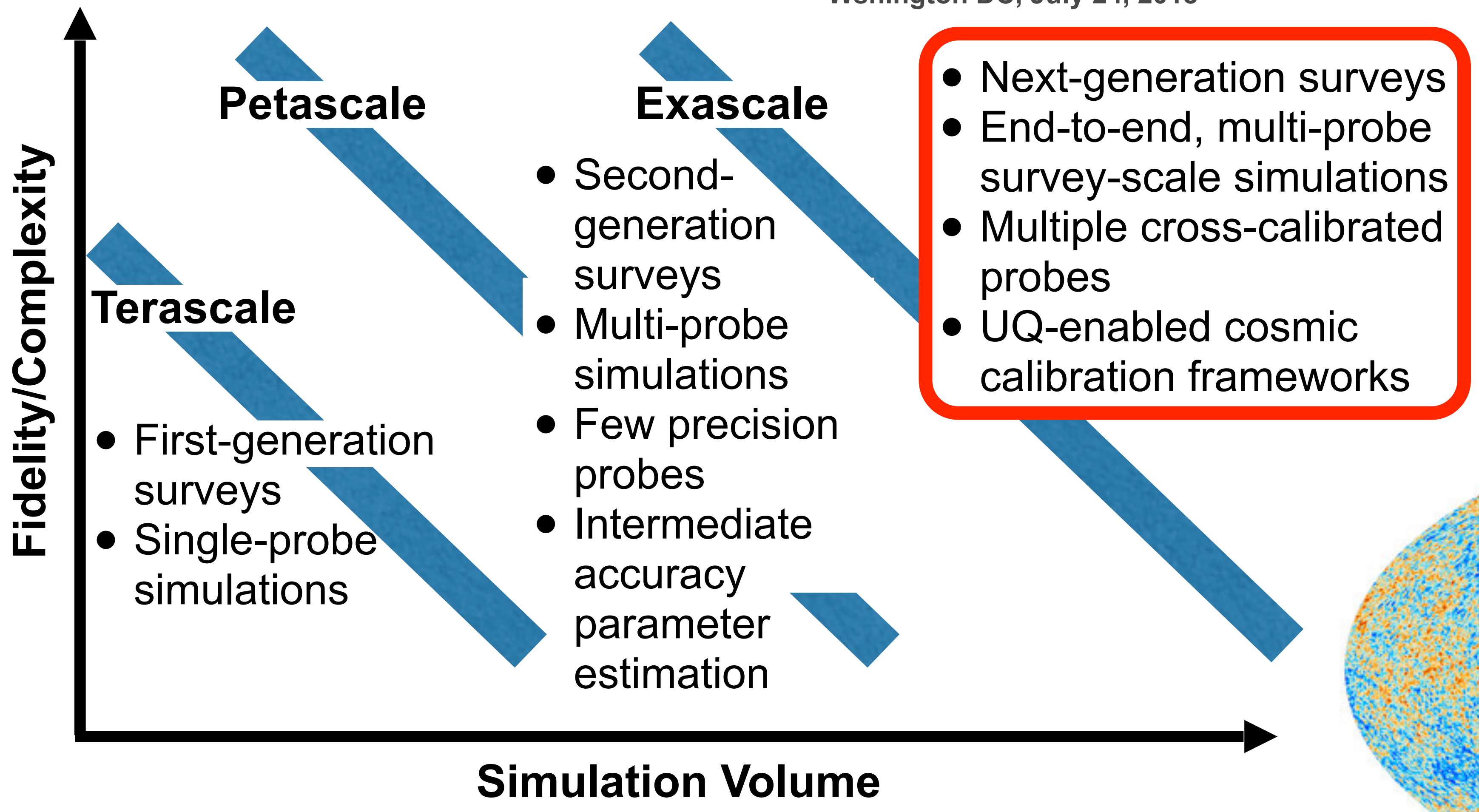
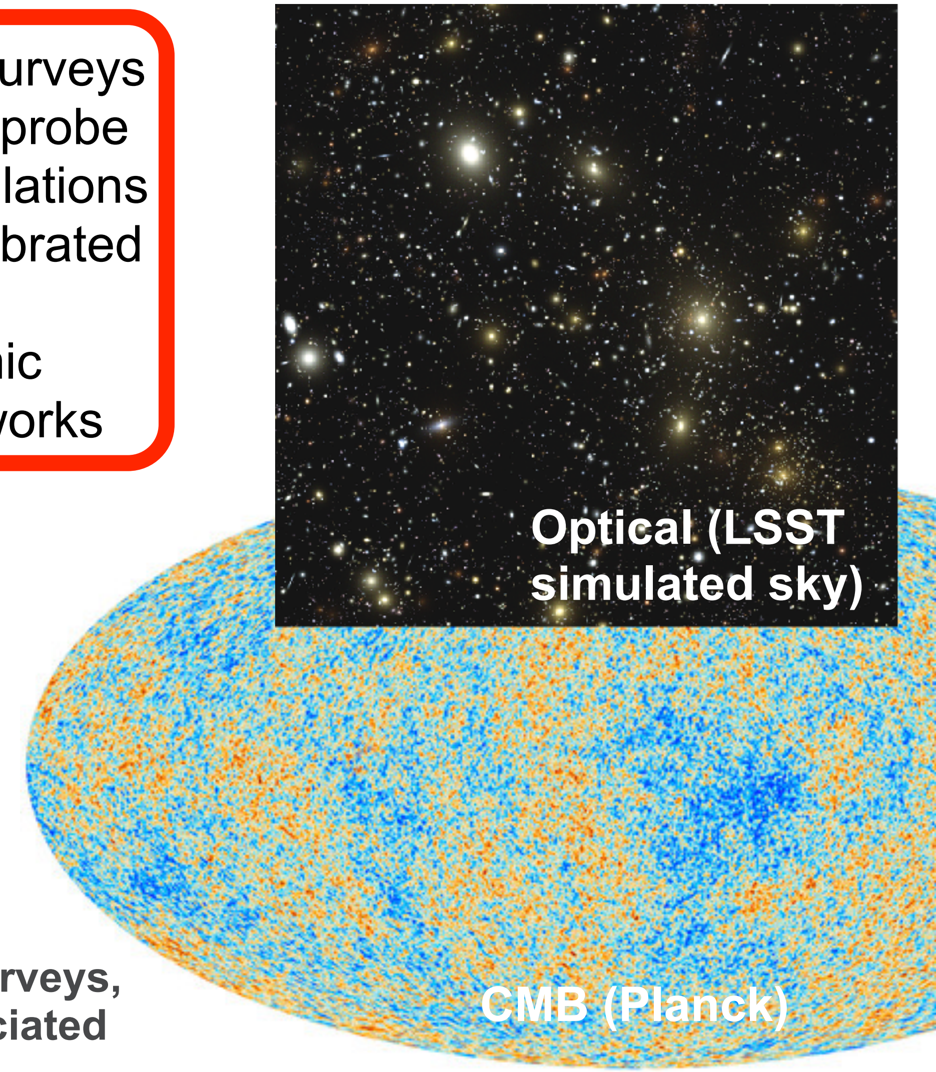
Salman Habib, SciDAC PI Meeting
Wshington DC, July 24, 2018

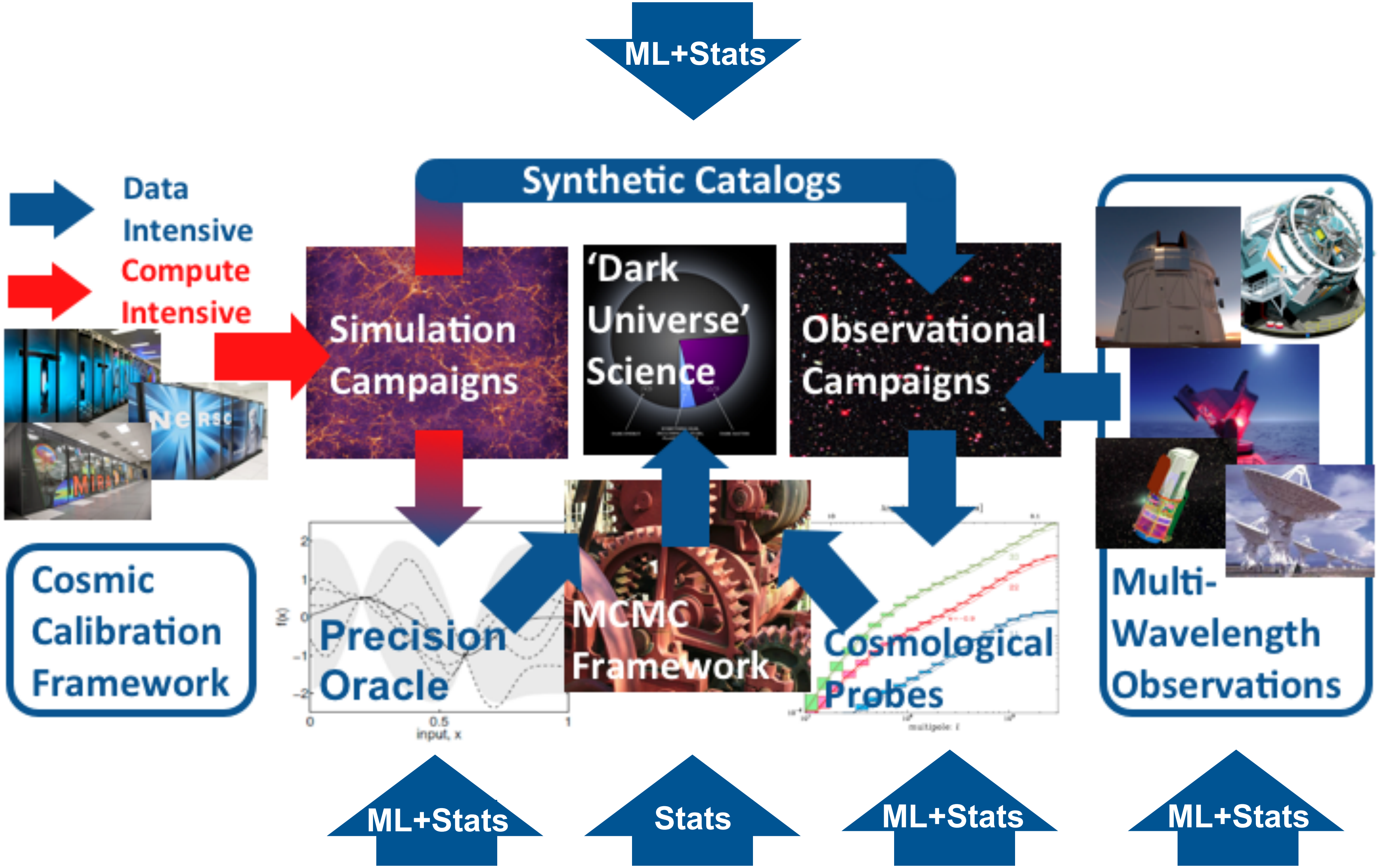
http://press3.mcs.anl.gov/cpac/projects/scidac/





Computational context for Cosmic Frontier science with cosmological surveys, also showing the growing role of data-intensive computing and the associated development of advanced machine learning and statistical methods

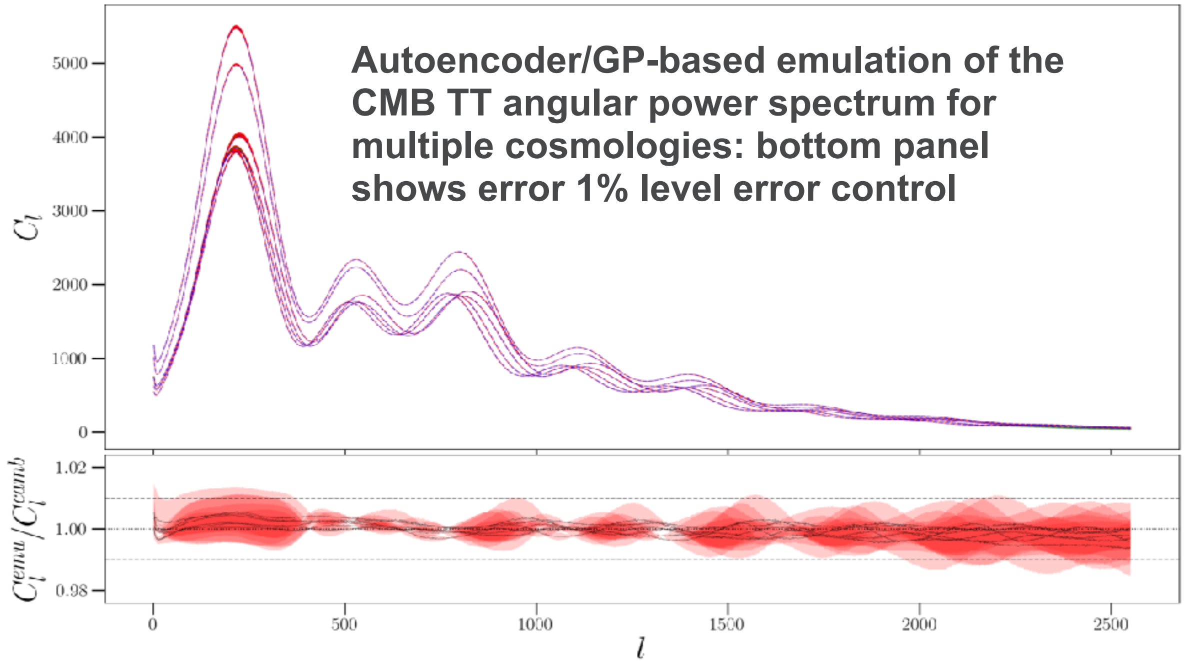
Science with Surveys: Extreme-Scale Computing meets Statistics and Machine Learning



- **Modern Precision Cosmology:** Use of HPC resources as high-fidelity, large data-volume sources for state-of-the-art data-intensive statistical and machine learning (ML) methods
- **'Stats at Scale':** Need to speed up methods by ***many orders of magnitude*** to enable dealing with datasets in the multi-PB to EB era
- **SciDAC-3:** Work on emulators is enabling a new era in cosmological analysis

Precision CMB Emulation

- **Science Target:** Precision fast prediction tools via emulators built on a large simulated dataset for South Pole Telescope and future CMB-S4 mission data analysis, speed-up requirement: factor of ~1000
- **Methodology:**
  - Large training/validation data set generated using the CAMB code
  - Dimensional reduction via unsupervised learning
  - High-dimensional non-parametric regression
  - HIgh-accuracy posterior error controls
- **ML/DL method:**
  - Variational autoencoder and PCA-based dimensional reduction methods compared (similar results)
  - Sensitivity analyis via autoencoder-based nonlinear dimension reduction
  - Gaussian Process-based interpolation for both reduction methods
- **Results achieved:**
  - Emulator with factor of **~2000** speed-up compared to CAMB with 1% errors over the desired dynamic range (Top figure; paper in prep.)



Autoencoder/GP-based emulation of the CMB TT angular power spectrum for multiple cosmologies: bottom panel shows error 1% level error control

Toy 2-d dimensionally-reduced models showing the difference between autoencoding (left) and PCA (right)

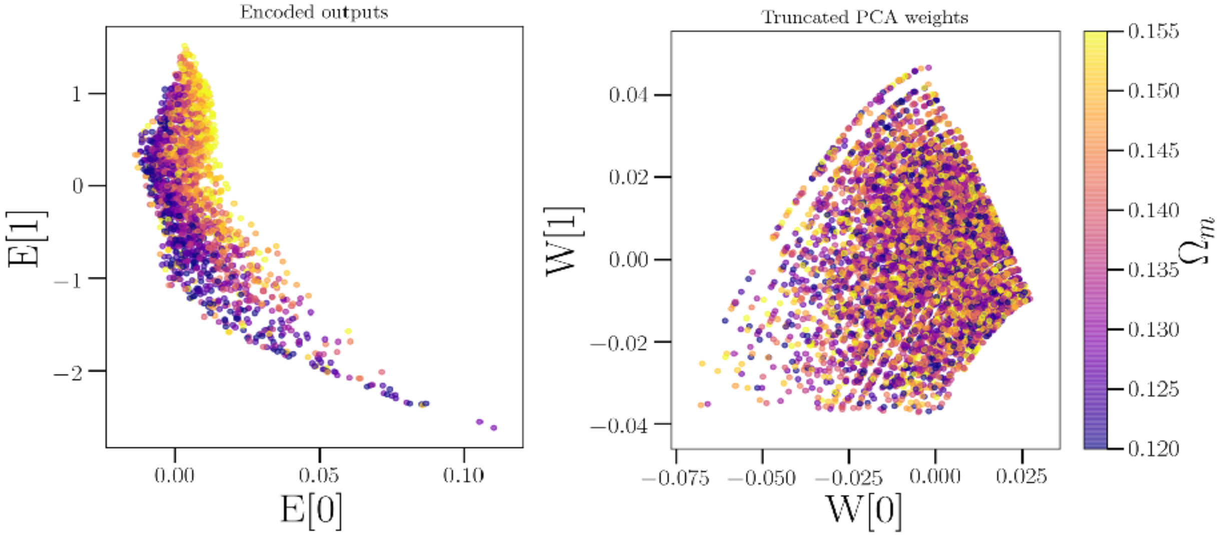
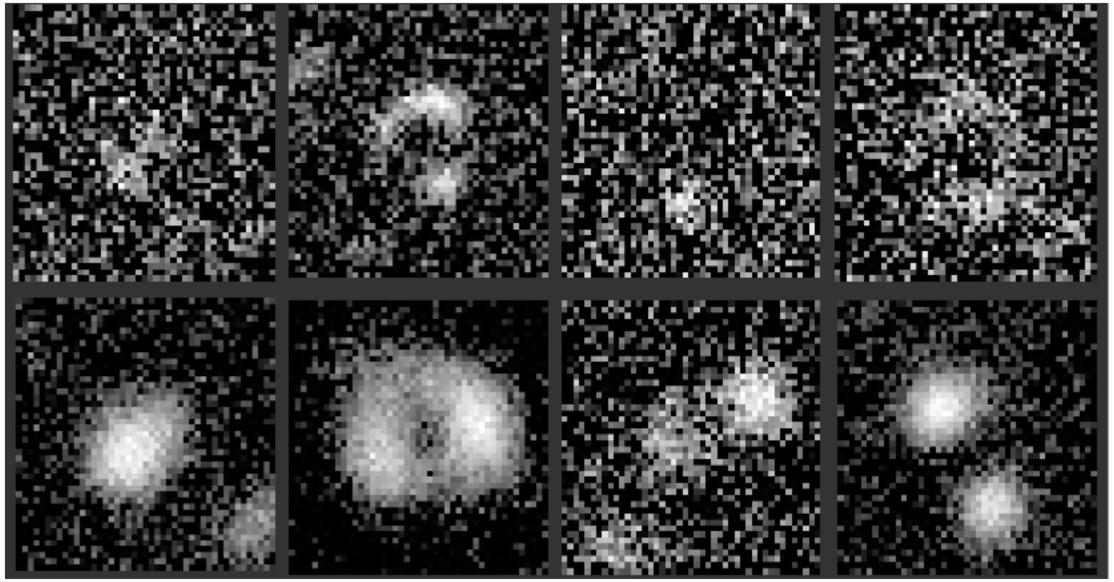
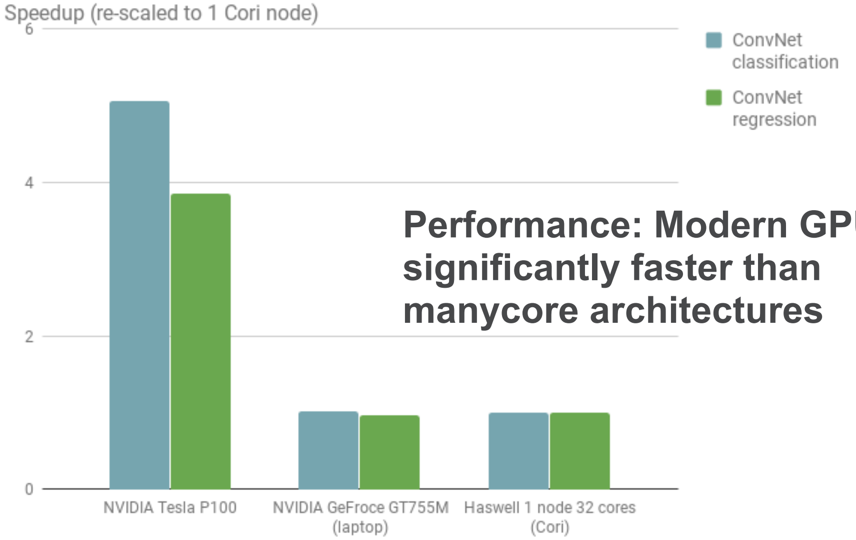


Image Classification/Regression for Strong Lensing

- **Science Target:** Search for strong lensing of galactic sources by intervening galaxies (~100K expected in LSST) for precision cosmology measurements; Deep CNN regression for lens properties
- **Methodology:**
  - Large synthetic data set based on full ray tracing algorithm with 1) model halo mass distribution as lenses and 2) halos from cosmological simulations, realistic telecope properties (pixelization, noise, etc.); single as well as stacked images
  - DL techniques for classification, regression, and other applications (denoising, deblending, —)
- **ML/DL method:**
  - Deep CNN classification/regression
  - GANs for fast generation of images
- **Results achieved:**
  - 80-90% accuracy with very fast classification time (10 microsecs per image)
  - Regression testing underway



Single and stacked noisy lensed training images for LSST

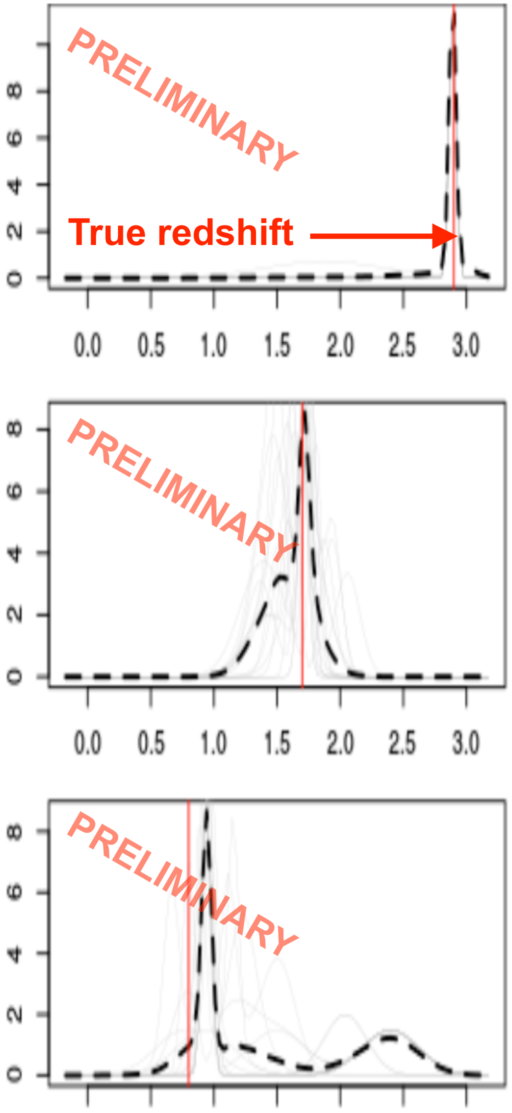


Performance: Modern GPUs significantly faster than manycore architectures

ML/DL-Based Photometric Redshift Estimation

Argonne NATIONAL LABORATORY
BERKELEY LAB
BROOKHAVEN NATIONAL LABORATORY
Los Alamos NATIONAL LABORATORY EST. 1943
VIRGINIA TECH.

- **Science Target:** Estimation of galaxy redshift distribution conditioned on photometric information, morphology, and spatial correlations; application to LSST
- **Methodology:**
  - Large synthetic data set based on a set of realistic templates
  - ML techniques for classification (hidden space variables), use of mixture models; Bayesian learning for posterior PDFs
  - Techniques for outlier rejection
- **ML/DL method:**
  - Mixture models to follow galaxy sub-populations
  - Autoencoders for hidden space variable searches
  - Various Gaussian Process-based approaches
  - Bayesian Adaptive Regression Tree (BART) methods
- **Results achieved:**
  - Multiple synthetic data sets constructed
  - Initial anlyses with different methods underway



Multi-GP approach estimated PDFs and comparisons to training set z_true

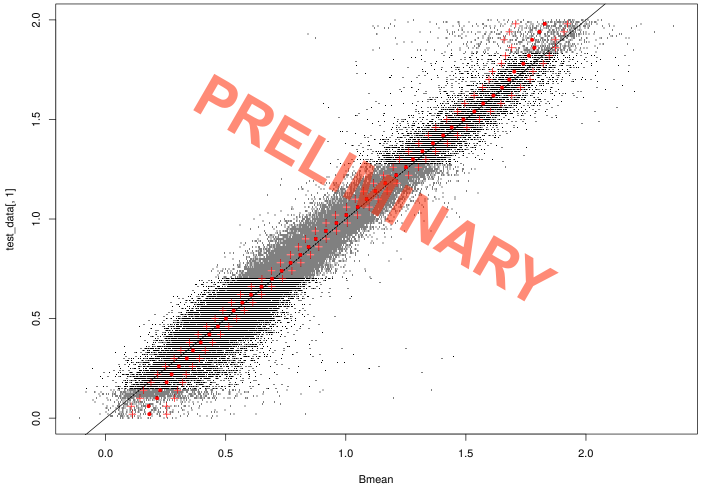
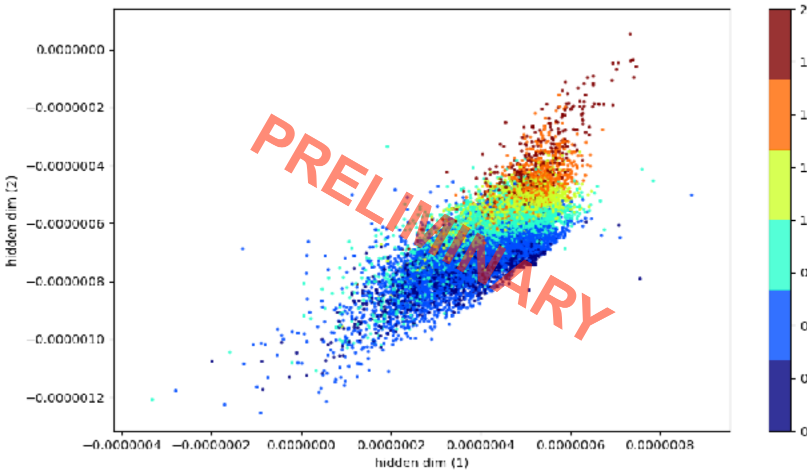


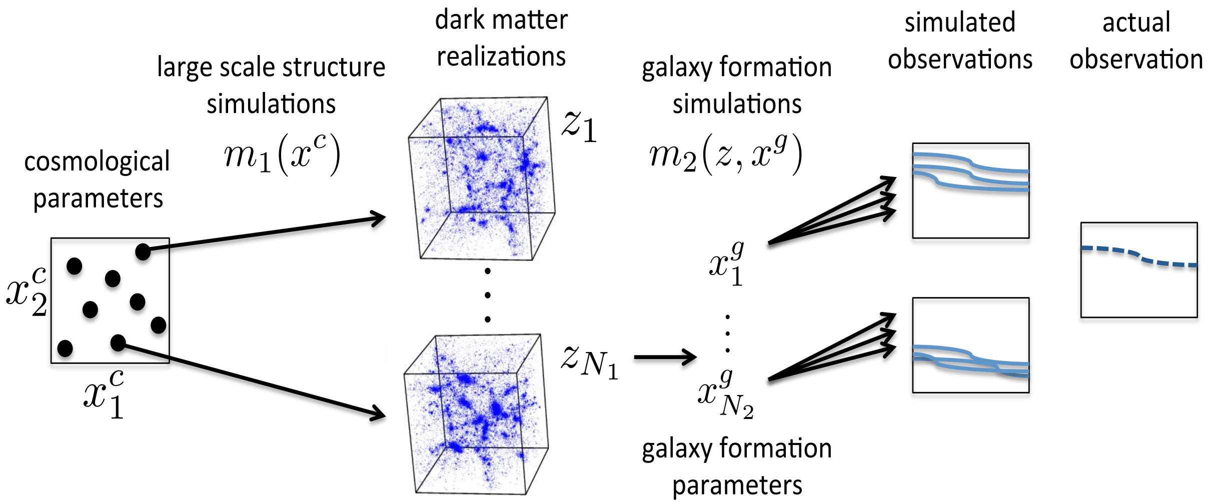
Photo-z estimates with BART



Hidden space variables w/ autoencoder

Other Topics; Future Work

- **Emulation Landscape:** ***1)*** Extend work on summary statistics to problems with significantly higher dimensionality, *O*(10) to *O*(100); ***2)*** Multi-fidelity emulation; ***3)*** Develop new methods for applications to likelihood-free scenarios (e.g., semi-analytic galaxy modeling); ***4)*** Fast generation of multiple realizations of 'raw' sky data (e.g., synthetic catalog/image emulation, prediction of dust maps from 21cm)
- **Image Applications:** Image cross-validation, source de-blending algorithms, application to calibration studies
- **ML/DL Methods on HPC Platforms:** Work on scaling up ML and statistical methods on HPC platforms with GPU acceleration (e.g., Cooley@ALCF, Summit@OLCF)
- **Stats meets ML:** Improve methods by incorporating model information into 'black box' techniques; incorporate optimization methods into Bayesian calibration



Catalog-level, emulation-aided, 'full' forward modeling approach to cosmological inference