Computer Model Calibration: Bayesian Methods for Combining Simulations and Experiments for Inference and Prediction

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Example

- The Lyon-Fedder-Mobary (LFM) model simulates the interaction of solar wind plasma in the magnetosphere

- We see this as the Aurora Borealis

- Have a computer model that attempts to capture the main features of this phenomenon

- Outputs are large 3-dimensional space-time fields or extracted features thereof

- Computer model has three inputs: $\theta = (\alpha, \beta, R)$

Example

- Field observations available from the Polar Ultraviolet Imager satellite

- Computer model is assumed to capture all salient features of the solar wind interactions, up to random error

- However, the inputs ($\theta = (\alpha, \beta, R)$) are not known

- Scientific problem: estimate $\theta = (\alpha, \beta, R)$

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Basic inverse problem – Statistical formulation

$$y_s(t) = \eta(t)$$

$$y_f(\theta) = \eta(\theta) + \epsilon$$

- Where,
  - y_f system response
  - y_s simulator response at input t
  - θ calibration parameters
  - ε random error

Have data from 2 separate sources – computer model and field observations

Problem is to estimate the calibration parameters

Solutions

- Many different solutions to such problems… can you think of one?
- Suppose the computer model is fast?
- Suppose the computer model is slow?

Model calibration – Statistical formulation

$$y_s(x,t) = \eta(x,t)$$

$$y_f(x,\theta) = \eta(x,\theta) + \epsilon$$

- Where,
  - x model or system inputs;
  - y_f system response
  - y_s simulator response
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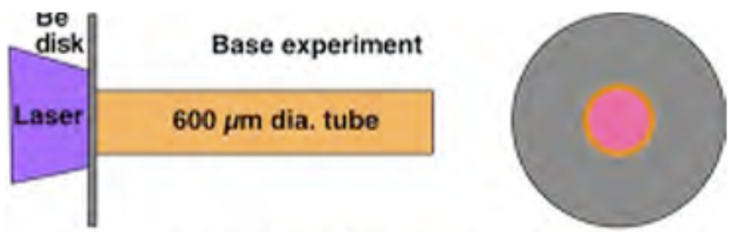
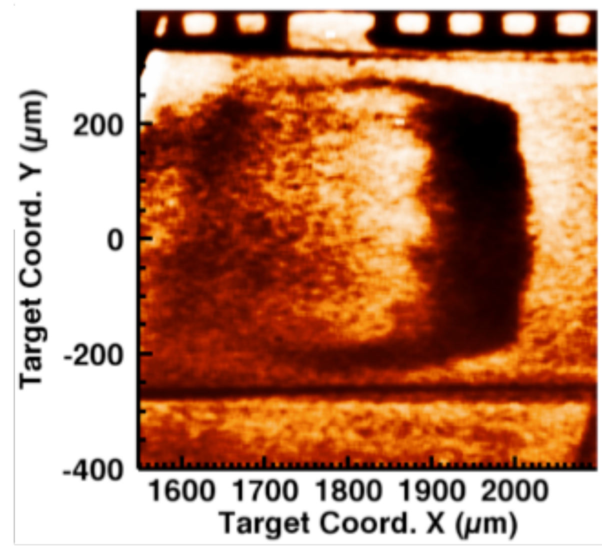
Example: Radiative shock experiment

A conceptually simple experiment

– Launch a thin Be plasma down a shock tube at ~ 200 km/s

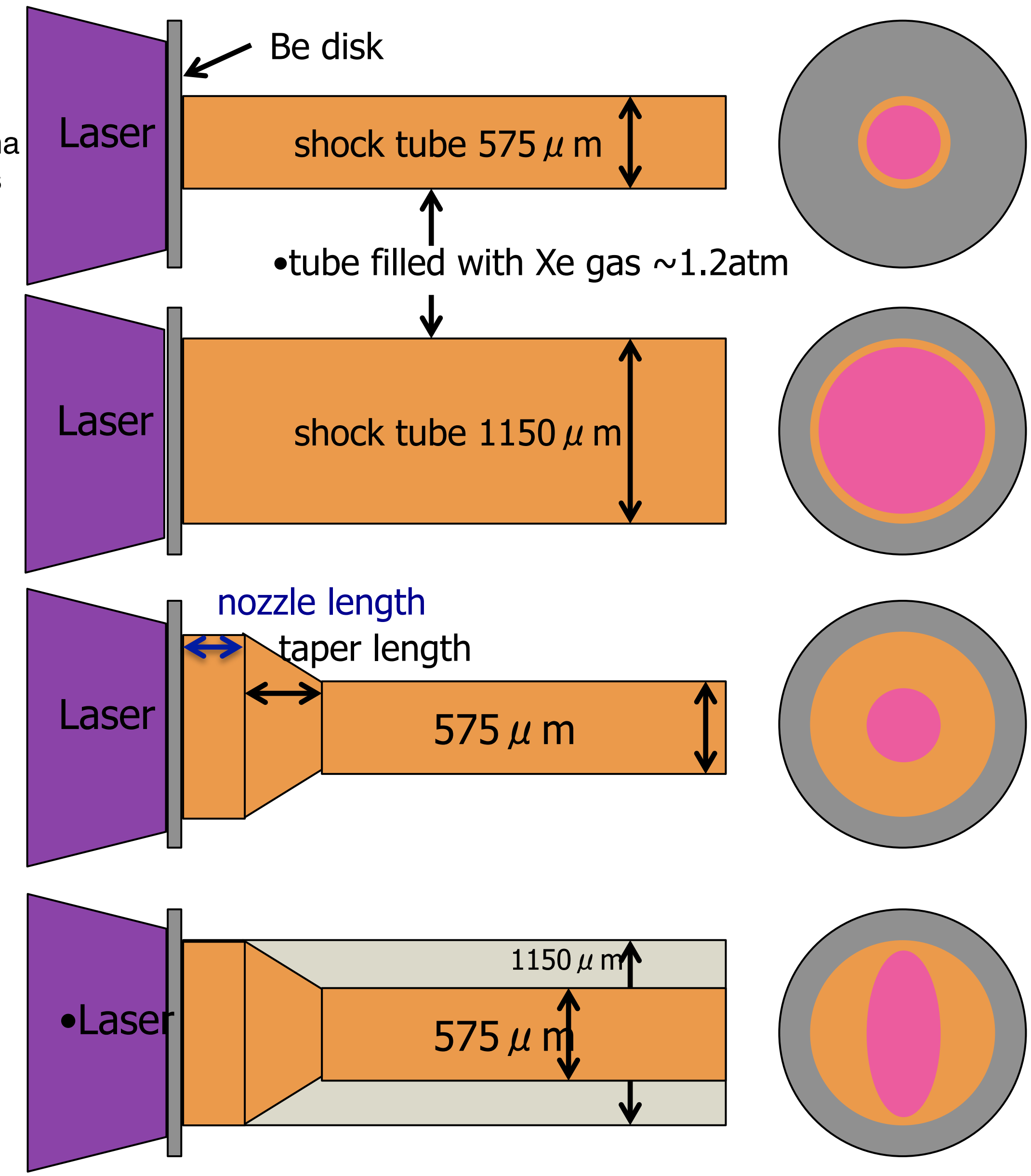




A radiative shock is a wave in which both hydrodynamic and radiation transport physics play a significant role in the shock's propagation and structure

Application

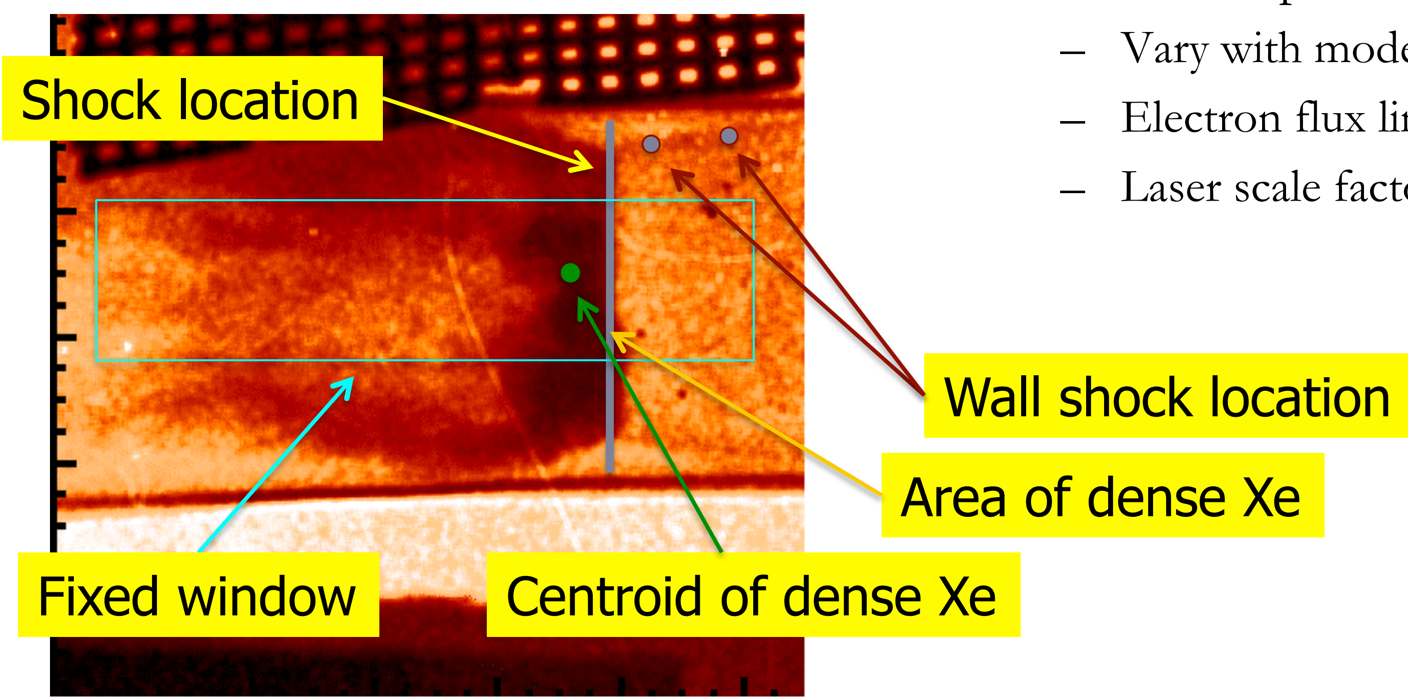
- Initial experiments:
  - 1 ns, 3.8 kJ laser irradiates Be disk➔ plasma down Xe gas filled shock tube at ~ 200 km/s
  - Circular tube; diam = 575µm
  - Timing 13-14 ns
- Additional experiments
  - Laser energy ~ 3.8kJ
  - Circular tube; diam = 575, 1150µm
  - Timing 13,20,26 ns
- Nozzle experiments
  - Laser energy ~ 3.8kJ
  - nozzle length = taper length = 500µm
  - Circular tube; diam = 575µm
  - Timing 26 ns
- Extrapolation experiments (5th year)
  - Laser energy ~ 3.8kJ
  - **Elliptical** tube; diam = 575-1150µm
  - Aspect ratio = 2
  - Includes nozzle in shock tube
  - Timing 26 ns



Have several outputs & inputs

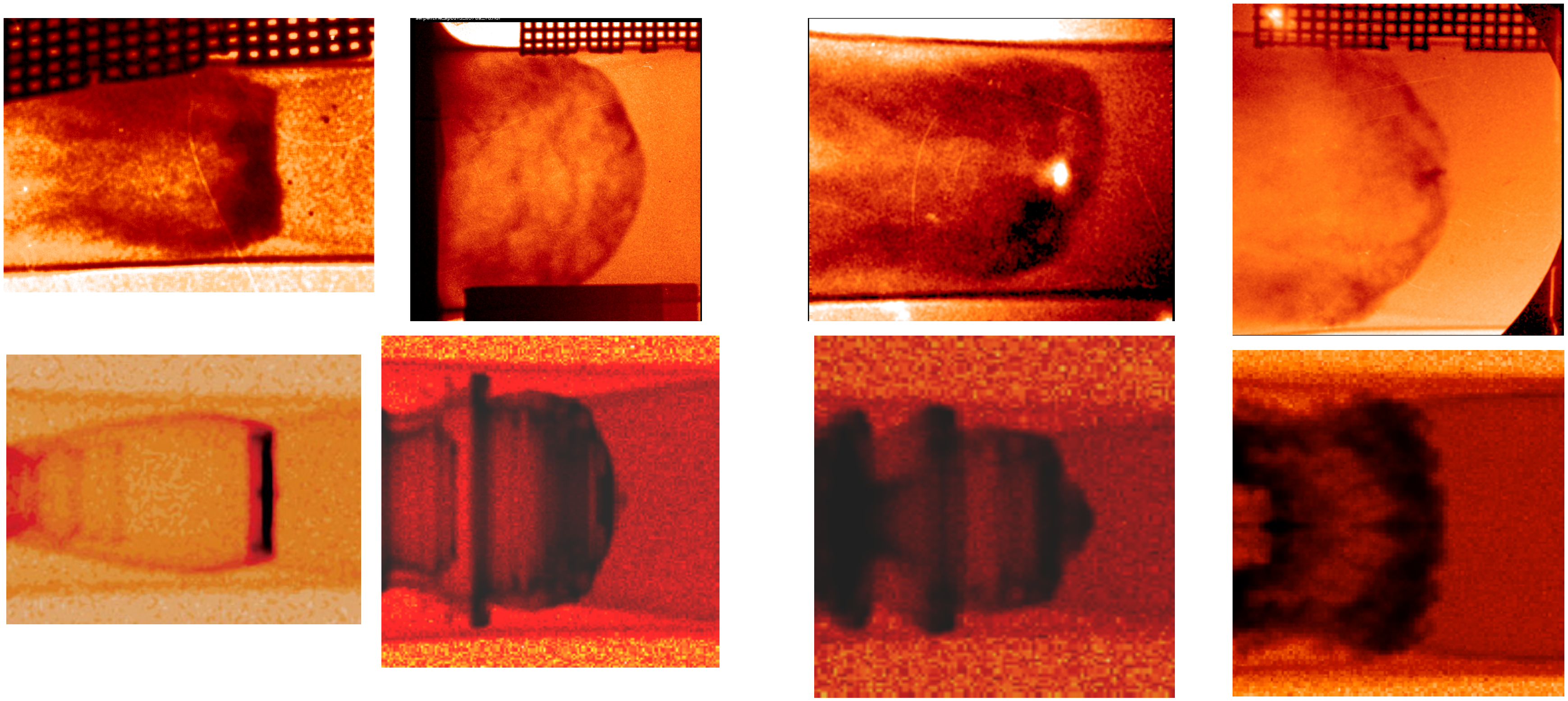
- Outputs (y)
  - Shock location
  - Shock breakout time
  - Wall shock location
  - Axial centroid of Xe
  - Area of dense Xe

- Inputs (x)
  - Observation time
  - Laser energy
  - Be disk thickness
  - Xe gas pressure
  - Tube geometry
- Calibration parameters (θ)
  - Vary with model
  - Electron flux limiter
  - Laser scale factor



We can measure and we can compute

600 μm tube | 1200 μm tube | Circular nozzle | Elliptical nozzle



Goal is to predict elliptical tube quantities of interest and uncertainty, without using any data from elliptical tube experiments

- Shocks at 13 ns

Data

- Have observations from 1-D CRASH model and experiments

- Experiment data:
  - 9 experiments
  - experiment variables: Be thickness, Laser Energy, Xe pressure and Time
  - responses: Shock location

- 1-D CRASH Simulations
  - 320 simulations, varied over 8 inputs
  - experiment variables: Be thickness, Laser Energy, Xe pressure and Time
  - calibration parameters: Be Gamma, Be OSF, Xe Gamma, Xe OSF
  - response: Shock location

Use observations and simulations for prediction in real world

- Have simulations from the CRASH code
- Have observations from laboratory experiments
- Want to combine these sources of data to make prediction of the real-world process ... Also have to estimate the calibration parameters

- Additional complicating factor, the computer model is not an exact representation of the mean of the physical system… darn!

- **Approach:** Model calibration (Kennedy and O'Hagan, 2001; Higdon et al., 2004)

Model calibration – Statistical formulation

$$
\begin{aligned}
y_s(x,t) &= \eta(x,t) \\
y_f(x,\theta) &= \eta(x,\theta) + \delta(x) + \varepsilon
\end{aligned}
$$

- Where,
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Model calibration – Statistical formulation

$$y_s(x,t) = \boxed{\eta(x,t)}$$
$$y_f(x,\theta) = \boxed{\eta(x,\theta)} + \delta(x) + \varepsilon$$

Shared signal

Model calibration – Statistical formulation

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y_s(x,t) &= \eta(x,t) \\
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Discrepancy

Model calibration – Statistical formulation

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Gaussian process models

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Back to Gaussian process models

- $y(x_i) = \mu + z(x_i)$

- $z(x_i) \sim N(0, \sigma_z^2)$
- $cor\left((z(x_i), z(x_j)\right) = e^{-\sum_{k=1}^{d} \theta_k (x_{ik} - x_{jk})^2}$
- $z(x) \sim N(0_n, \sigma_z^2 R)$
- $y(x) \sim N(\mu 1_n, \sigma_z^2 R)$

Gaussian process model for the emulator in this setting

- $y_s(x_i, t_i) = \mu + z(x_i, t_i)$

- $z(x_i, t_i) \sim N(0, \sigma_z^2)$
- $cor\left((z(x_i), z(x_j)\right) = e^{-\sum_{k=1}^{d} \theta_k (x_{ik} - x_{jk})^2 - \sum_{k=1}^{d'} \omega_k (t_{ik} - t_{jk})^2}$
- $z(x, t) \sim N(0_n, \sigma_z^2 R)$
- $y(x, t) \sim N(\mu 1_n, \sigma_z^2 R)$

Have Gaussian process model for the discrepancy

- $\delta(x_i) \sim N(0, \sigma_\delta^2)$
- $cor\left((\delta(x_i), \delta(x_j)\right) = e^{-\sum_{k=1}^{d} \gamma_k (x_{ik} - x_{jk})^2}$
- $\delta(x) \sim N(0_m, \sigma_\delta^2 R_\delta) = N(0_m, \Sigma_\delta)$

Hierarchical model is used to combine simulations and observations

- View computational model as a draw of a random process (like before)
- Denote vectors of simulation trials as and field measurements as y_s & y_f
- Suppose that these are *n* and *m*-vectors respectively

$\longrightarrow$

- Can combine sources of information using a single GP

$$\begin{aligned} y_s(x,t) &= \eta(x,t) \\ y_f(x,\theta) &= \eta(x,\theta) + \delta(x) + \varepsilon \end{aligned}$$

$$y = \begin{pmatrix} y_s \\ \\ y_f \end{pmatrix} \sim N\left(\mu,\ \Sigma_\eta + \Sigma_\delta + \Sigma_\varepsilon\right)$$

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$$
y = \begin{pmatrix} y_s \\ \\ y_f \end{pmatrix} \sim N\left(\mu, \Sigma_\eta + \Sigma_\delta + \Sigma_\varepsilon\right)
$$

Contains correlations between all sources of data via the joint signal in the computer model

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Problem… correlations involving field trials have $t = \theta$

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Only operates on the field data

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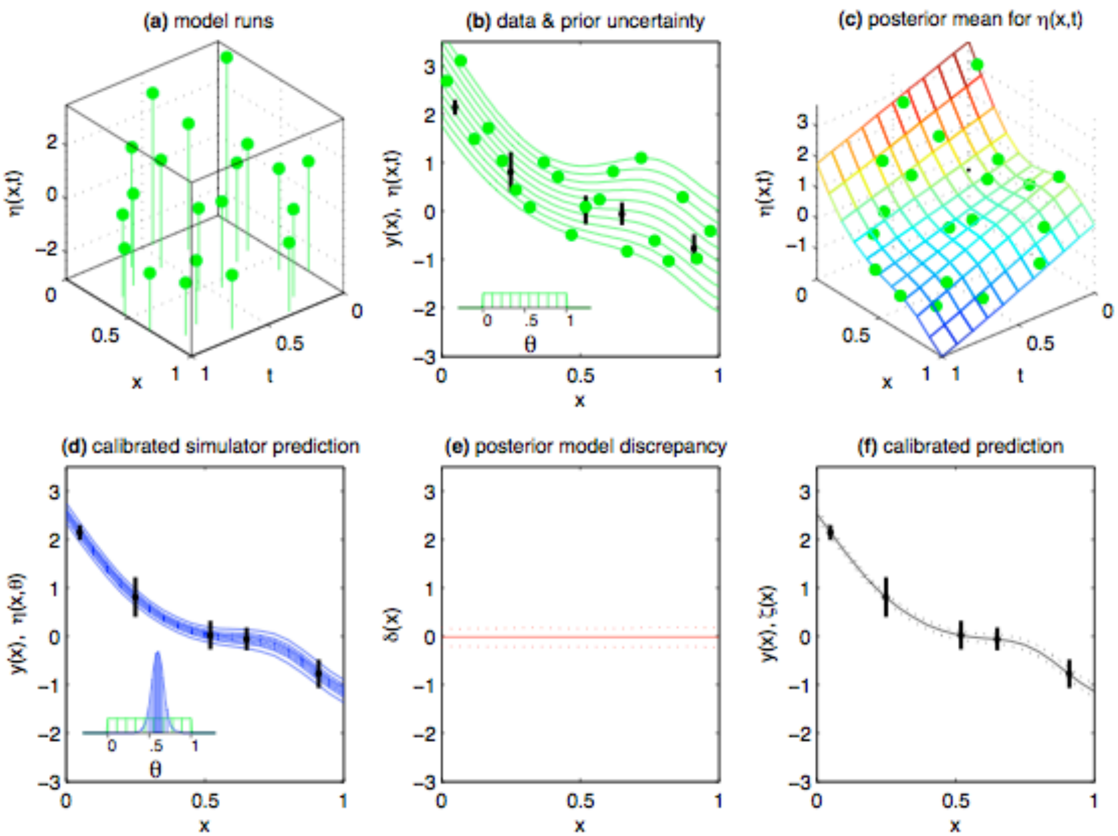
Calibration idea: No discrepancy model

(Plot taken shamelessly from Dave Higdon)



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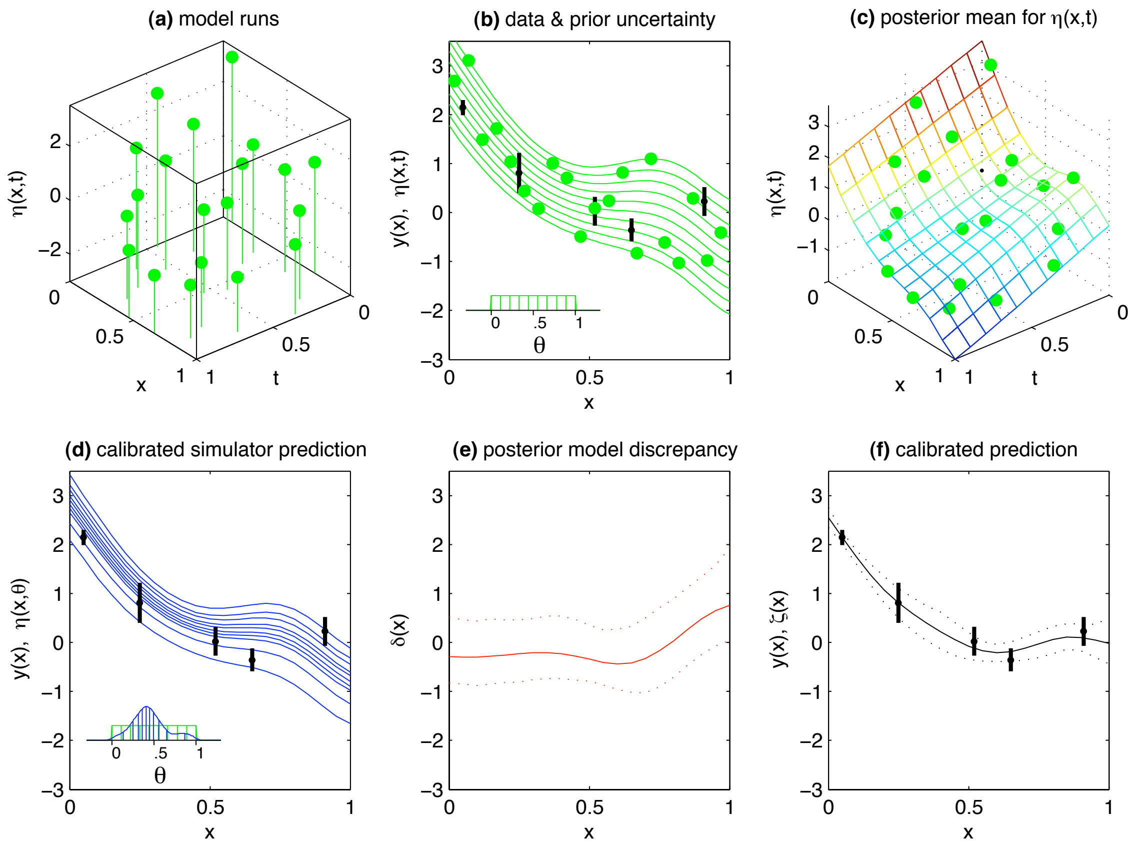
Calibration idea: Discrepancy model

(Plot taken shamelessly from Dave Higdon)



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Comments

- Interpretation of unknown constants can change
- Without discrepancy: estimating unknown physical constants
- With discrepancy: selecting tuning constants that best fit the model

Estimation

- What parameters do we have to estimate?

Estimation

- Can apply Bayes' Rule:

$$[A|B] = \frac{[B|A][A]}{[B]}$$

Ignoring statistical model parameters for the moment…

- In the unbiased case for a fast simulator,

$$[\theta|\eta, y_f] \propto [y_f|\eta, \theta][\eta|\theta][\theta]$$

- For the simulators we have been considering, use an emulator in place of computer model… basic idea

$$[\eta|\theta] \to [\hat{\eta}|\theta, y_s]$$

$$[\theta|\hat{\eta}, y_f] \propto [y_f|\hat{\eta}, \theta][\hat{\eta}|\theta, y_s][\theta]$$

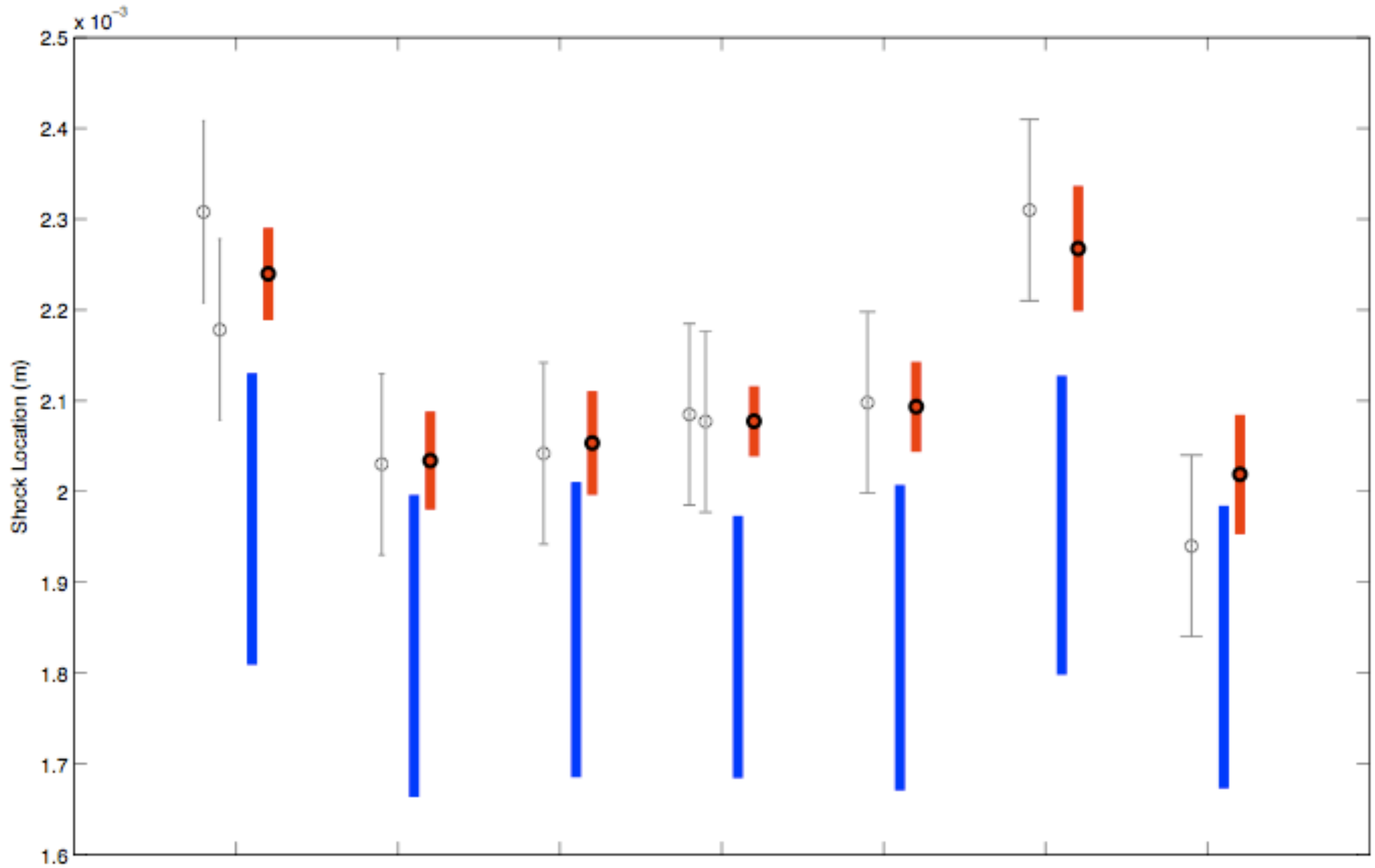
Estimation

- How could we put this together for the CRASH problem?

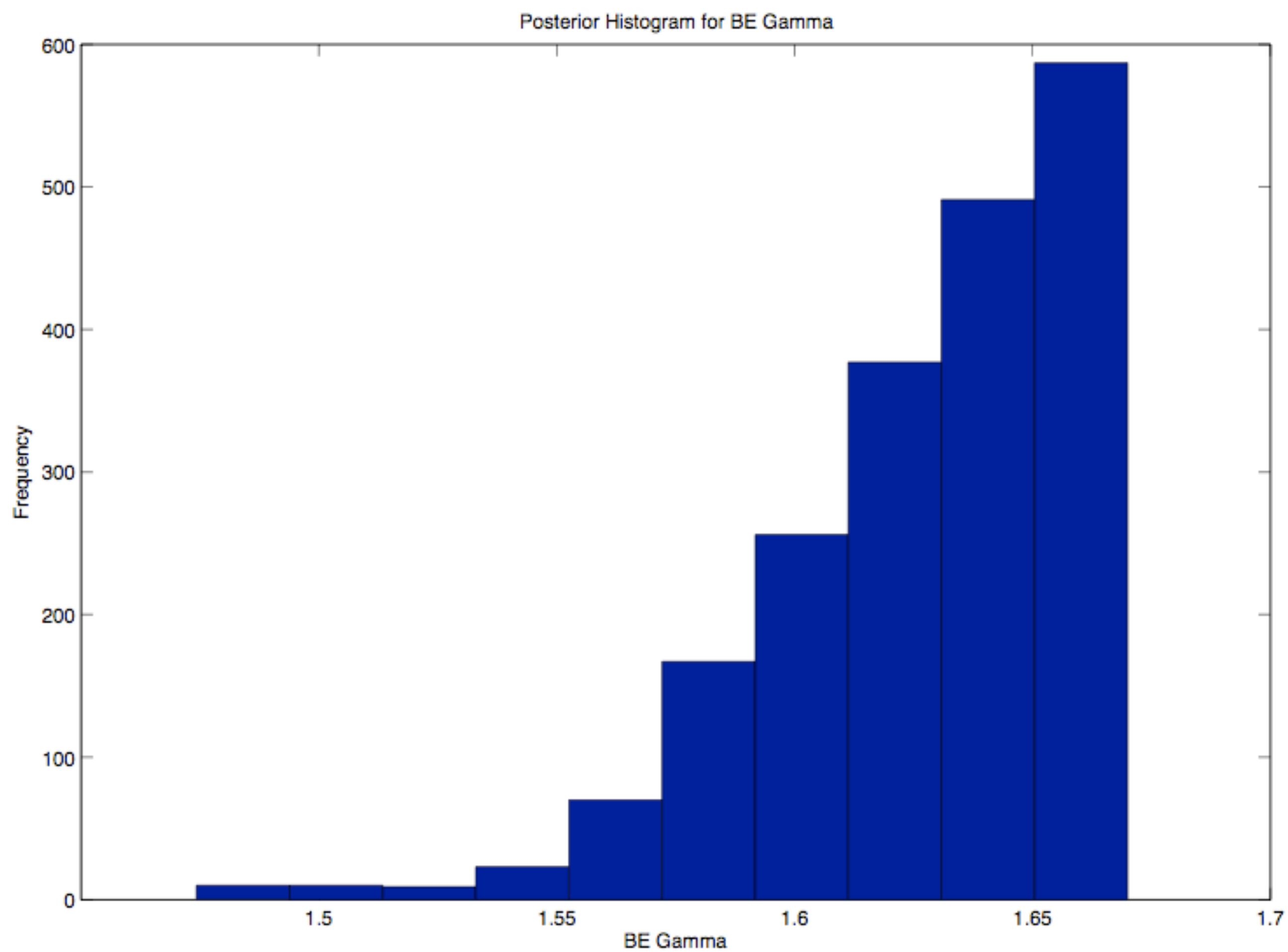
Back to CRASH

- Inverted-gamma priors for variance components
- Gamma priors for the correlation parameters
- Log-normal priors for the calibration parameters
- Samples from the posterior are generated through MCMC… anyone know how to do this?

CRASH predictions



Calibration - BE Gamma



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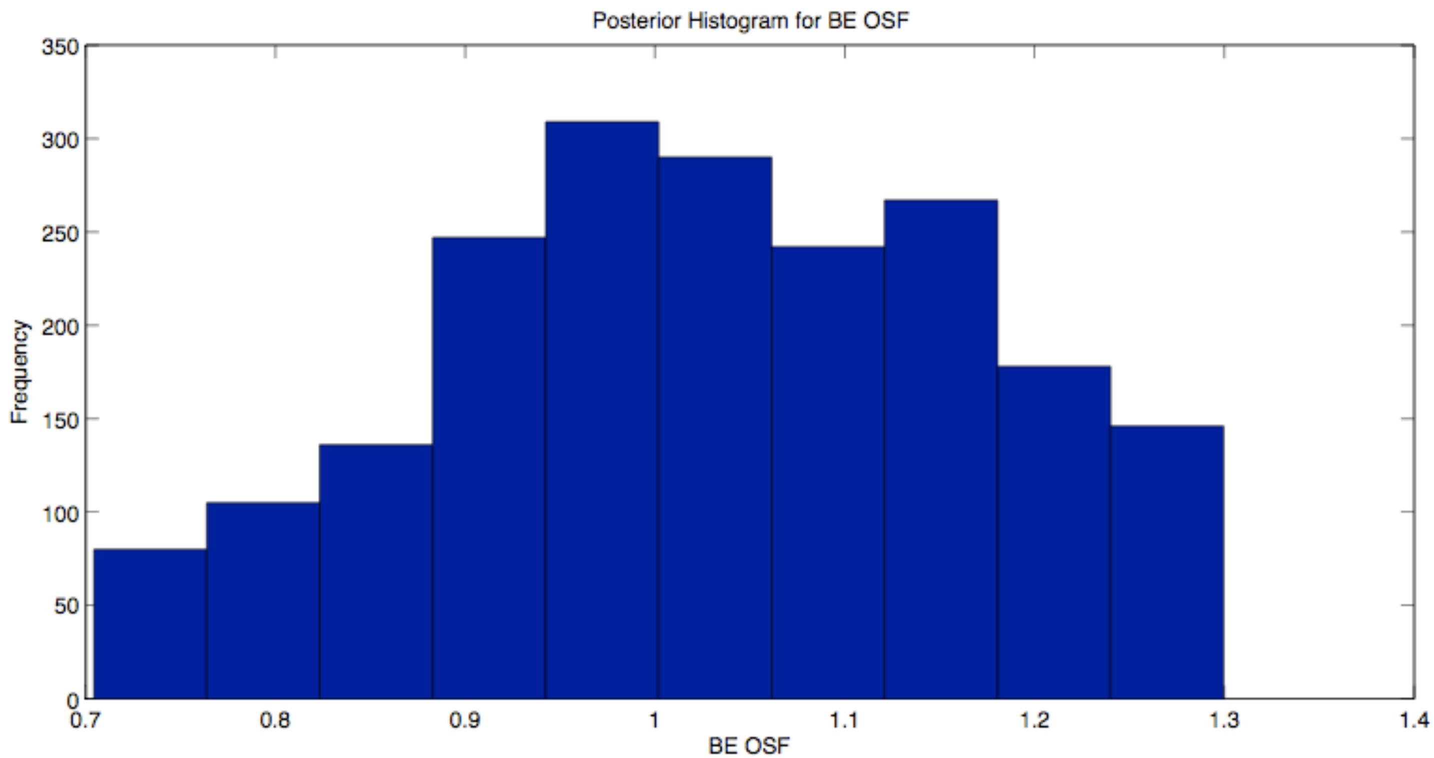
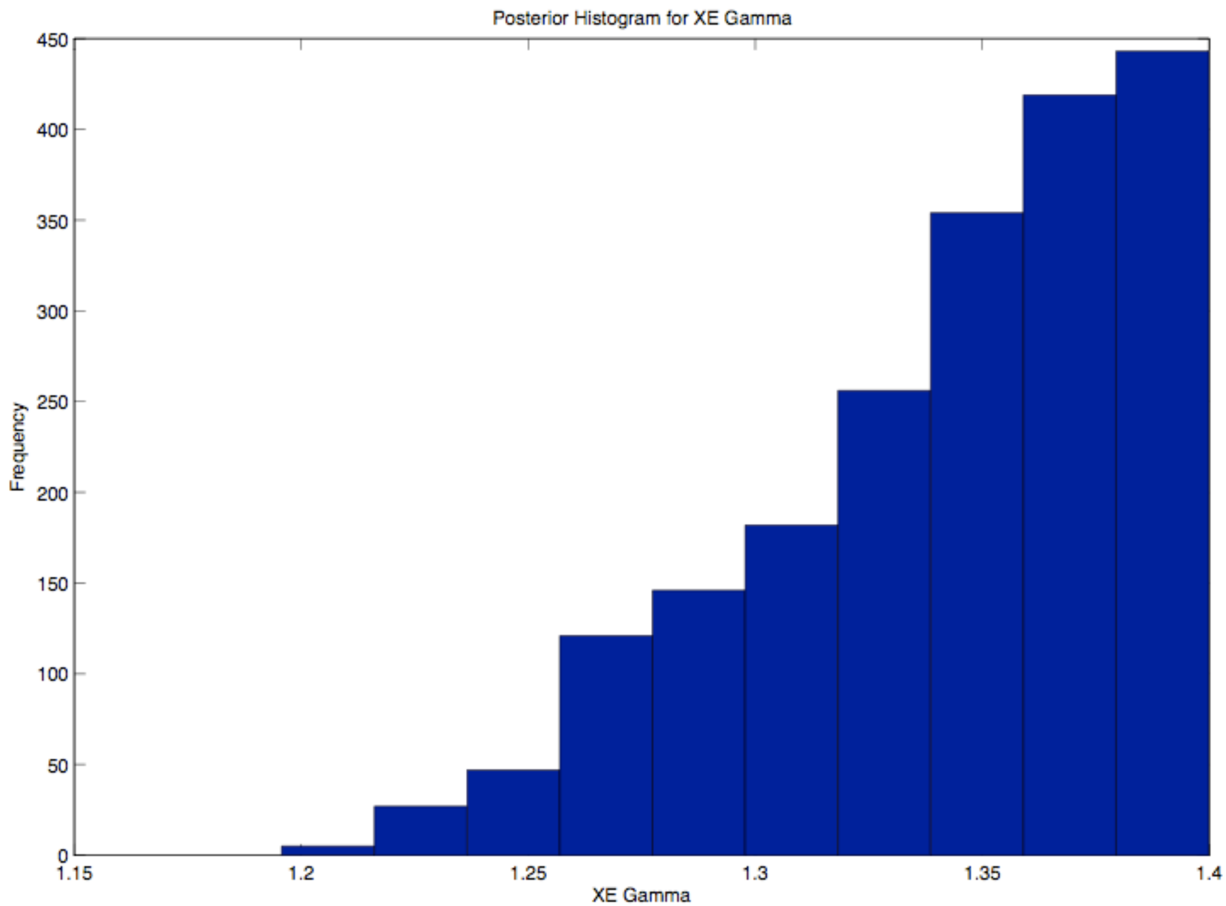
Calibration - BE OSF



Calibration - XE Gamma



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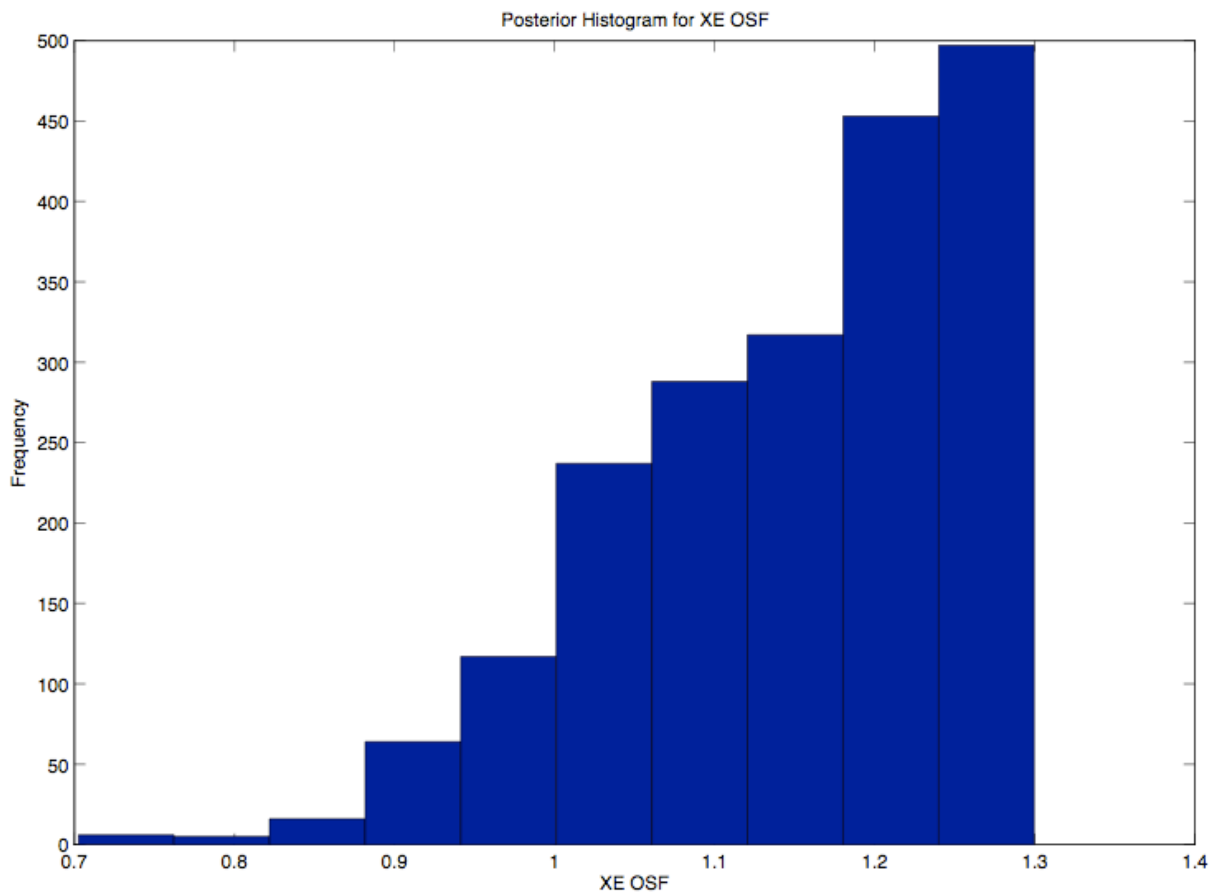
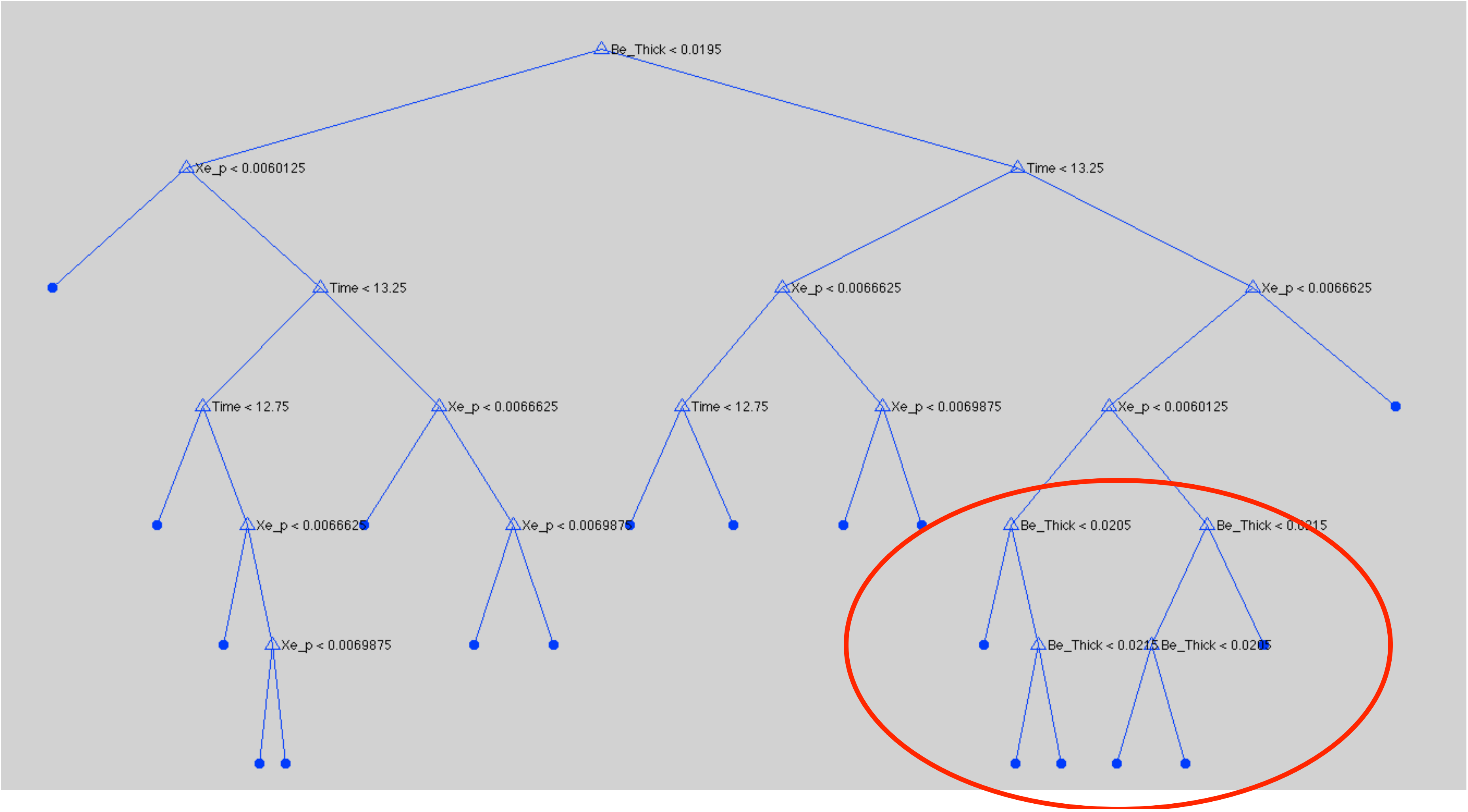
Calibration - XE OSF



Exploring the discrepancy

- The CRASH project was an ongoing endeavor
- Computer codes were being developed
- Idea is to use the statistical model to inform code development
- Predicted the discrepancy over a 4-d grid
- Used posterior mean surface

Discrepancy



- Reasons for the discrepancy
  - It was interesting that the discrepancy is always positive
  - Incorrect radial loss of energy results in Xe that is too hot in front of the shock, and that systematically messes up the shock speed
  - The region where the discrepancy is highest is thought to be the region where Xe pressure is largely going to impact
  - Why might this be a crazy approach to explore the discrepancy?