# *Density Estimation Framework for Model Error Assessment*

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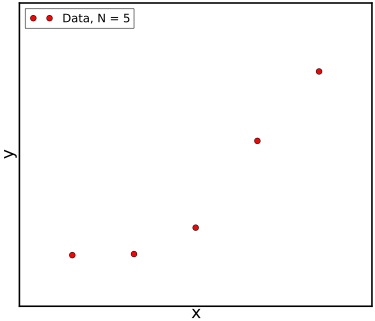
# Motivation

- 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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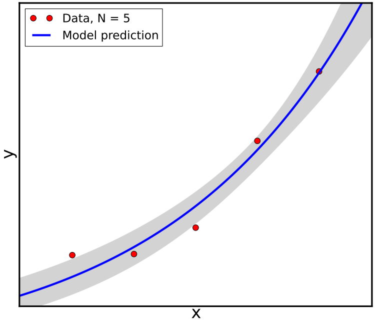


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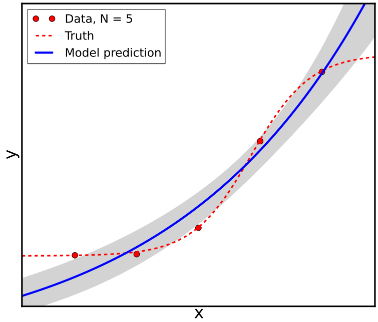


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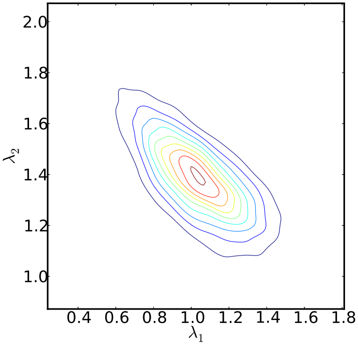


Calibrated parameters

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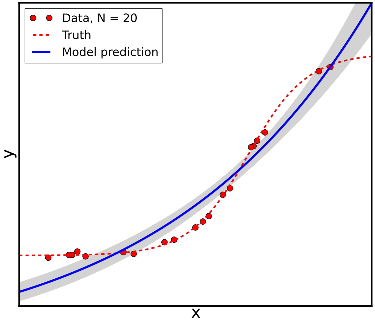


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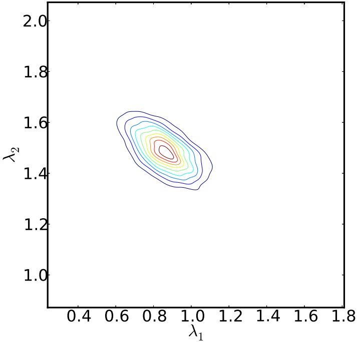


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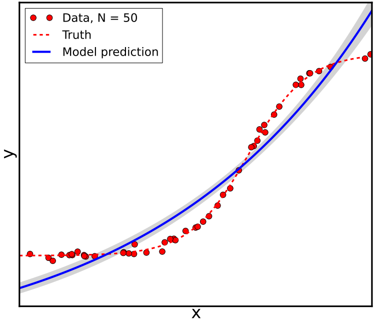


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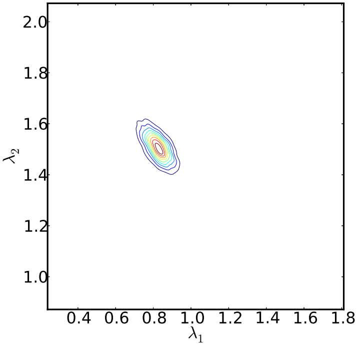



Calibrated parameters

- 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

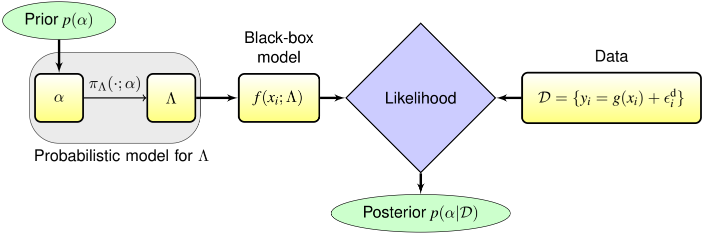
$$y_i = \underbrace{f(x_i;\lambda) + \delta(x_i)}_{\text{truth}} + \epsilon_i^{\mathrm{d}}$$

- Explicit additive statistical model for model error $\delta(x)$ Kennedy-O'Hagan (2001).
- Calibrated predictive model $\quad y_{mod}(x) = f(x;\lambda) + \delta(x)$
- Potential violation of physical constraints
  - *e.g.* incompressible flow: $\nabla \bullet v = 0$
- Disambiguation of model error $\delta(x_i)$ and data error $\epsilon_i^{\mathrm{d}}$
- 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* (PDF): inserting randomness on the outputs has issues, so...
- Cast input parameters $\lambda$ as a random variable $\Lambda$
  *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 $\Lambda$, not parameter $\lambda$
- Back to calibration: parameterize $\pi_\Lambda(\cdot; \alpha)$ and calibrate for $\alpha$
  - 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 $\lambda$ as a random variable $\Lambda$
  *Black-box*
  $$y_i = f(x_i; \Lambda)$$
- Calibration turns into density estimation for the PDF of $\Lambda$
- Polynomial Chaos $\Lambda = \sum_{k=0}^{K} \alpha_k \Psi_k(\xi)$
- Back to parameter estimation, now for $\alpha = (\alpha_0, \dots, \alpha_K)$
- Bayesian setting
  $$\underbrace{p(\alpha|\mathcal{D})}_{\text{Posterior}} \propto \underbrace{L_{\mathcal{D}}(\alpha)}_{\text{Likelihood}} \underbrace{p(\alpha)}_{\text{Prior}}$$
  - Likelihood $L_{\mathcal{D}}(\alpha) = p(\mathcal{D}|\alpha) = p(y_1, \dots, y_N|\alpha)$

# Approximate Bayesian Computation (ABC)

Employ a kernel density as a pseudo-likelihood to enforce select constraints:

- Uncertain prediction $p(y|D)$ is centered on the data
  - With $\mu_i(\alpha) = \mathrm{E}_\xi[f(x_i, \lambda(\xi;\alpha))]$:

    minimize $\| \mu_i(\alpha) - y_{\mathrm{data},i} \|_2^2$

- The width of the distribution $p(y|D)$ is consistent with the spread of the data around the nominal model prediction
  - With $\sigma_i^2(\alpha) = \mathrm{V}_\xi[f(x_i, \lambda(\xi,\alpha))]$:

    minimize $\| \sigma_i(\alpha) - \gamma|\mu_i(\alpha) - y_{\mathrm{data},i}| \|_2^2$

  - $\gamma$ is a factor that specifies the desired match between $\sigma_i$ and the discrepancy $|\mu_i(\alpha) - y_{\mathrm{data},i}|$, on average

# ABC Likelihood

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

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

where $\epsilon$ controls the severity of the consistency control

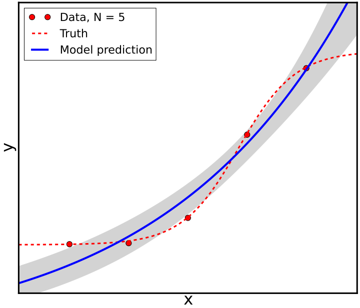
Propose the Gaussian kernel density:

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

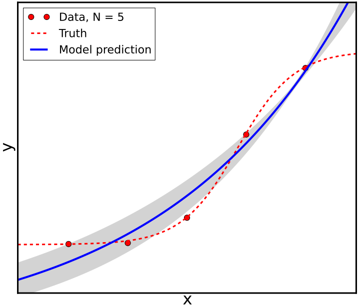
# Predictions account for model error: example 1

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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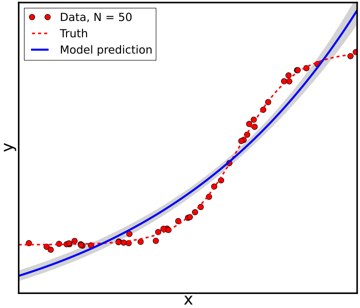


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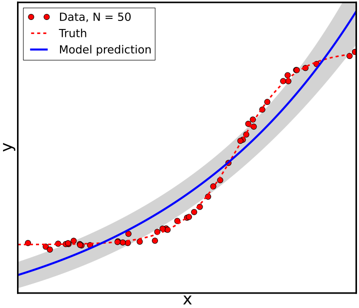

# Predictions account for model error: example 2

Calibrating single-exponential models
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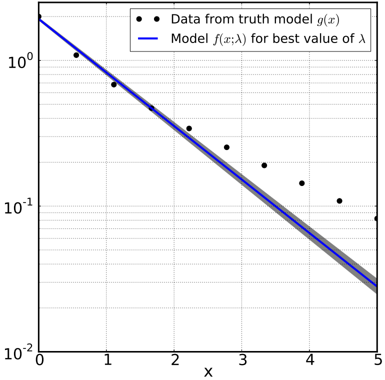
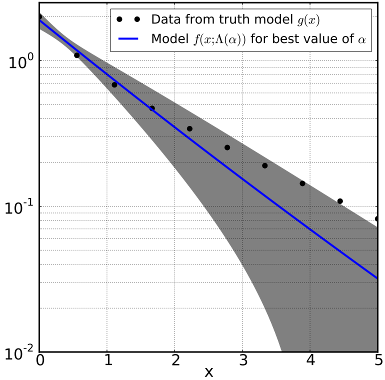



Linear-exponential $f(x,\lambda) = e^{\lambda_1+\lambda_2 x}$



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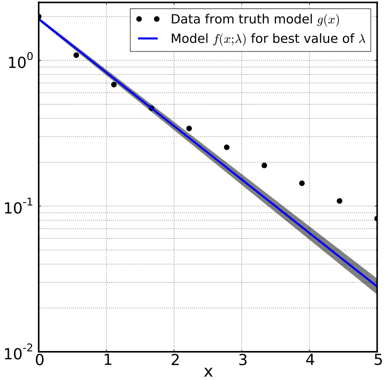
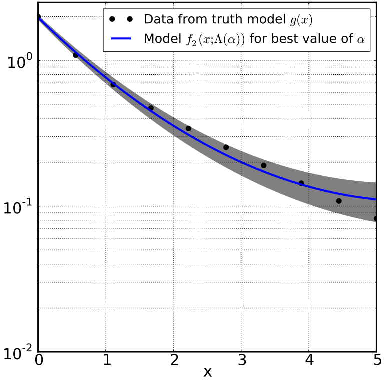



Quadratic-exponential $f_2(x,\lambda) = e^{\lambda_1+\lambda_2 x+\lambda_3 x^2}$



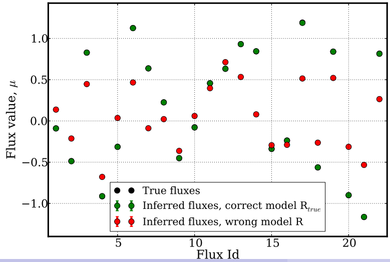
# TransCom3 Experiment of $CO_2$ Flux Inversion

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

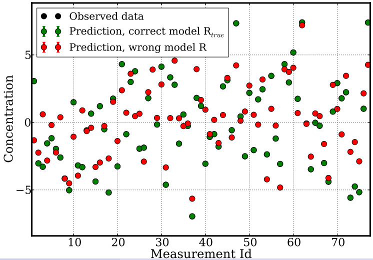
- Observations $\mathbf{d}$ at $N = 77$ sites around the world
- Inverse problem: find fluxes $\mathbf{s}$ at $M = 22$ locations
- Linearized 'response' model $\mathbf{R}$, such that $\mathbf{d} \approx \mathbf{Rs}$

- Model $\mathbf{R}$ is never perfect thus contaminating the inversion
- The inferred values of $\mathbf{s}$ compensate for model deficiencies
- Synthetic study: assume data comes from a true model $\mathbf{R}_{\text{true}}$ with exact flux values: $\mathbf{d} = \mathbf{R}_{\text{true}}\mathbf{s}_{\text{exact}}$

Additive Gaussian error




Embedded model error



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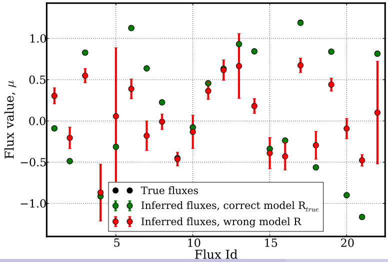


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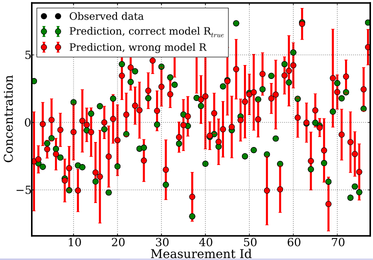
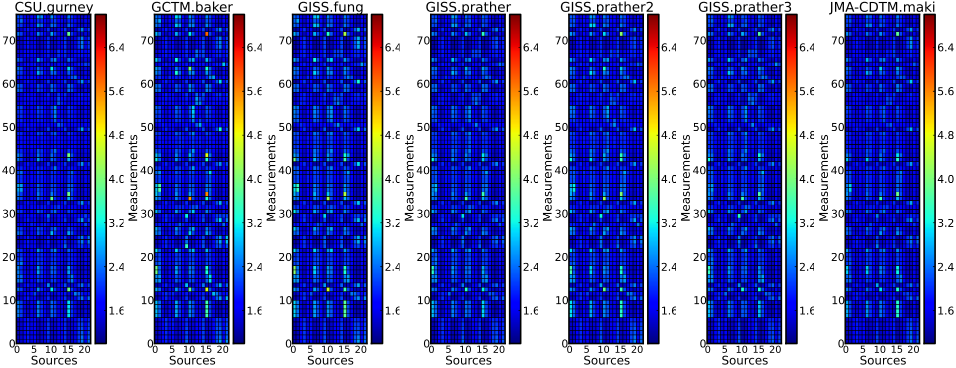


# Consider 14 different response models $\mathbf{R}$




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

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

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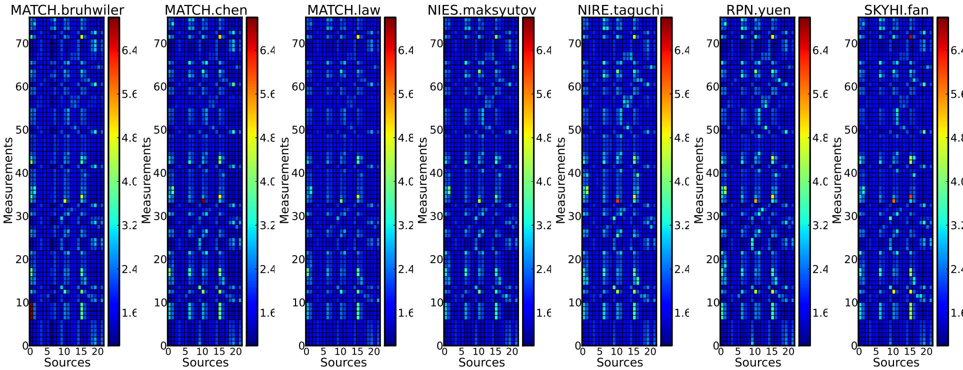


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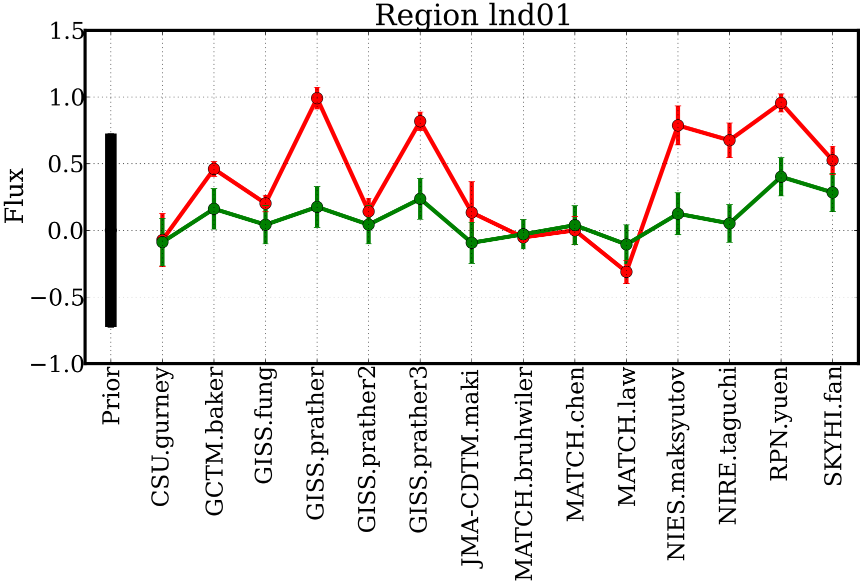
# Inferred fluxes show less variability across models



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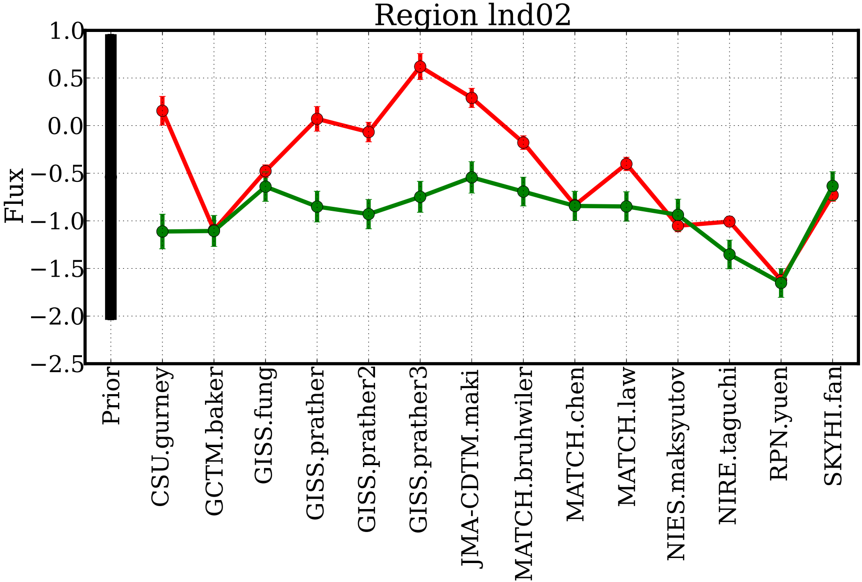

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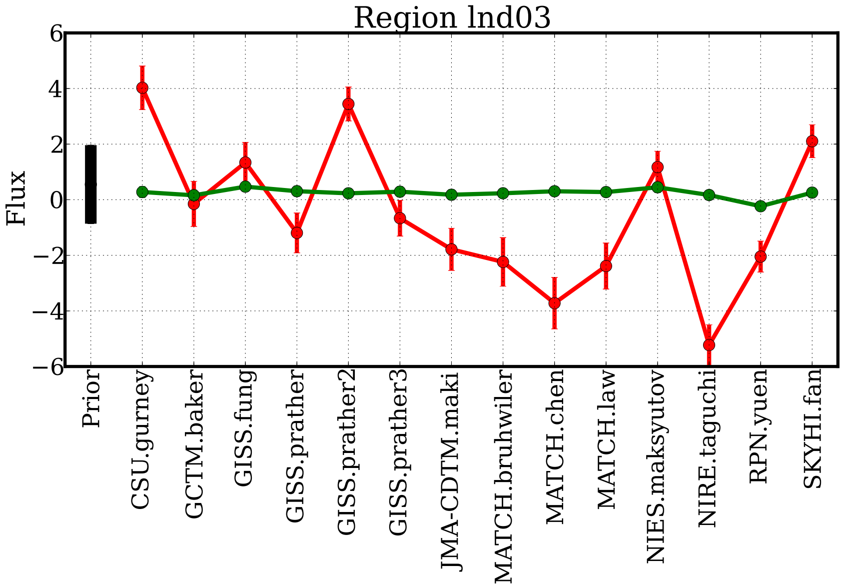

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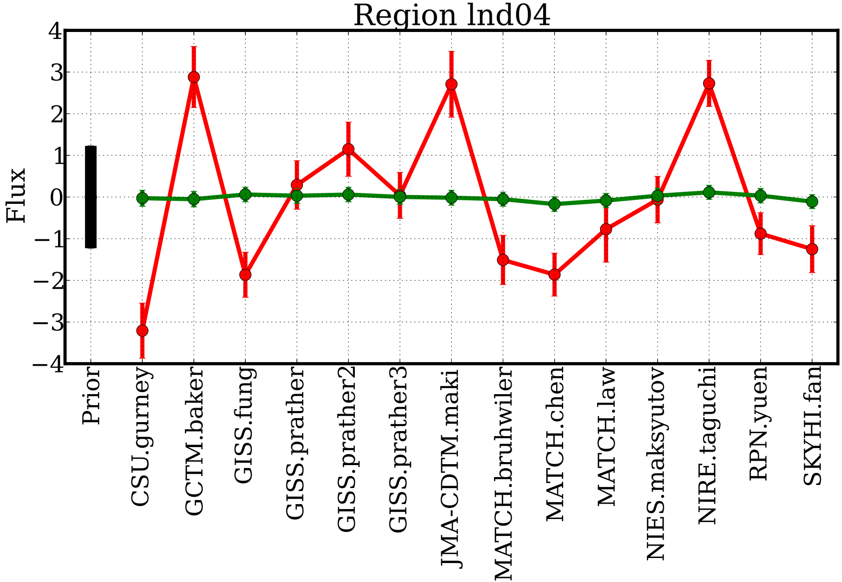

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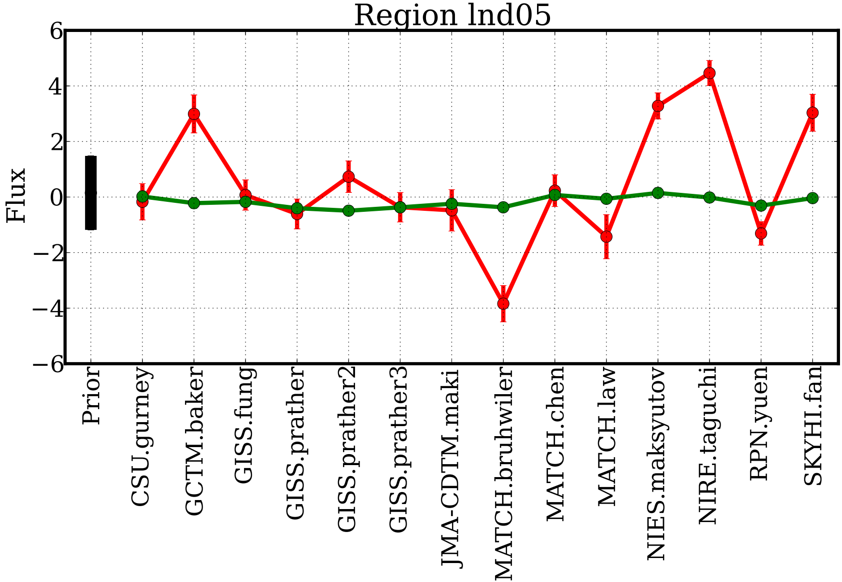

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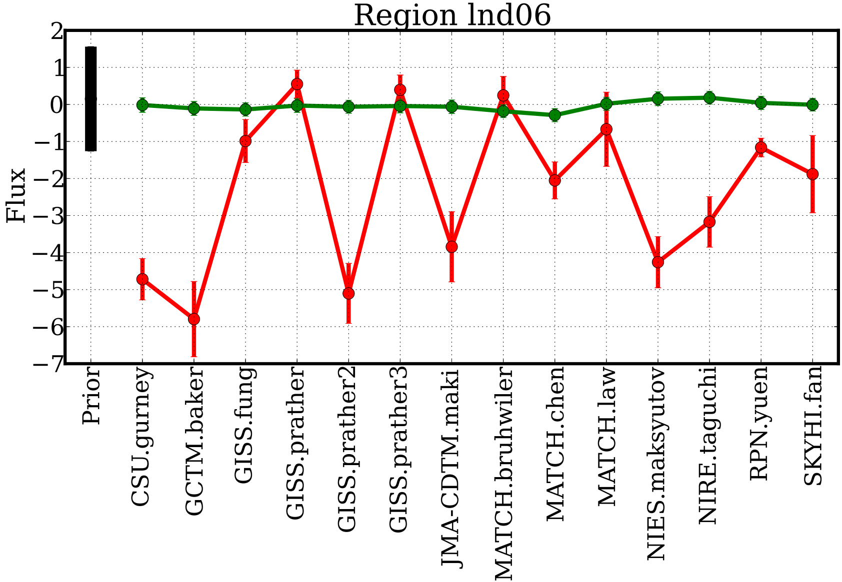

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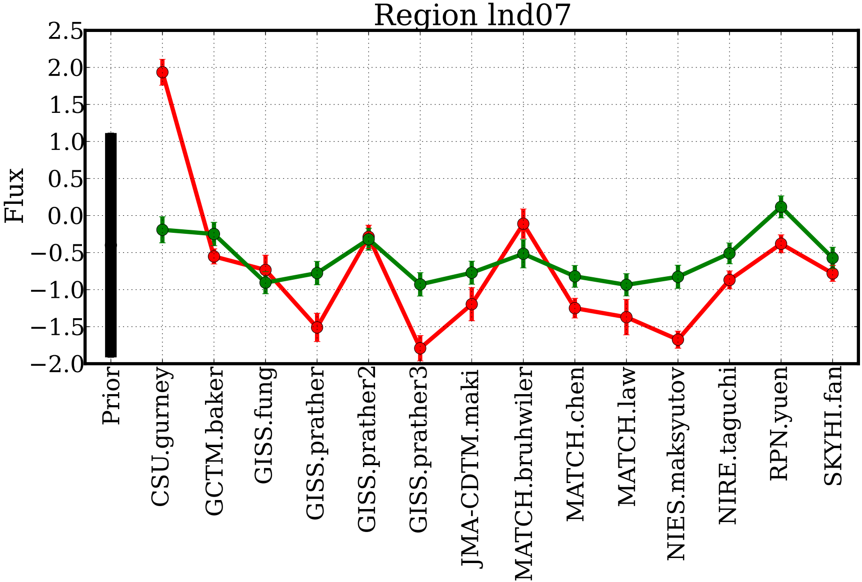

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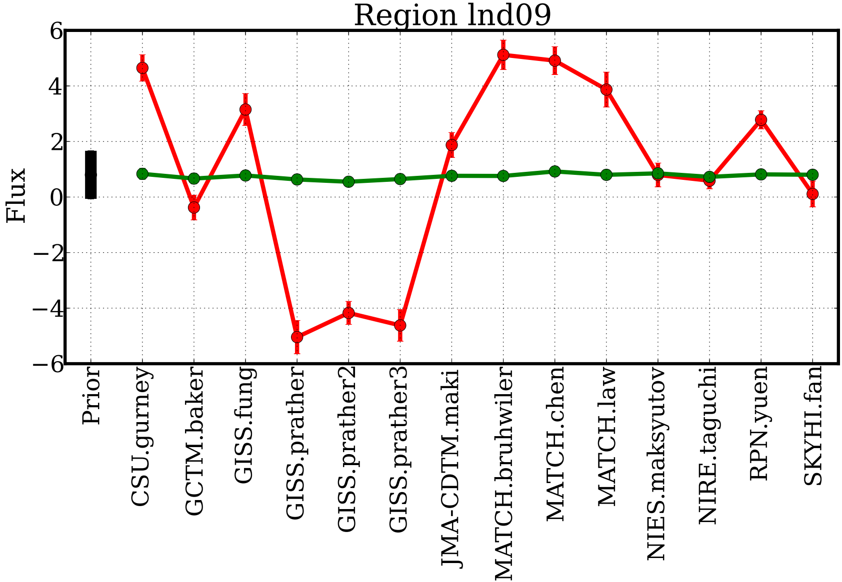

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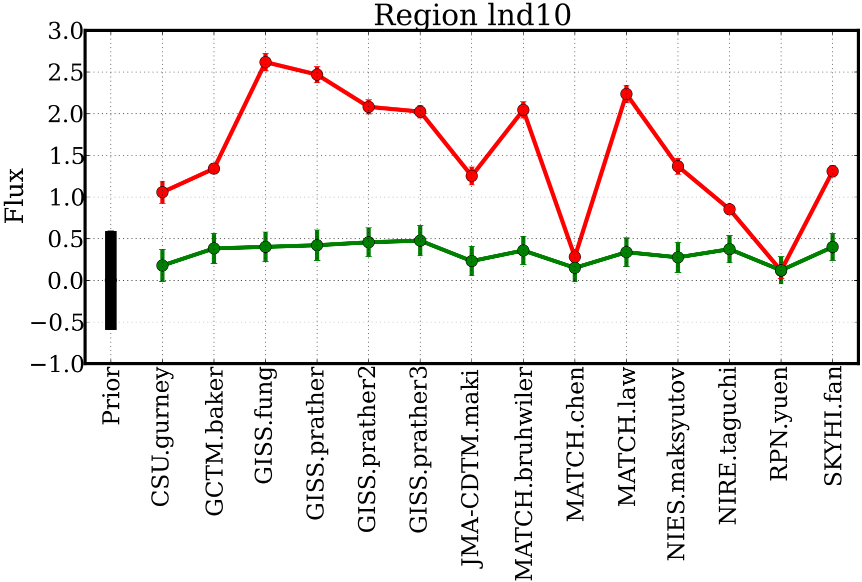

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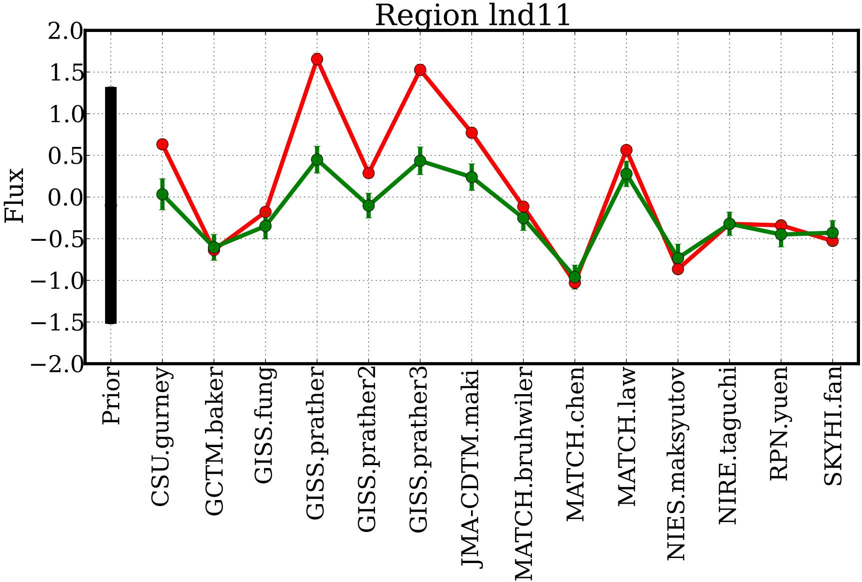

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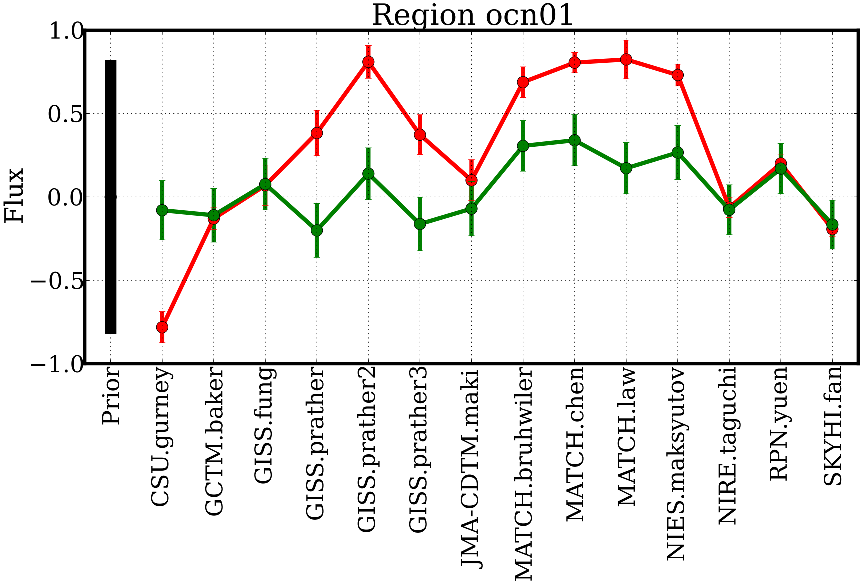

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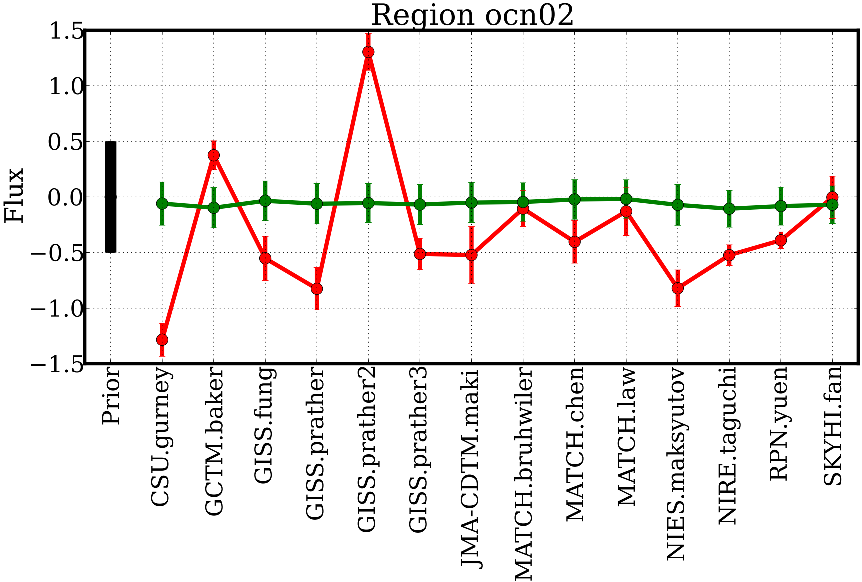

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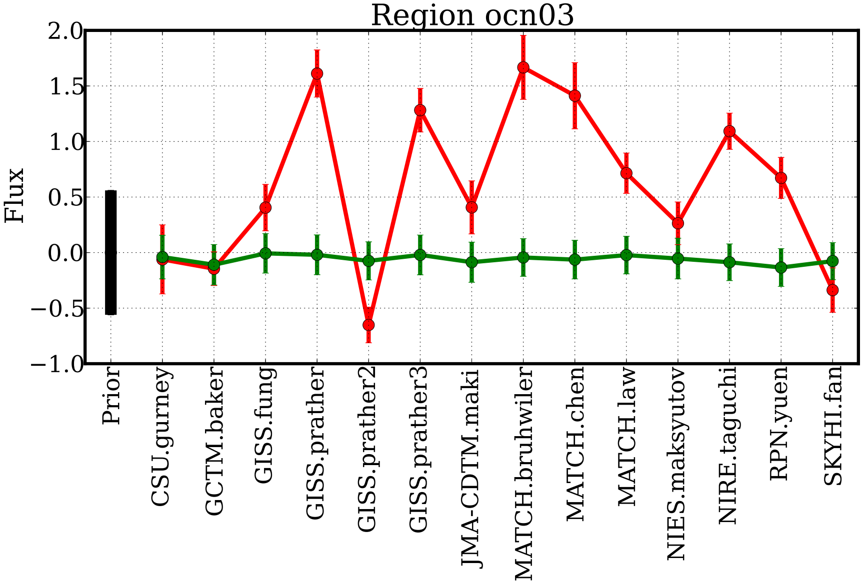

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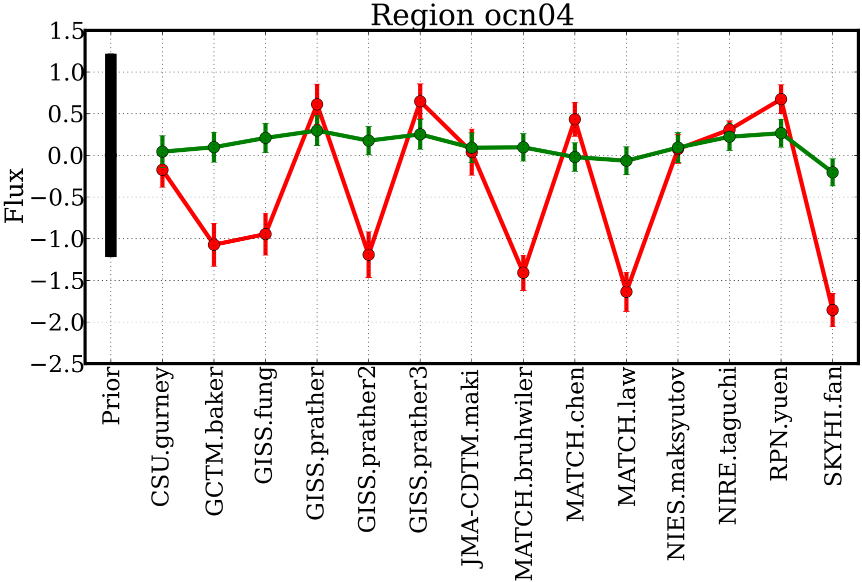

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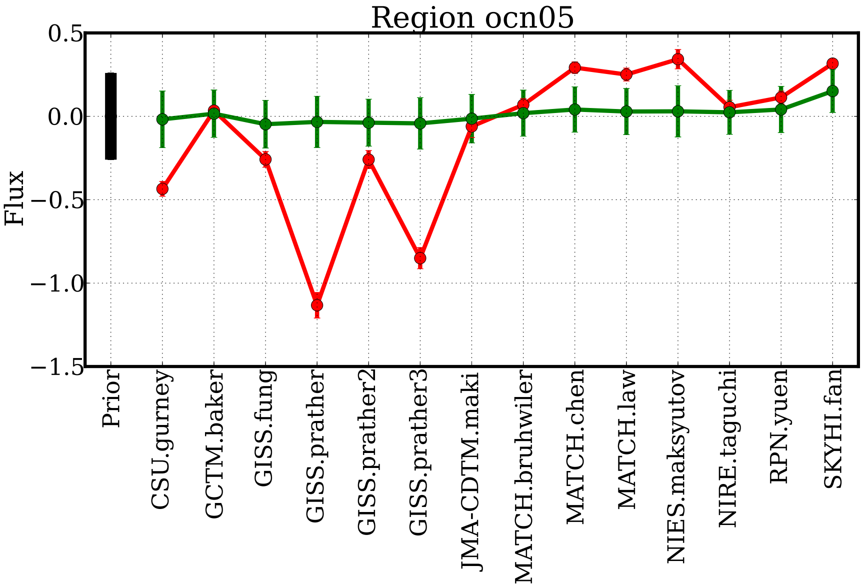

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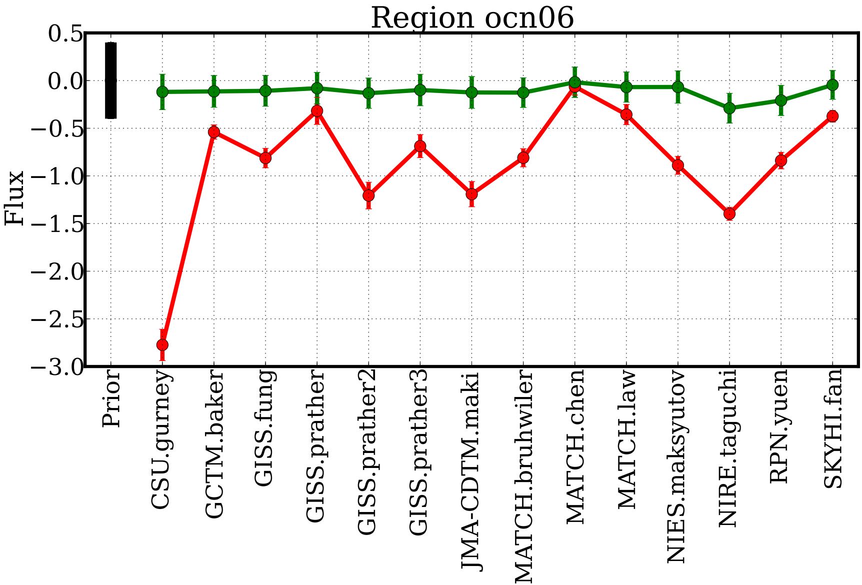

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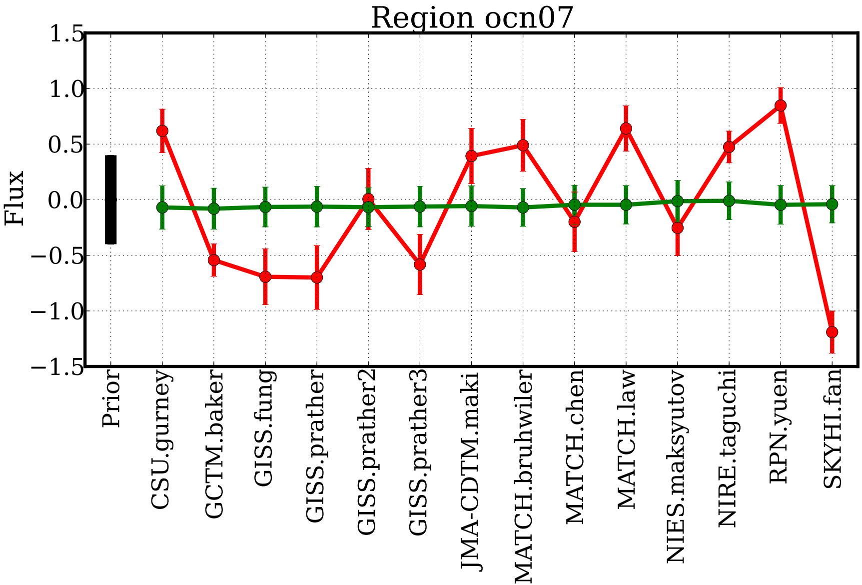

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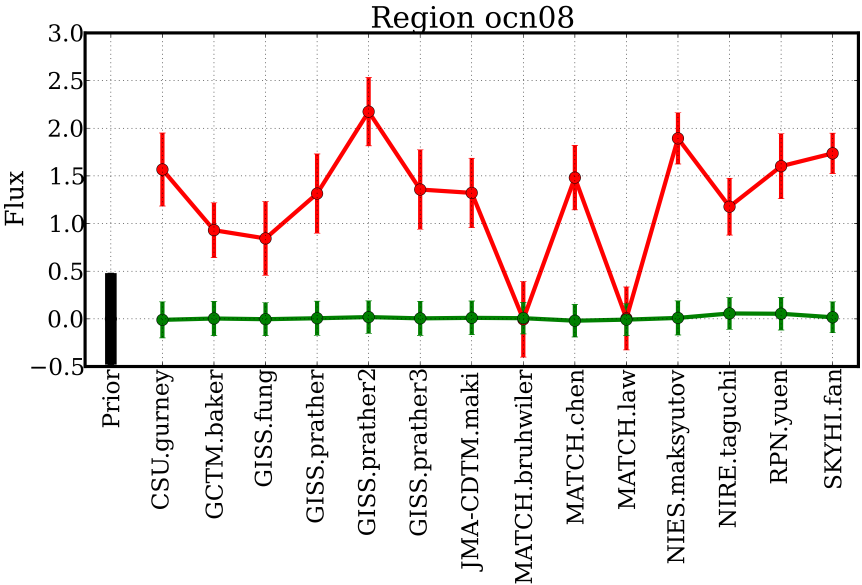

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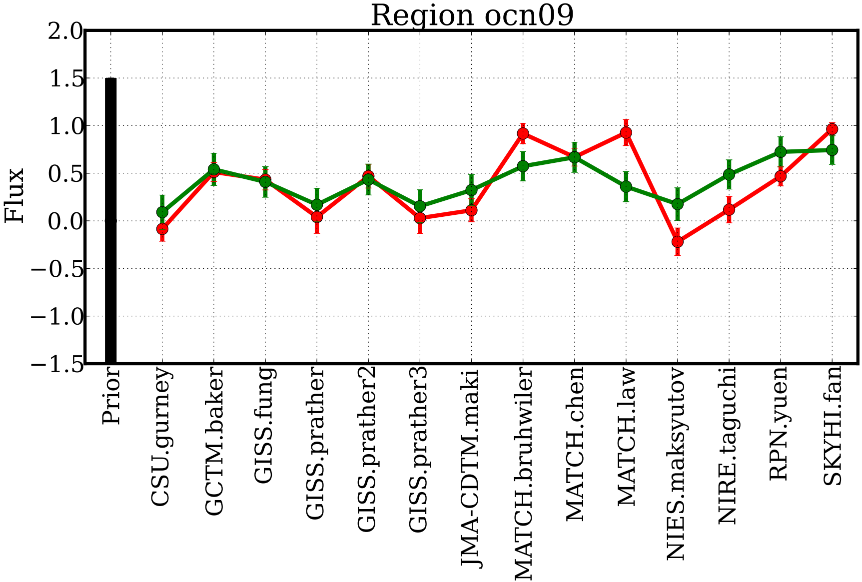

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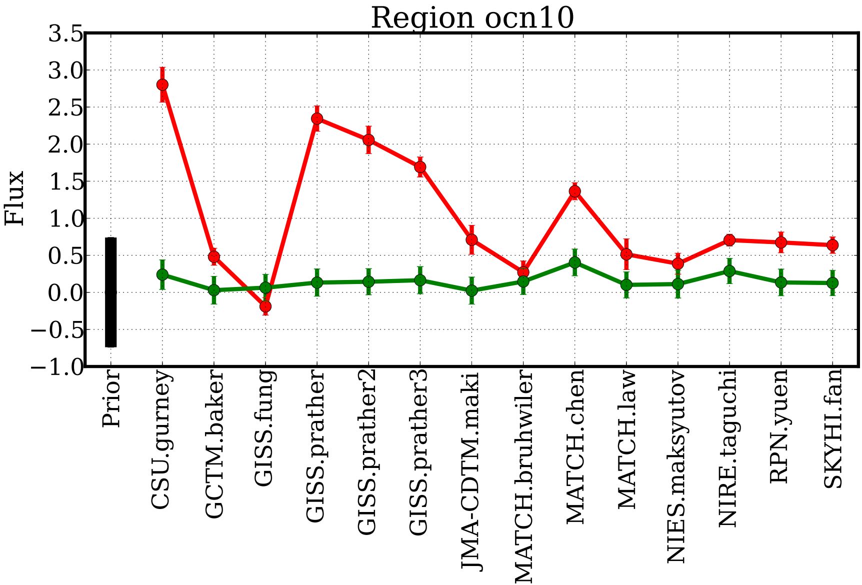

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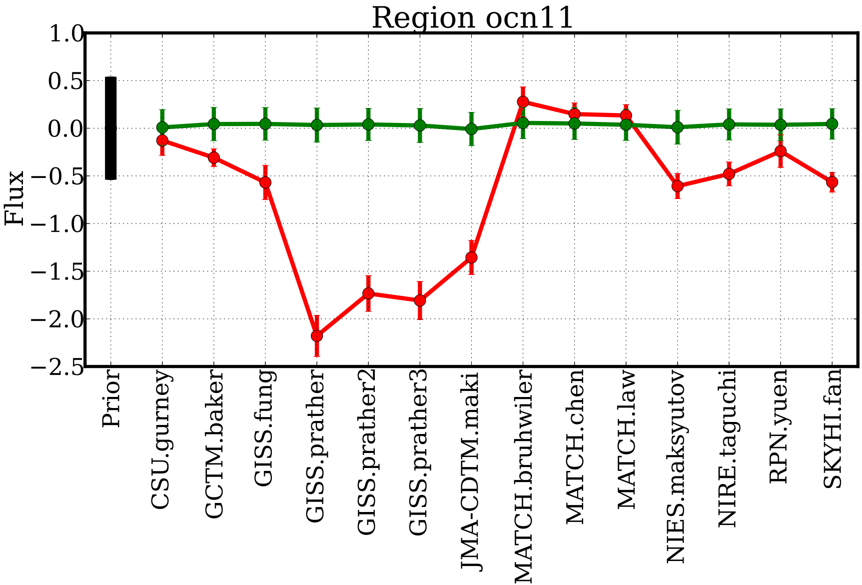

# Summary

- 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

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- In the simplest setting, cast $\lambda$ as a random variable $\Lambda$
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  - Likelihood $L_{\mathcal{D}}(\alpha) = p(\mathcal{D}|\alpha) = p(y_1, \ldots, y_N|\alpha)$

# 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 $\lambda$ along with those of $\delta(x)$, $\epsilon_i^{\mathrm{d}}$