Accelerating HEP Science: Inference and Machine Learning at Extreme Scales

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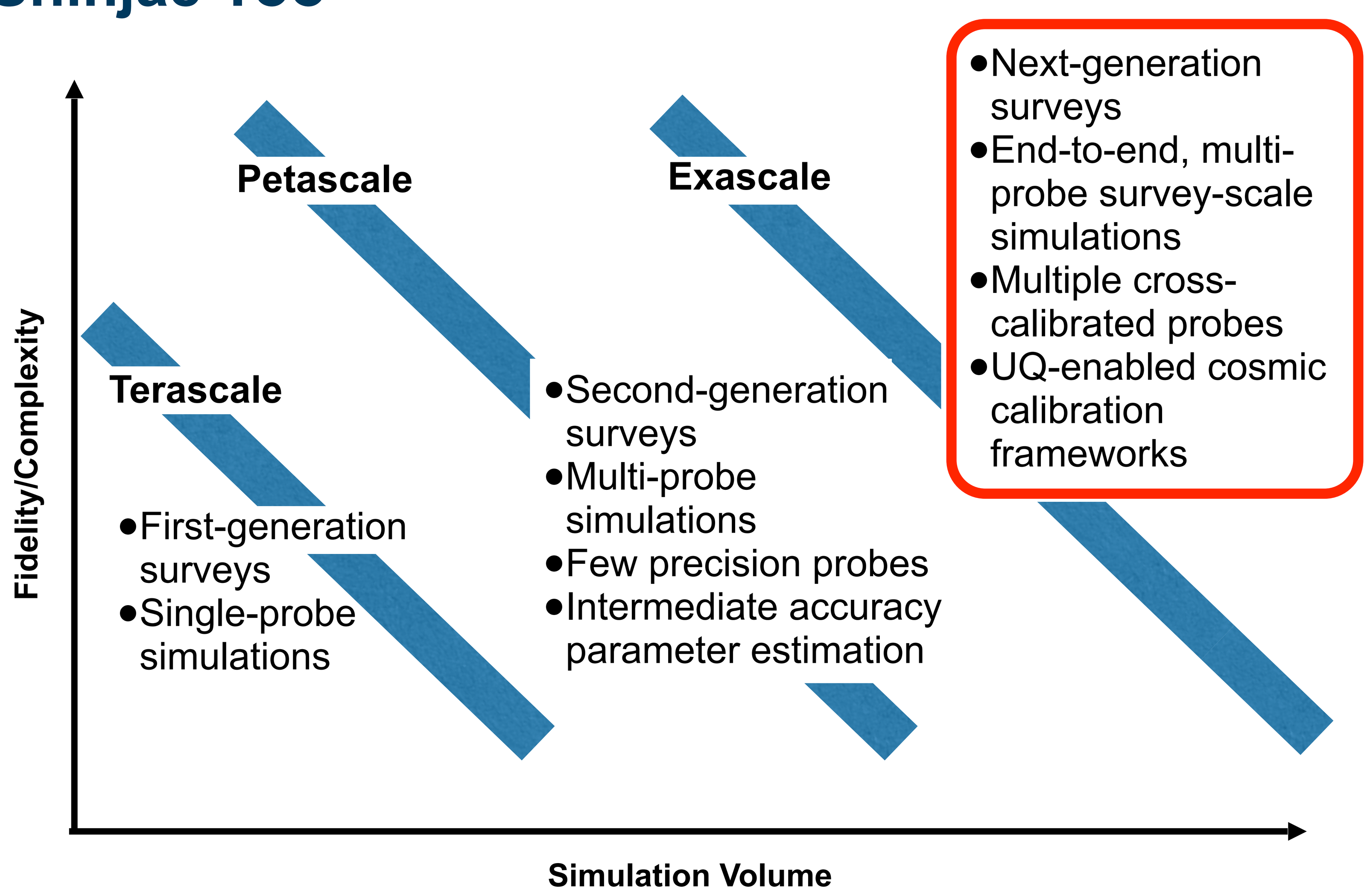
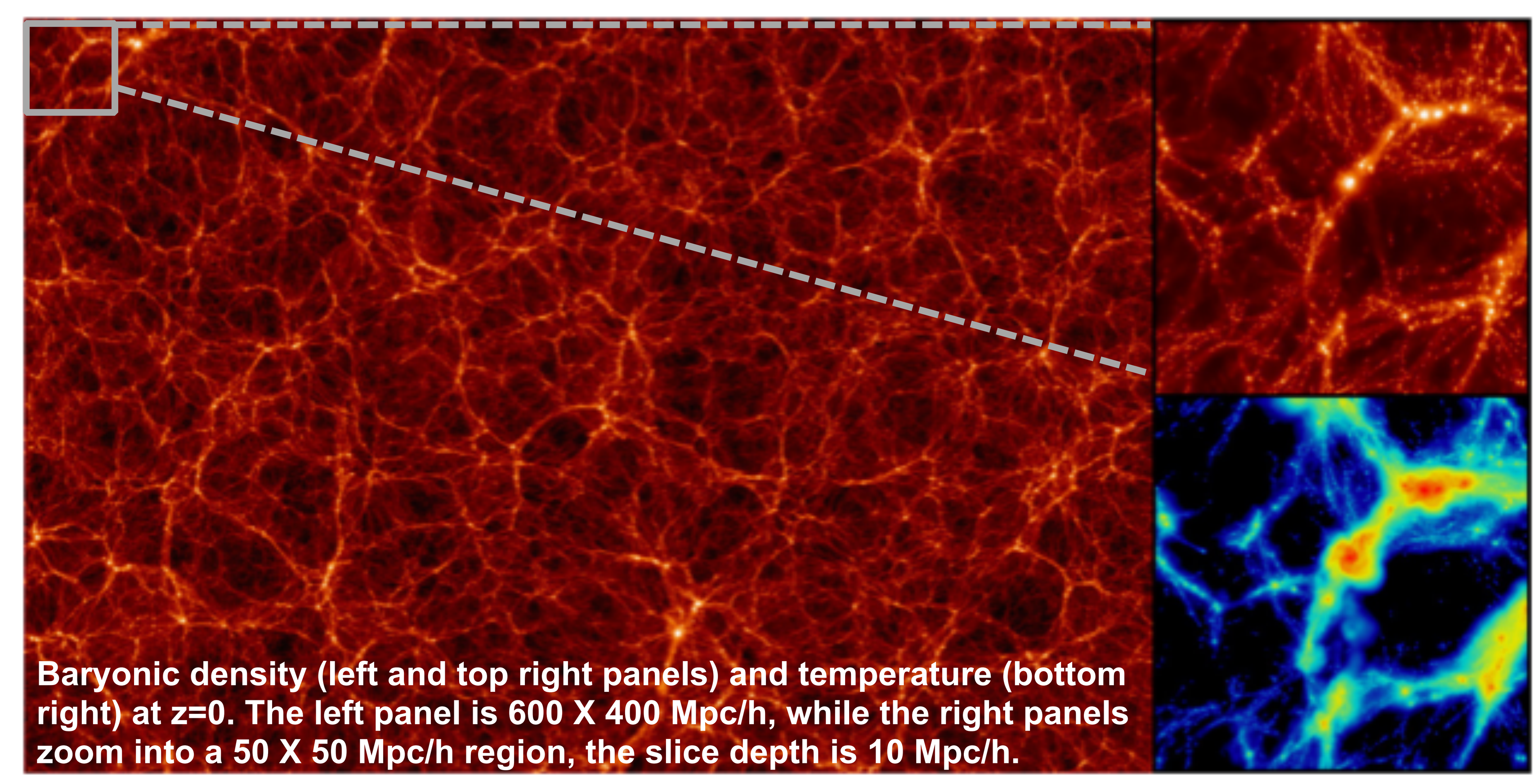
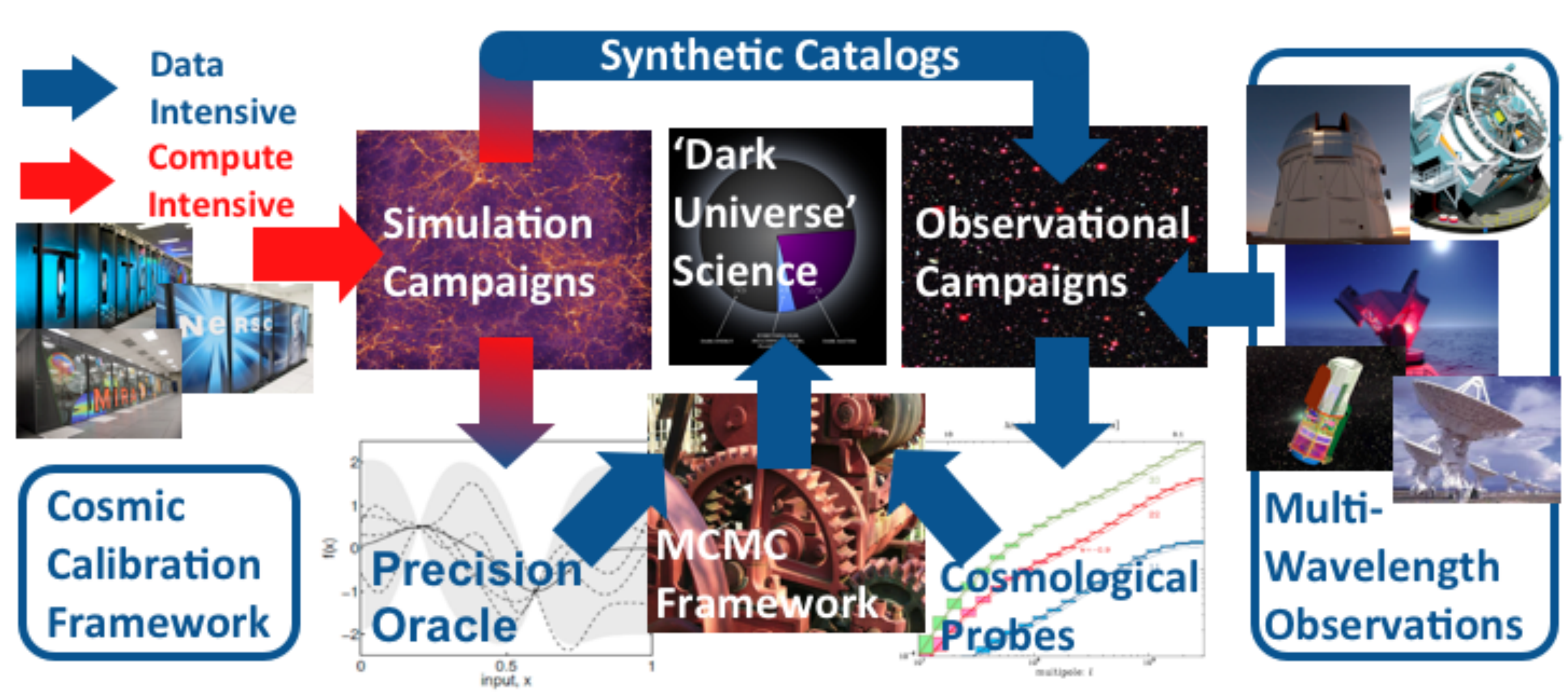


- **Simulations and Sky Surveys**
  - **Sky surveys** can measure certain cosmological statistics (including cross-correlations) at the 1% level or better; scientific inference from these measurements is strongly limited by shortcomings in theory and modeling
  - **Exascale simulations**, constructed from improved theory and modeling approaches (including subgrid modeling), implemented with new algorithms, and melded with advanced V&V and UQ protocols have the potential to fill current simulation gaps for a number of cosmological probes



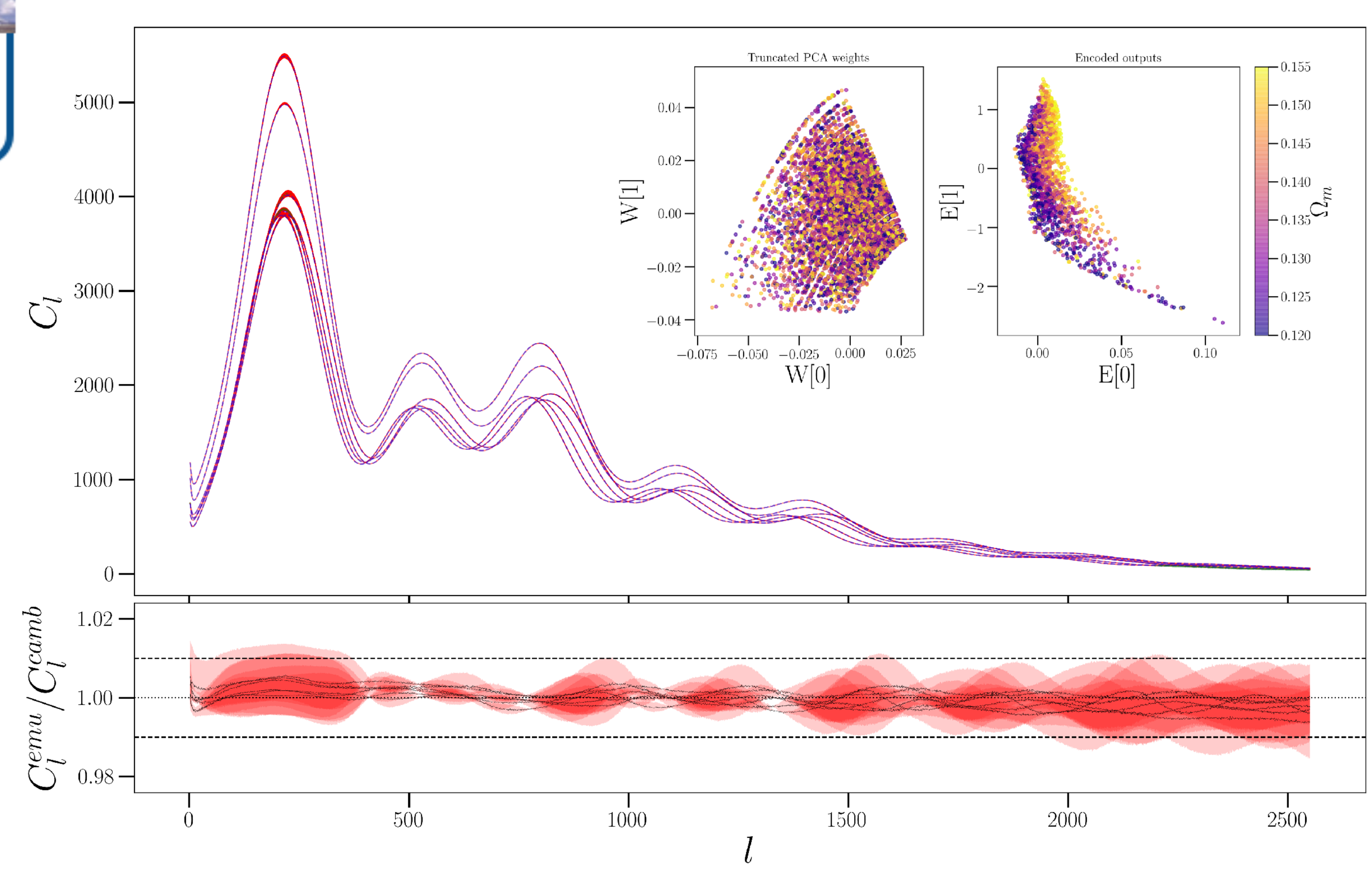
Baryonic density (left and top right panels) and temperature (bottom right) at z=0. The left panel is 600 X 400 Mpc/h, while the right panels zoom into a 50 X 50 Mpc/h region, the slice depth is 10 Mpc/h.

BorgCube: First large-scale CRK-HACC simulation containing 2 X 2304^3 dark matter plus baryonic particles in a cubic volume of side length 800 Mpc/h.

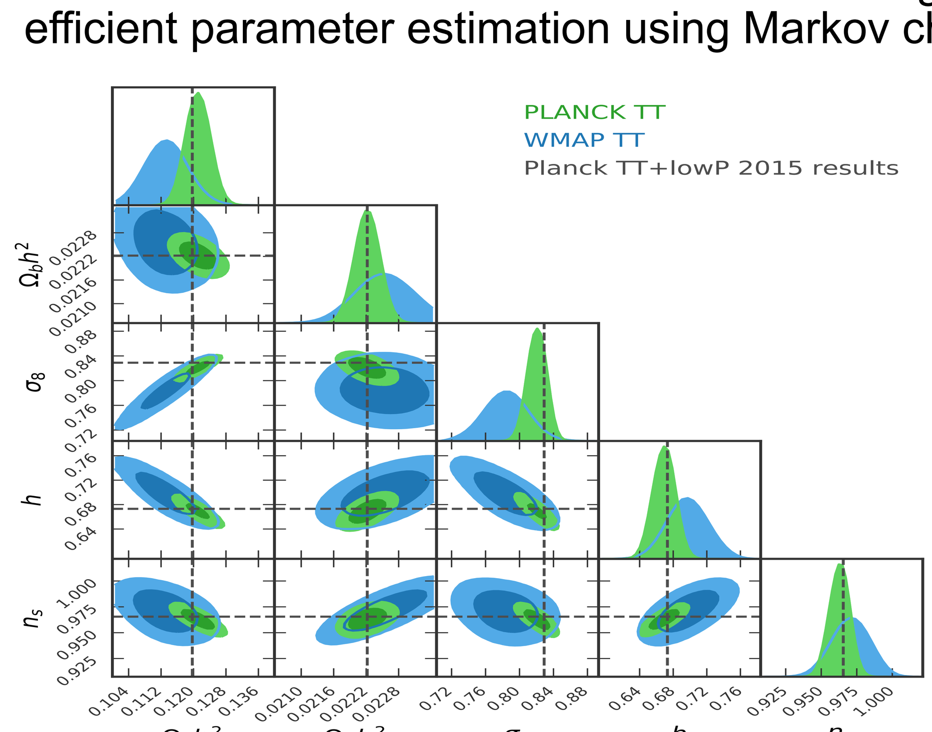


Cosmological Scientific Inverse Problem: Data and information flow in a precision cosmology application using emulators built using modern statistical and machine learning methods; these techniques can also be used to efficiently generate synthetic galaxy catalogs.

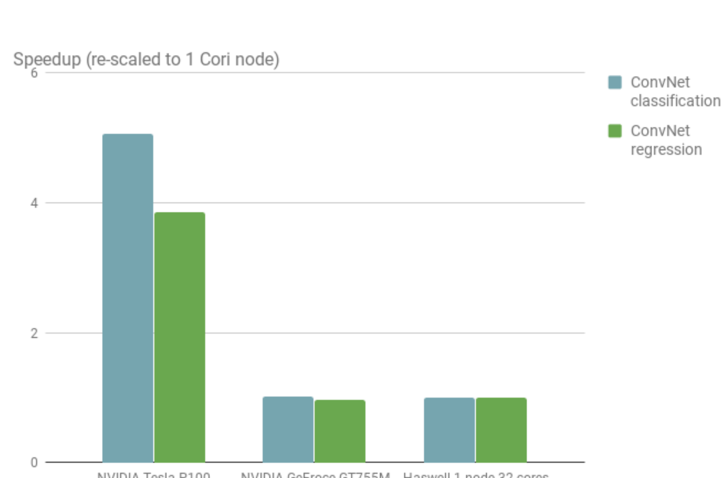
- **Emulation using Variational Autoencoders**
  - **Dimensional Reduction** is used in constructing emulators to make Gaussian process-based interpolation numerically tractable; traditionally this has been done using Principal Component Analysis (PCA). In initial work, we have shown that accurate emulators can be constructed using autoencoders; the resulting emulators are ~2000 times faster than the original code, allowing for very efficient parameter estimation using Markov chain Monte Carlo



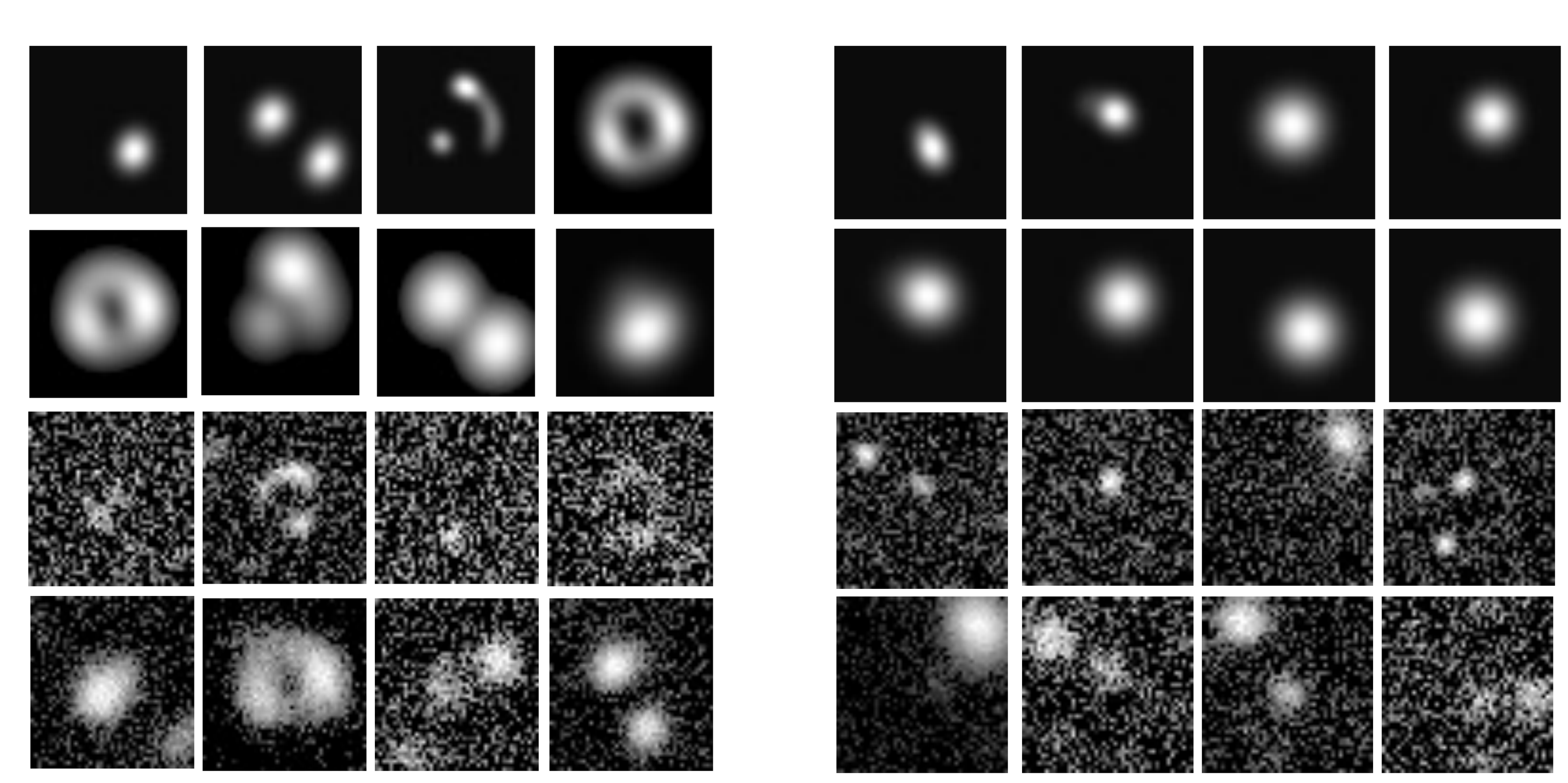
Cosmic Microwave Background Emulation: Angular power spectrum for multiple cosmologies with 5 free parameters, exact and emulated spectra superimposed; dimensional reduction was perfromed using a variational autoencoder. The 1% error behavior is evident in the lower panel. The insets show a comparison of a 2-D PCA dimensional reduction (left) versus an autoencoder (right).



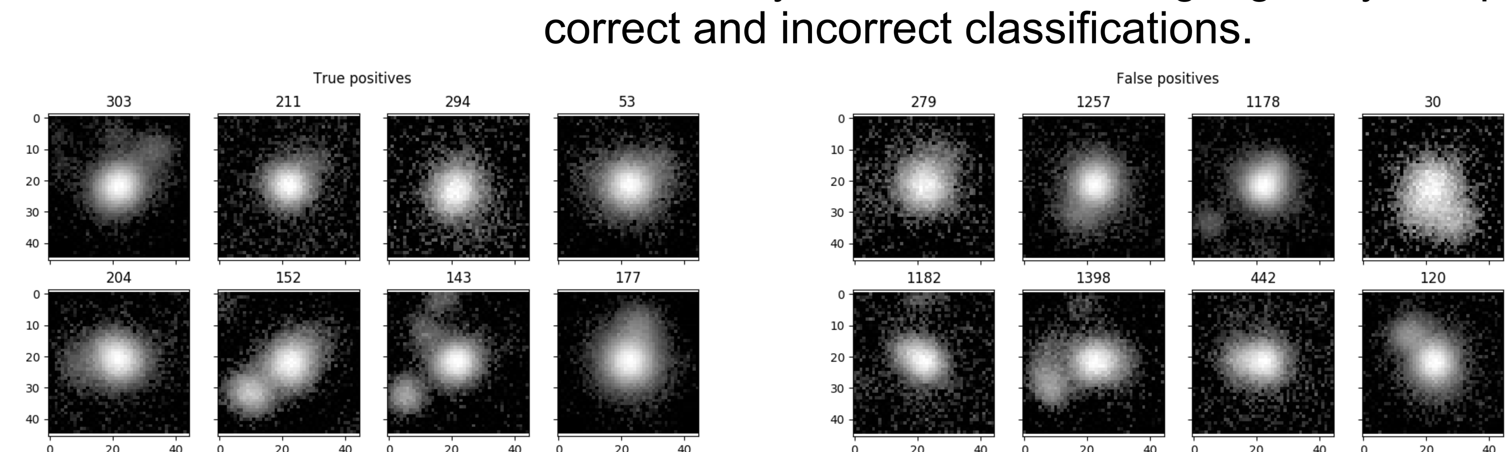
Cosmological Parameters: Emulator-based MCMC results for cosmological parameters from WMAP and Planck satellite observations of the CMB thermal anisotropy power spectrum. Emulators have been constructed for the polarization and cross-power spectra and wil be used for analysis of South Pole Telescope (SPT) datasets.



Strong Lensing Image Classification: Strongly-lensed background galaxies have distorted shapes (arc-like to rings) but these are hard to discern in the presence of noise and can be confused with non-lensed background objects — with billions of candidates in future surveys, the task is beyond human capability. A CNN-based classifier was developed using noisy simulated images, achieving 80-90% accuracy with a classifcation time of only 10 microseconds per image using state-of-the-art GPUs. The difficulty of the task can be gauged by comparing correct and incorrect classifications.



Strong Lensing Image Classification: Left — lensed examples, top two rows (noiseless), bottom two rows with sky noise; right — coreesponding unlensed images. Convolutional neural networks were trained on a large number of simulated images for fast classification tasks.



Correct and Incorrect Image Classification: Left — correct classifications, right incorrect.