Density Estimation Framework for Model Error Assessment

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B. van Bloemen Waanders, H. Michelsen, R. Bambha

Sandia National Laboratories
Livermore, CA
Albuquerque, NM

AGU Fall Meeting
San Francisco
December 15-19, 2014

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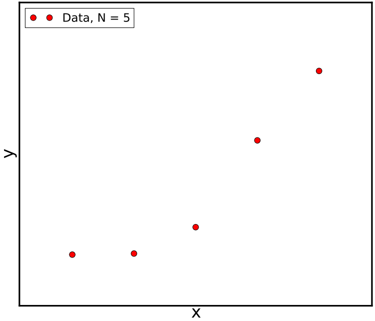
- DOE Office of Advanced Scientific Computing Research (ASCR), Scientific Discovery through Advanced Computing (SciDAC)
- Sandia National Labs Laboratory Directed Research and Development (LDRD) Program
- DOE Office of Basic Energy Sciences (BES), Div. of Chem. Sci., Geosci., & Biosci.

Motivation

- All models are wrong, but some are useful *[George Box]*
- Models of physical systems rely on
  - Presumed theoretical framework
  - Mathematical formulation
  - Simplifying assumptions, parameterizations
  - Numerical discretization of governing equations
  - Computational software & hardware
- Model error is frequently non-negligible
- Estimating model error is useful for
  - Model validation
  - Model comparison
  - Scientific discovery and model improvement
  - Reliable computational predictions

Motivation



Model-data fit

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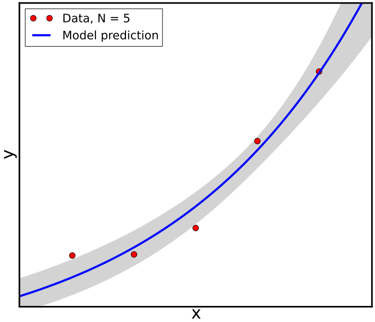

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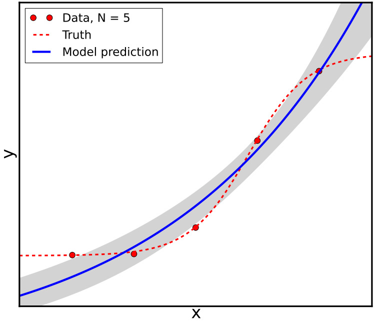

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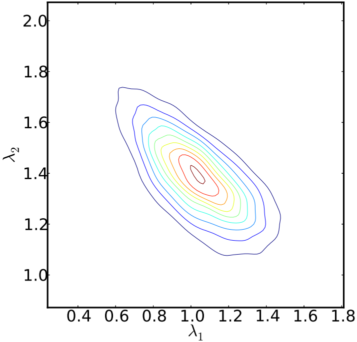

Calibrated parameters

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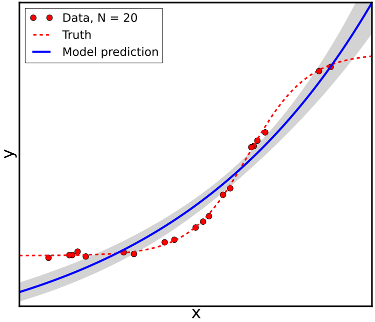

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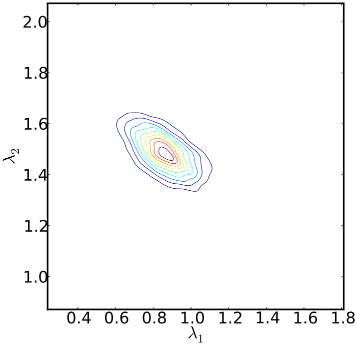

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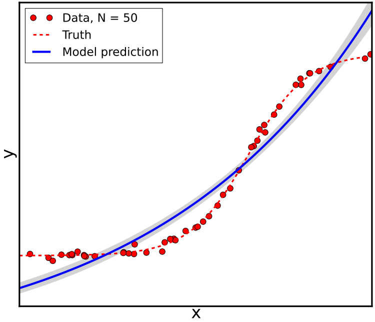

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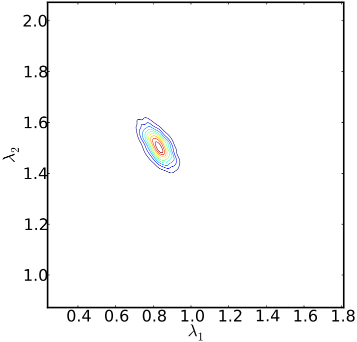


Calibrated parameters

- If the model has structural errors, more data does not help!
- We target model-vs-truth discrepancy

State-of-the-art: Issues for physical models

$$y_i = \underbrace{f(x_i; \lambda) + \delta(x_i)}_{\text{truth}} + \epsilon_i^{\text{d}}$$

- Explicit additive statistical model for model error $\delta(x)$ Kennedy-O'Hagan (2001).
- Calibrated predictive model $y_{mod}(x) = f(x; \lambda) + \delta(x)$

- Potential violation of physical constraints
  - *e.g.* incompressible flow: $\nabla \bullet v = 0$
- Disambiguation of model error $\delta(x_i)$ and data error ϵ_i^{d}
- Calibration of model error on measured observable does not impact the quality of model predictions on other QoIs

Model error embedding: key idea

- Ideally, modelers want predictive *errorbars*:
  inserting randomness on the outputs has issues, so...
- Cast input parameters λ as a random variable Λ
  Black-box

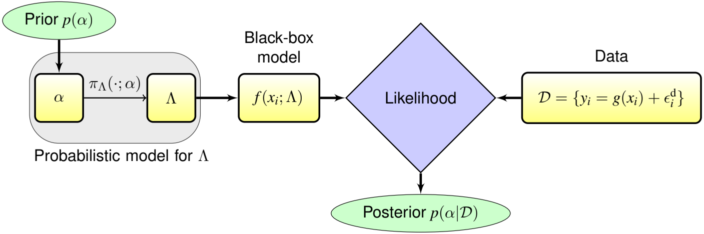
$$y_i = f(x_i; \Lambda) + \epsilon_i^{\mathrm{d}}$$

- More generally, explore additional parameterizations,
  Extra 'physics'

$$y_i = \tilde{f}(x_i; \lambda, \Theta) + \epsilon_i^{\mathrm{d}}$$

- Calibration turns into density estimation
  - Object of inference is PDF of Λ, not parameter λ
- Back to calibration: parameterize $\pi_\Lambda(\cdot; \alpha)$ and calibrate for α
  - E.g. Multivariate Normal, or Polynomial Chaos

Model error embedding: features



- Embed model error in specific submodel phenomenology
    - a modified transport or constitutive law
    - a modified formulation for a material property
- Allows placement of model error term in locations where key modeling assumptions and approximations are made
    - as a correction or high-order term
    - as a possible alternate phenomenology
- Naturally preserves model structure and physical constraints

Model error embedding: Bayesian formulation

- Consider the simplest setting with no data noise, *i.e.* $\epsilon_i^{\mathrm{d}} = 0$.
- In the simplest setting, cast λ as a random variable Λ
  Black-box $$y_i = f(x_i; \Lambda)$$
- Calibration turns into density estimation for the PDF of Λ
- Polynomial Chaos parameterization for $\Lambda = \sum_{k=0}^{K} \alpha_k \Psi_k(\xi)$
- Back to parameter estimation, now for $\alpha = (\alpha_0, \ldots, \alpha_K)$

- Bayesian setting $$\underbrace{p(\alpha|\mathcal{D})}_{\text{Posterior}} \propto \underbrace{L_{\mathcal{D}}(\alpha)}_{\text{Likelihood}} \underbrace{p(\alpha)}_{\text{Prior}}$$
  - Full Likelihood $L_{\mathcal{D}}(\alpha) = p(\mathcal{D}|\alpha) = p(y_1, \ldots, y_N|\alpha)$
  - Marginalized Likelihood $L_{\mathcal{D}}(\alpha) \approx \prod_{i=1}^{N} p(y_i|\alpha)$
  - ABC Likelihood, see next

ABC Likelihood

With $\rho(\mathcal{S})$ being a metric of the statistic $\mathcal{S}$, use the kernel function as an ABC likelihood:

$$L_{\mathrm{ABC}}(\alpha) = \frac{1}{\epsilon} K\left(\frac{\rho(\mathcal{S})}{\epsilon}\right)$$

where ϵ is a ‘tolerance’ parameter. Require

- Uncertain prediction $p(y|D)$ is centered on the data
- The width of the distribution $p(y|D)$ is consistent with the spread of the data around the nominal model prediction

Propose the Gaussian kernel density:

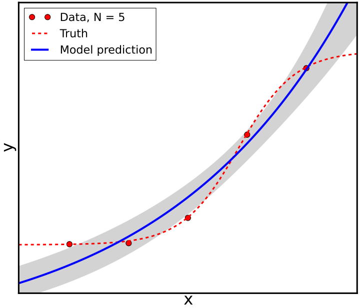
$$L_{\mathrm{ABC}}(\alpha) = \frac{1}{\epsilon\sqrt{2\pi}} \prod_{i=1}^{N} \exp\left(-\frac{(\mu_i(\alpha) - y_i)^2 + (\sigma_i(\alpha) - \gamma|\mu_i(\alpha) - y_i|)^2}{2\epsilon^2}\right)$$

Predictive moments: $\mu_i(\alpha) = \mathrm{E}_\Lambda[f(x_i;\Lambda)]$ $\sigma_i^2(\alpha) = \mathrm{V}_\Lambda[f(x_i,\Lambda)]$

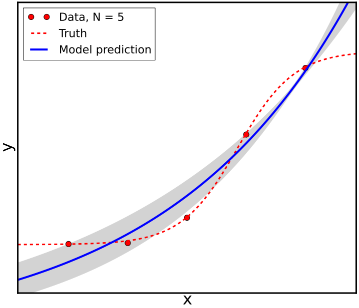
Predictions account for model error: example 1

Calibrating an exponential model $f(x;\lambda_1,\lambda_2) = \lambda_2 e^{\lambda_1 x} - 2$
with data from a hyperbolic tangent model $g(x) = \tanh(3(x-0.3))$

Additive Gaussian error



Embedded model error



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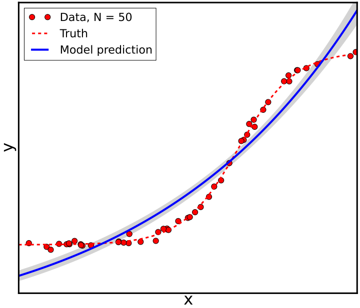

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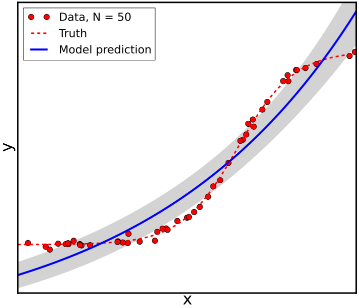
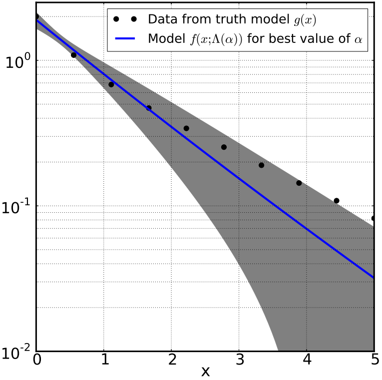


Predictions account for model error: example 2

Calibrating single-exponential models
with data from a double exponential model $g(x) = e^{-0.5x} + e^{-2x}$

Linear-exponential $f(x,\lambda) = e^{\lambda_1 + \lambda_2 x}$



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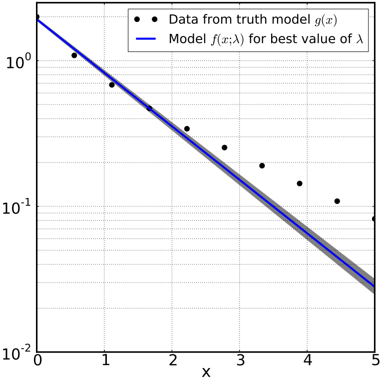

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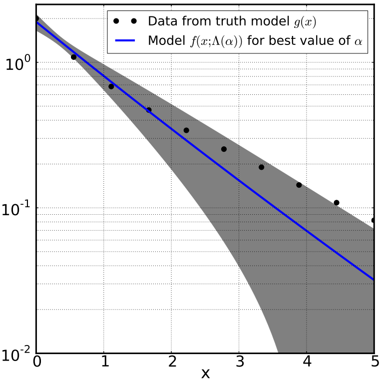
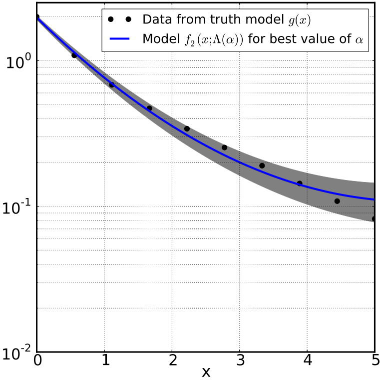


Quadratic-exponential $f_2(x,\lambda) = e^{\lambda_1 + \lambda_2 x + \lambda_3 x^2}$



TransCom3 Experiment of CO_2 Flux Inversion

[Gurney *et al.*, Tellus B, 2003]

- Observations $\mathbf{d}$ at $N = 77$ sites around the world
- Inverse problem: find fluxes $\mathbf{s}$ at $M = 22$ locations
- Linearized 'response' model $\mathbf{R}$, such that $\mathbf{d} \approx \mathbf{R}\mathbf{s}$

$$\mathbf{d} = \mathbf{R}\mathbf{s} + \epsilon_{\mathbf{d}}$$

- Model $\mathbf{R}$ is never perfect thus contaminating the inversion
- The inferred values of $\mathbf{s}$ compensate for model deficiencies
- $\epsilon_{\mathbf{d}}$ is meant to capture data errors, but is 'entangled' with model errors

TransCom3 Experiment of CO_2 Flux Inversion

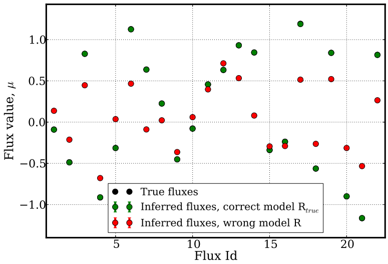
[Gurney *et al.*, Tellus B, 2003]

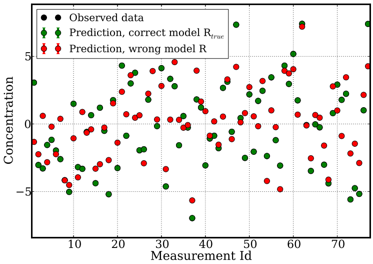
- Synthetic study: assume no measurement error
- Generate data from a true model $\mathbf{R}_{\text{true}}$ with exact flux values:

$$\mathbf{d} = \mathbf{R}_{\text{true}}\mathbf{s}_{\text{exact}}$$

- Infer $\mathbf{s}$
  - with the true model $\mathbf{d} \approx \mathbf{R}_{\text{true}}\mathbf{s}$, or
  - with a wrong model $\mathbf{d} \approx \mathbf{R}\mathbf{s}$

Additive Gaussian error





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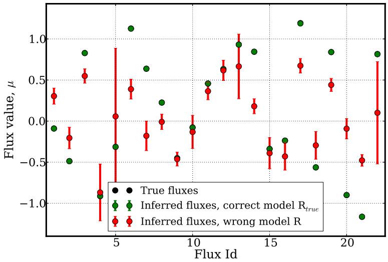
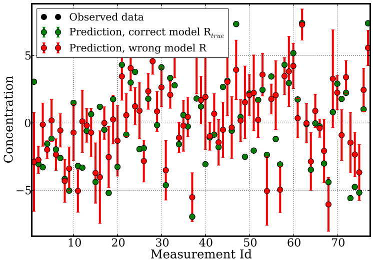
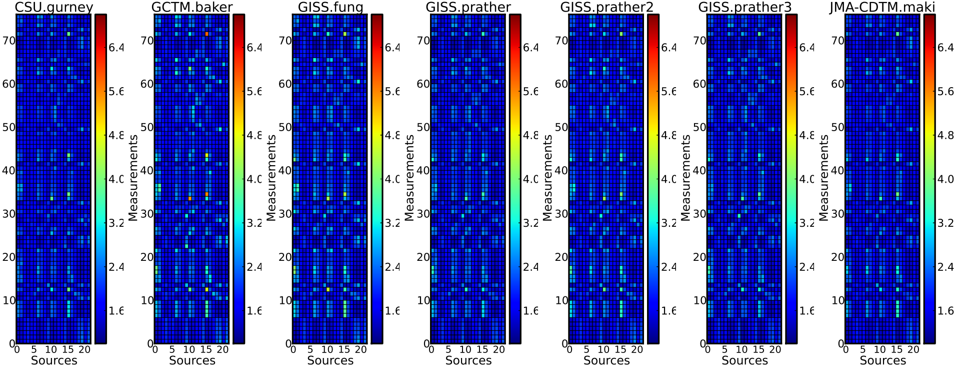
Embedded model error





Consider 14 different response models $\mathbf{R}$



Infer fluxes $\mathbf{s}$, given measurements $\mathbf{d}$ to satisfy $\mathbf{d} \approx \mathbf{Rs}$

- Conventional additive Gaussian error (least-squares): $\mathbf{d} = \mathbf{Rs} + \xi$
- Embed probabilistic model for fluxes s: $\mathbf{d} = \mathbf{R}(\mu_\mathbf{s} + \mathbf{C_s}\xi)$

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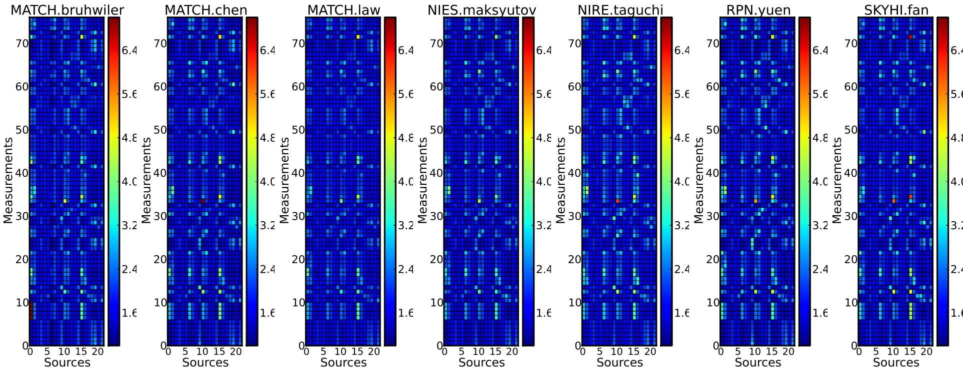

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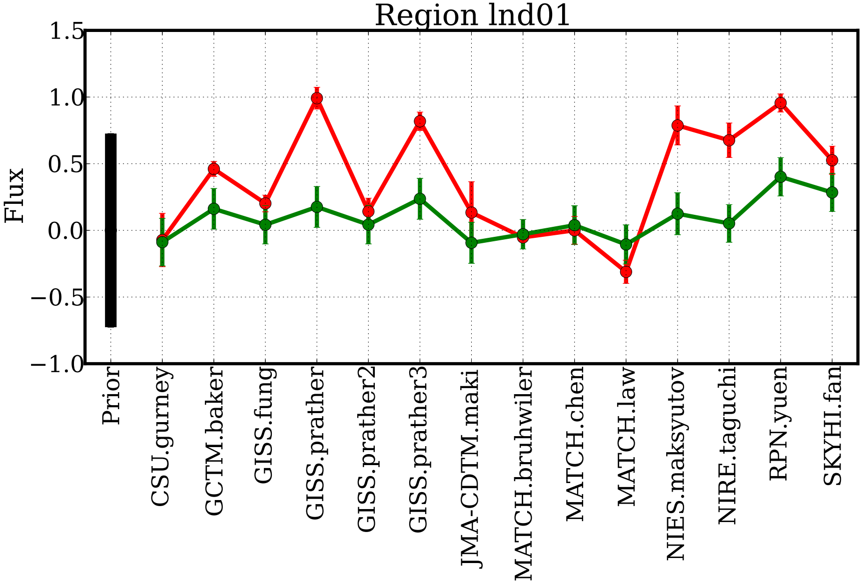
Inferred fluxes show less variability across models



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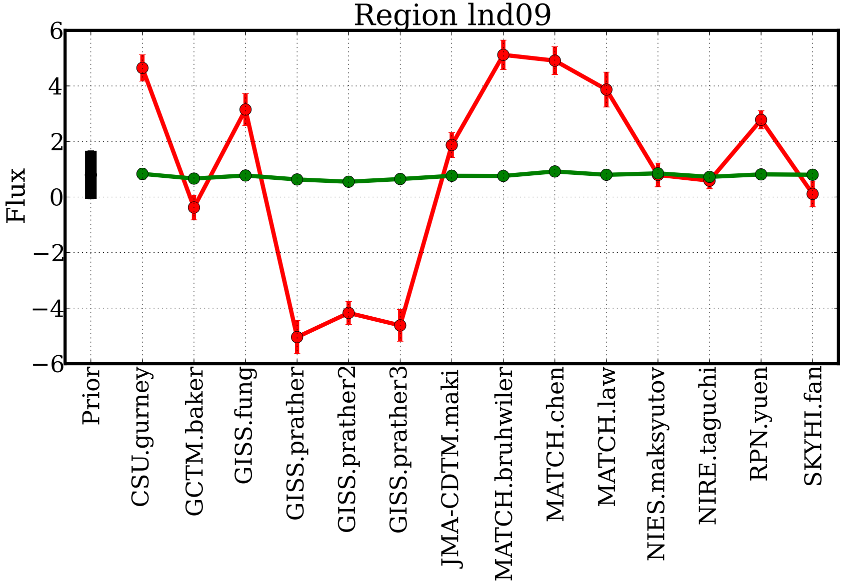

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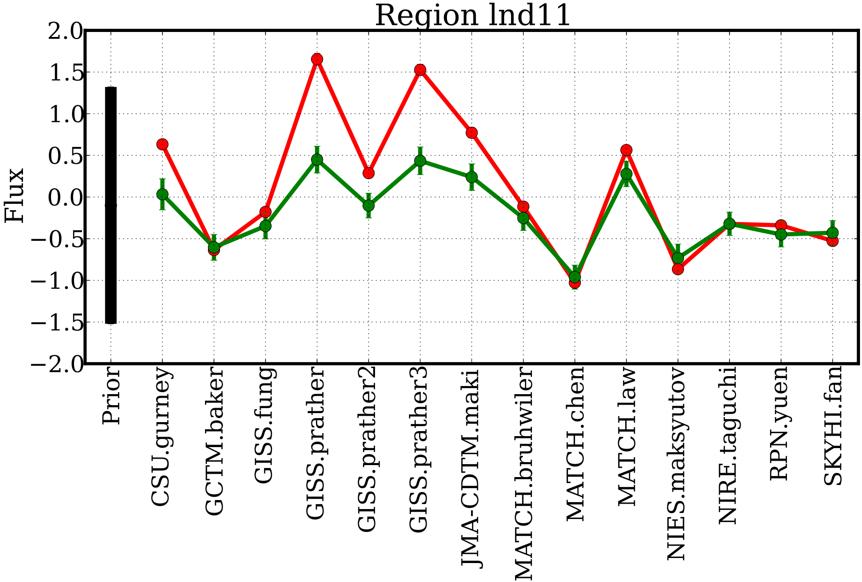

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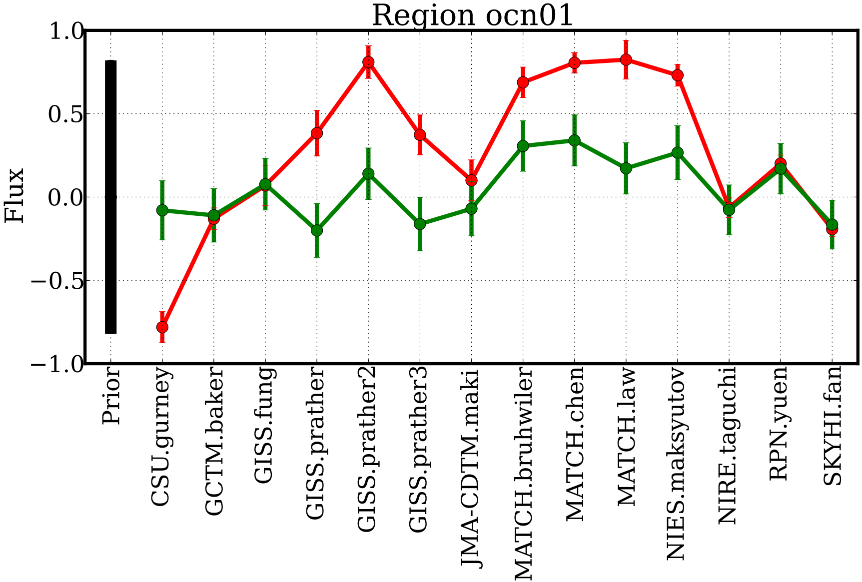

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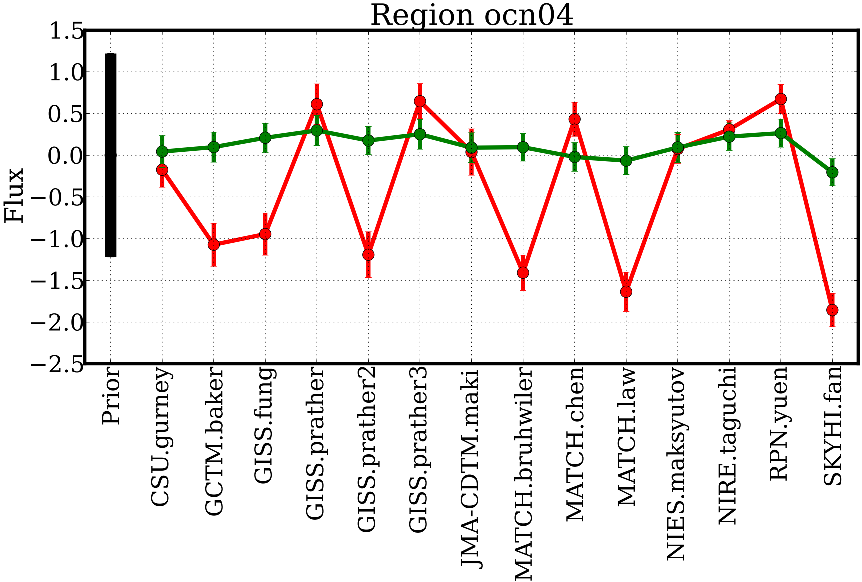

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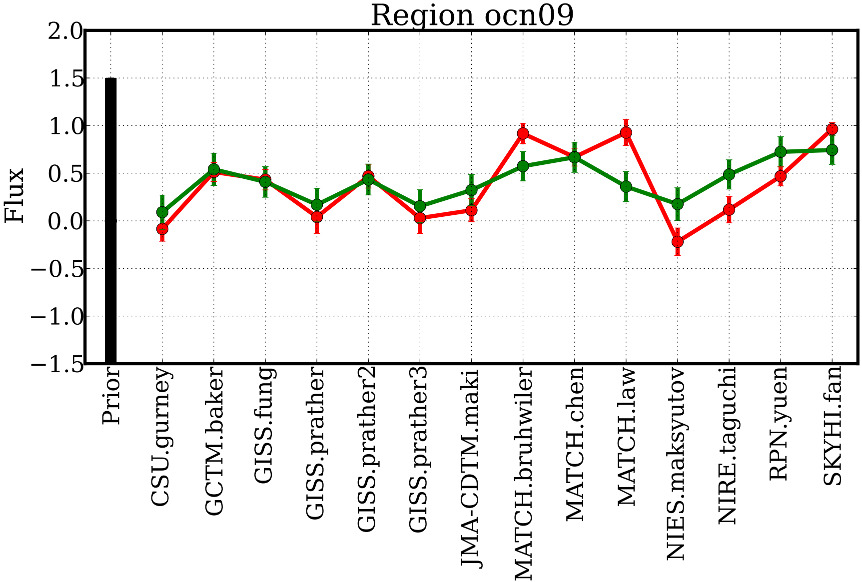

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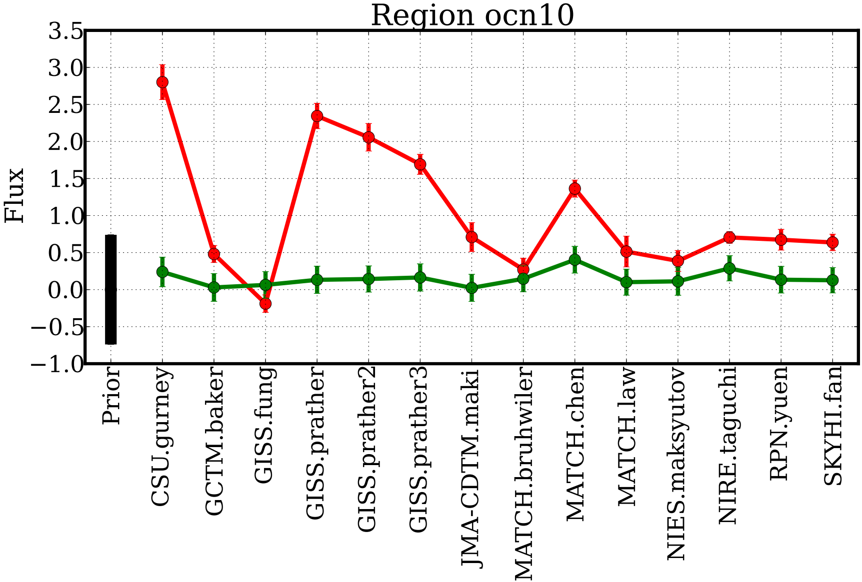

Summary

- A method for dealing with model discrepancy error that is targeted at physical models
- Reformulate the calibration as a density estimation problem
- Bayesian machinery to find parameters of the PDFs
- Approximate Bayesian Computation (ABC) targets constraints of interest to the modeler
- Model-to-model calibration
- (in progress) Extension to include data noise

- K. Sargsyan, H. Najm, and R. Ghanem. "On the Statistical Calibration of Physical Models". *International Journal for Chemical Kinetics*, in review.

Thank You

Model error embedding: Bayesian formulation

- Consider the simplest setting with no data noise, *i.e.* $\epsilon_i^{\mathrm{d}} = 0$.
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  Black-box
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  - ABC Likelihood, see next

Data-Model-Truth

- Measurements

$$\overset{\text{data}}{y_i} \;=\; \overset{\text{truth}}{g(x_i)} \;+ \overset{\text{data error}}{\epsilon_i^{\mathrm{d}}}$$

- Model

$$\overset{\text{truth}}{g(x_i)} = \overset{\text{model}}{f(x_i;\lambda)} \;+\; \overset{\text{model error}}{\delta(x_i)}$$

- Total error budget

$$y_i = \underbrace{f(x_i;\lambda) + \delta(x_i)}_{\text{truth } g(x_i)} + \epsilon_i^{\mathrm{d}}$$

Statistical modeling of errors in calibrating $f(x;\lambda)$

Data Error: $\epsilon_i^{\mathrm{d}} \sim \mathrm{N}(0,\sigma^2)$

Model Error: $\delta(x) \sim \mathrm{GP}(\mu(x), C(x,x'))$

Estimate model parameters λ along with those of $\delta(x)$, ϵ_i^{d}