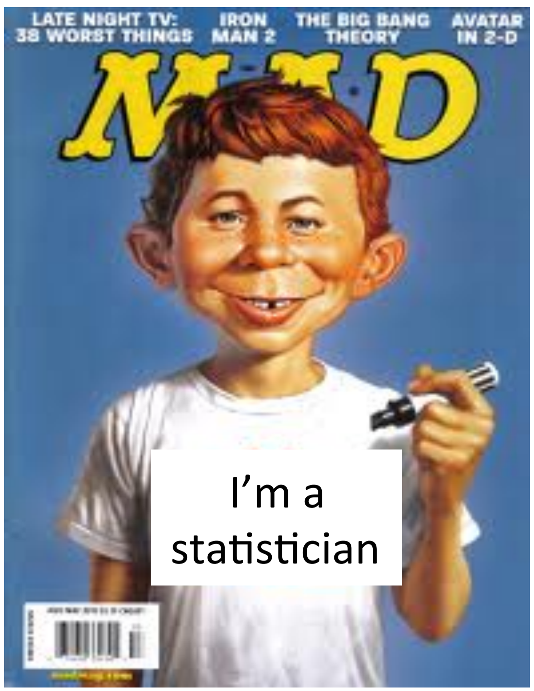
A statistical perspective of validation and UQ

Dave Higdon, Statistical Sciences, Los Alamos National Laboratory



August 5, 2011

The Mathematics of Changing Your Mind

By JOHN ALLEN PAULOS

THE THEORY THAT WOULD NOT DIE

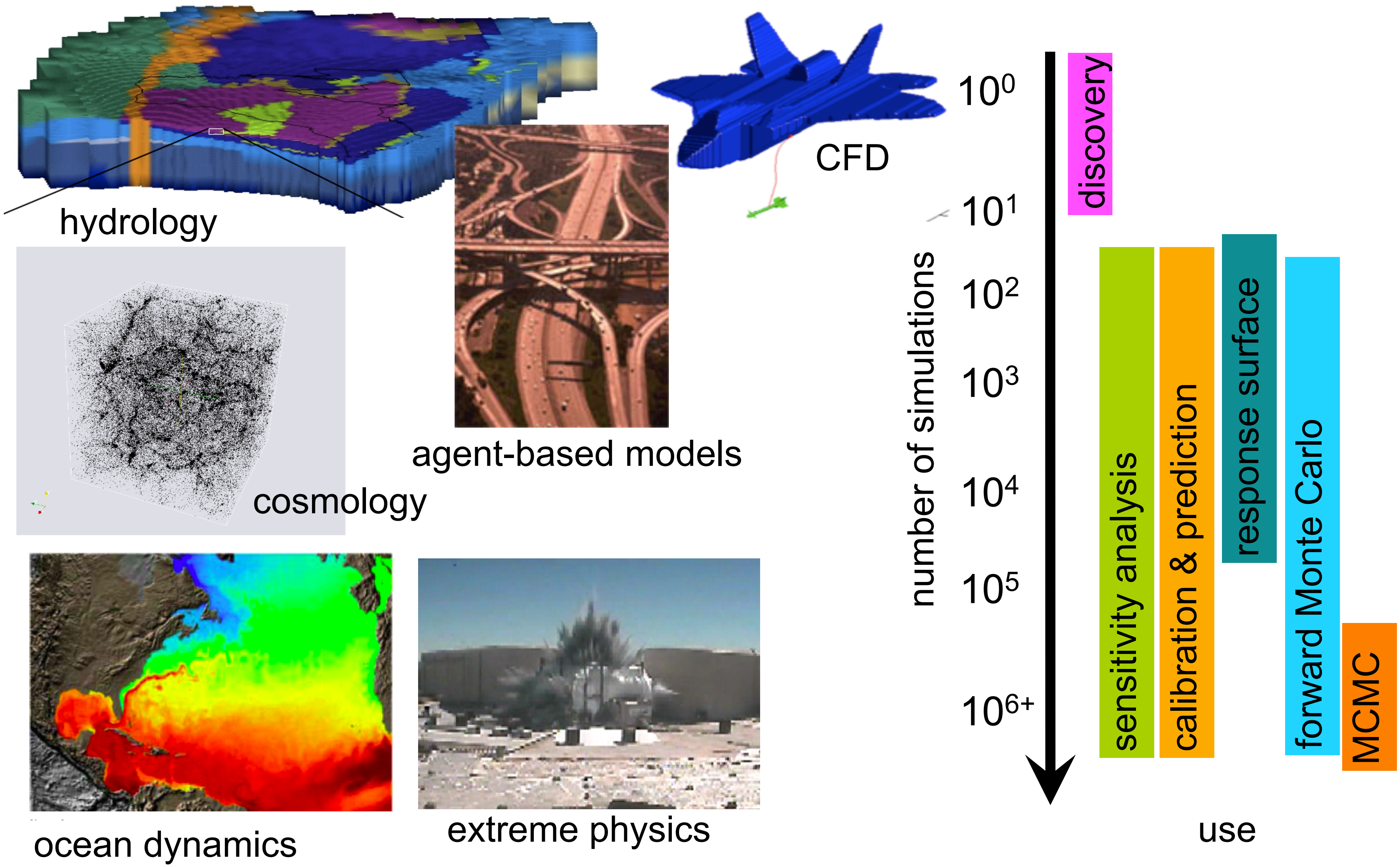
How Bayes' Rule Cracked the Enigma Code, Hunted Down Russian Submarines and Emerged Triumphant From Two Centuries of Controversy

By Sharon Bertsch McGrayne

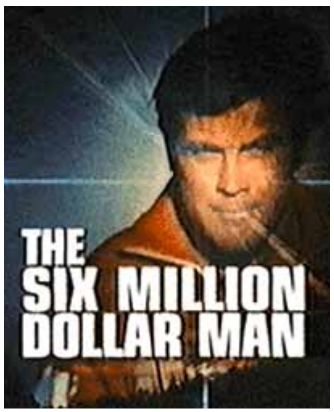
Sharon Bertsch McGrayne introduces Bayes's theorem in her new book with a remark by John Maynard Keynes: "When the facts change, I change my opinion. What do you do, sir?"

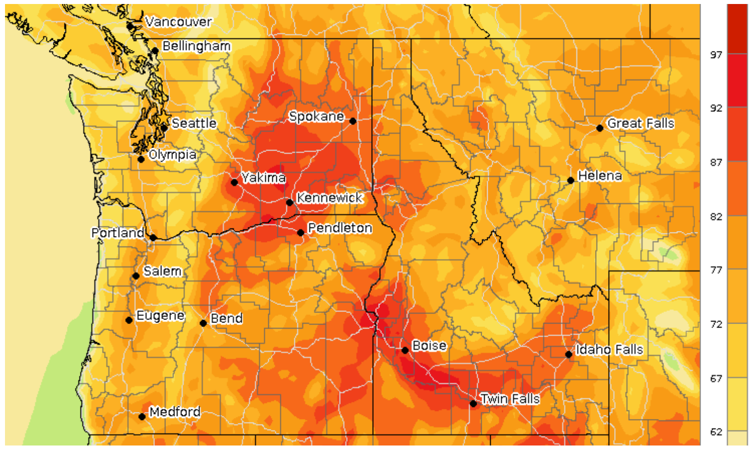
Bayes's theorem, named after the 18th-century Presbyterian minister Thomas Bayes, addresses this selfsame essential task: How should we modify our beliefs in the light of additional information? Do we cling to old assumptions long after they've become untenable, or abandon them too readily at the first

Computational models

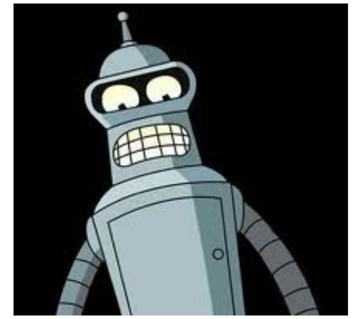


Model-based prediction & quantifying uncertainties

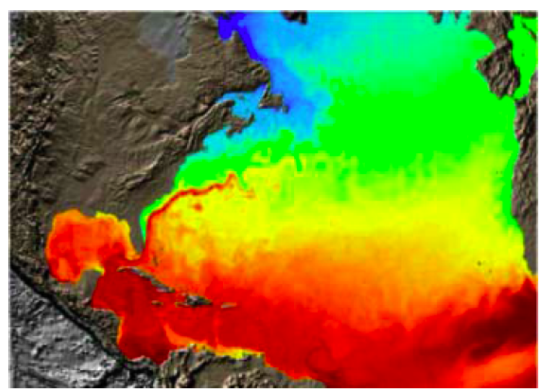




Combination of physical data & computational model

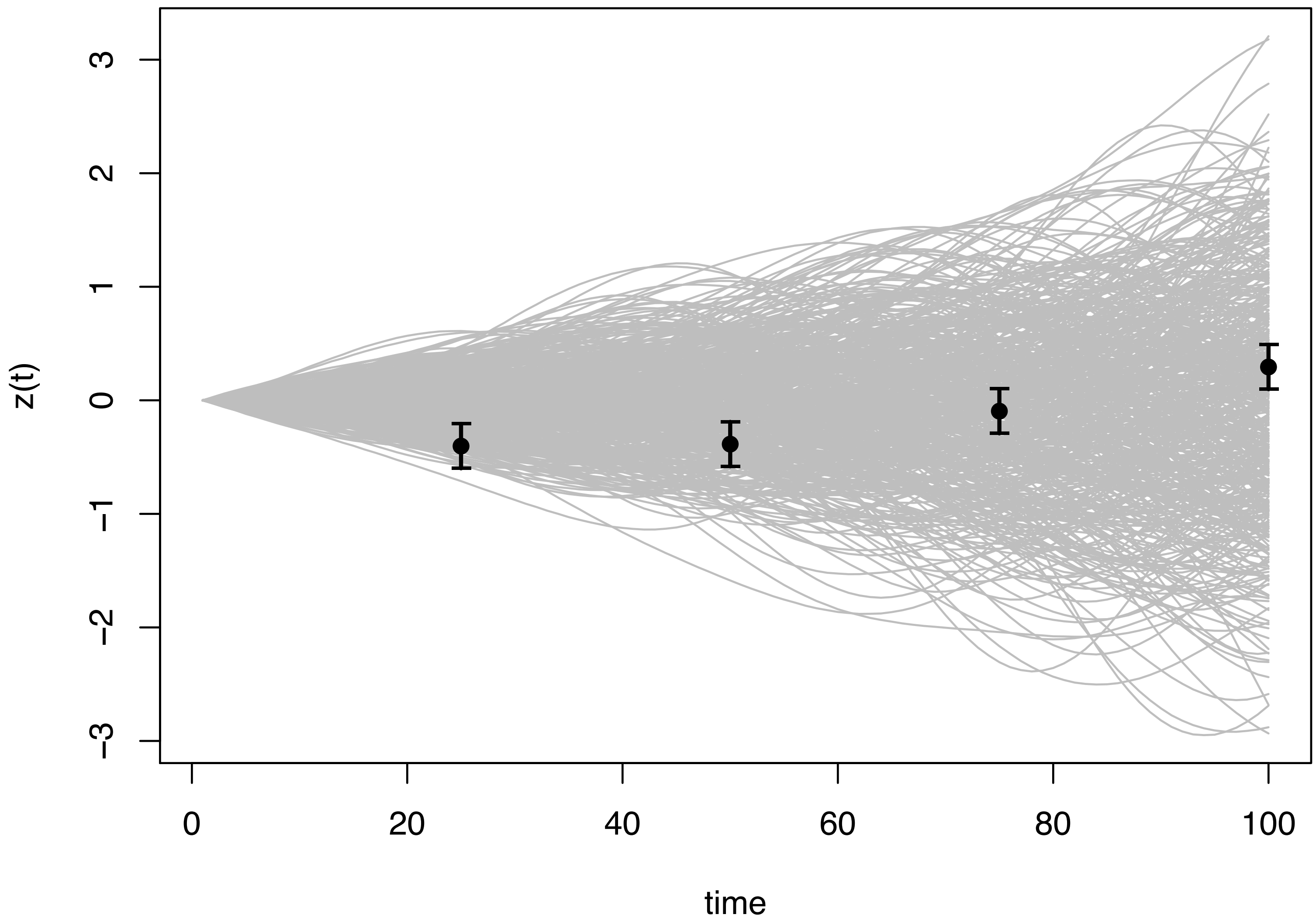


Estimate input settings & let it go

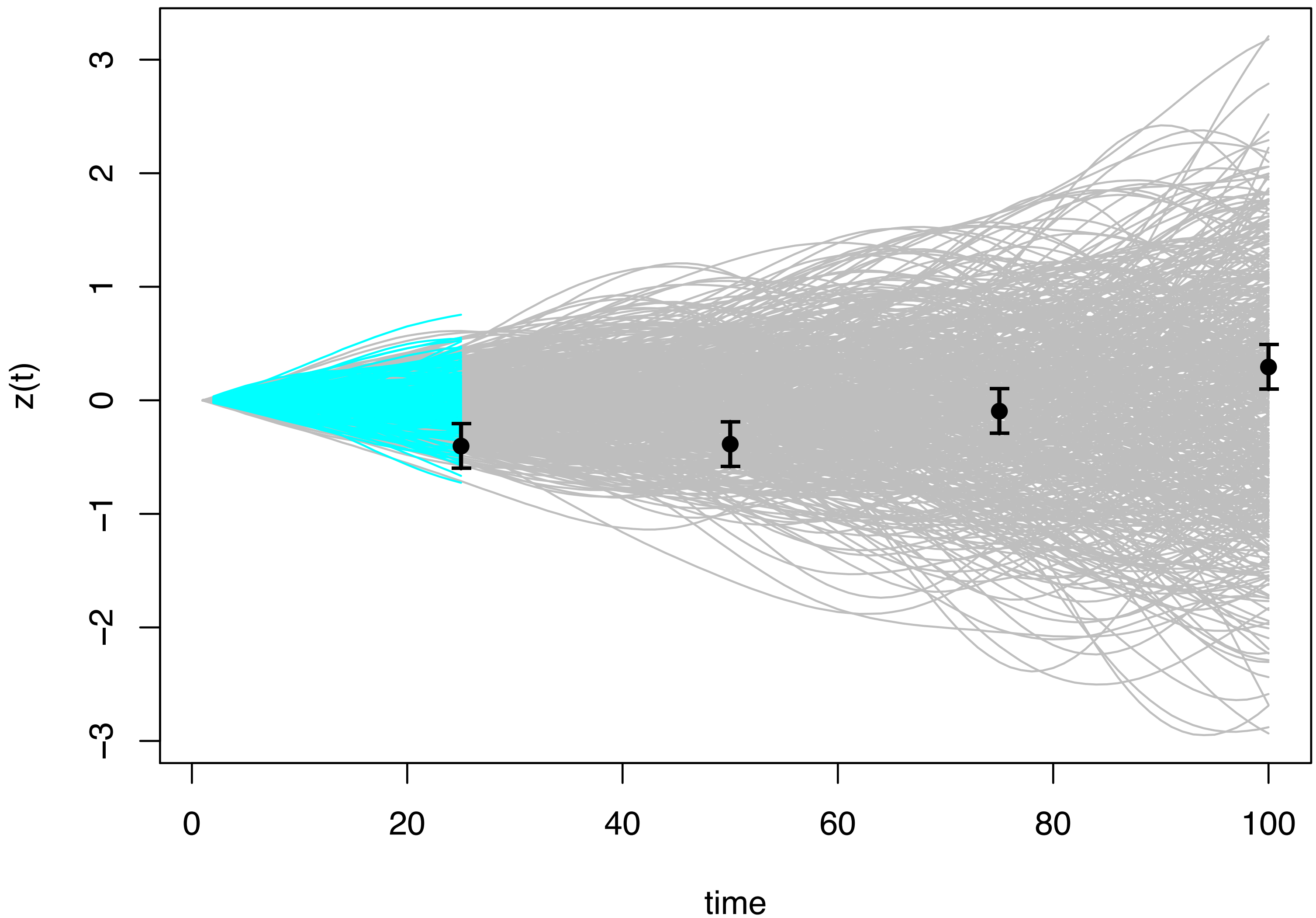


North Atlantic temperatures

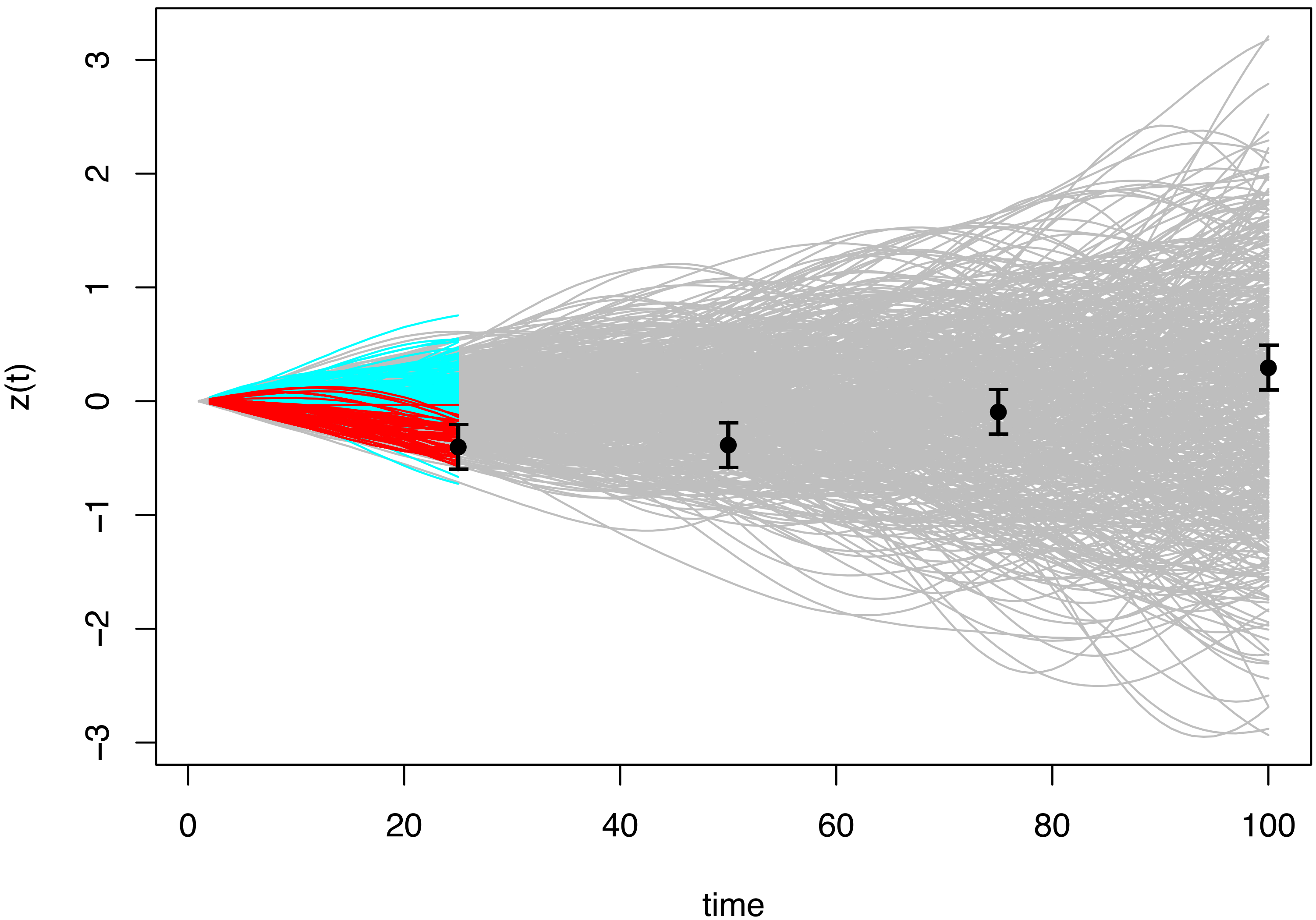
Sequential Buld-up (i.e. building cyborgs)



Sequential Buld-up (i.e. building cyborgs)



Sequential Buld-up (i.e. building cyborgs)



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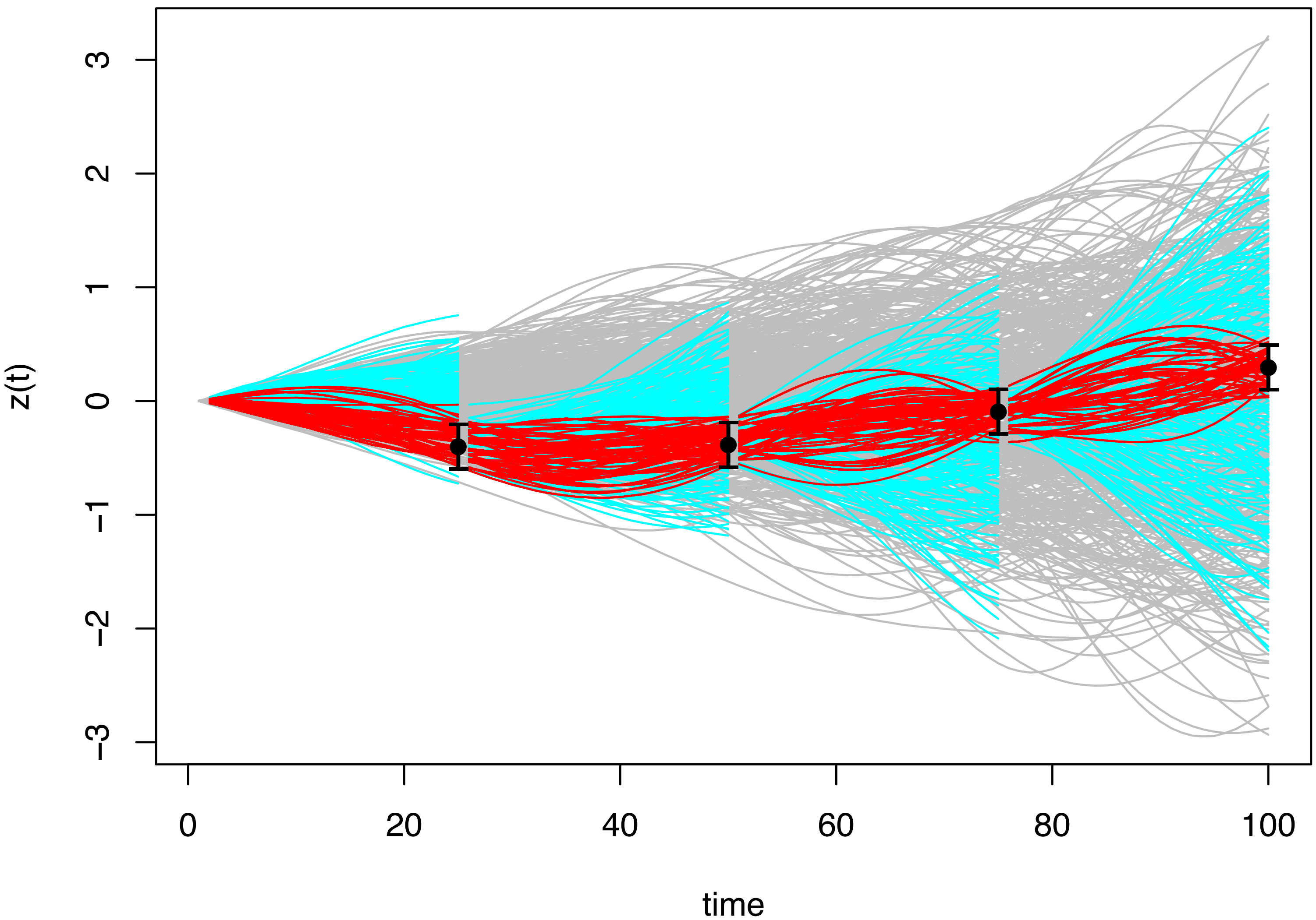
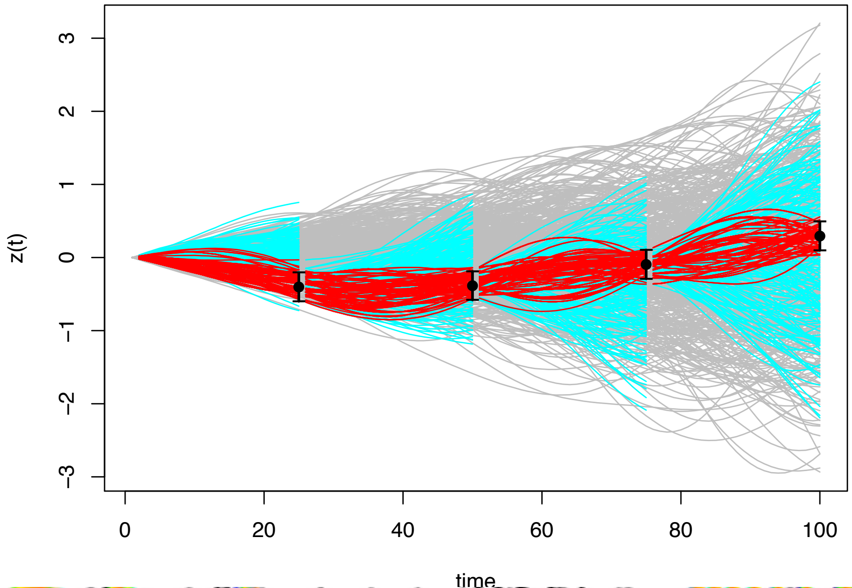
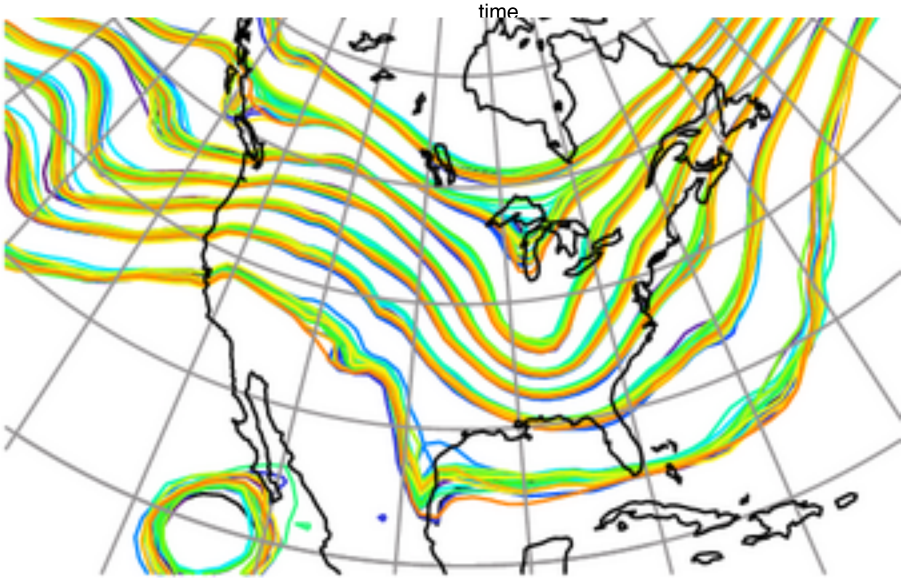


Building cyborgs

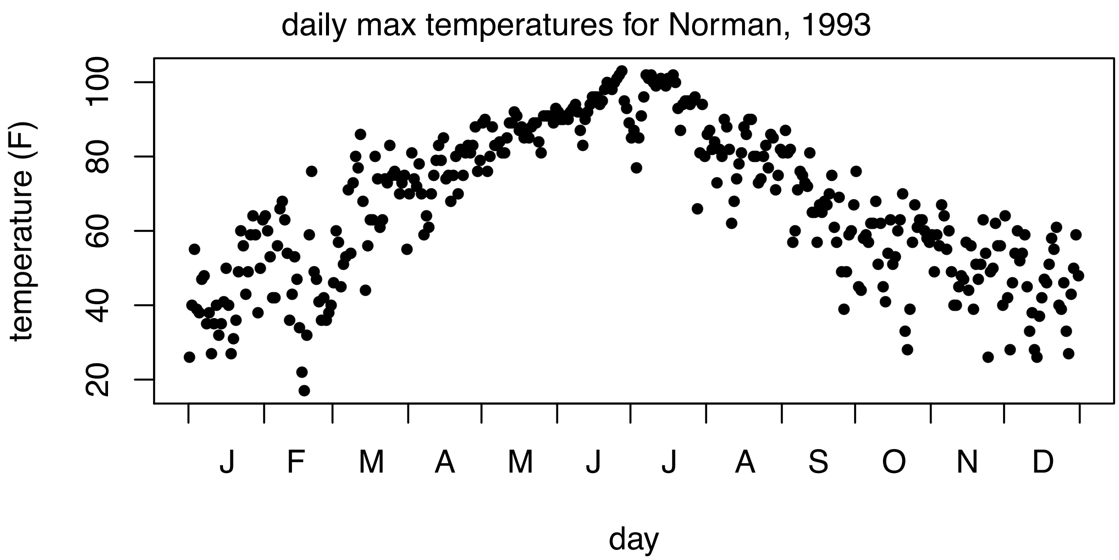


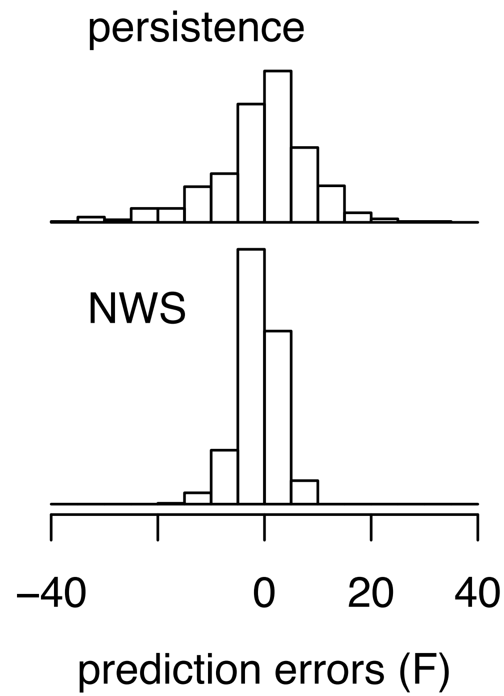


500 hPa height contours from 20 different members of an ensemble assimilation with an atmospheric model.

- Recurring data source is required
- A model that can easily be reseeded; with little sensitivity for past history
- Model must have some description of randomness / flexibility within it.
- Need to be able to adjust system state to be consistent with physical observations
- Can recover from aphysical perturbations
- Ideally, observations are the same as the QoI to be predicted.
- Weather, oil recovery, target tracking, seasonal climate, GHG emissions, …
- Methods: Kalman filter, Ensemble Kalman filter, particle filter, Bayesian/ variational approaches (e.g. 4-d Var).

Models can give more accurate predictions than empirical analyses



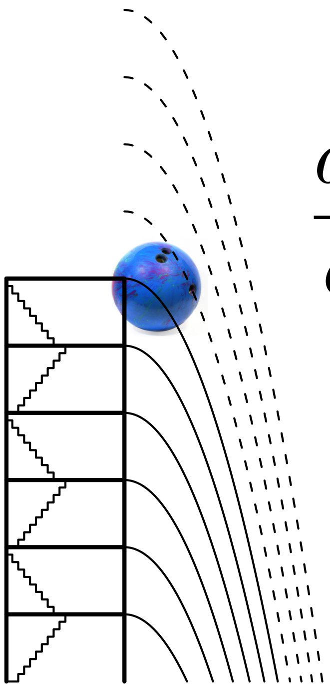


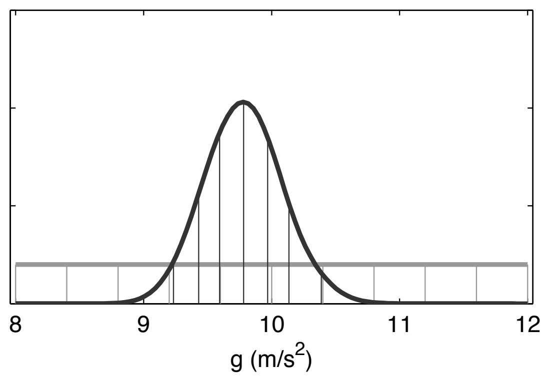
- model-based weather predictions give more reliable weather forecasts than empirical, model free forecasts
- uncertainty regarding these forecasts can be assessed looking at historical prediction accuracy
- many engineering regulations are based on extreme value statistics which assume an unchanging climate.

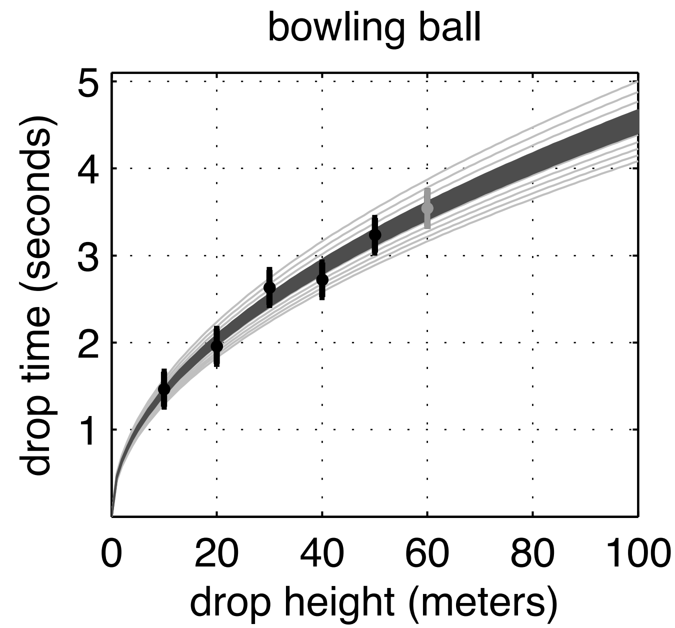
One-day-ahead forecasts:
The National Weather Service's model-based forecast is more accurate than predicting today's temperature with yesterday's temperature. Histograms summarize forecast errors over 1993.

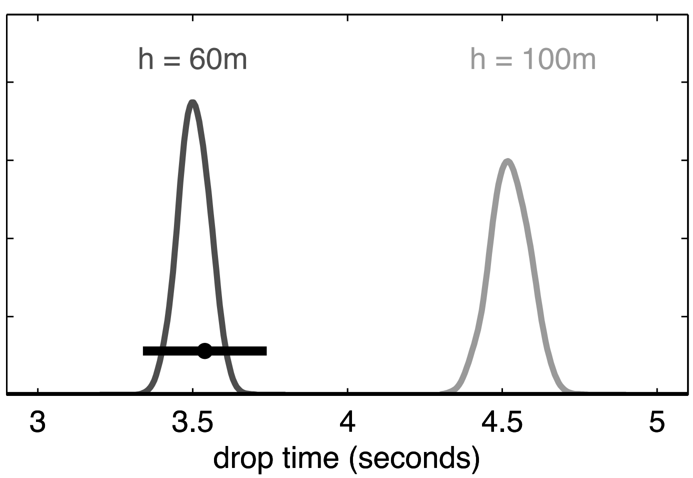
Simple robot problem I

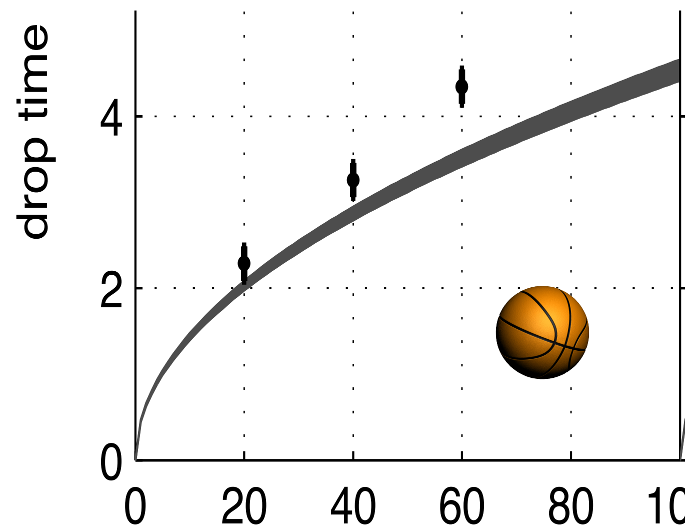
$$\frac{d^2h}{dt^2} = g$$



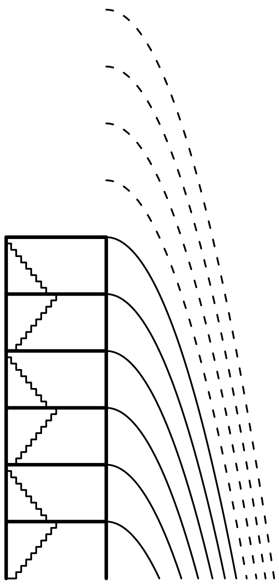


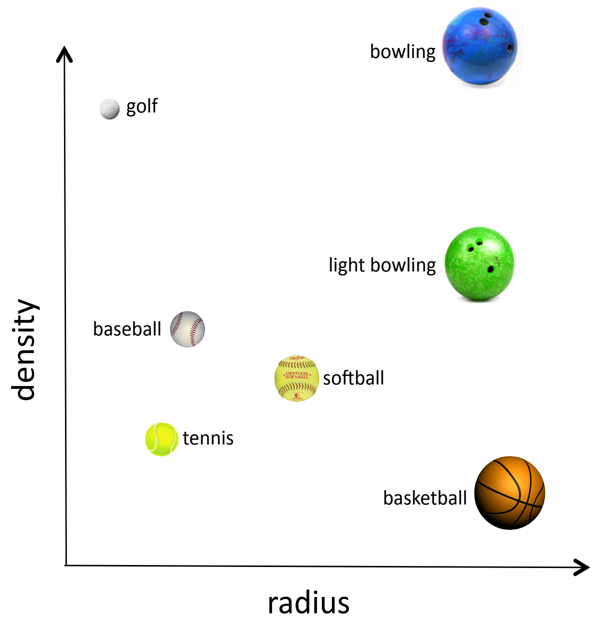




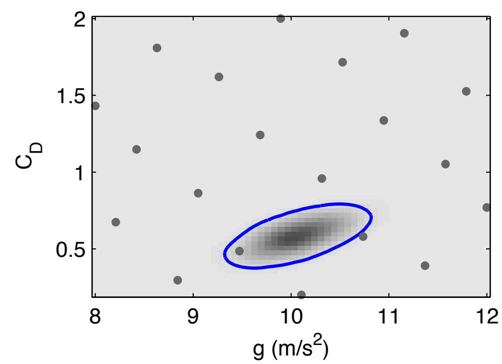


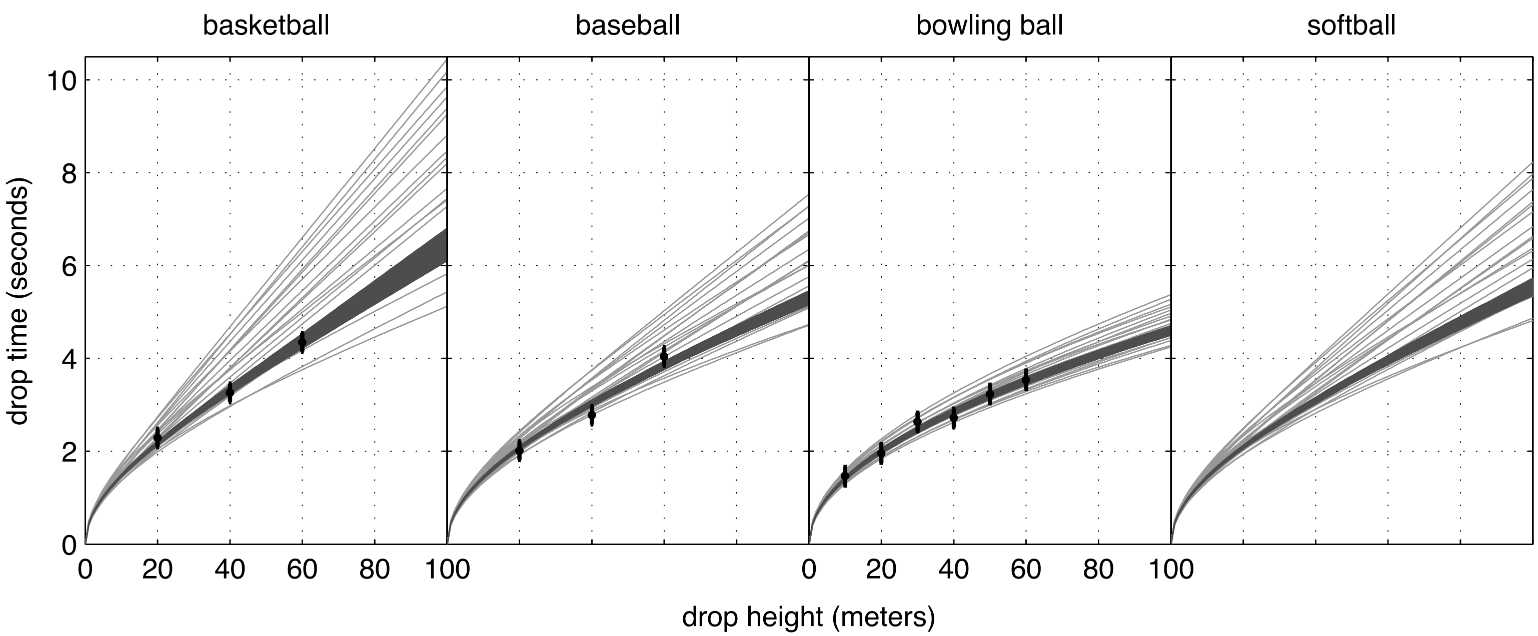
Simple robot problem II



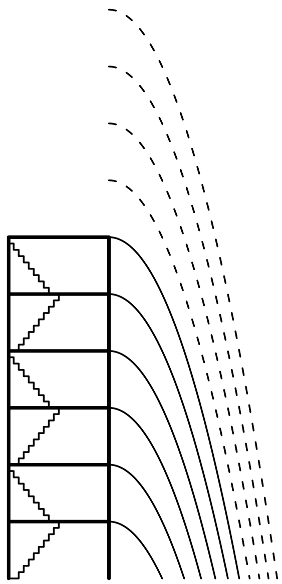


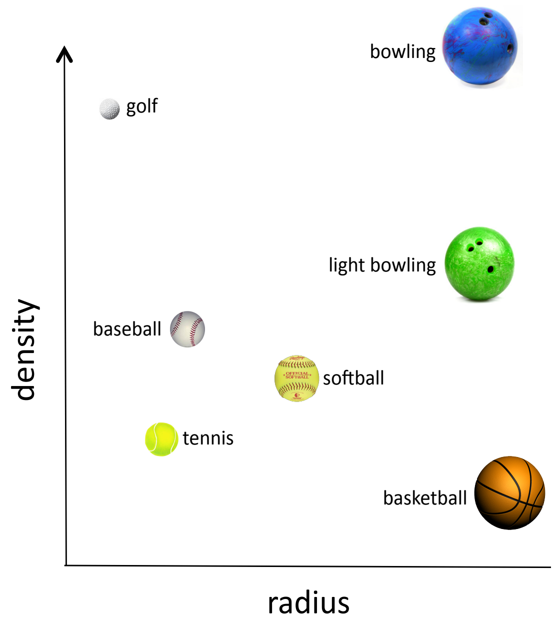
$$\frac{d^2h}{dt^2} = g - \frac{C_D}{2} \frac{3\rho_{\text{air}}}{4R_{\text{ball}}\rho_{\text{ball}}} \left(\frac{dh}{dt}\right)^2$$





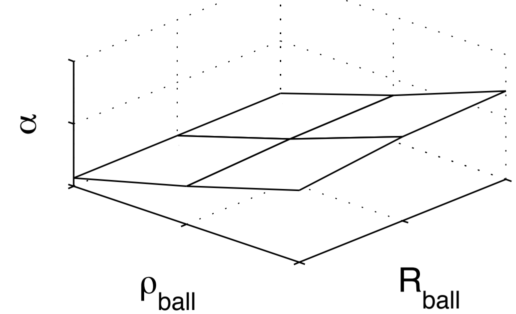
Simple robot problem III

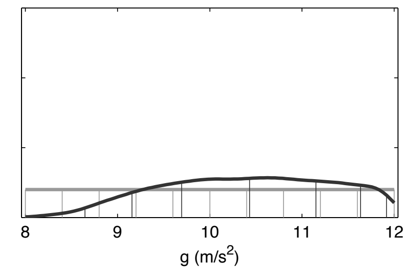


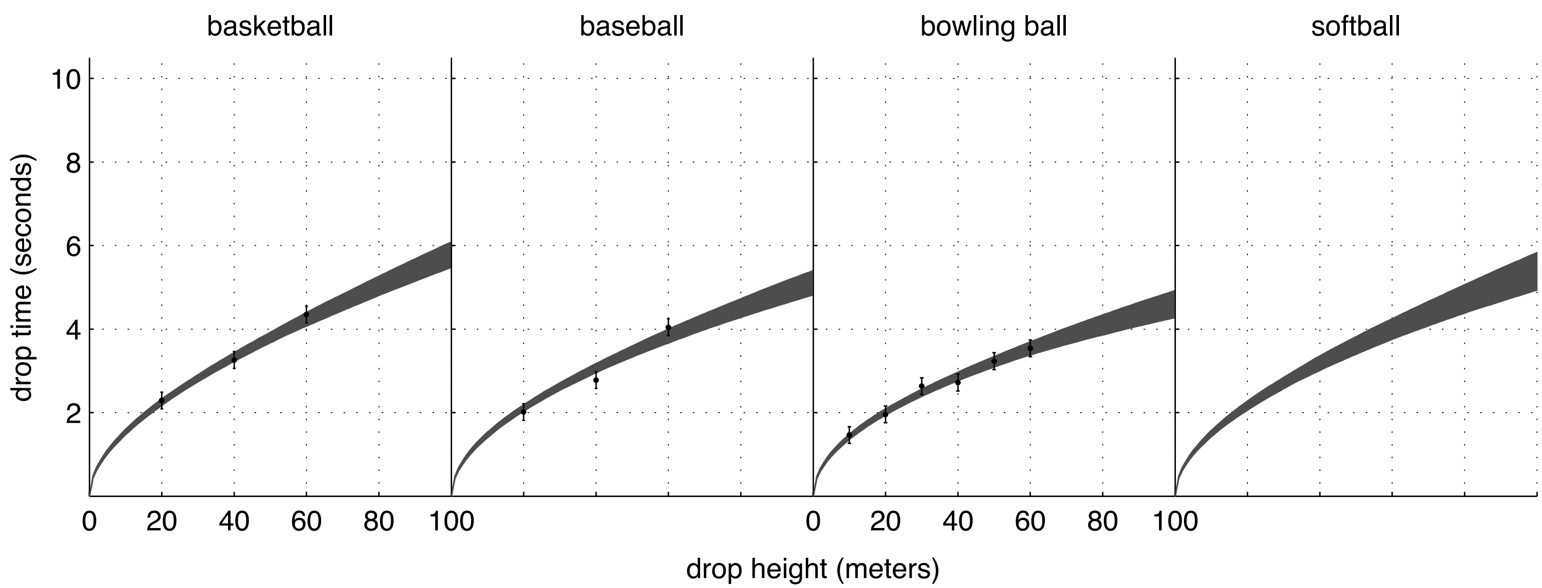


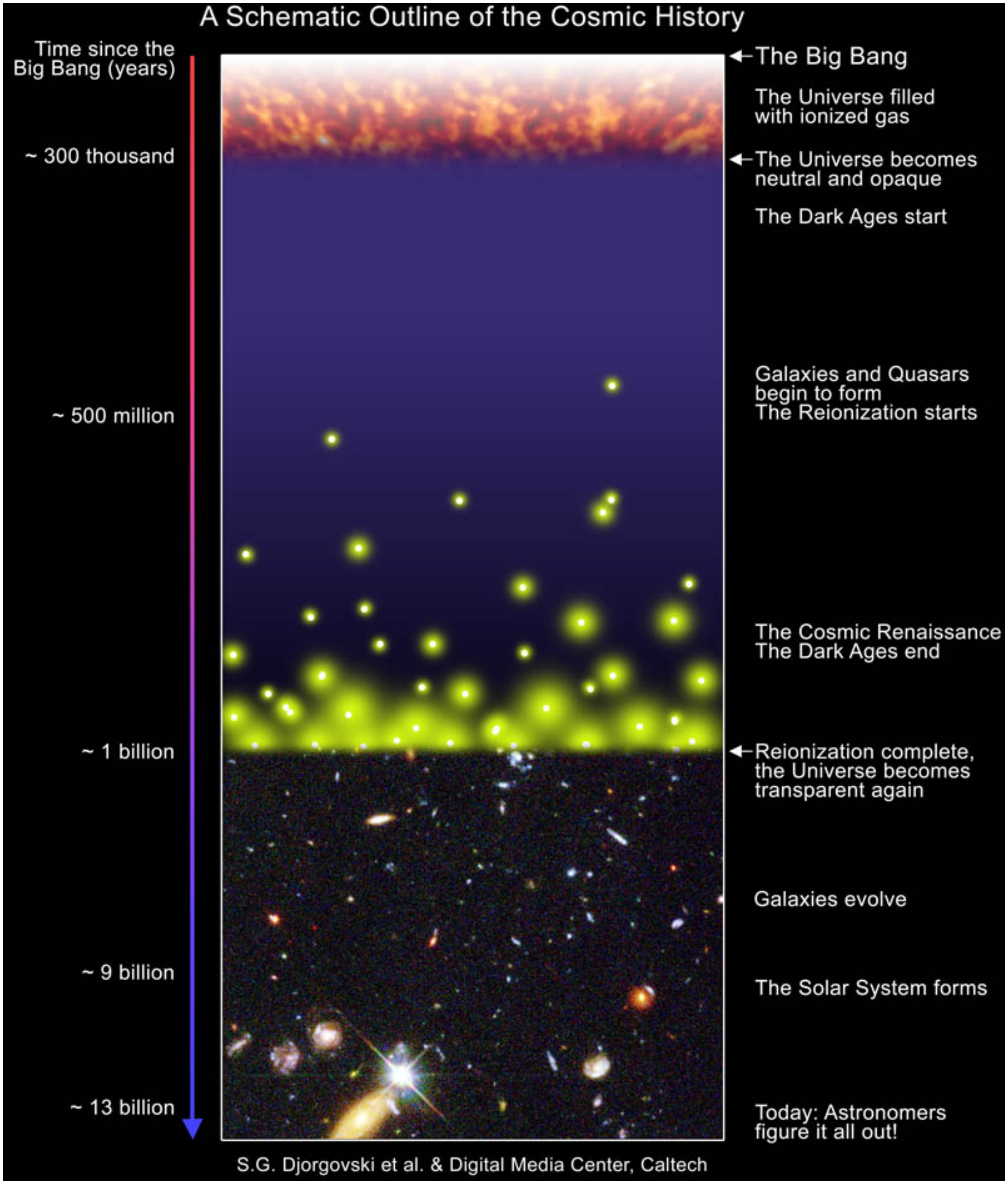
$$\frac{d^2h}{dt^2} = g$$

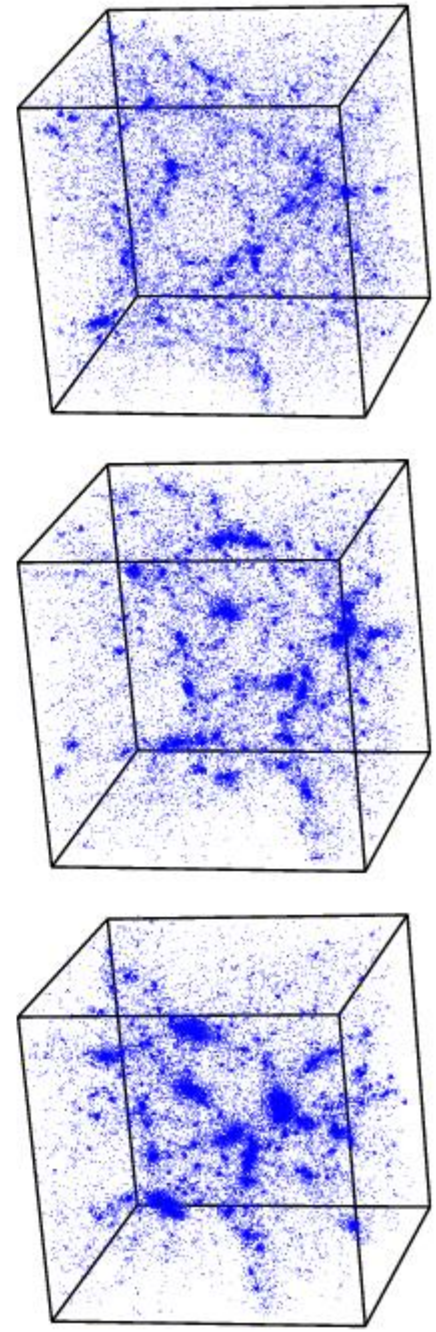
drop time = simulated drop time + α × drop height





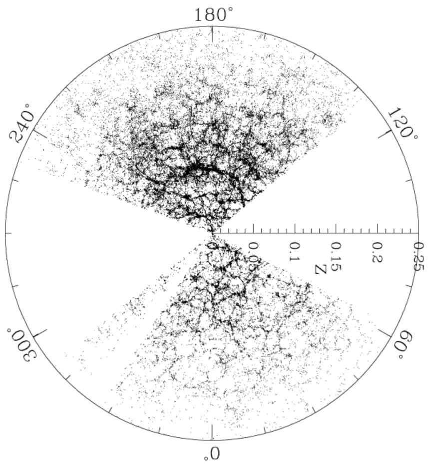


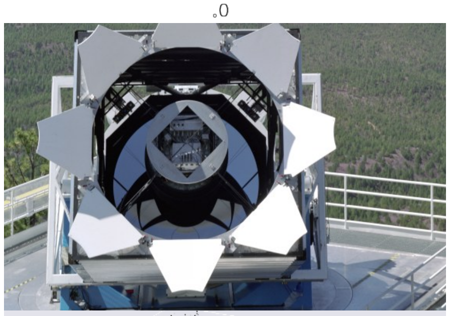


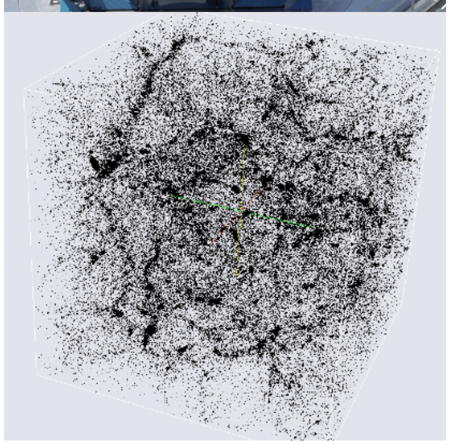


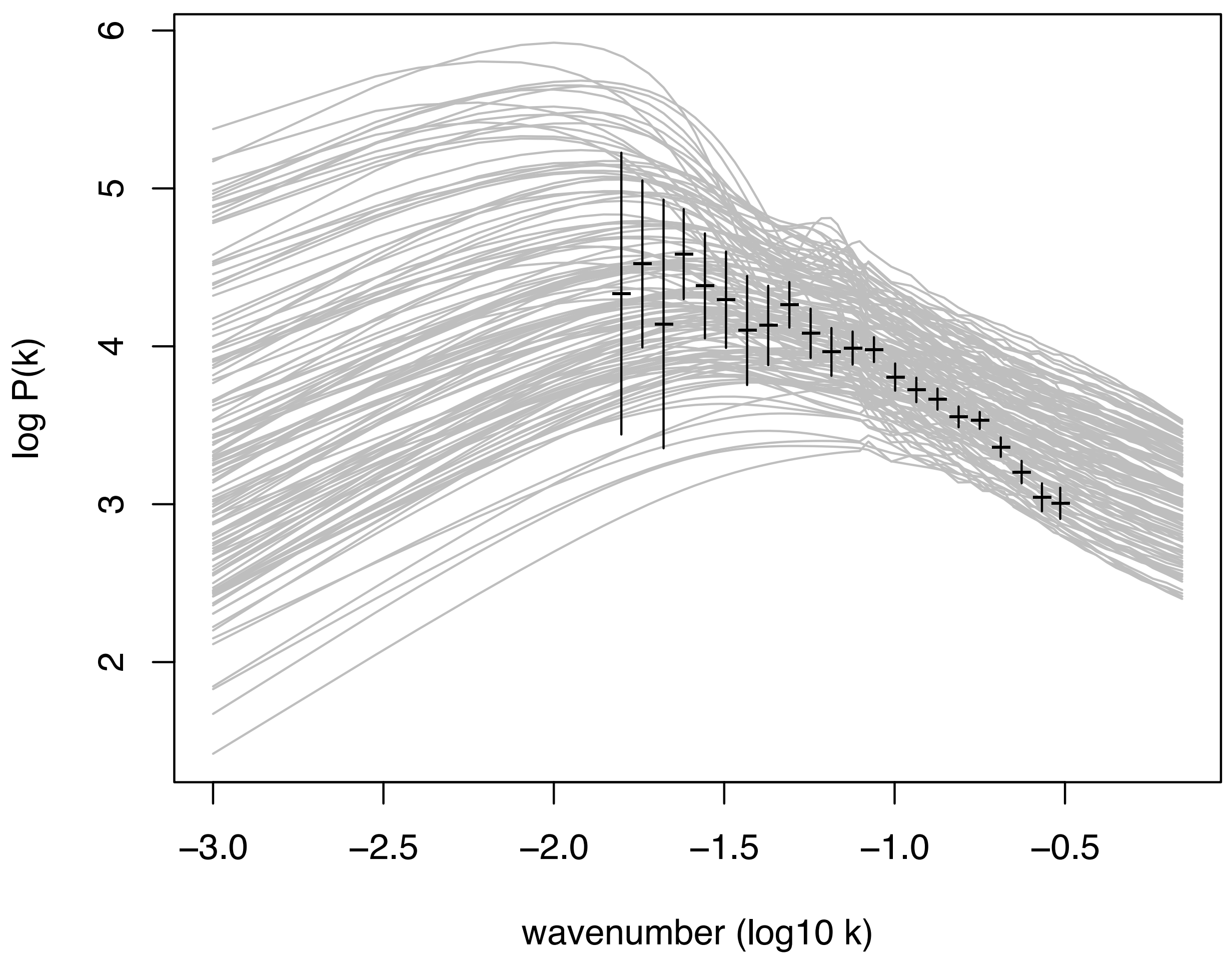
Cloud-in-cell FFT-based Poisson solver; 512^3, 1024^3 and 2048^3 particles

Sloan Digital Sky Survey

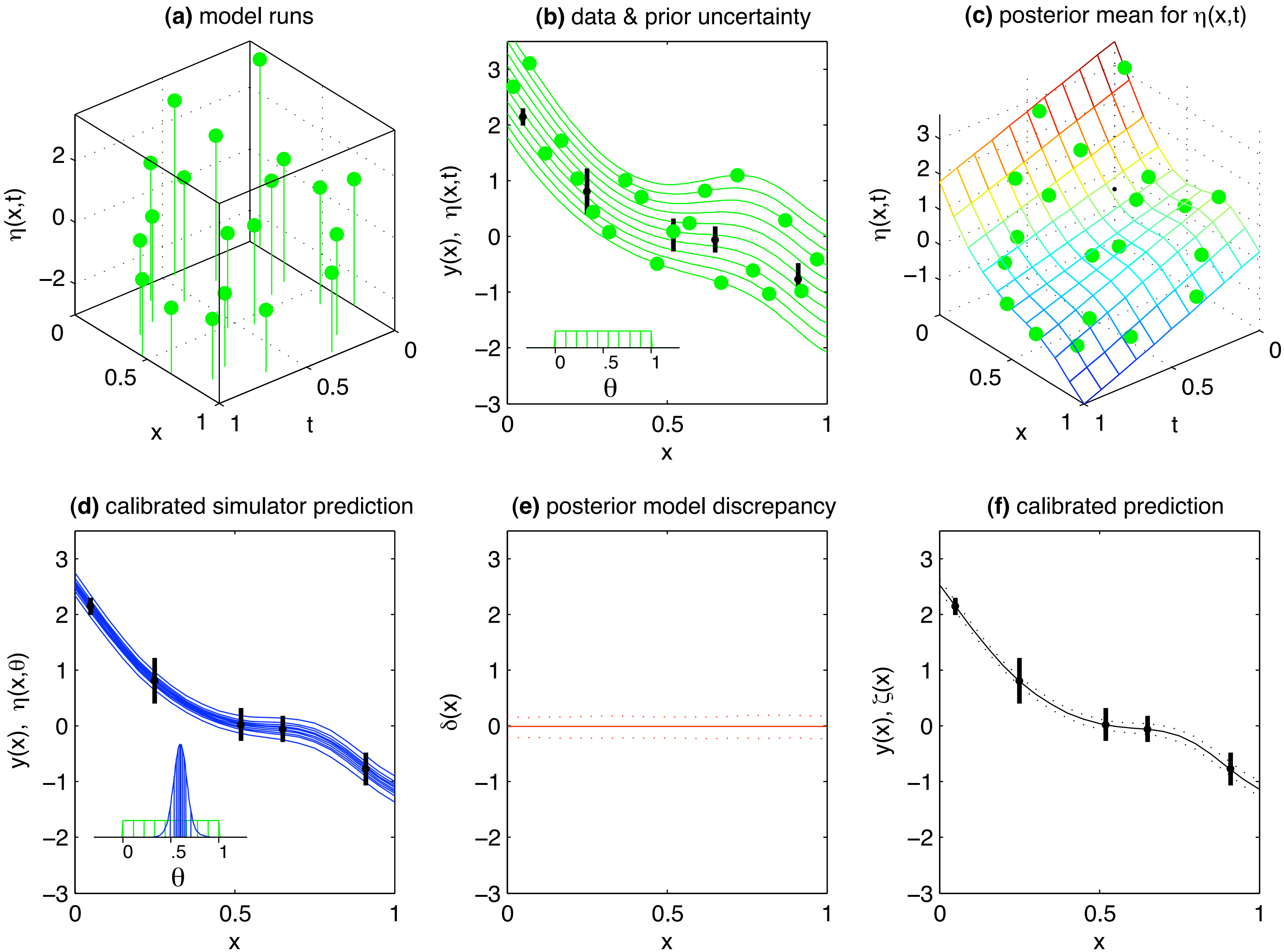




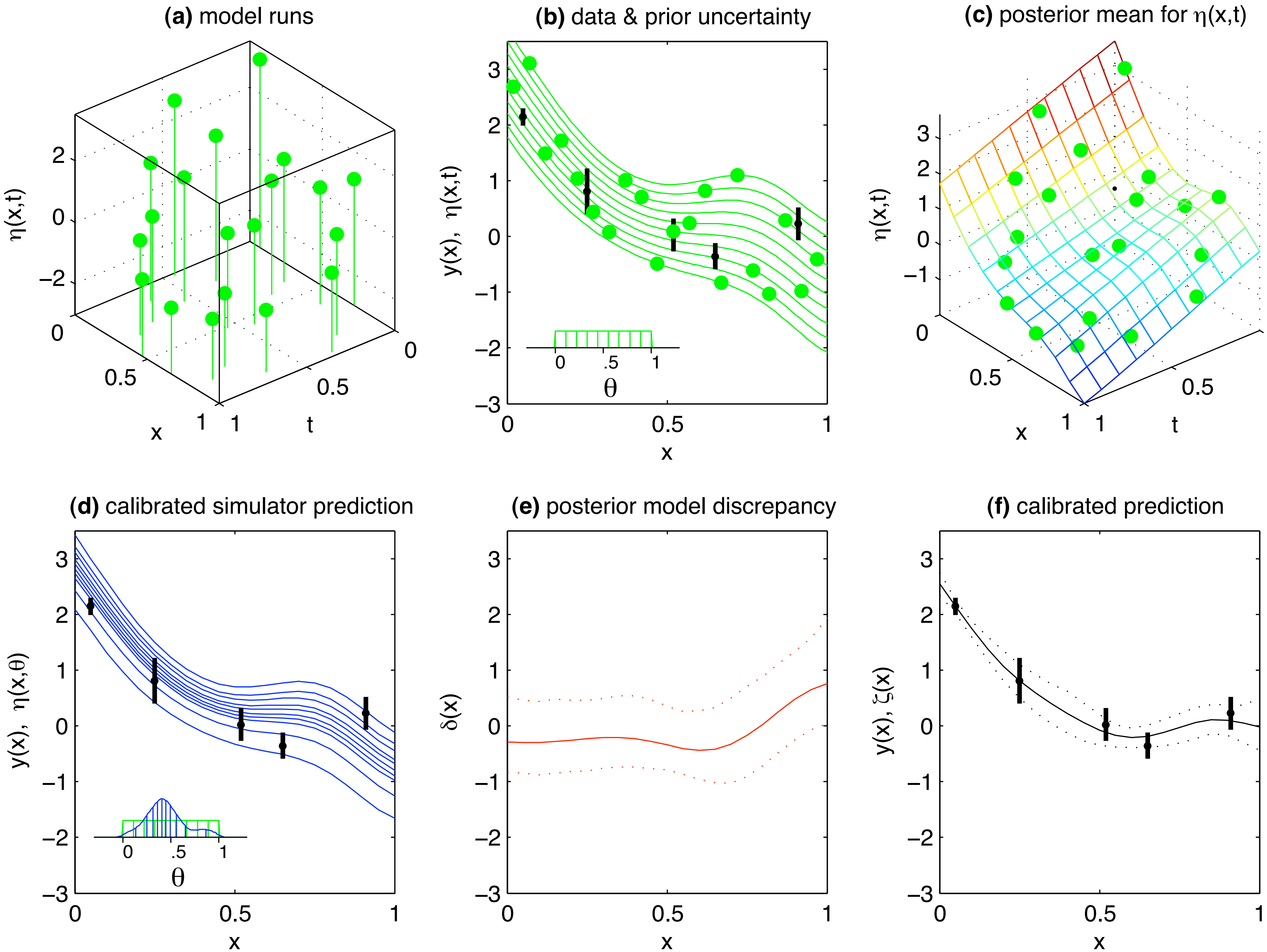




Statistical framework $y(x_i) = \eta(x_i, \theta) + \delta(x_i) + \epsilon_i$

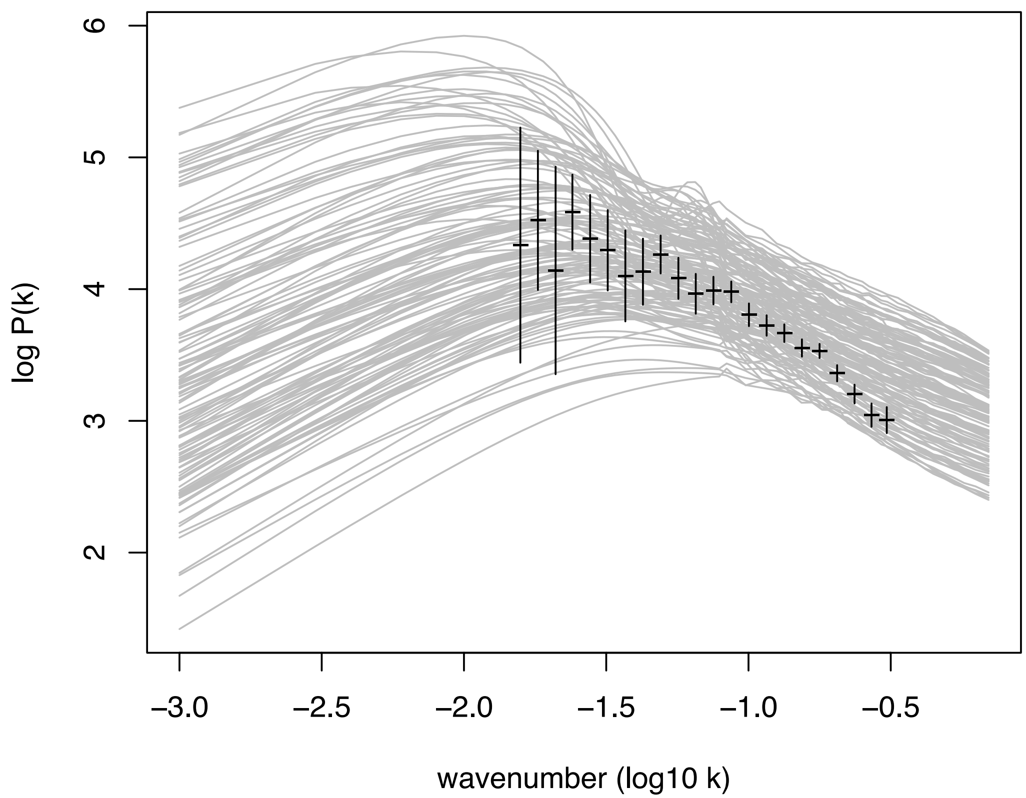


Statistical framework $y(x_i) = \eta(x_i, \theta) + \delta(x_i) + \epsilon_i$

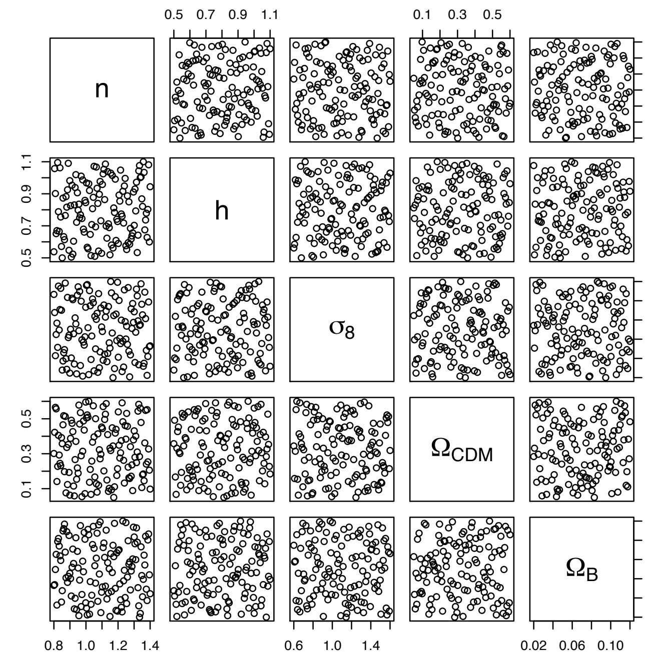


Data, parameter ranges, and simulations

Physical observations and simulations



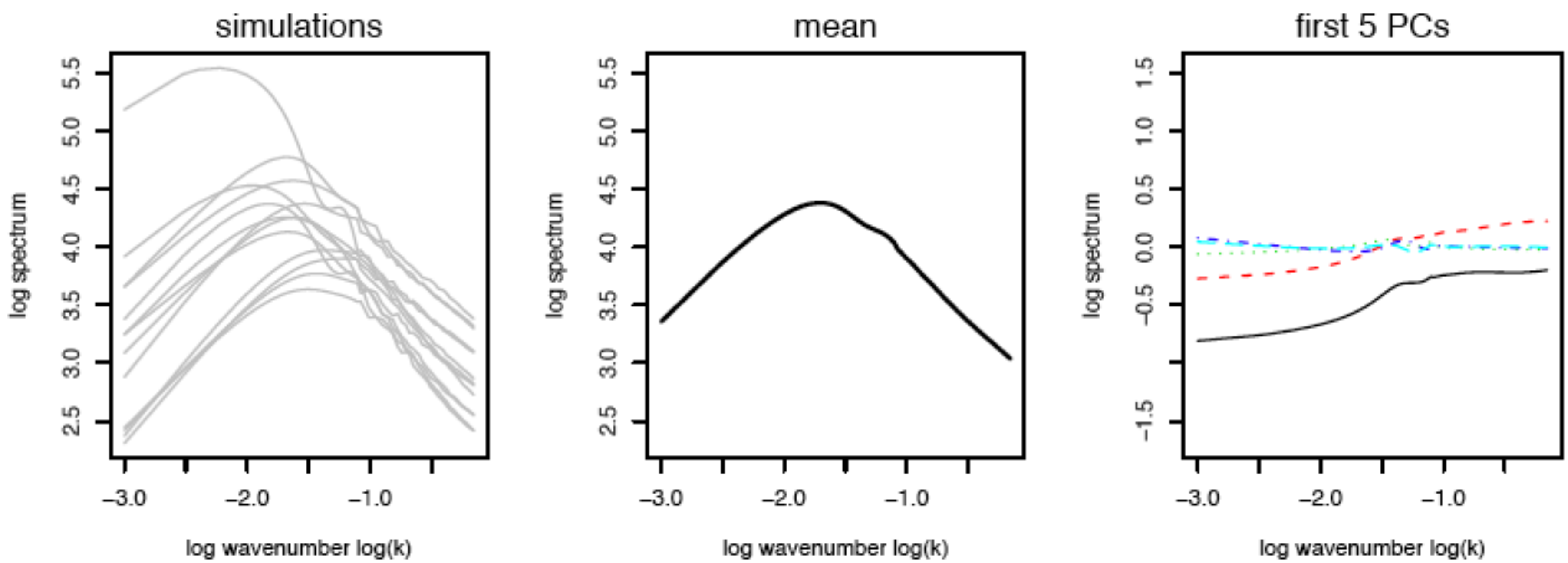
OA-LHS 128 run design



Calibration parameter ranges	
Spectral index	0.8 to 1.4
Hubble parameter	0.5 to 1.1
Sigma 8	0.6 to 1.6
Omega CDM	0051 to 0.6
Omega baryon	0.02 to 0.12

Basis representation of simulated spectra

Basis representation for matter power spectra.



Power spectra are represented as a function of the 5-d input parameters θ and PC basis functions $\phi_j(k)$:

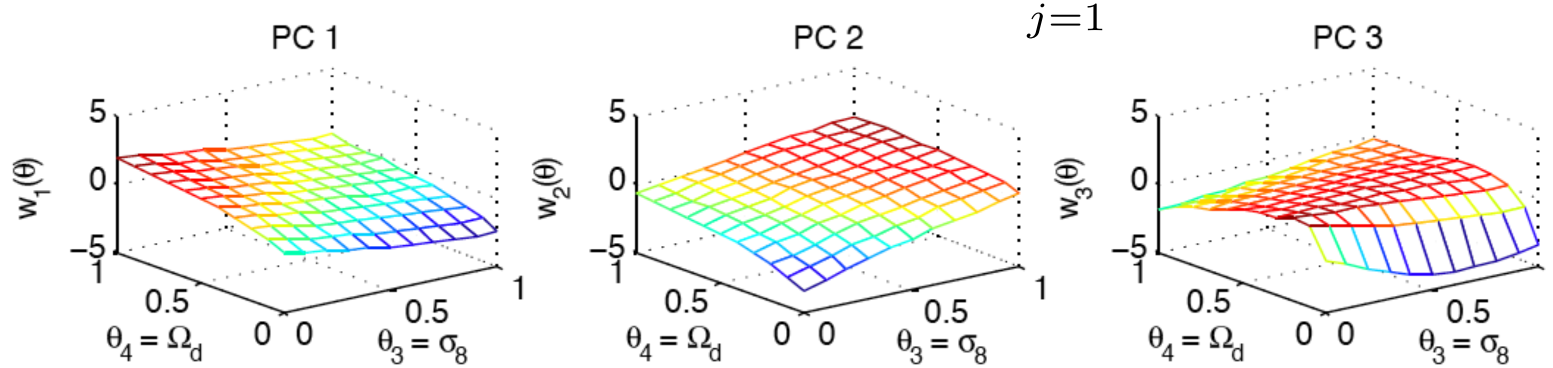
$$\widehat{\eta}(\theta; k) = \sum_{j=1}^{p_\eta} w_j(\theta)\phi_j(k)$$

Gaussian process model to emulate multivariate simulation output

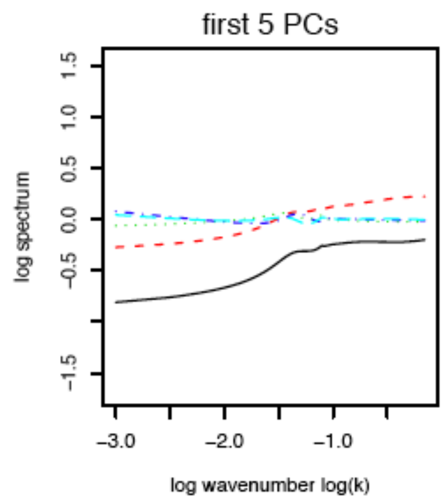
Gaussian process (GP) models are used to estimate the weights $w_j(\theta)$ at untried settings

$$\eta(\theta;k) = \sum_{j=1}^{p_\eta} w_j(\theta)\phi_j(k)$$

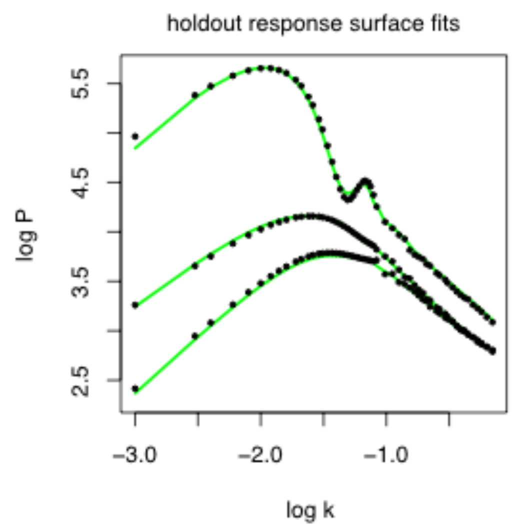
GP models $w_j(\theta)$



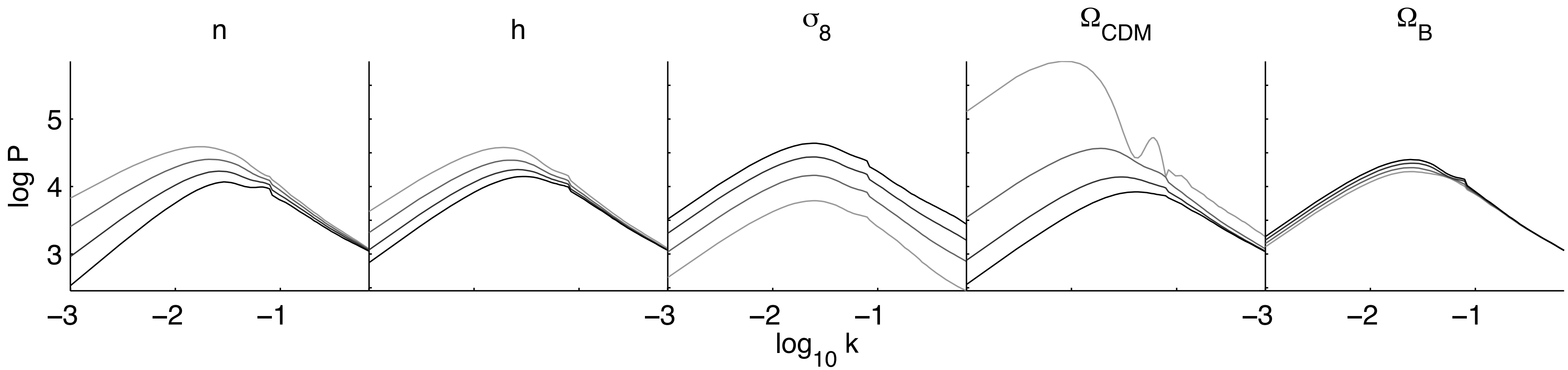
Bases $\phi_j(\theta)$



Prediction at new θ



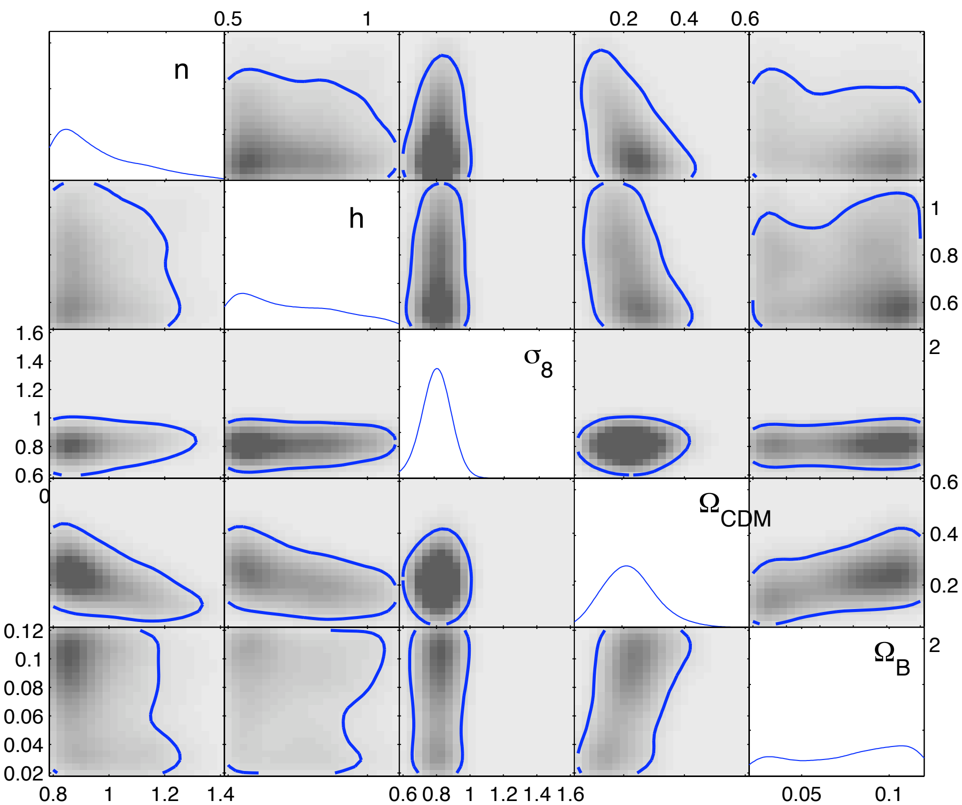
Simulator emulation and sensitivity



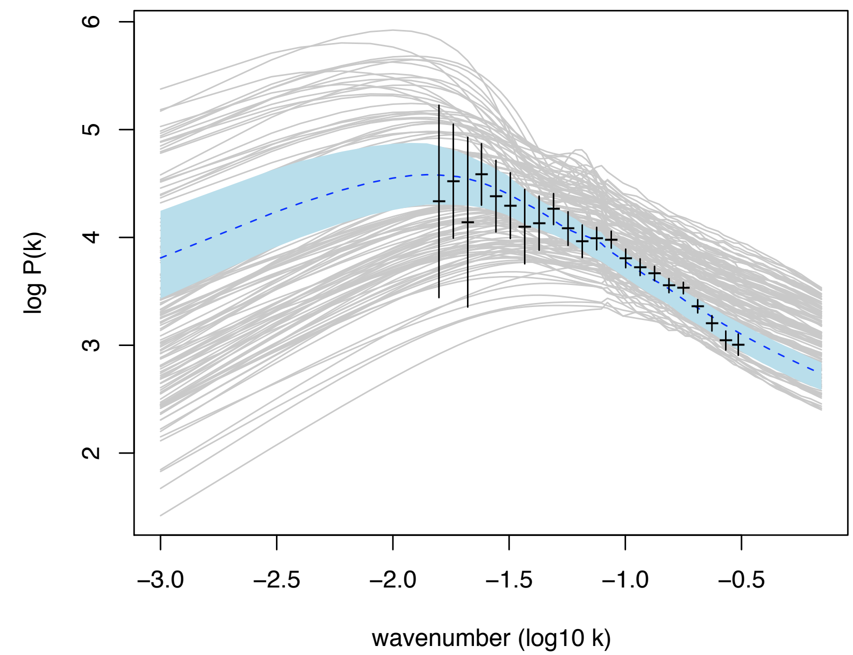
- Changes in emulator prediction as each parameter is varied while holding the others at their midpoint
- Note, σ_8 Ω_{CDM} have the largest effect on log P

Calibration results using physical observations

Posterior distribution of cosmological parameters

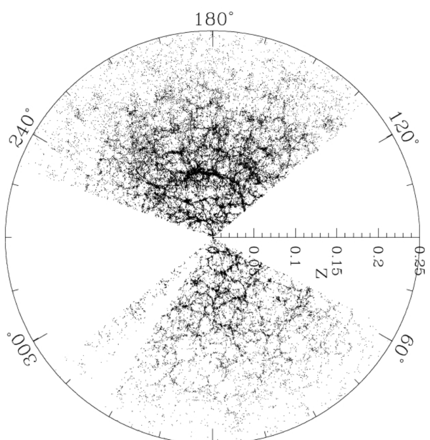


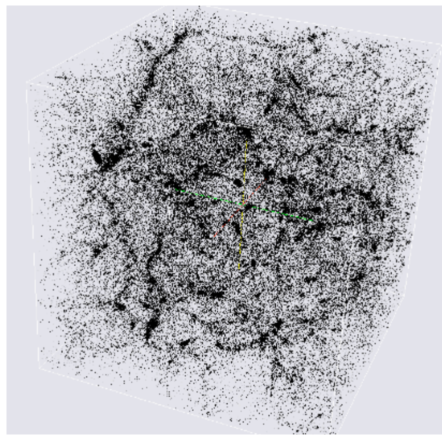
Resulting fit and uncertainty for the matter power spectrum

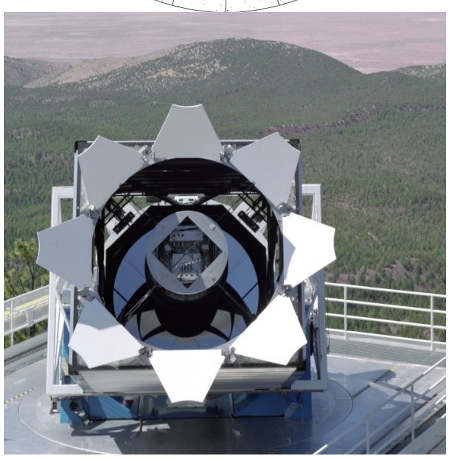


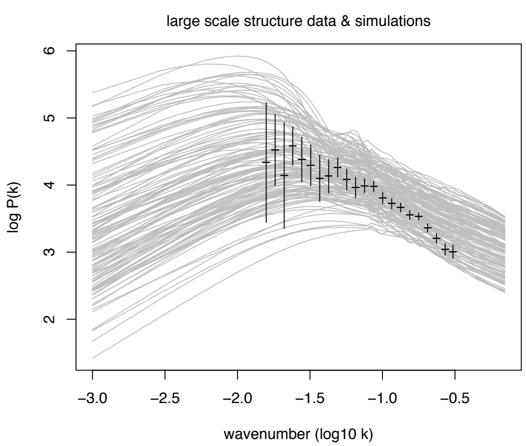
Methodology allows combining multiple computational models and data sources

Sloan Digital Sky Survey

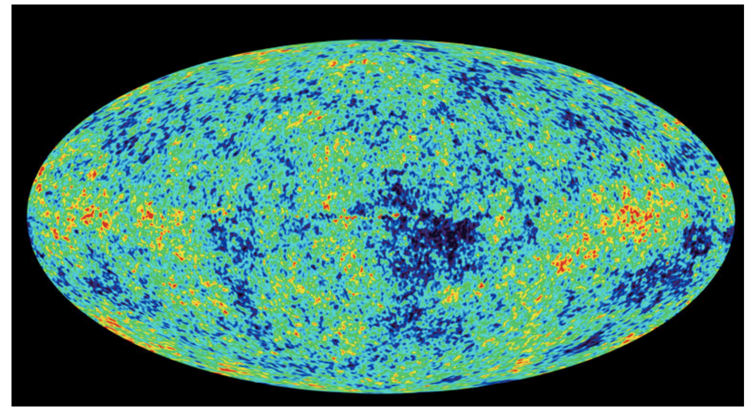


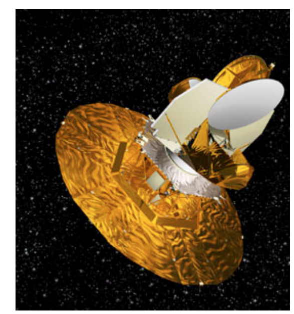


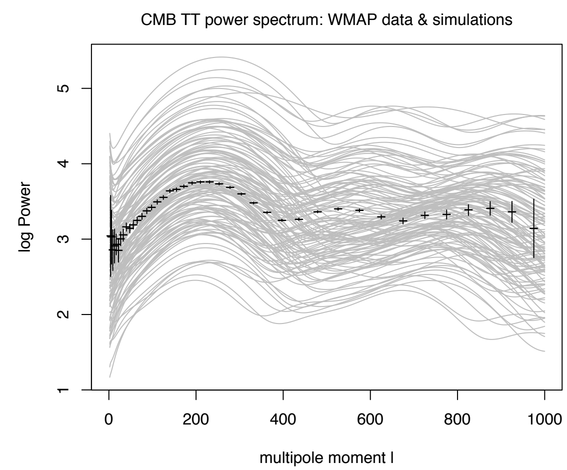




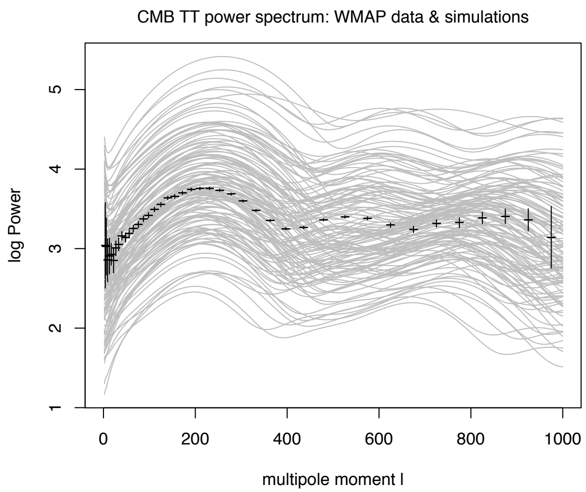
Wilkinson microwave anisotropy probe

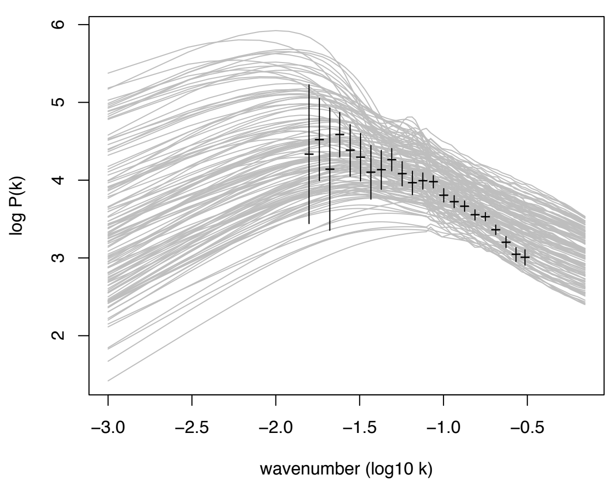


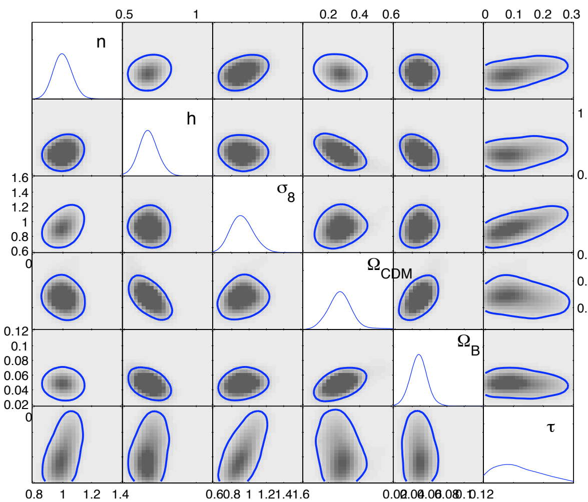


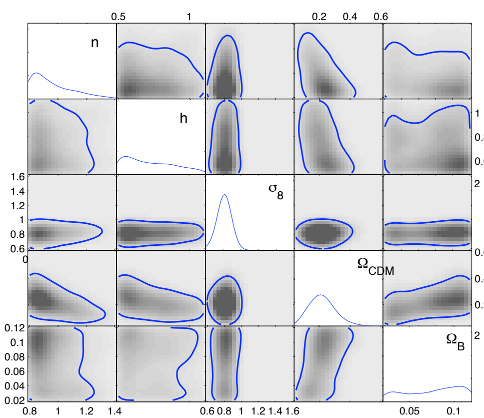


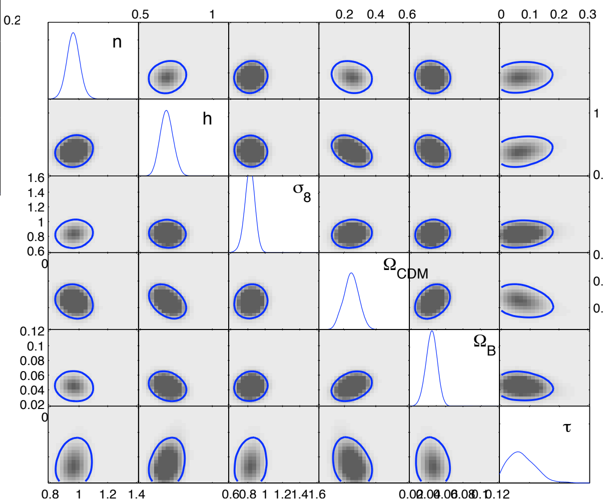
Combined WMAP & SDSS analysis





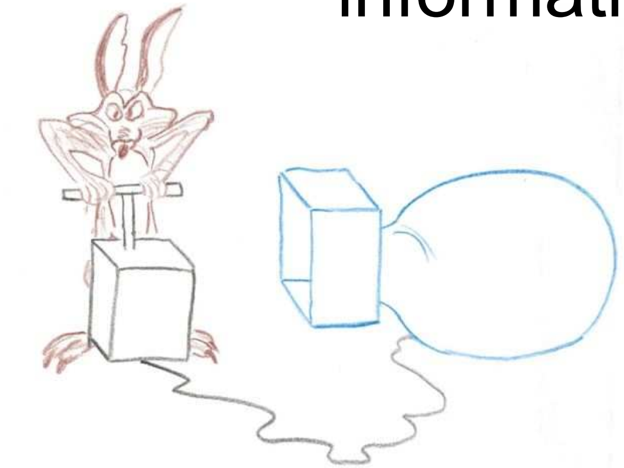


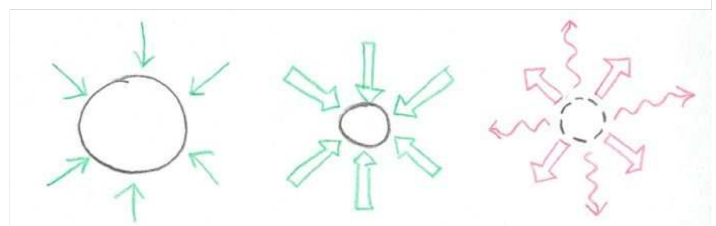


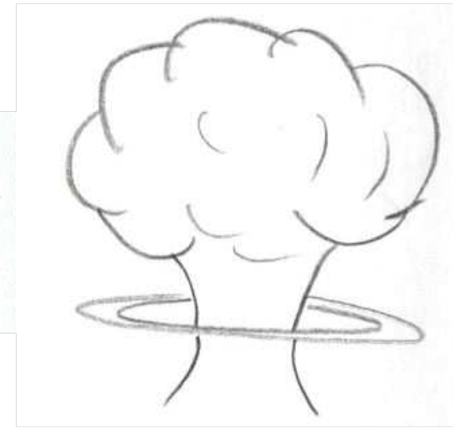


Combining information from both data sources sharpens inference on ΛCDM parameters

UQ in support of NW assessment combines information from many data sources







time

detonation | implosion | nuclear yield

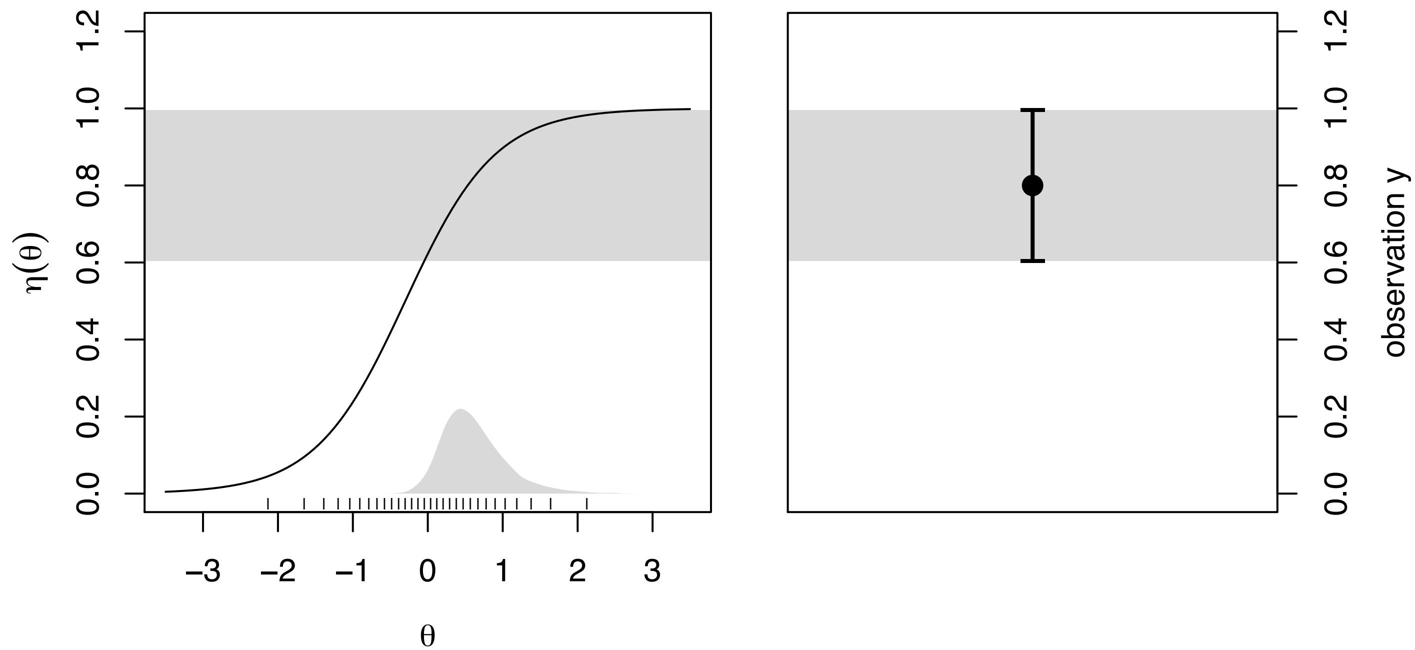
implosion experiments

sub-critcal experiments

historical nuclear tests

off-line experiments
materials, equations of state (EOS), high explosive (HE)

Simple, 1-d inverse problem: $y = \eta(\theta) + \epsilon$



Prior model

$$\pi(\theta) \propto \exp\left\{-\frac{1}{2}\theta^2\right\}$$

Observation model:

$$L(y|\theta) \propto \exp\left\{-\frac{1}{2\sigma^2}(y-\eta(\theta))^2\right\}$$

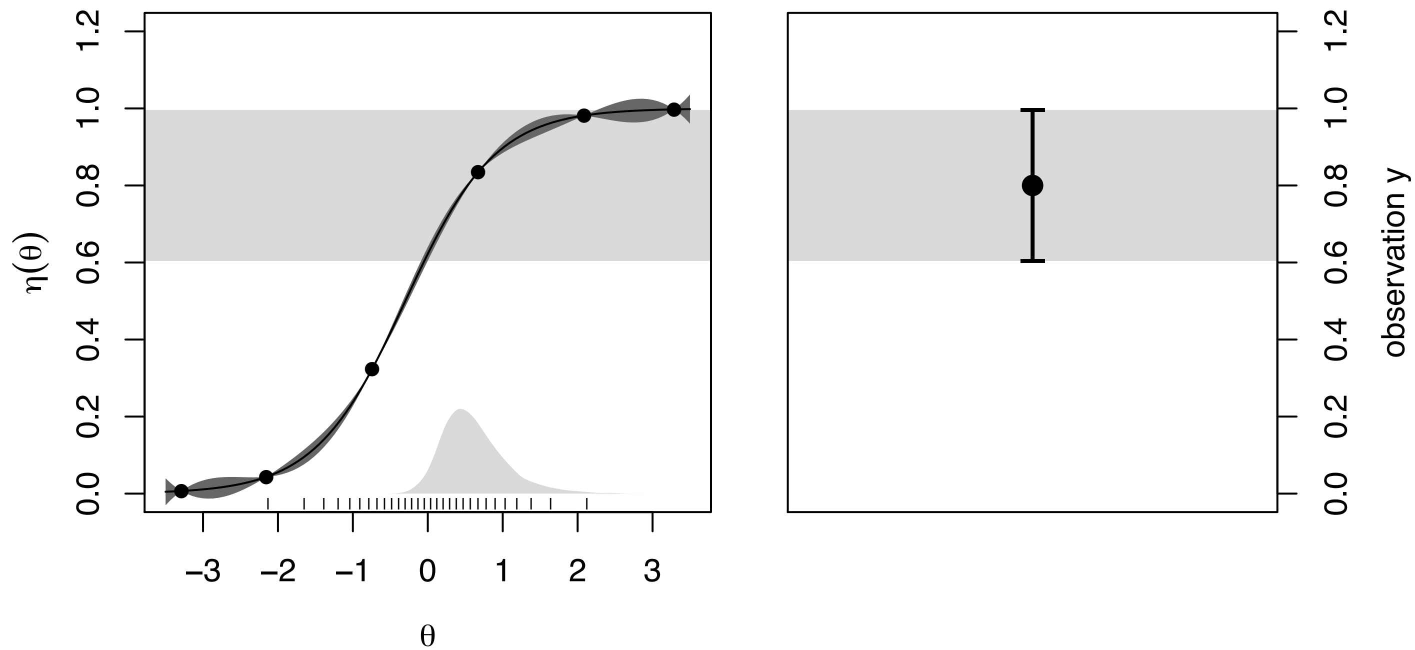
Computational model

$$\eta(\cdot)$$

Posterior

$$\pi(\theta|y) \propto L(y|\theta) \times \pi(\theta)$$

Using a Gaussian Process Emulator



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Observation model:

$$L(y|\theta) \propto \exp\left\{-\frac{1}{2\sigma^2}(y-\eta(\theta))^2\right\}$$

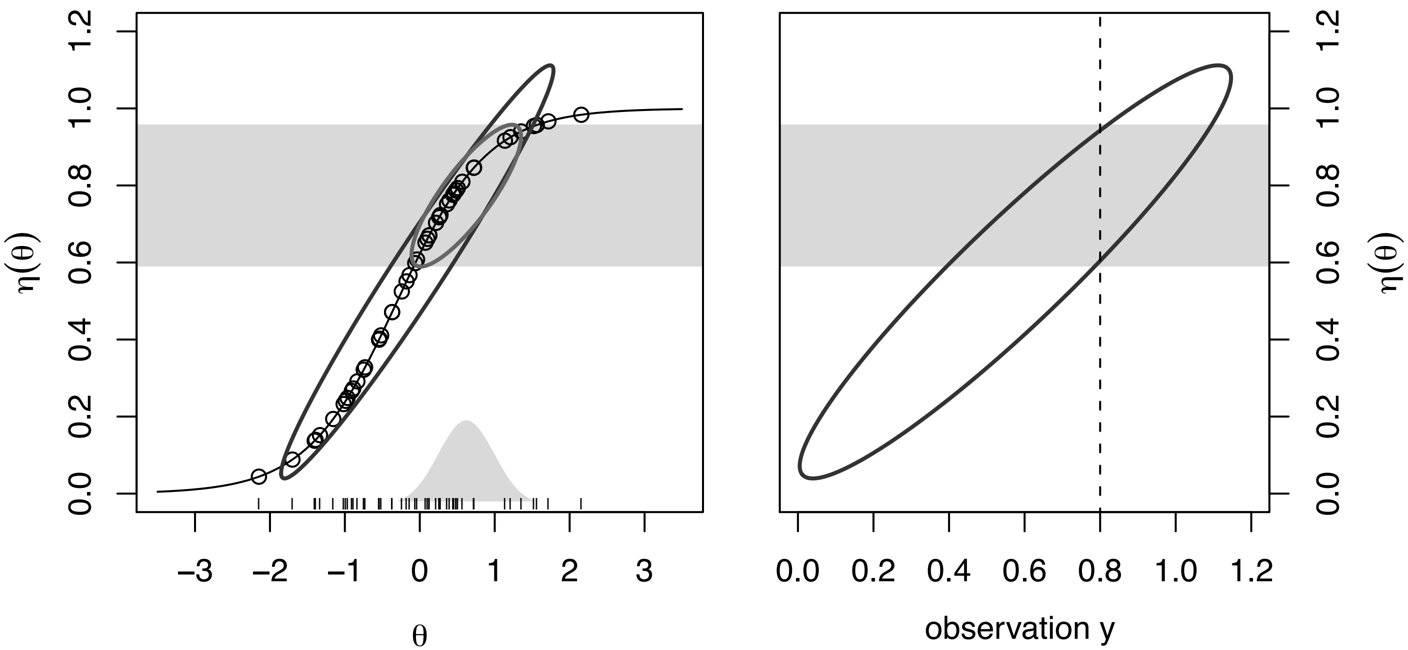
Computational model

$$\eta(\cdot) \sim GP(\mu(\cdot), C(\cdot,\cdot))$$

Posterior

$$\pi(\theta,\eta(\cdot)|y) \propto L(y|\theta,\eta(\cdot)) \times \pi(\theta) \times \pi(\eta(\cdot))$$

Ensemble Kalman smoother: normal version



Prior model

$$\begin{pmatrix}\theta \\ \eta(\theta)\end{pmatrix} \sim N(\mu_{\mathrm{pr}}, \Sigma_{\mathrm{pr}})$$

Observation model:

$$\begin{pmatrix}\theta \\ \eta(\theta)\end{pmatrix} \sim N\left(\mu_{\mathrm{obs}} = \begin{pmatrix}\star \\ y\end{pmatrix}, \Sigma_{\mathrm{obs}}^{-1} = \begin{pmatrix}0 & 0 \\ 0 & \sigma_y^{-2}\end{pmatrix}\right)$$

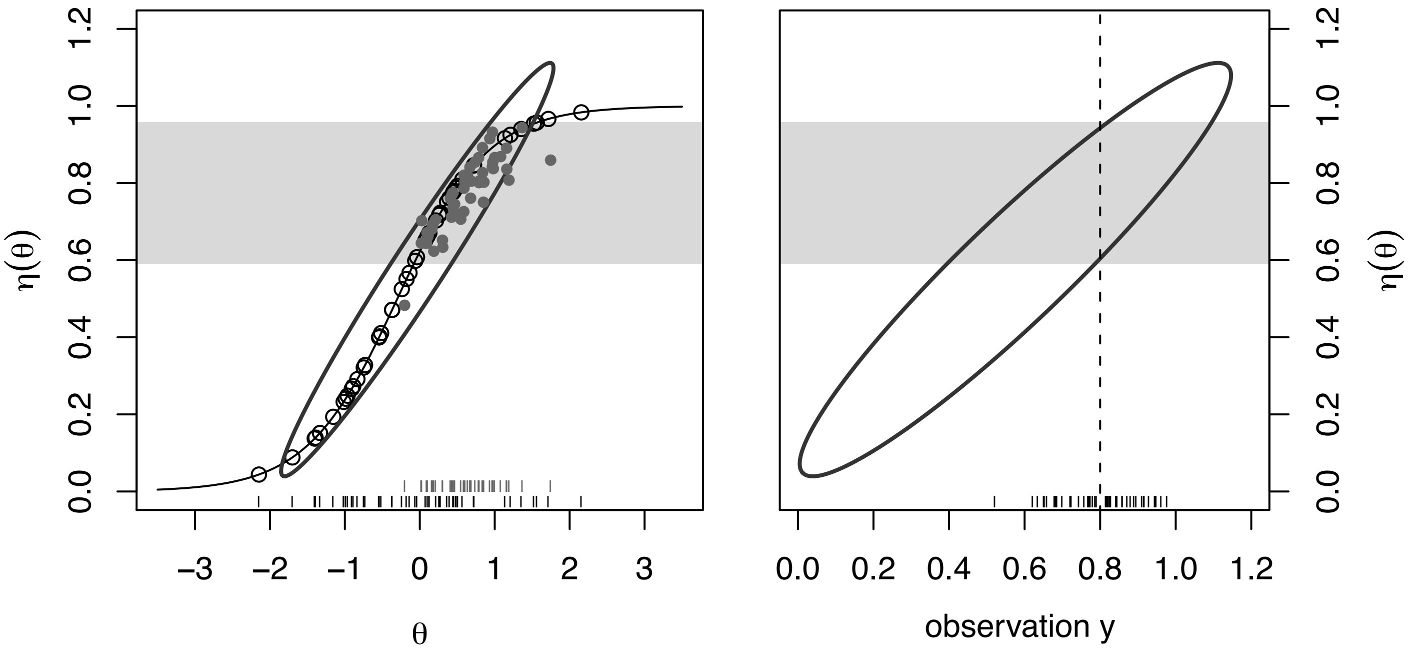
Posterior

$$\begin{pmatrix}\theta \\ \eta(\theta)\end{pmatrix} \sim N(\mu_{\mathrm{post}}, \Sigma_{\mathrm{post}})$$

$$\Sigma_{\mathrm{post}}^{-1} = \Sigma_{\mathrm{pr}}^{-1} + \Sigma_{\mathrm{obs}}^{-1}$$

$$\mu_{\mathrm{post}} = \Sigma_{\mathrm{post}}(\Sigma_{\mathrm{pr}}^{-1}\mu_{\mathrm{pr}} + \Sigma_{\mathrm{obs}}^{-1}\mu_{\mathrm{obs}})$$

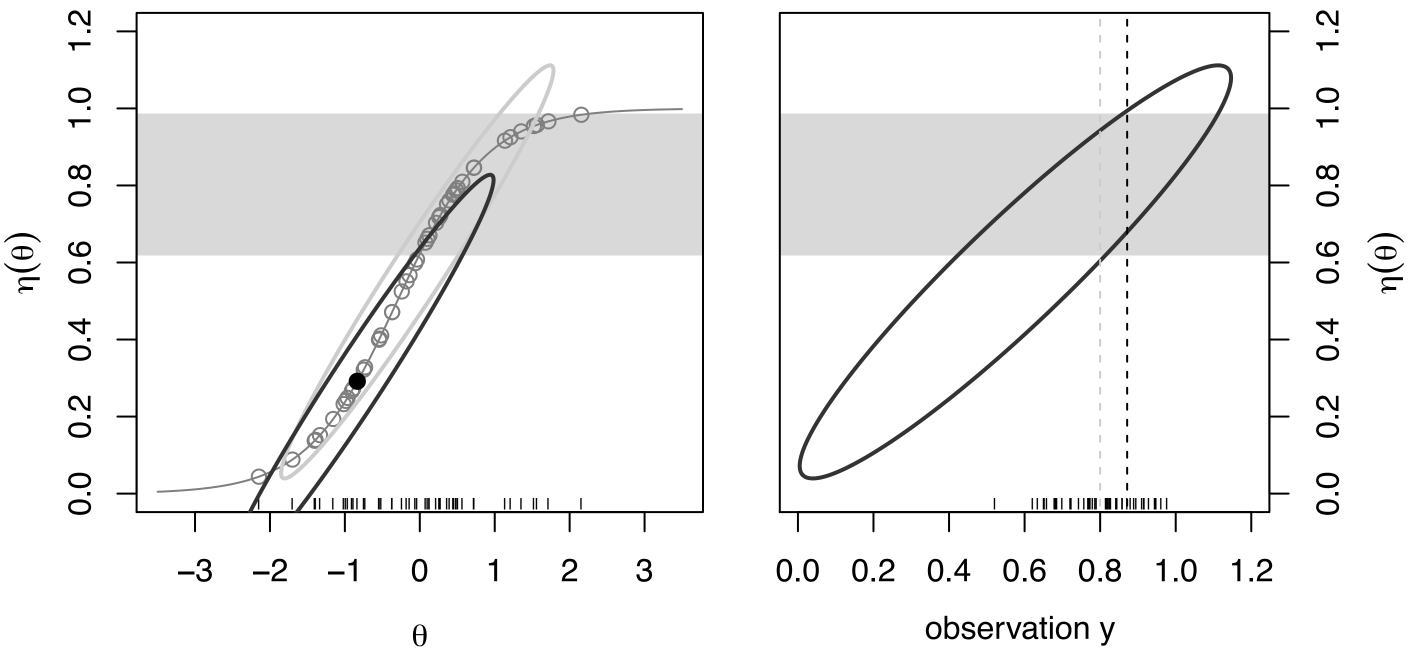
Ensemble Kalman smoother: ensemble version



Perturb each pair $\begin{pmatrix}\theta_k \\ \eta(\theta_k)\end{pmatrix} \to \begin{pmatrix}\theta \\ \eta(\theta)\end{pmatrix}_k$ so that the sample $\begin{pmatrix}\theta \\ \eta(\theta)\end{pmatrix}_1, \ldots, \begin{pmatrix}\theta \\ \eta(\theta)\end{pmatrix}_m$ is an approximate collection of draws from the posterior distribution.

Use posterior mean induced by combining these two (random) information sources: $\begin{pmatrix}\theta_k \\ \eta(\theta_k)\end{pmatrix} \sim N(\mu_{\mathrm{pr}}, \Sigma_{\mathrm{pr}})$ and $y_k \sim N(y, \sigma_y^2)$.

Ensemble Kalman smoother: ensemble version



Perturb each pair $\begin{pmatrix}\theta_k \\ \eta(\theta_k)\end{pmatrix} \to \begin{pmatrix}\theta \\ \eta(\theta)\end{pmatrix}_k$ so that the sample $\begin{pmatrix}\theta \\ \eta(\theta)\end{pmatrix}_1, \ldots, \begin{pmatrix}\theta \\ \eta(\theta)\end{pmatrix}_m$ is an approximate collection of draws from the posterior distribution.

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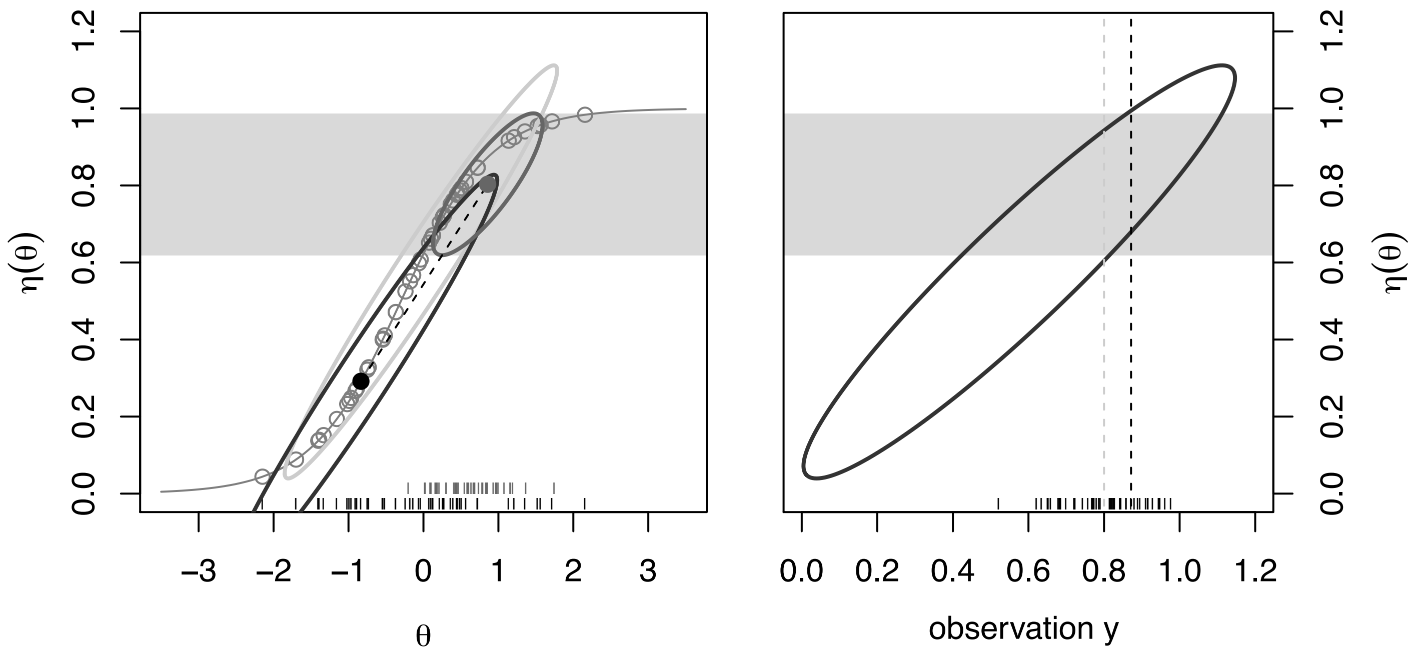
Ensemble Kalman smoother: ensemble version



Perturb each pair $\begin{pmatrix}\theta_k \\ \eta(\theta_k)\end{pmatrix} \rightarrow \begin{pmatrix}\theta \\ \eta(\theta)\end{pmatrix}_k$ so that the sample $\begin{pmatrix}\theta \\ \eta(\theta)\end{pmatrix}_1, \ldots, \begin{pmatrix}\theta \\ \eta(\theta)\end{pmatrix}_m$ is an approximate collection of draws from the posterior distribution.

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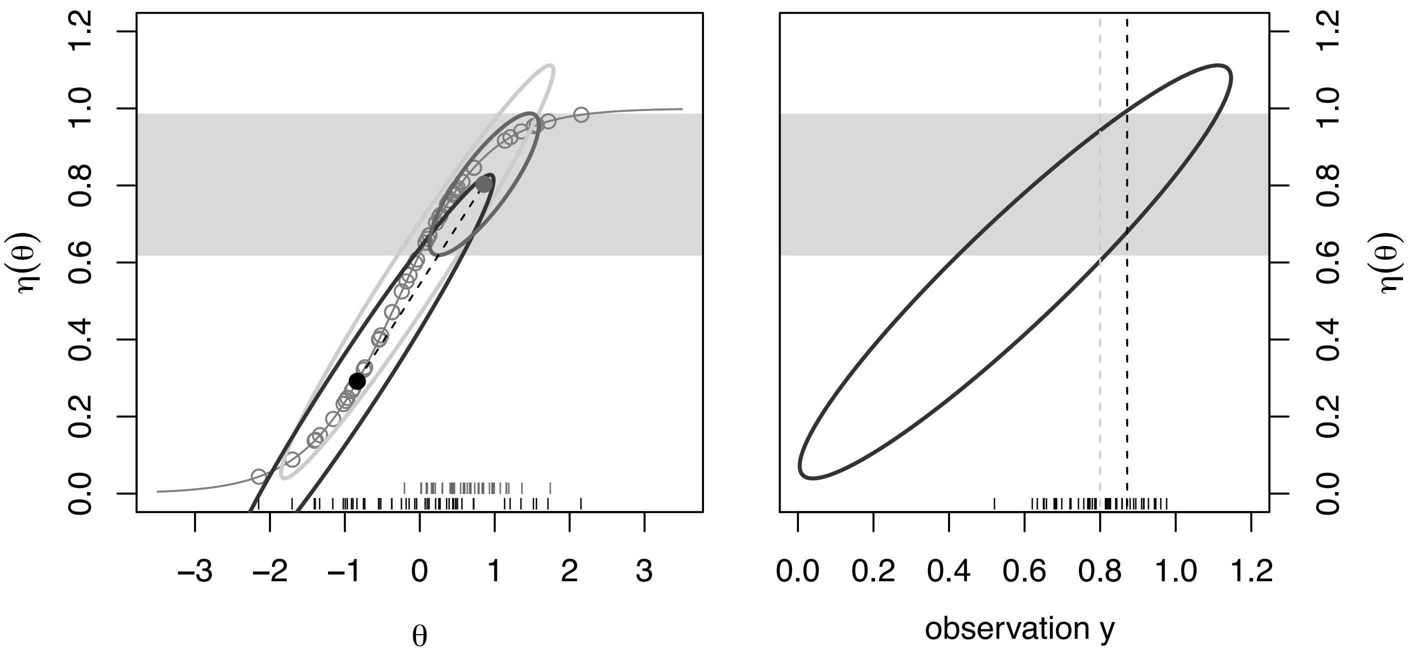
Ensemble Kalman smoother: ensemble version



Prior model: centered @ k^{th} ensemble

Observation model with perturbed data $y_k \sim N(y, \sigma^2)$

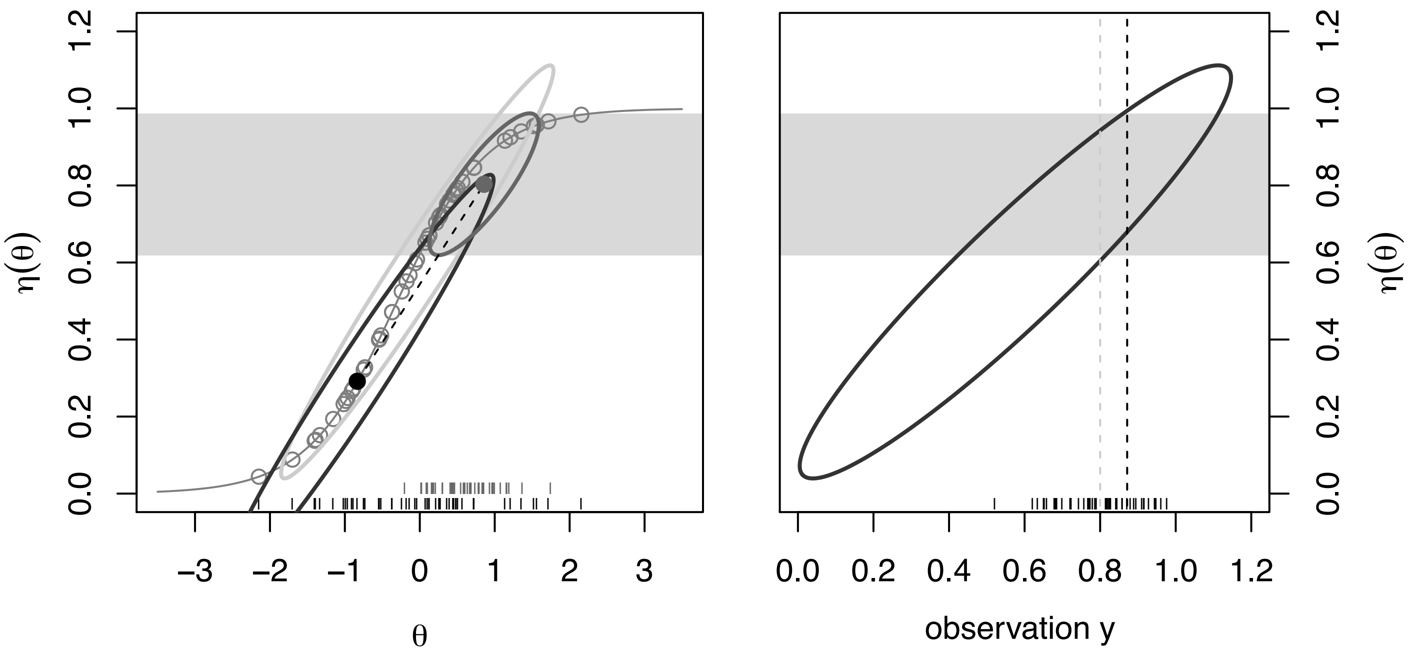
$$\begin{pmatrix} \theta \\ \eta(\theta) \end{pmatrix}_k \sim N\left(\begin{pmatrix} \theta_k \\ \eta(\theta_k) \end{pmatrix}, \Sigma_{\text{pr}} \right)$$

$$\begin{pmatrix} \theta \\ \eta(\theta) \end{pmatrix}_k \sim N\left(\mu_{\text{obs}} = \begin{pmatrix} \star \\ y_k \end{pmatrix}, \Sigma_{\text{obs}}^{-1} = \begin{pmatrix} 0 & 0 \\ 0 & \sigma_y^{-2} \end{pmatrix} \right)$$

Set k^{th} ensemble value to the posterior mean

$$\begin{pmatrix} \theta \\ \eta(\theta) \end{pmatrix}_k = \left(\Sigma_{\text{pr}}^{-1} + \Sigma_{\text{obs}}^{-1}\right)^{-1} \left(\Sigma_{\text{pr}}^{-1} \begin{pmatrix} \theta_k \\ \eta(\theta_k) \end{pmatrix} + \Sigma_{\text{obs}}^{-1} \begin{pmatrix} \star \\ y_k \end{pmatrix} \right)$$

Ensemble Kalman smoother: ensemble version



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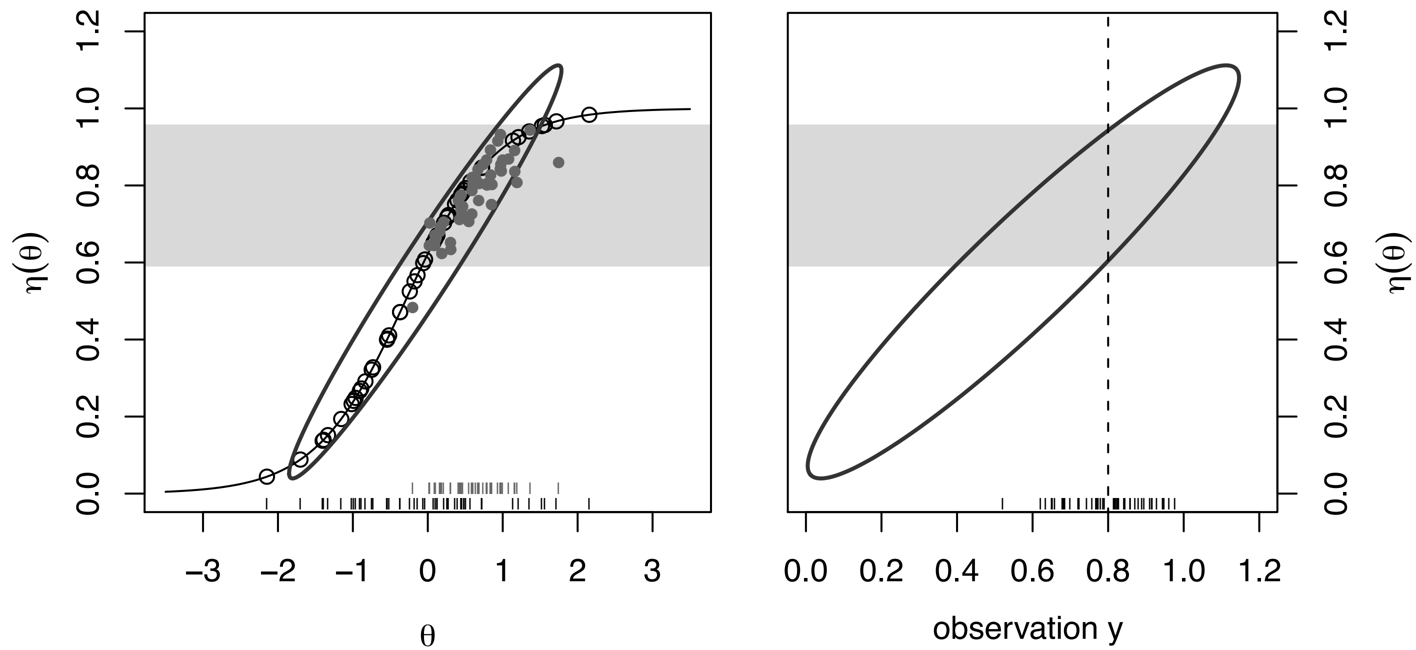
Observation model with perturbed data $y_k \sim N(y, \sigma^2)$

$$\begin{pmatrix}\theta \\ \eta(\theta)\end{pmatrix}_k \sim N\left(\mu_{\text{obs}} = \begin{pmatrix}\star \\ y_k\end{pmatrix}, \Sigma_{\text{obs}}^{-1} = \begin{pmatrix}0 & 0 \\ 0 & \sigma_y^{-2}\end{pmatrix}\right)$$

Set k^{th} ensemble value to the posterior mean (using Kalman gain)

$$\begin{pmatrix}\theta \\ \eta(\theta)\end{pmatrix}_k = \begin{pmatrix}\theta_k \\ \eta(\theta_k)\end{pmatrix} + \Sigma_{\text{pr}}\mathcal{O}'(\mathcal{O}\Sigma_{\text{pr}}\mathcal{O}' + \mathcal{O}\Sigma_{\text{obs}}\mathcal{O}')^{-1}(y_k - \eta(\theta_k))$$

Ensemble Kalman smoother: ensemble version



Prior model: centered @ k^{th} ensemble

$$\begin{pmatrix} \theta \\ \eta(\theta) \end{pmatrix}_k \sim N\left(\begin{pmatrix} \theta_k \\ \eta(\theta_k) \end{pmatrix}, \Sigma_{\text{pr}} \right)$$

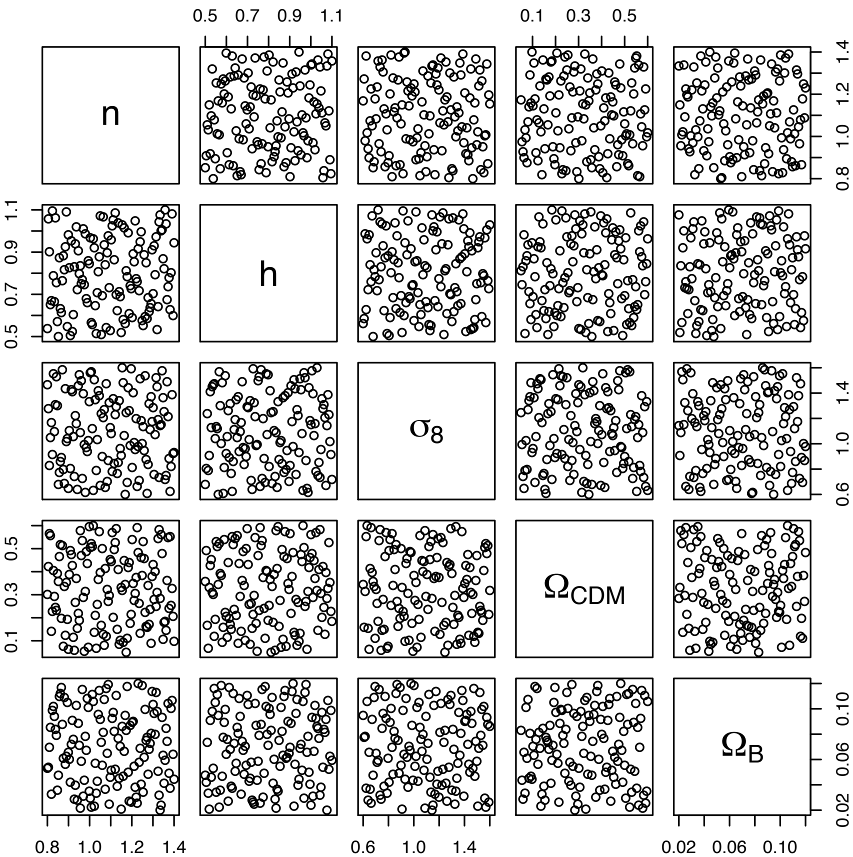
Observation model with perturbed data $y_k \sim N(y, \sigma^2)$

$$\begin{pmatrix} \theta \\ \eta(\theta) \end{pmatrix}_k \sim N\left(\mu_{\text{obs}} = \begin{pmatrix} \star \\ y_k \end{pmatrix}, \Sigma_{\text{obs}}^{-1} = \begin{pmatrix} 0 & 0 \\ 0 & \sigma_y^{-2} \end{pmatrix} \right)$$

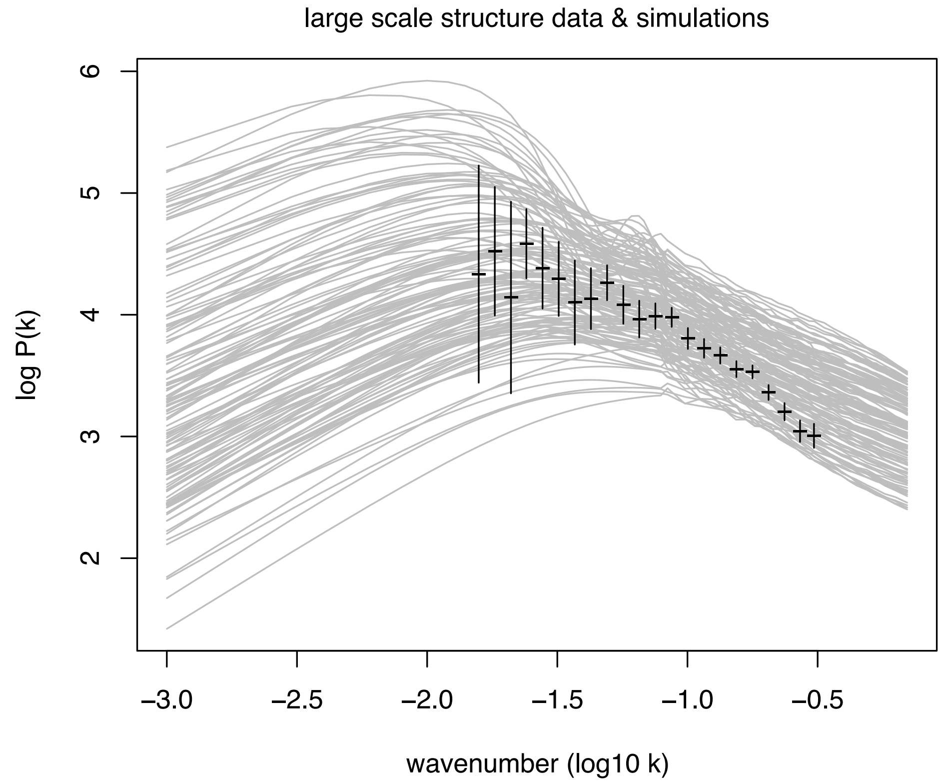
Set k^{th} ensemble value to the posterior mean

$$\begin{pmatrix} \theta \\ \eta(\theta) \end{pmatrix}_k = \left(\Sigma_{\text{pr}}^{-1} + \Sigma_{\text{obs}}^{-1} \right)^{-1} \left(\Sigma_{\text{pr}}^{-1} \begin{pmatrix} \theta_k \\ \eta(\theta_k) \end{pmatrix} + \Sigma_{\text{obs}}^{-1} \begin{pmatrix} \star \\ y_k \end{pmatrix} \right)$$

Cosmology application: large scale structure

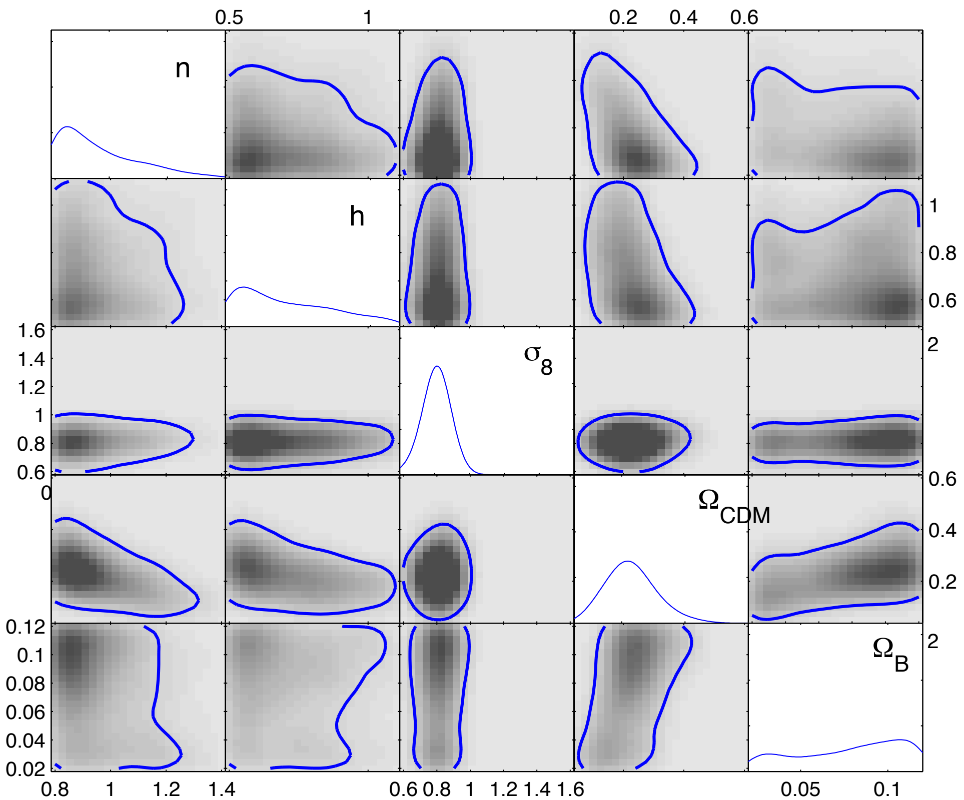


Ensemble parameter design

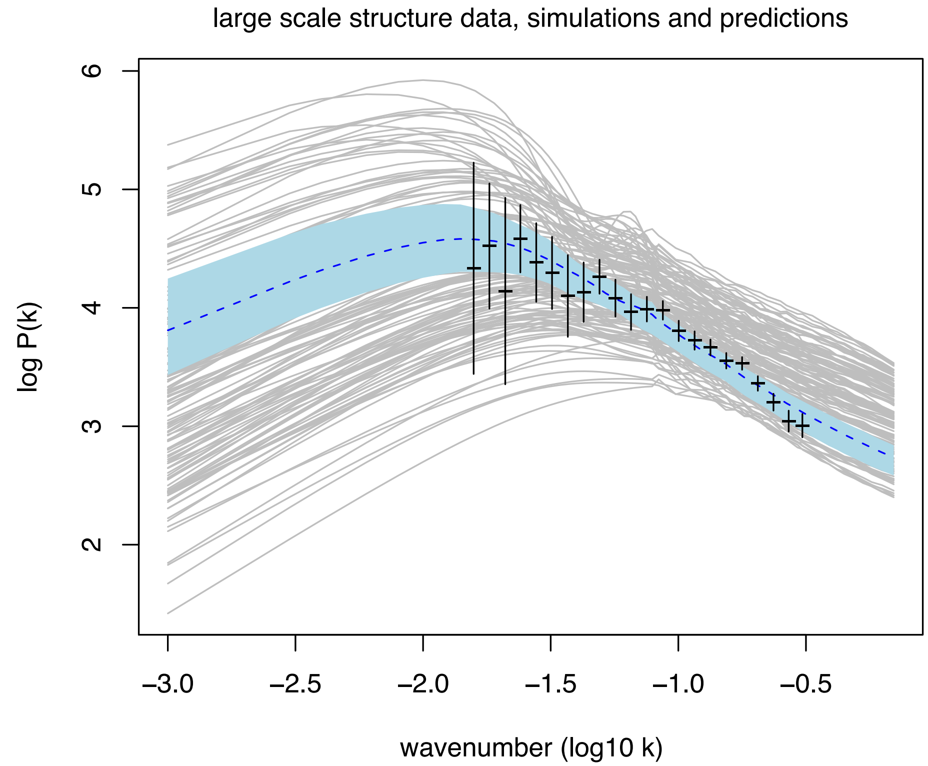


Resulting Matter Spectra & Data

Cosmology application: large scale structure



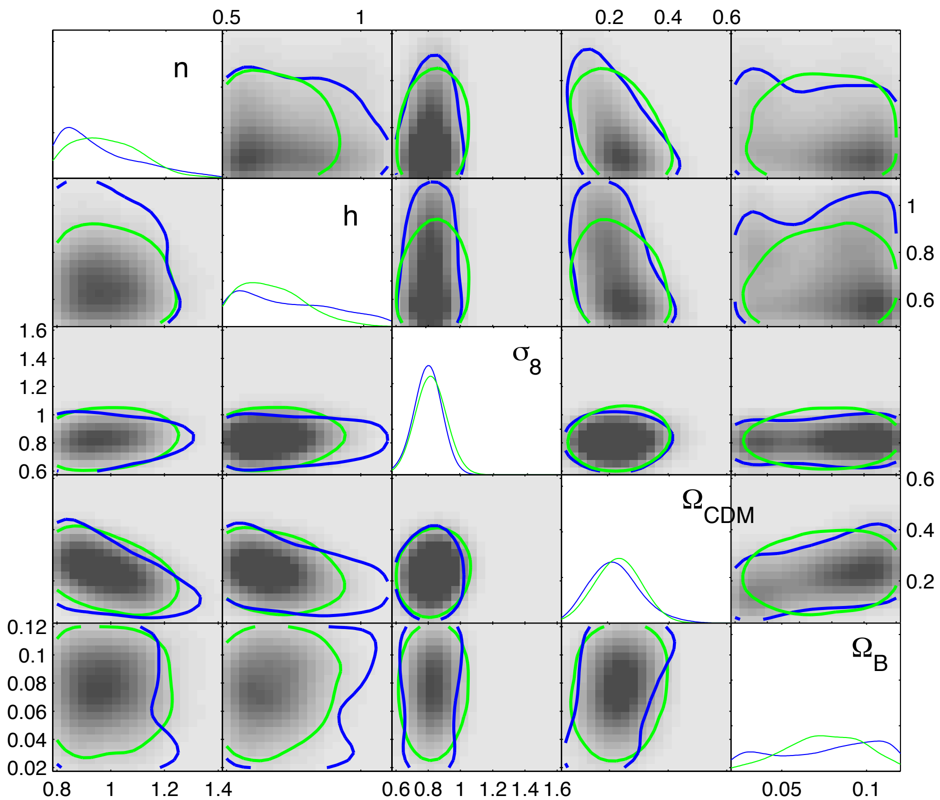
Posterior Parameter Density



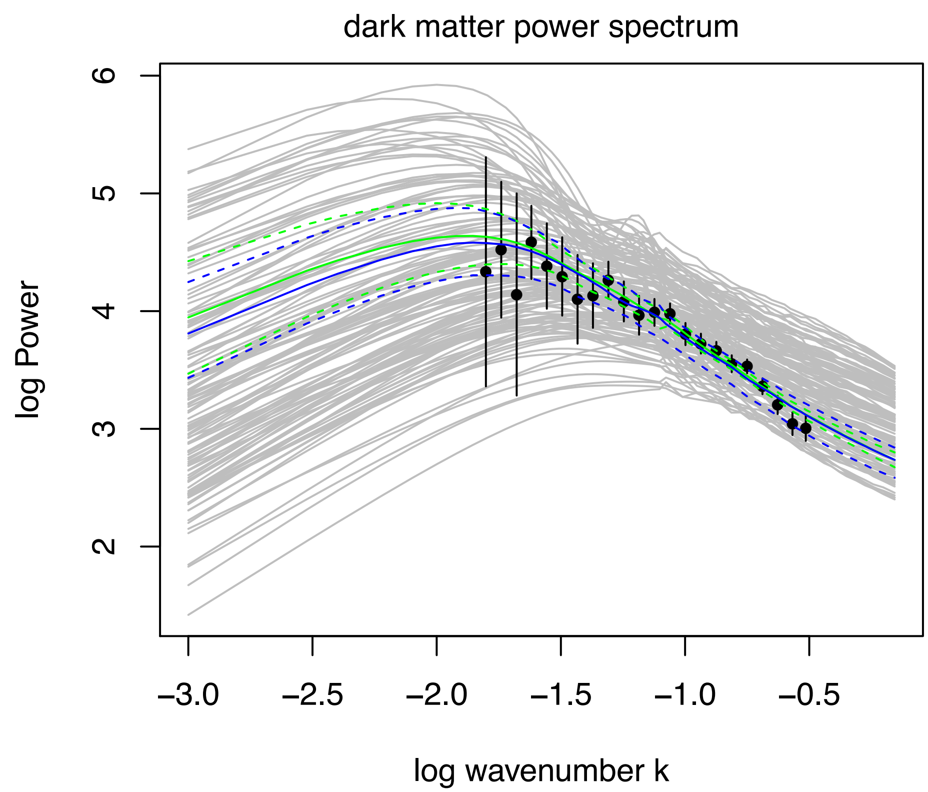
Matter Spectrum Estimate

GP-based Emulator

Cosmology application: large scale structure



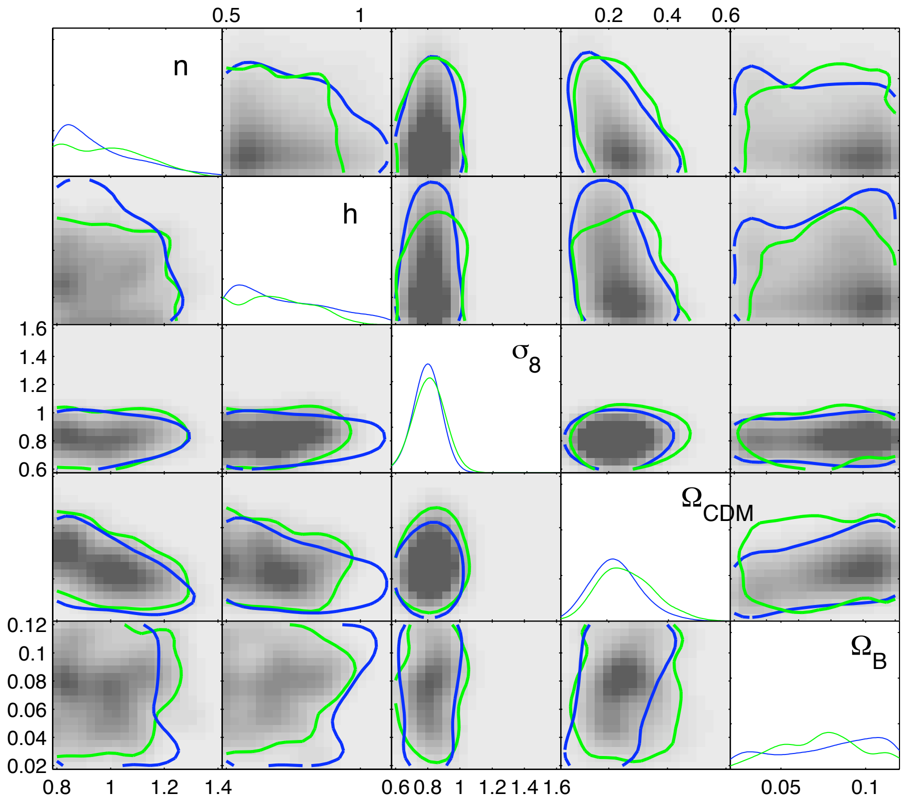
Posterior Parameter Density



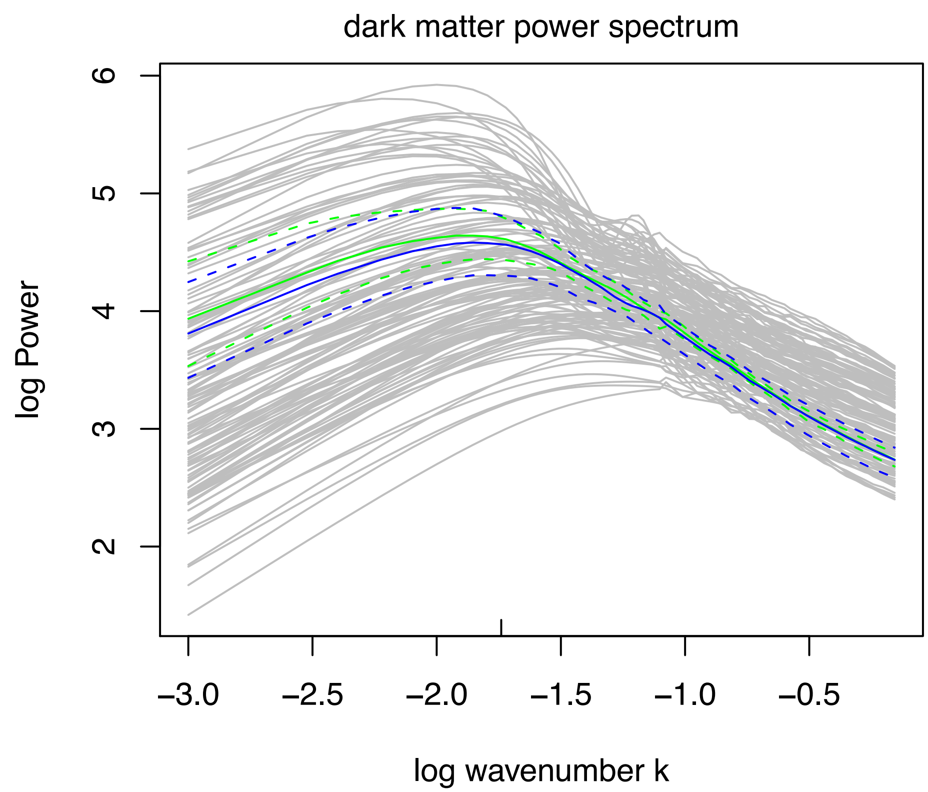
Matter Spectrum Estimate

GP-based Emulator vs. EnKS (normal)

Cosmology application: large scale structure



Posterior Parameter Density



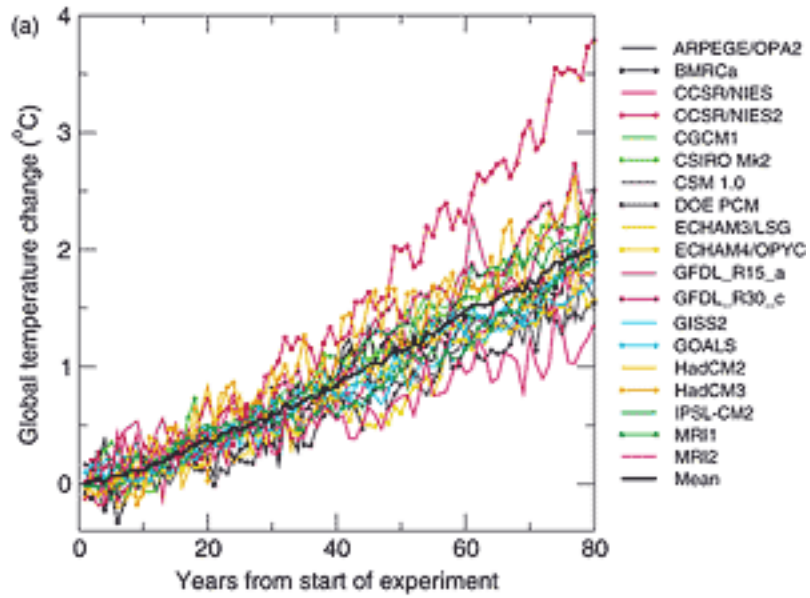
Matter Spectrum Estimate

GP-based Emulator vs. EnKS (ensemble)

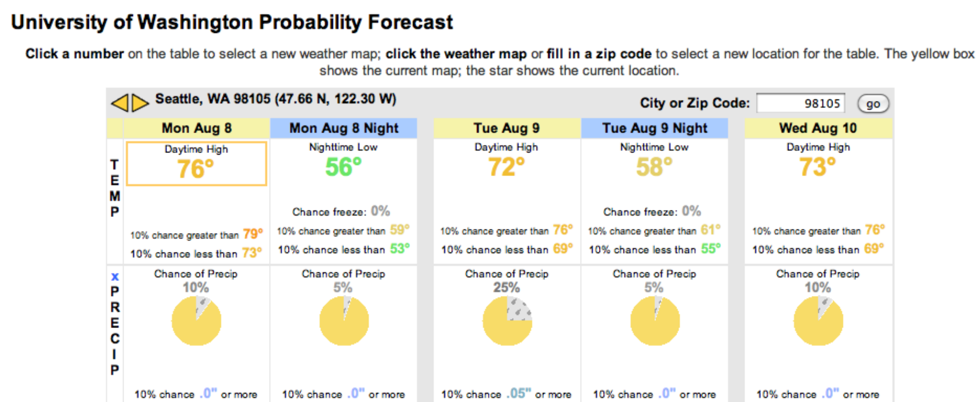
Multi-model ensembles

- To get at structural error (discrepancy or model-form error)
- Typically combined using Bayesian model averaging, mixture of experts, …
- Notable successes in cyborg applications
- Difficult in extrapolations – models not independently centered around the truth
- Can ensembles of models be constructed with assessing model error in mind?

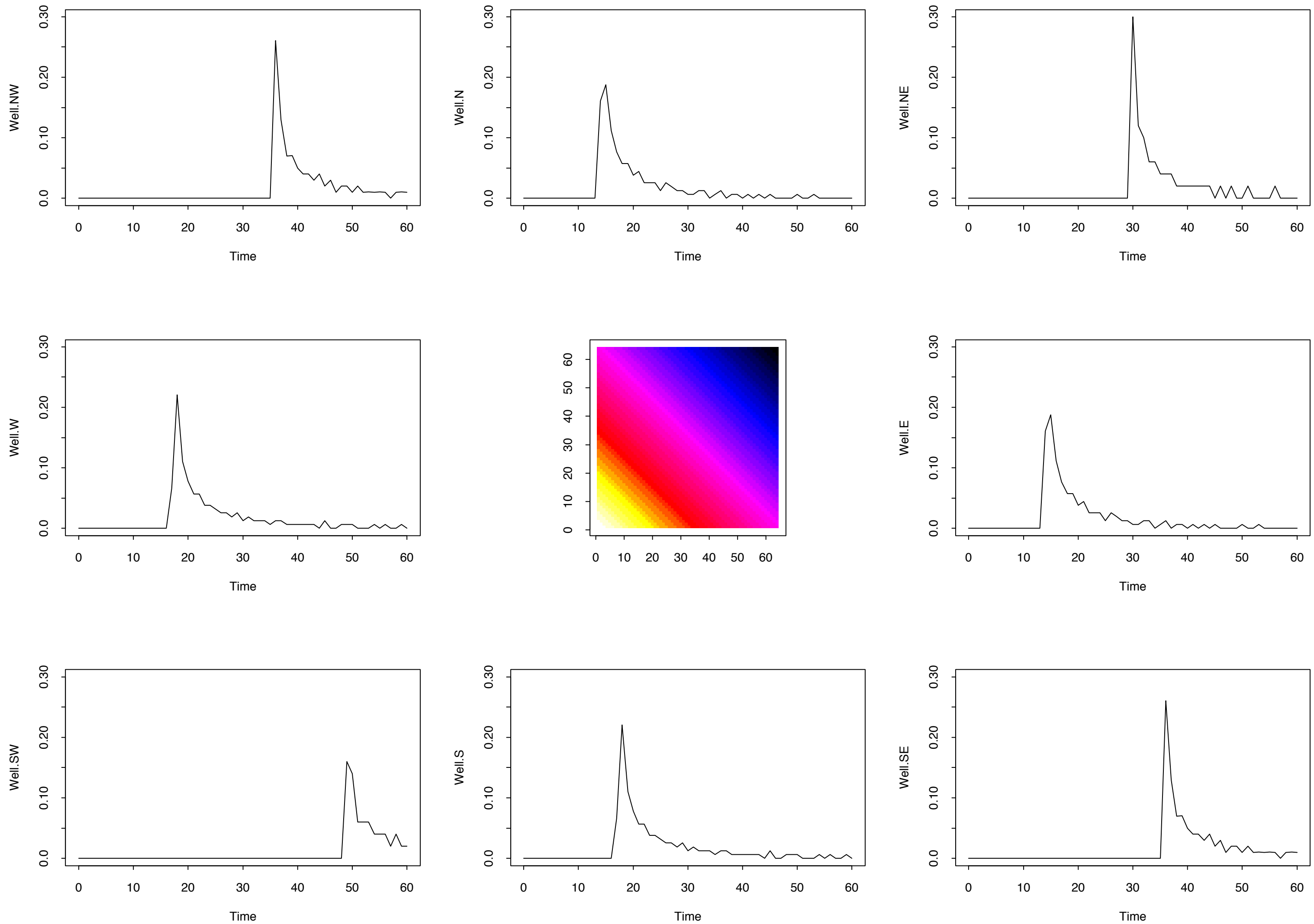
IPCC



Probcast: Gneiting and Raftery (2005+)

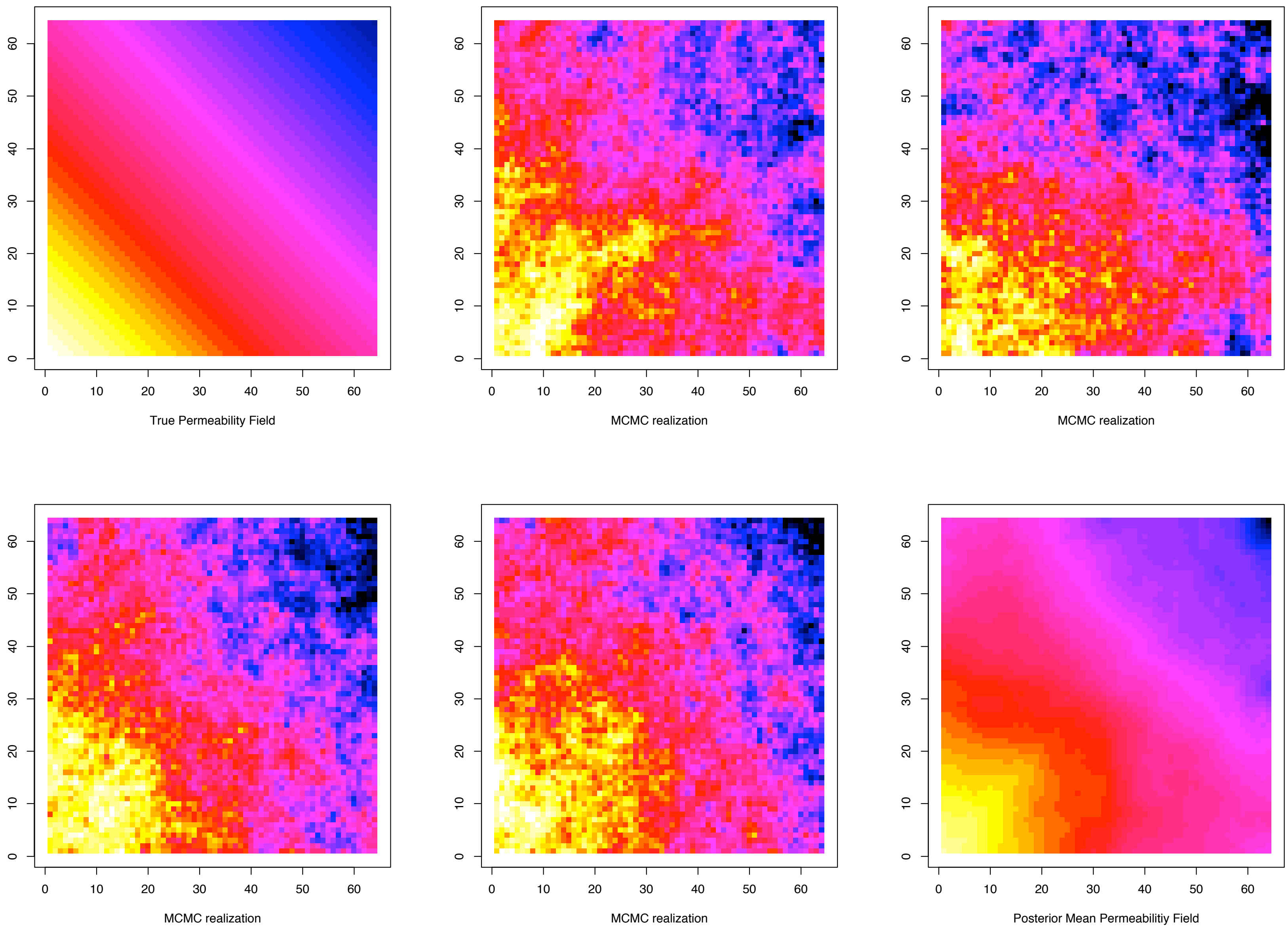


Highly parameterized model from hydrology



$$\pi(\theta|y) \propto L(y|\eta(\theta)) \times \pi(\theta) \qquad \pi(\theta|y) \propto \prod_{i=1}^{8} \exp\{\frac{1}{2\sigma^2}(y_i - \eta(\theta)_i)\} \times \exp\{\theta^T W \theta\}$$

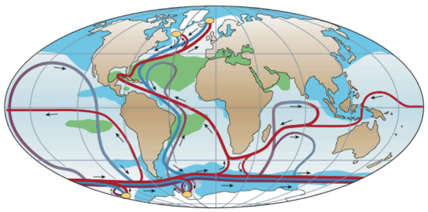
Samples from the posterior distribution



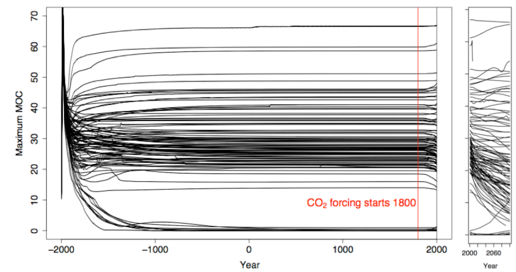
Rare, high consequence events

- PRA ideas:
  - Scenarios
  - consequences
  - chances
- Often involves catastrophic failure – a difficult process to model
- Rare ➔ estimation of small probabilities
- Rare ➔ difficult to compare to reality
- Difficult in extrapolation applications – are all important processes in the model?
- Build models to cater to such events?

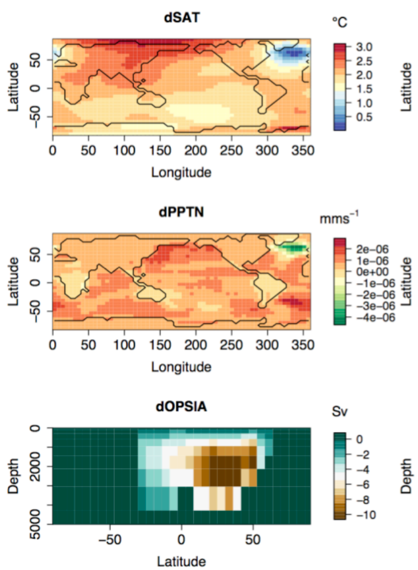
Hunting down high-consequence events: collapse of MOC circulation in 2100



Goal: estimate 33%-tile of MOC reduction in 2100 given a particular carbon



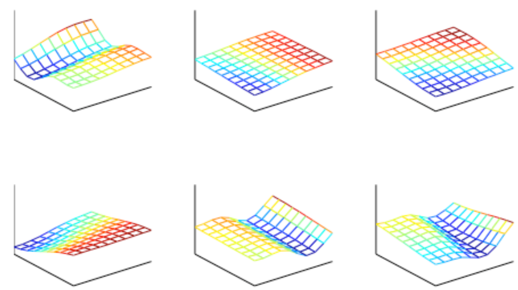
Track MOC strength over time for an ensemble of climate simulations varying 8 different inputs



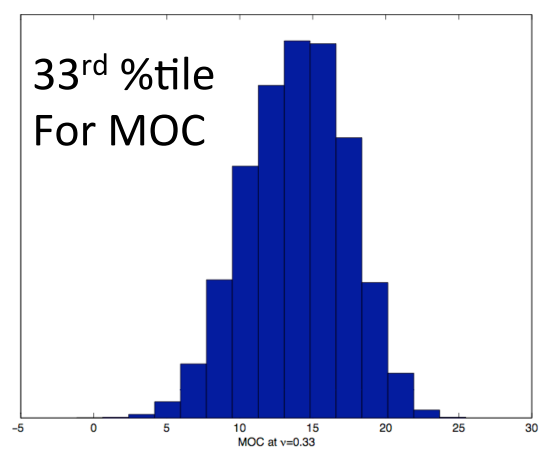
Use GENIE-1, a medium complexity climate model

64 long. X 30 lat. X 8 depth.

Use scalar measure of MOC strength.

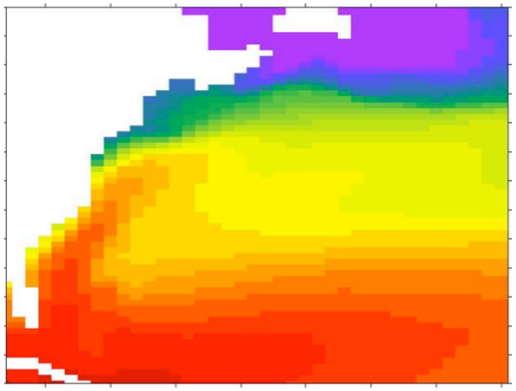


Estimate response surface of MOC strength at 2100 as a function of the 8-d inputs



Resulting estimate of the 33rd %-tile of MOC strength in 2100. This estimate uses prior uncertainties elicited via expert judgment.

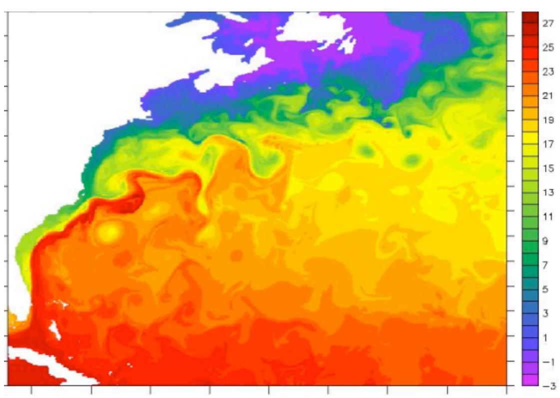
IPCC class ocean model
for climate simulations



1.0º×1.0º grid

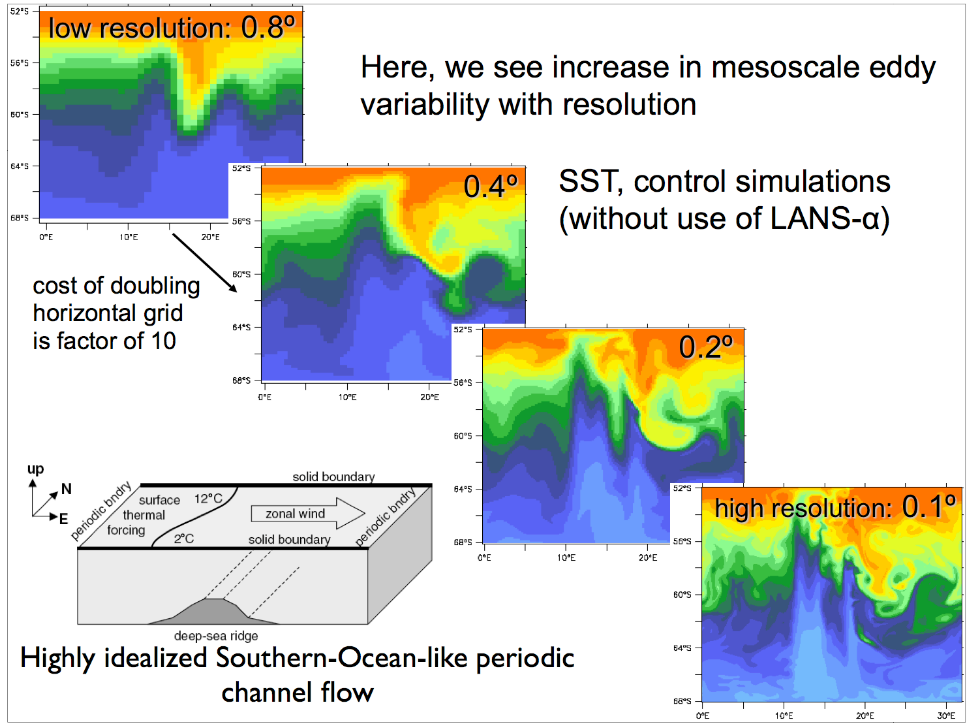
Factor of ~10 additional computational effort for each doubling of resolution

Strongly eddying simulation



0.1º×0.1º grid

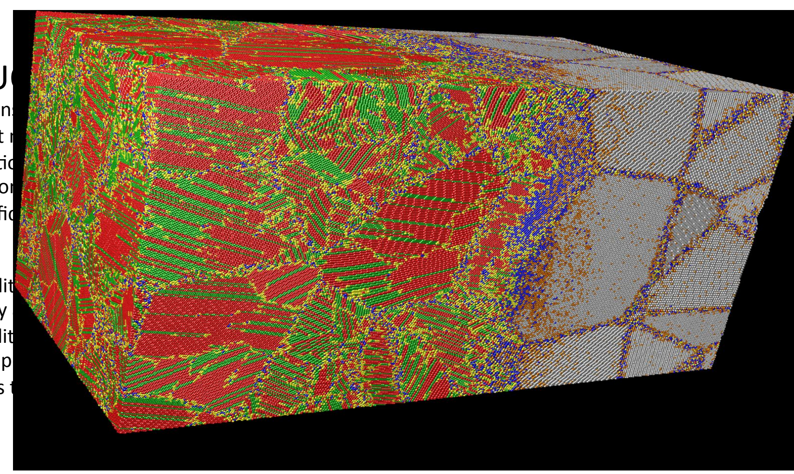
Bridging Resolutions



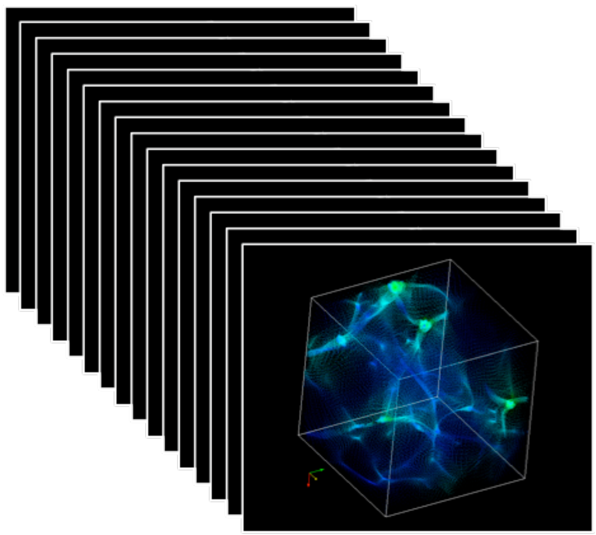
Highly idealized Southern-Ocean-like periodic channel flow

The U … tion from
simulation…
• The first … ings using a
combinatio…
• The seco … y features of
the high fi…

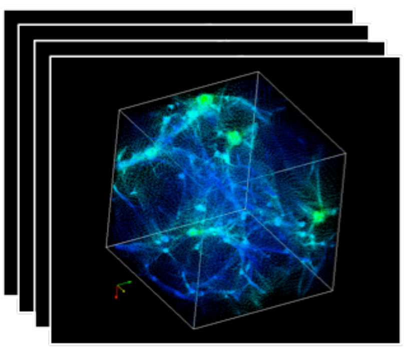
High fideli … UQ tasks such as
sensitivity … runs is infeasible for
high-fideli … er resolution runs we
have the p … he computational
resources …



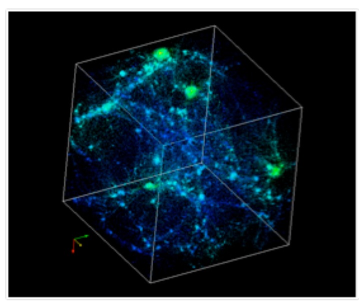
Multiple Runs at Multiple Resolutions



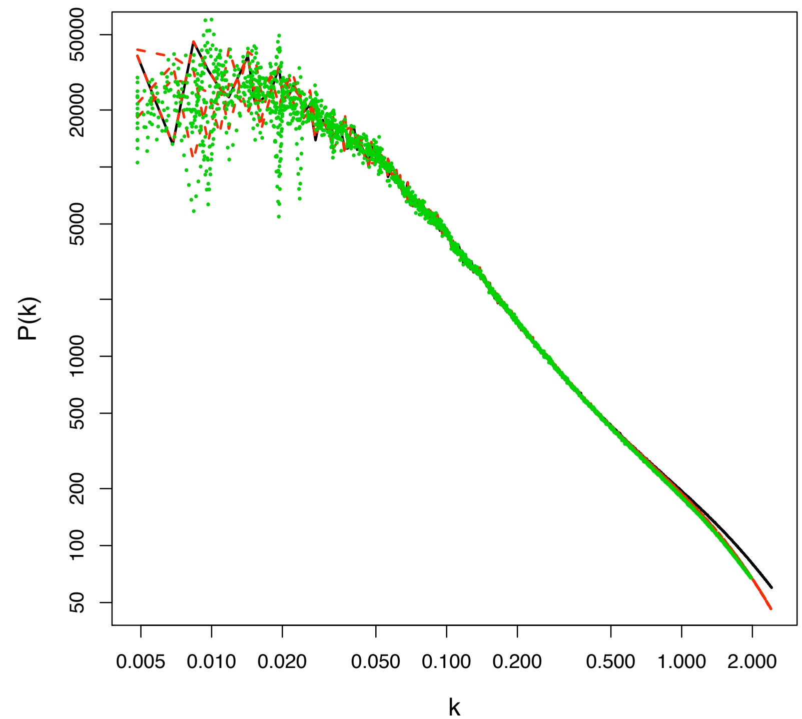
16 simulations



4 simulations



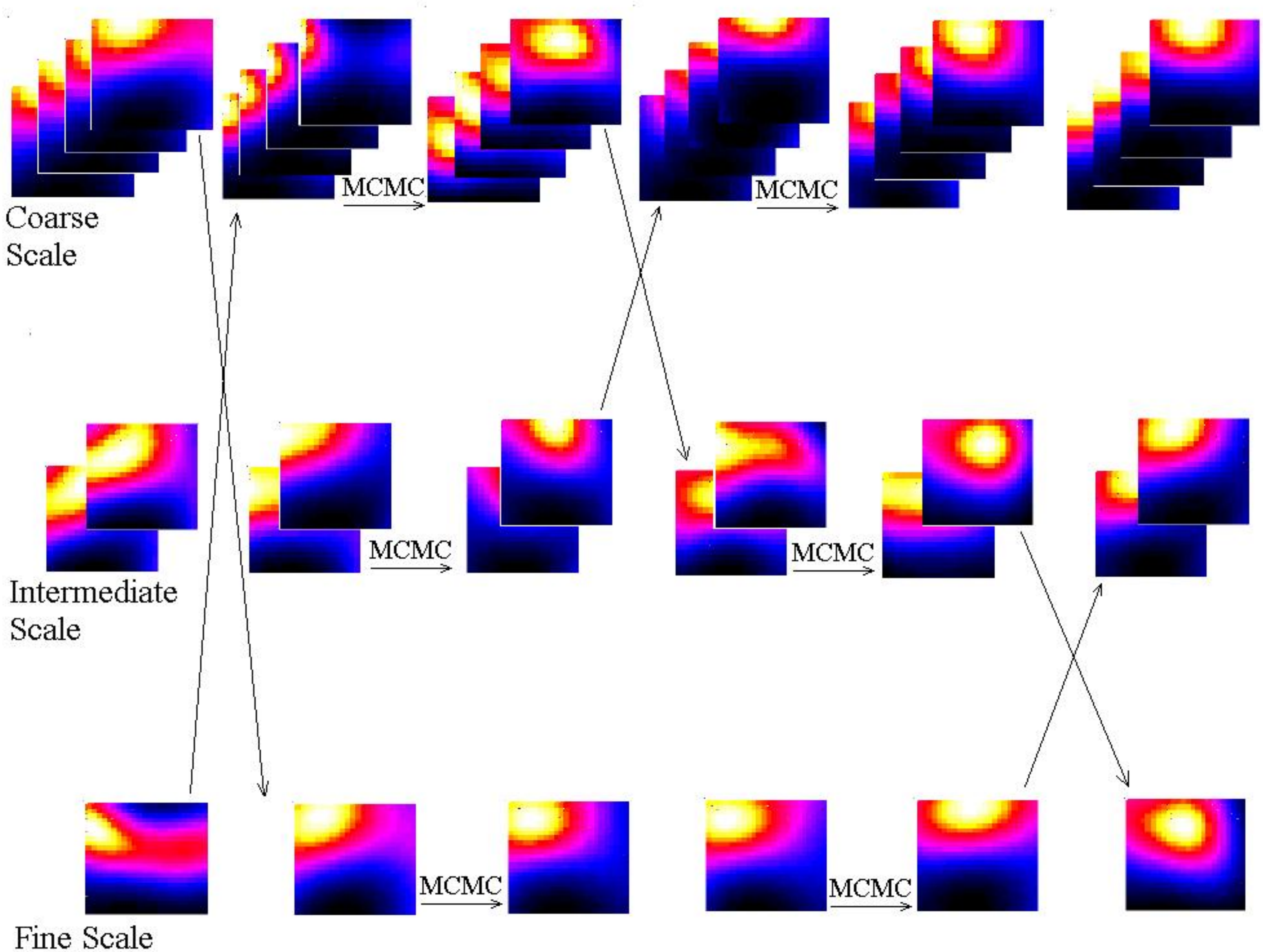
1 simulation



16 random initializations
> 20 TB to store simulation output

37 + 1 cosmologies; Cloud-in-cell FFT-based Poisson solver; 512^3, 1024^3 and 2048^3 particles

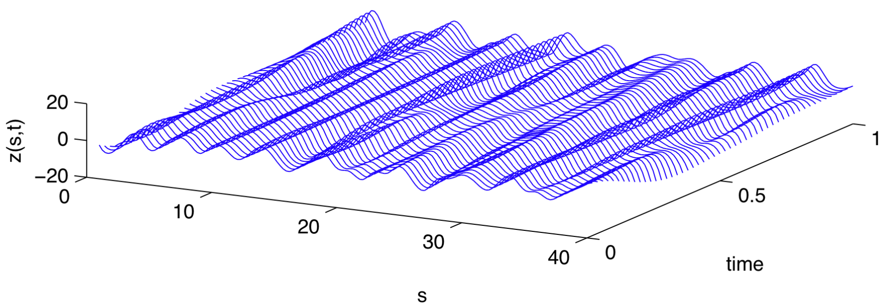
Multiple fidelities can speed up sampling uncertainties



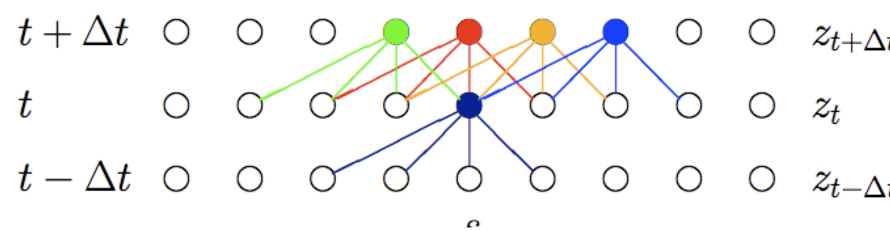
Exchange traditional computational models for UQ friendly implementations

PDE Solver

$$\frac{\partial}{\partial t} z(s,t) = [z(s+1,t) - z(s-2,t)]z(s-1,t) - z(s,t) + F$$



Markov Random Field



Constructing forward models and adjoints

- Very informative in high-dimensional problems
- Can help in building response surface
- Can facilitate MCMC or other UQ algorithms

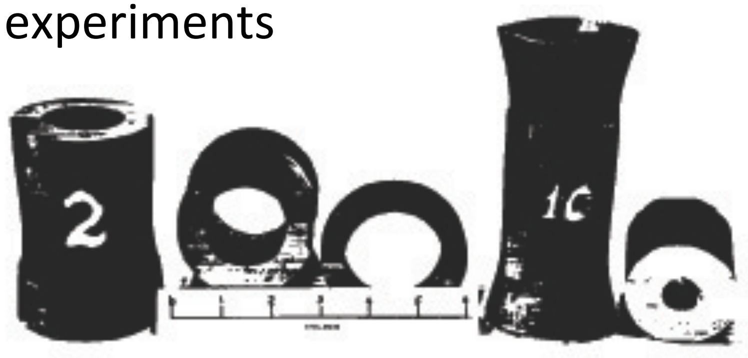
Exploiting new, heterogeneous, high performance computing architectures

Ending thoughts on calibration & UQ

- Design – choosing input settings at which to run model
  - Adaptive approaches
  - Searching for high-consequence events
- Dealing with extrapolations
  - Need to understand what predictions are/are not extrapolations
  - Need to mark out conditions in which model predictions can be trusted
  - Multiple model approaches
  - Theoretical approaches (e.g. bounding tail probabilities, bounding model errors)
- Making use of lower fidelity and/or reduced models to speed up exploration of input space
- Resource allocation
  - What new data sources impact uncertainties? By how much?
  - What is the most cost effective way to reduce our uncertainties?
- Other settings:
  - Physically constrained models and limited amounts of data vs. weaker, empirical models with large amounts of physical observations.

Implosion experiments at LANL

Neddermeyer’s 1943 implosion experiments



2005 implosion experiment at the DARHT facility

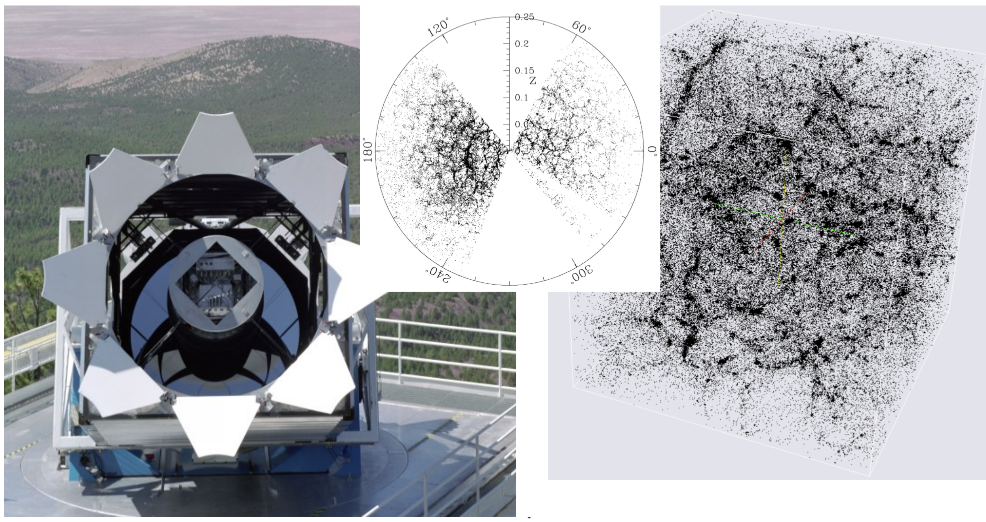
This basic template for cosmology is applicable in other scientific investigations

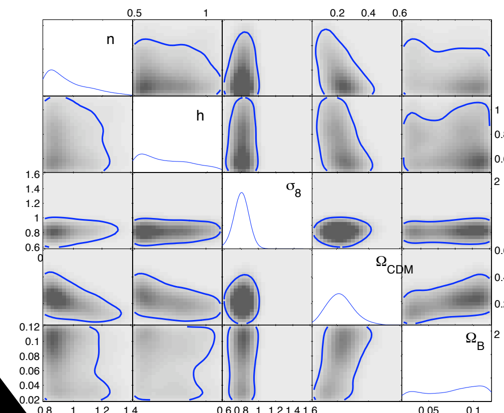
Observation/experiment

simulations

Calibration: finding parameter settings consistent with observations

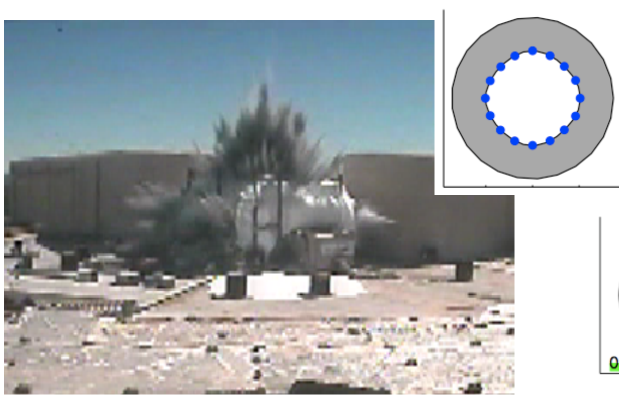
large scale structure of universe



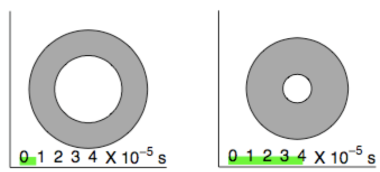


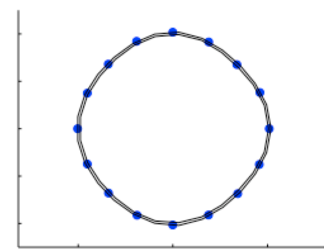
prediction uncertainties

Hydrodynamic behavior



notional data & simulations





Statistical framework $y(x_i) = \eta(x_i, \theta) + \epsilon_i$