On Combining Functional Experimental Data and Computer Simulations

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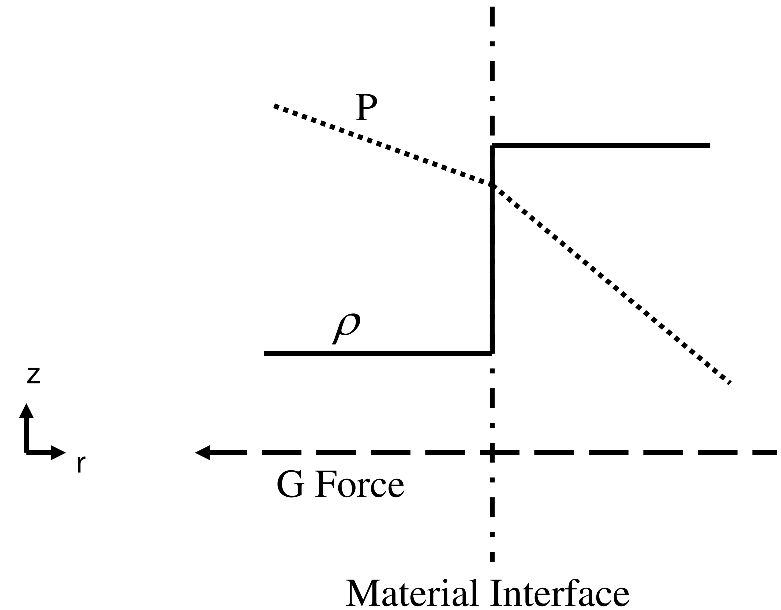
Outline

- Overview of Fluid Instability Model
- Overview of Statistical Framework
- Experimental Design
- Sensitivity Analysis
- Example: Linear Electric Motor Experiments

Fluid Instabilities

R-T test problem



- Rayleigh-Taylor (R-T) instability

$\longrightarrow$ occurs at perturbed interface between light and heavy fluid

$\longrightarrow$ density and pressure gradients are opposite

$\longrightarrow$ acceleration or buoyancy driven

- Rictmyer-Meshkov (R-M) instability

$\longrightarrow$ occurs at perturbed interface between two distinct fluids

$\longrightarrow$ density and pressure gradients are mis-aligned

$\longrightarrow$ driven by impulsive acceleration at the interface

k-L Model: Hydrodynamic Equations in Cylindrical Coordinates

Mass: $$\frac{D\rho}{Dt} = -\rho\frac{1}{r}\left[\frac{\partial(ru)}{\partial z} + \frac{\partial(rv)}{\partial r}\right]$$

u velocity: $$\rho\frac{Du}{Dt} = -\frac{1}{r}\frac{\partial(rP)}{\partial z}$$

v velocity: $$\rho\frac{Dv}{Dt} = \frac{1}{r}\left[-\frac{\partial(rP)}{\partial r} + P\right]$$

Internal Energy: $$\rho\frac{De}{Dt} = -P\left[\frac{\partial u}{\partial z} + \frac{\partial v}{\partial r} + \frac{v}{r}\right] + \frac{1}{r}\left[\frac{\partial}{\partial r}\left(r\mu_t\frac{\partial e}{\partial r}\right) + \frac{\partial}{\partial z}\left(r\mu_t\frac{\partial e}{\partial z}\right)\right] - \rho S_k$$

Mass Fraction: $$\rho\frac{DX}{Dt} = \frac{1}{r}\left[\frac{\partial}{\partial r}\left(r\mu_t\frac{\partial X}{\partial r}\right) + \frac{\partial}{\partial z}\left(r\mu_t\frac{\partial X}{\partial z}\right)\right]$$

$$\frac{D}{Dt} = \frac{\partial}{\partial t} + u\frac{\partial}{\partial z} + v\frac{\partial}{\partial r}$$

k-L Model: Turbulence Parameters

- Sub-grid model for describing R-T and Richtmyer-Meshkov (R-M) instabilities
- k represents kinetic energy of unthermalized and unresolved turbulence
- L represents length scale of turbulent eddies

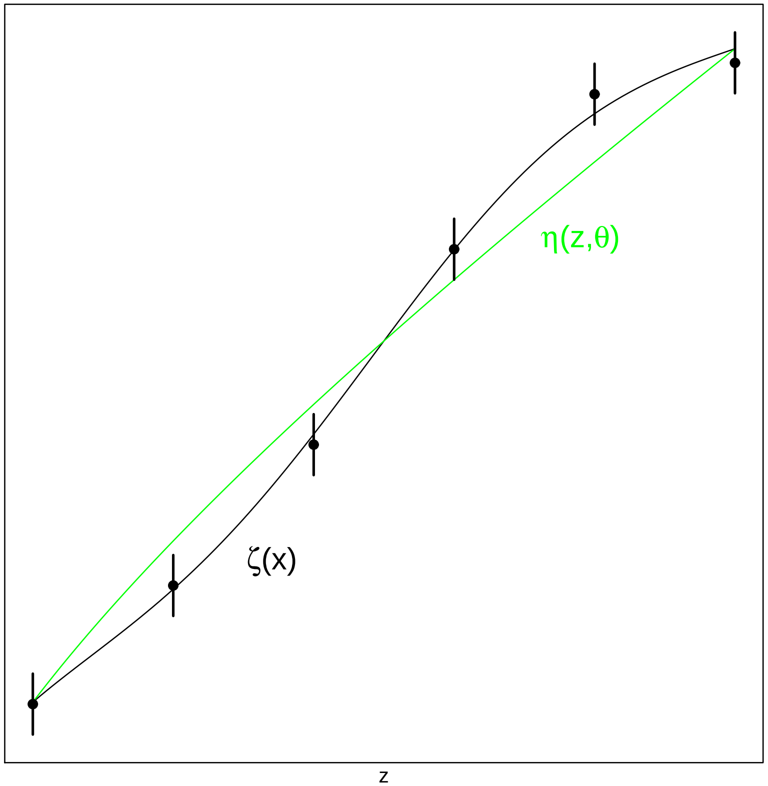
L equation: $\rho\frac{DL}{Dt} = \frac{1}{r}\left[\frac{\partial}{\partial r}\left(r\mu_t\frac{\partial L}{\partial r}\right) + \frac{\partial}{\partial z}\left(r\mu_t\frac{\partial L}{\partial z}\right)\right] + \rho S_L$

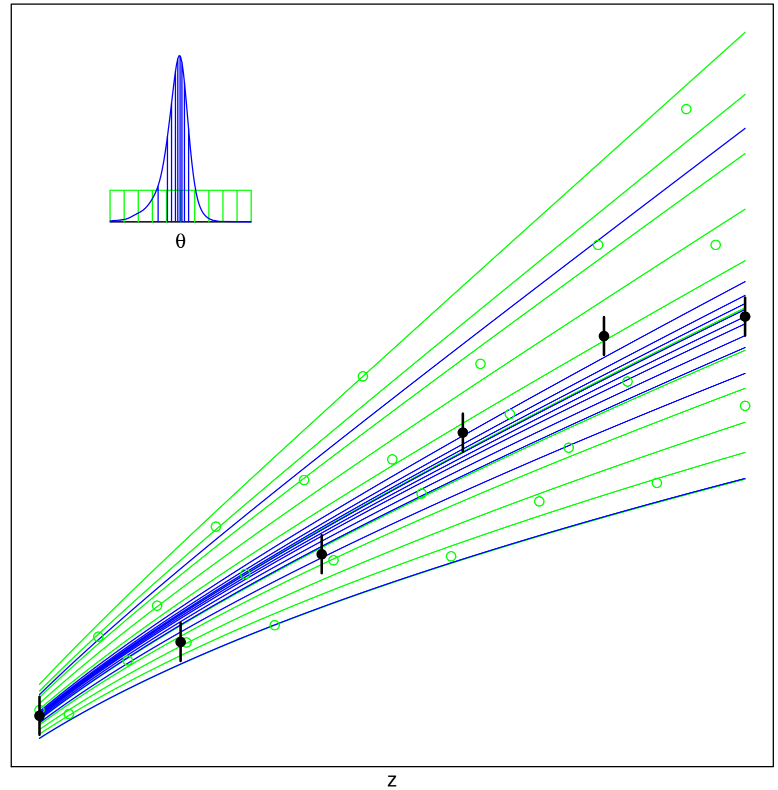
k equation: $\rho\frac{Dk}{Dt} = -\frac{2}{3}\rho k\left[\frac{\partial u}{\partial z} + \frac{\partial v}{\partial r} + \frac{v}{r}\right] + \frac{1}{r}\left[\frac{\partial}{\partial r}\left(r\mu_t\frac{\partial k}{\partial r}\right) + \frac{\partial}{\partial z}\left(r\mu_t\frac{\partial k}{\partial z}\right)\right] + \rho S_k$

Source terms: $S_L = \sqrt{2k} + \frac{L}{r}\left[\frac{\partial(rv)}{\partial r} + \frac{\partial(ru)}{\partial z}\right] \qquad S_k = \sqrt{2k}\left[C_B A a - \frac{C_D k}{L}\right]$

Turbulent eddy viscosity: $\mu_t = C_T \rho L \sqrt{2k}$

Outline of Statistical Framework I





- $y(x) = \zeta(x) + \epsilon(x)$

$\longrightarrow$ $\zeta(x)$: mean system output

$\longrightarrow$ $\epsilon(x)$: observational error

- $\eta(z, \theta)$: computer model evaluated at best θ

- Use field data $\boldsymbol{y}$ to calibrate θ

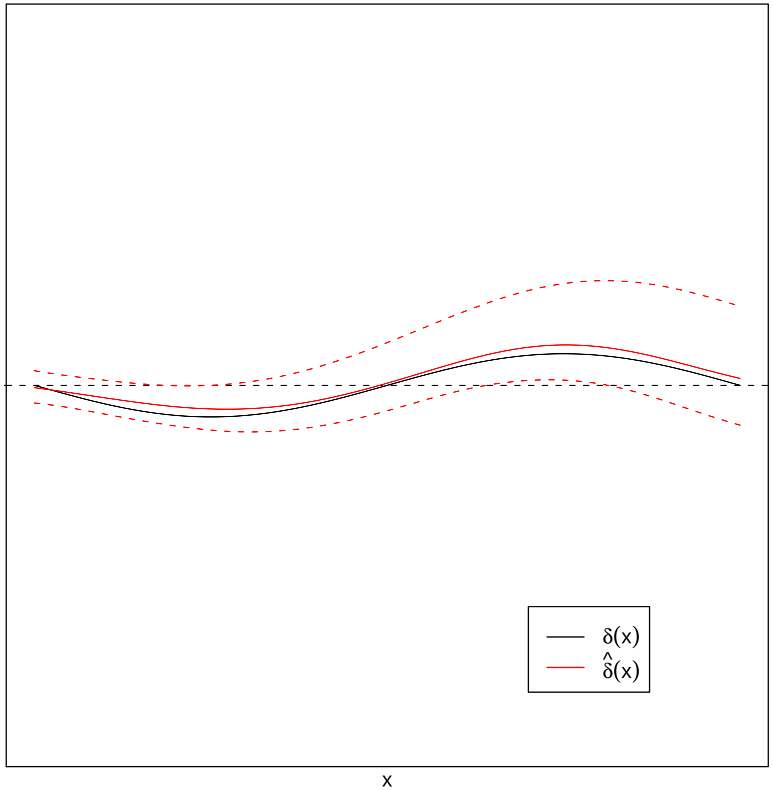
$\longrightarrow$ prior (green); posterior (blue)

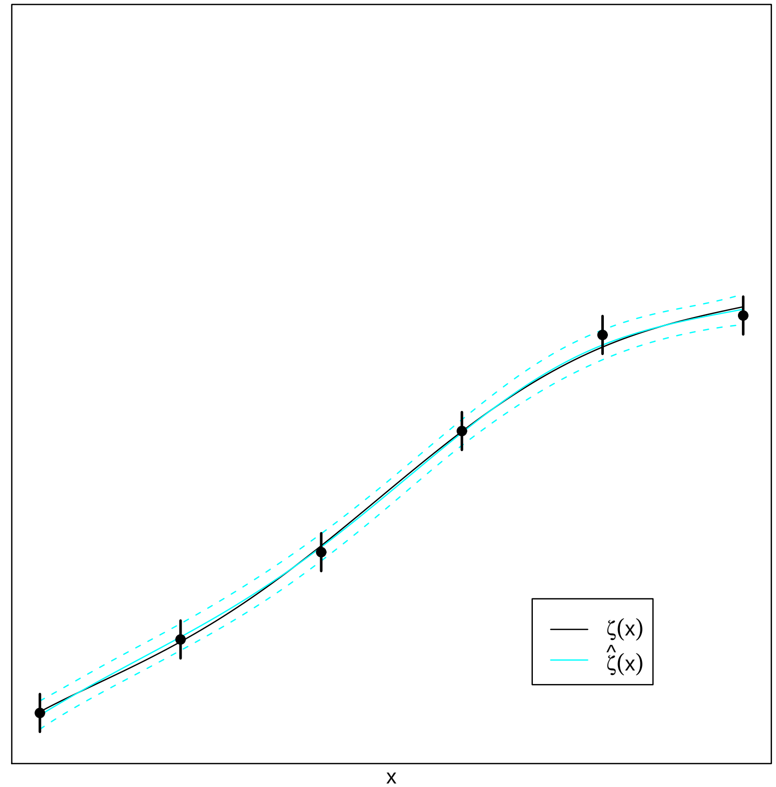
- Response surface model

$\longrightarrow$ experiment design (circles)

$\longrightarrow$ predictions

Outline of Statistical Framework II





- Inference for discrepancy

$\longrightarrow$ $\delta(x) = \zeta(x) - \eta(x, \theta)$

$\longrightarrow$ true $\delta(x)$ (black)

$\longrightarrow$ posterior mean (solid red)

$\longrightarrow$ 5/95 pointwise intervals (dashed red)

- Inference for system

$\longrightarrow$ adjusts for code inadequacy

$\longrightarrow$ true $\zeta(x)$ (black)

$\longrightarrow$ posterior mean (solid cyan)

$\longrightarrow$ 5/95 pointwise intervals (dashed cyan)

Specifics of Statistical Framework I

- Statistical model for functional experimental data:

$$\boldsymbol{y}(\boldsymbol{x}) = \boldsymbol{\eta}(\boldsymbol{x},\boldsymbol{\theta}) + \boldsymbol{\delta}(\boldsymbol{x}) + \boldsymbol{\epsilon}(\boldsymbol{x})$$

$\longrightarrow$ Continuous function of input variables or multivariate collection of features

- Functional code output $\boldsymbol{\eta}(\boldsymbol{x},\boldsymbol{\theta})$

$\longrightarrow$ Response surface surrogate for slow codes (e.g. 2-d)

$\longrightarrow$ Represent $\boldsymbol{\eta}$ in terms of a basis decomposition:

$$\boldsymbol{\eta}(\boldsymbol{x},\boldsymbol{\theta}) = \boldsymbol{k}_1 w_1(\boldsymbol{x},\boldsymbol{\theta}) + \cdots + \boldsymbol{k}_{p_\eta} w_{p_\eta}(\boldsymbol{x},\boldsymbol{\theta})$$

- Flexibility in choice of $\boldsymbol{k}_i$

$\longrightarrow$ general $\Rightarrow$ orthogonal $\Rightarrow$ principal components

- Statistical model for $w_i(\boldsymbol{x},\boldsymbol{\theta})$: GP($\boldsymbol{\rho}_{wi}$; λ_{wi})

$\longrightarrow$ Gaussian process (GP): response surface model for smooth functions

$\longrightarrow$ mean zero; covariance

$$C((\boldsymbol{x},\boldsymbol{\theta}),(\boldsymbol{x}^*,\boldsymbol{\theta}^*)) = \frac{1}{\lambda_{wi}} \prod_{j=1}^{n_x} \rho_{wi,j}^{4(x_j - x_j^*)^2} \prod_{j=1}^{n_\theta} \rho_{wi,j+n_x}^{4(\theta_j - \theta_j^*)^2}, \quad \rho_{wi} = \exp(-\beta_{wi}/4)$$

$\longrightarrow$ $\{w(\boldsymbol{x}_1,\boldsymbol{\theta}_1),\ldots,w(\boldsymbol{x}_m,\boldsymbol{\theta}_m)\}$ is multivariate normal for any m

Specifics of Statistical Framework II

• Functional discrepancy $\boldsymbol{\delta}(\boldsymbol{x})$

→ Discrepancy defined through difference $\boldsymbol{\zeta}(\boldsymbol{x}) - \boldsymbol{\eta}(\boldsymbol{x}, \boldsymbol{\theta})$, evaluated at "best", unknown tuning parameter $\boldsymbol{\theta}$

→ Represent $\boldsymbol{\delta}$ in terms of a basis decomposition:

$$\boldsymbol{\delta}(\boldsymbol{x}) = \boldsymbol{d}_1 v_1(\boldsymbol{x}) + \cdots + \boldsymbol{d}_{p_\delta} v_{p_\delta}(\boldsymbol{x})$$

• Localized basis functions often chosen for $\boldsymbol{d}_i$

→ allow for lack of smoothness in discrepancy, eg. kernel basis

→ allow for calibration to multiple features simultaneously, eg. unit vectors

• Statistical model for $v_i(\boldsymbol{x})$: GP($\boldsymbol{\rho}_v$; λ_v)

→ Groups of coefficients may have their own specific GP parameters

• $\boldsymbol{\delta}(\cdot)$ independent of $\boldsymbol{\eta}(\cdot)$

• Statistical model for $\boldsymbol{\epsilon}(\boldsymbol{x})$: Gaussian white noise (GP($\mathbf{0}$; λ_ϵ))

→ may need to accommodate correlated errors for some applications

• $\boldsymbol{\epsilon}(\cdot)$ independent of $\boldsymbol{\eta}(\cdot)$ and $\boldsymbol{\delta}(\cdot)$

• Extension of Kennedy and O'Hagan (2001)

→ Basis decompositions ease computational effort relative to standard Kennedy and O'Hagan implementation

Bayesian Framework

- Prior distributions: $\pi(\boldsymbol{\theta})\,, \pi(\boldsymbol{\rho}_w)\,, \pi(\lambda_w)\,, \pi(\boldsymbol{\rho}_v)\,, \pi(\lambda_v)\,, \pi(\lambda_\epsilon)$
- Likelihood function: $L(\boldsymbol{y}_1, \ldots, \boldsymbol{y}_n, \Xi | \boldsymbol{\theta}, \{\boldsymbol{\rho}_w\}, \{\lambda_w\}, \boldsymbol{\rho}_v, \lambda_v, \lambda_\epsilon)$

$\longrightarrow$ multivariate normal likelihood

- Priors in practice:

$\longrightarrow$ Correlation parameters ($\boldsymbol{w}$ and $\boldsymbol{v}$)

$$\pi(\boldsymbol{\rho}) \propto \prod_{j=1}^{n_\rho} (1-\rho_j)^{(b_\rho - 1)}\,, 0 < \rho_j \leq 1$$

  – Control degree of prior smoothness (variable importance)

$\longrightarrow$ Precision parameters ($\boldsymbol{w}$, $\boldsymbol{v}$, and ϵ)

$$\pi(\lambda) \propto \lambda^{(a_\lambda - 1)} \exp(-b_\lambda \lambda)\,,\ \lambda > 0$$

  – Set $a_w = b_w$ (prior mean 1; $b_w \uparrow \ \Rightarrow\ $ prior variance $\downarrow$)
  – Set $b_v \ll a_v$, i.e. noninformative with large prior mean
  – Settings for a_ϵ and b_ϵ depend on assumptions for observation error

- Inference objectives:

$\longrightarrow$ sensitivity analysis

$\longrightarrow$ posterior distribution of calibration parameters $\boldsymbol{\theta}$

$\longrightarrow$ predictive distribution for new experiment $\boldsymbol{y}(\boldsymbol{x}_0)$: $\pi(\boldsymbol{y}(\boldsymbol{x}_0) | \boldsymbol{y}_1, \ldots, \boldsymbol{y}_n, \Xi)$

Posterior Sampling

• Posterior is sampled via Metropolis MCMC. Let $\boldsymbol{\xi} = (\boldsymbol{\theta}, \{\boldsymbol{\rho}_w\}, \{\lambda_w\}, \boldsymbol{\rho}_v, \lambda_v, \lambda_\epsilon)$.

$\longrightarrow$ Begin with $\boldsymbol{\xi}^0$, set iteration counter $i = 1$

$\longrightarrow$ Generate candidate ξ_1^* from a symmetric distribution. Compute the acceptance ratio

$$\alpha(\xi_1^0, \xi_1^*) = \min\left(1, \frac{\pi((\xi_1^*, \boldsymbol{\xi}_{-1}^0)|\boldsymbol{y}, \boldsymbol{\eta})}{\pi(\boldsymbol{\xi}^0|\boldsymbol{y}, \boldsymbol{\eta})}\right)$$

and set

$$\xi_1^1 = \begin{cases} \xi_1^* \text{ with probability } \alpha(\xi_1^0, \xi_1^*) \\ \xi_1^0 \text{ otherwise} \end{cases}$$

$\longrightarrow$ At iteration i, scan through each parameter. Generate candidate ξ_j^* from a symmetric distribution. Compute the acceptance ratio

$$\alpha(\xi_j^{(i-1)}, \xi_j^*) = \min\left(1, \frac{\pi((\boldsymbol{\xi}^i_{\{1:(j-1)\}}, \xi_j^*, \boldsymbol{\xi}^{(i-1)}_{\{(j+1):\#\boldsymbol{\xi}\}})|\boldsymbol{y}, \boldsymbol{\eta})}{\pi((\boldsymbol{\xi}^i_{\{1:(j-1)\}}, \boldsymbol{\xi}^{(i-1)}_{\{j:\#\boldsymbol{\xi}\}})|\boldsymbol{y}, \boldsymbol{\eta})}\right)$$

and set

$$\xi_j^i = \begin{cases} \xi_j^* \text{ with probability } \alpha(\xi_j^{(i-1)}, \xi_j^*) \\ \xi_j^{(i-1)} \text{ otherwise} \end{cases}$$

$\longrightarrow$ Repeat this process for several thousand iterations, discarding initial pre-convergence samples

Optimal Symmetric Latin Hypercube (LH) Designs

- Optimize symmetric LH designs with respect to a distance-based criterion

$\longrightarrow$ spread points out in two-dimensional projections

- Start with a random, symmetric $N \times p$ LH design

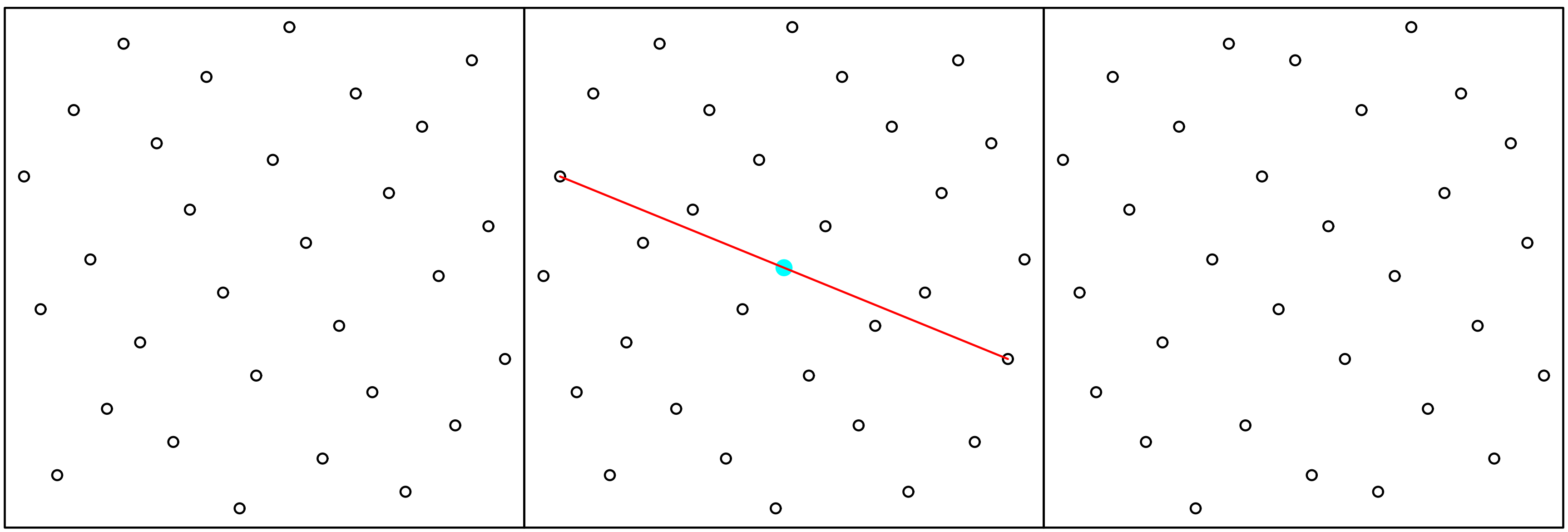
$\longrightarrow$ symmetry requires $(a_1, \ldots, a_p) \leftrightarrow (N+1-a_1, \ldots, N+1-a_p)$

- Two standard search algorithms

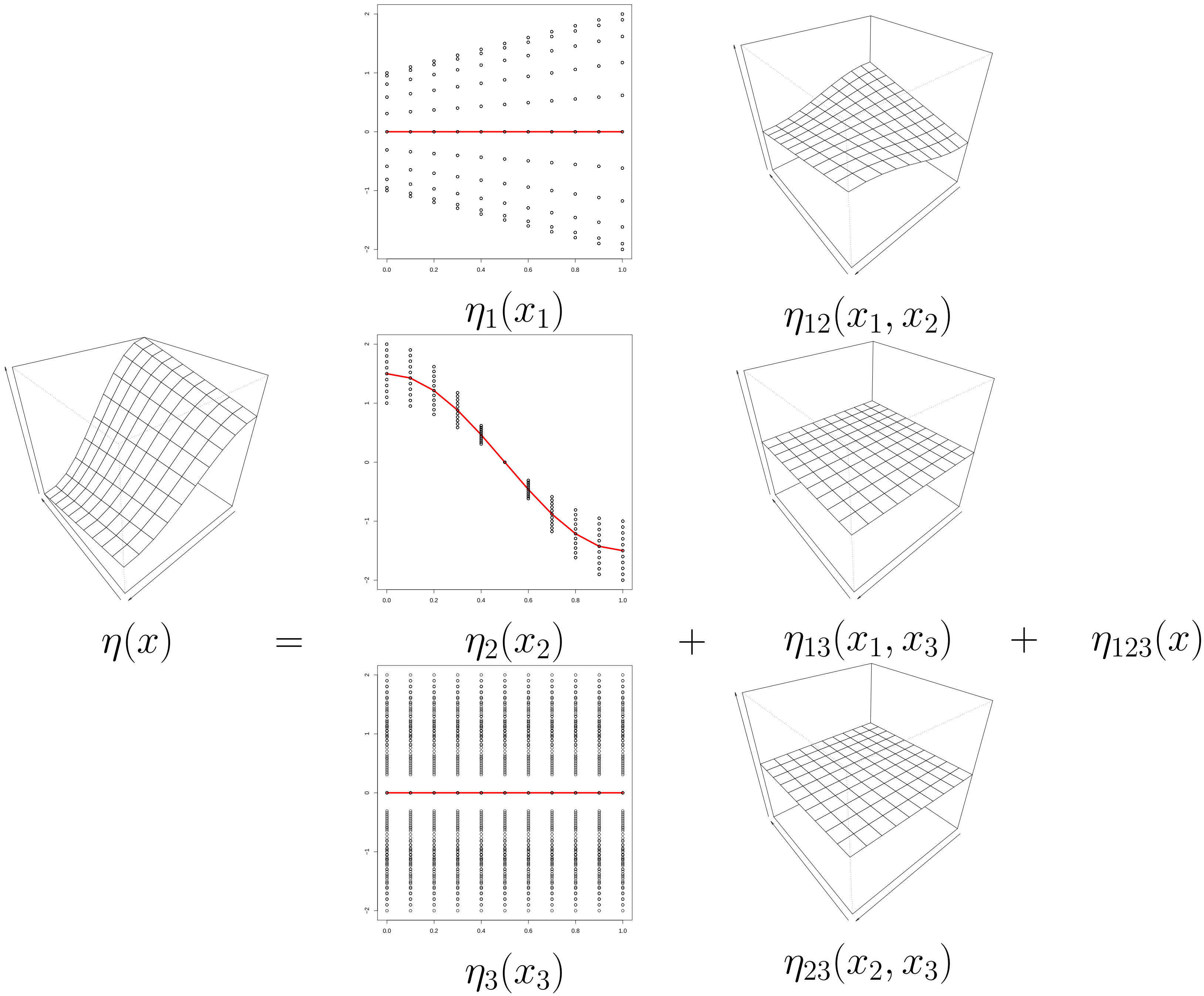
$\longrightarrow$ columnwise–pairwise (CP) algorithm [Ye, K., Li, W., Sudjianto, A. (2000)]

$\longrightarrow$ simulated annealing (SA) algorithm [Morris, M. and Mitchell, T. (1995)]

- Repeat optimization with multiple starting designs



Sobol' decomposition of $\eta(x_1, x_2, x_3) = (x_1 + 1)\cos(\pi x_2) + 0x_3$



Variance Based Global Sensitivity Analysis

- Sobol' unique function decomposition

$$\eta(x_1,\ldots,x_p) = \eta_0 + \sum_{j=1}^{p} \eta_j(x_j) + \sum_{1\le j<k\le p} \eta_{jk}(x_j,x_k) + \cdots + \eta_{1,2,\ldots,p}(x_1,x_2,\ldots,x_p)\,,$$

$$\eta_0 = \int_{[0,1]^p} \eta(x_1,\ldots,x_p)\,dx_1\cdots dx_p \text{ and } \int_0^1 \eta_{k_1,\ldots,k_s}(x_{k_1},\ldots,x_{k_s})dx_{k_i} = 0$$

for $i = 1,\ldots,s\,,\, s = 1,\ldots,p$ and $1 \le k_1 < \cdots < k_s \le p$

– orthogonal components

- Variance decompositon and sensitivity indices

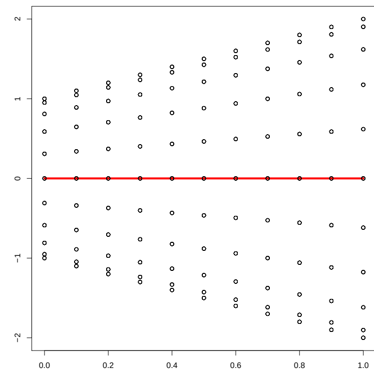
$$V = \sum_{j=1}^{p} V_j + \sum_{1\le j<k\le p} V_{jk} + \cdots + V_{1,2,\ldots,p}\,, \quad S_{k_1,\ldots,k_s} = \frac{V_{k_1,\ldots,k_s}}{V}$$

$$V = \int_{[0,1]^p} \eta^2(x)\,dx - \eta_0^2 \text{ and } V_{k_1,\ldots,k_s} = \int_{[0,1]^s} \eta^2_{k_1,\ldots,k_s}(x_{k_1},\ldots,x_{k_s})\,dx_{k_1}\cdots dx_{k_s}$$

- McKay correlation ratio

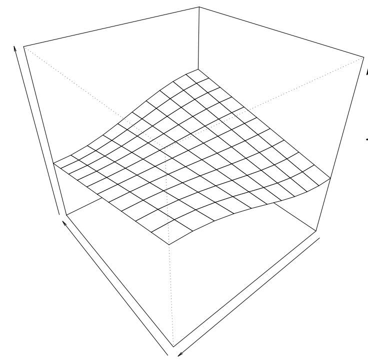
$$R^2_{k_1,\ldots,k_s} = \frac{\mathrm{Var}[\mathrm{E}(\eta(x)\,|\,x_{k_1},\ldots,x_{k_s})]}{V} = \sum_{i=1}^{s} \sum_{\omega\subset\{k_1,\ldots,k_s\};|\omega|=i} S_\omega$$

Sobol' decomposition of $\eta(x_1, x_2, x_3) = (x_1 + 1)\cos(\pi x_2) + 0x_3$



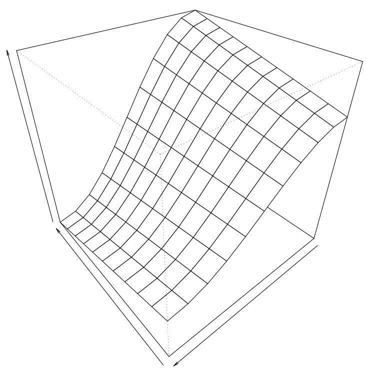
$S_1 = 0$
$R_1^2 = 0$

$\eta_1(x_1)$



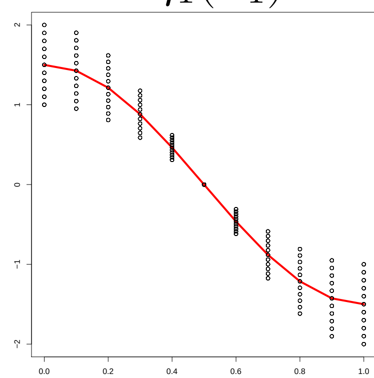
$S_{12} = .04$
$R_{12}^2 = 1$

$\eta_{12}(x_1, x_2)$



$\eta(x)$

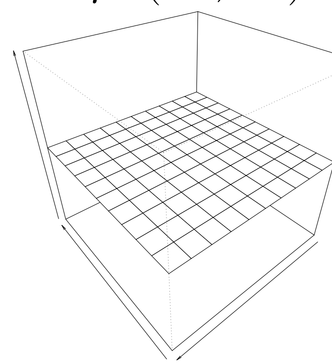
$=$



$S_2 = .96$
$R_2^2 = .96$

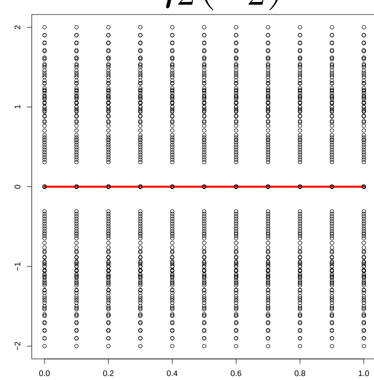
$\eta_2(x_2)$

$+$



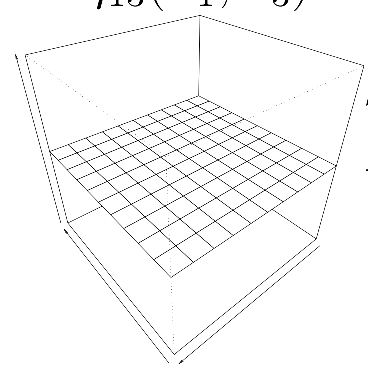
$S_{13} = 0$
$R_{13}^2 = 0$

$\eta_{13}(x_1, x_3)$



$S_3 = 0$
$R_3^2 = 0$

$\eta_3(x_3)$



$S_{23} = 0$
$R_{23}^2 = .96$

$\eta_{23}(x_2, x_3)$

Global Sensitivity Analysis for Functional Code Outputs

- Orthogonal basis representation

$$\boldsymbol{\eta}(x) = \boldsymbol{k}_1 w_1(x) + \cdots + \boldsymbol{k}_{p_\eta} w_{p_\eta}(x)$$

- Mean and total variance

$$\boldsymbol{\eta}_0 = \sum_{j=1}^{p_\eta} \boldsymbol{k}_j w_{j0} \quad \text{and} \quad V = \int_{[0,1]^p} \boldsymbol{\eta}^\top(x)\boldsymbol{\eta}(x)\,dx - \boldsymbol{\eta}_0^\top \boldsymbol{\eta}_0$$

- Main effect functions

$$\boldsymbol{\eta}(x_i) = \boldsymbol{k}_1 w_{1i}(x_i) + \cdots + \boldsymbol{k}_{p_\eta} w_{p_\eta i}(x_i)$$

- Main effect variance components and sensitivity indices

$$V_i = \sum_{j=1}^{p_\eta} \lambda_j V_{w_j,i} \text{ and } V = \sum_{j=1}^{p_\eta} \lambda_j V_{w_j} \text{ for } \lambda_j = \boldsymbol{k}_j^\top \boldsymbol{k}_j \Rightarrow S_i = V_i/V$$

- Two factor interaction effect functions

$$\boldsymbol{\eta}(x_h, x_i) = \boldsymbol{k}_1 w_{1,hi}(x_h, x_i) + \cdots + \boldsymbol{k}_{p_\eta} w_{p_\eta,hi}(x_h, x_i)$$

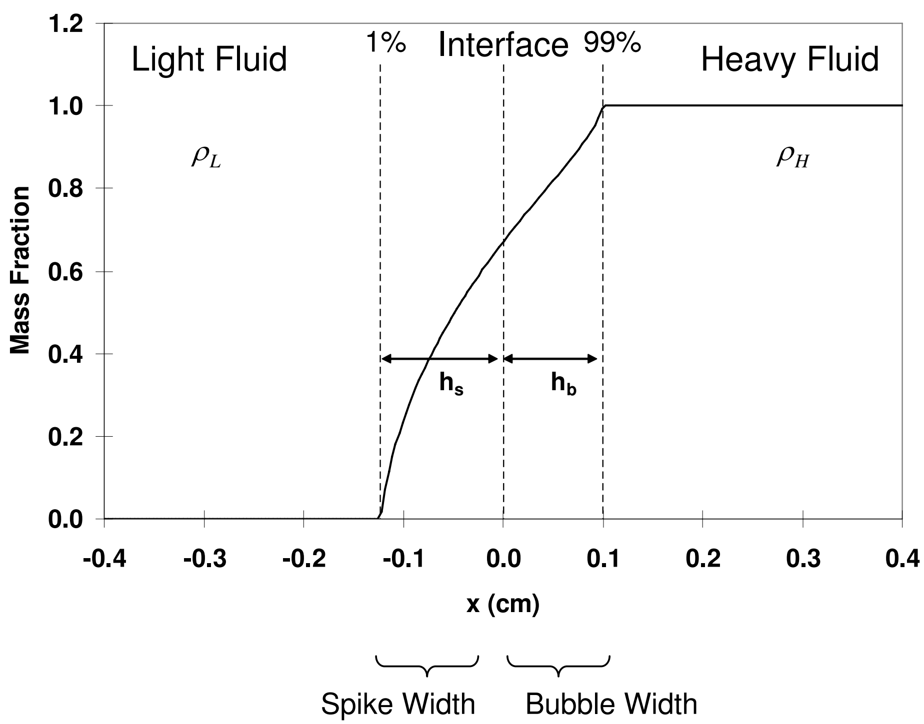
- Two-factor interaction effect variance components and sensitivity indices

$$V_{hi} = \sum_{j=1}^{p_\eta} \lambda_j V_{w_j,hi} \Rightarrow S_{hi} = V_{hi}/V$$

Calibration of k-L Turbulent Mix Model to Linear Electric Motor (LEM) Experiments

• Experiment: Electromagnetic force accelerates a sealed plastic fluid container
$\longrightarrow$ two immiscible fluids having specified Atwood number
$\longrightarrow$ optical diagnosis of fluid interpenetration using backlit photography and laser-induced fluorescence

• Calibrate three free parameters in numerical simulation model affecting fluid buoyancy, drag and turbulent eddy viscosity



• Atwood number: $A = \dfrac{\rho_H - \rho_L}{\rho_H + \rho_L}$

• R-T growth rate: $h = \alpha A g t^2$

• R-M growth rate:

$$h = h_0 \left(\frac{u_0 t}{h_0 \theta} + 1 \right)^{\theta}$$

Physics Model Calibration Parameters

Parameter	Description	Domain	
		Min	Max
C_T	turbulent eddy viscosity coefficient	0.01	1.0
C_B	buoyancy coefficient	0.2	2.0
C_D	fluid drag coefficient	0.6	6.0

- Turbulent eddy viscosity coefficient C_T

$\longrightarrow$ controls turbulent diffusion of material in fluid

$\longrightarrow$ affects turbulence on macroscopic scale (ie. mass fraction, internal energy, pressure)

$\longrightarrow$ diffusive effect on k; $C_T \uparrow \;\Rightarrow\; \alpha \uparrow$

- Buoyancy coefficient C_B

$\longrightarrow$ affects turbulence on microscopic scale

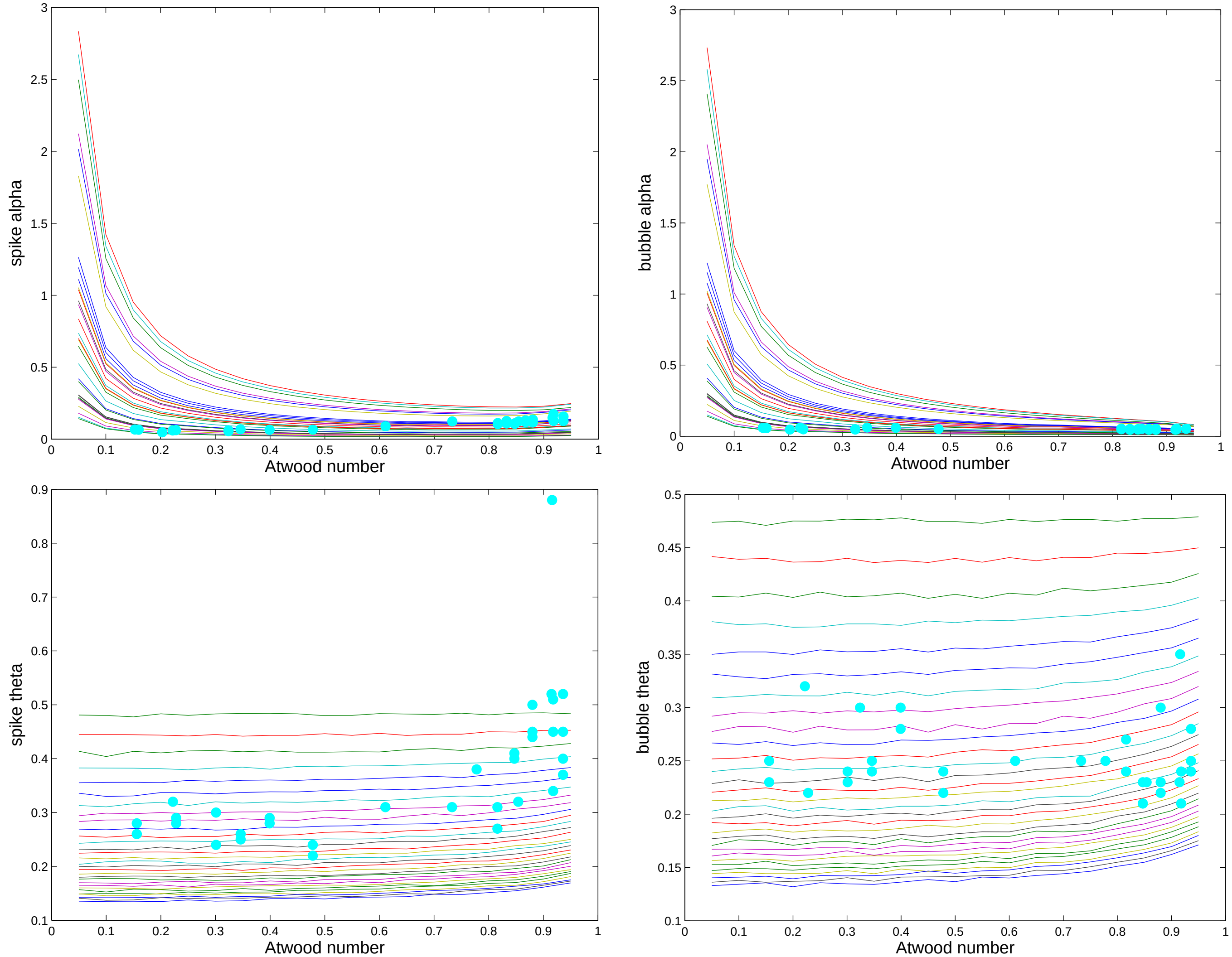
$\longrightarrow$ affects production of k at interface; $C_B \uparrow \;\Rightarrow\; \alpha \uparrow$

- Fluid drag coefficient C_D

$\longrightarrow$ affects turbulence on microscopic scale

$\longrightarrow$ affects production of k at interface; $C_D \uparrow \;\Rightarrow\; \alpha \downarrow$, $\theta \downarrow$

Simulator and Experimental Data



- "Optimal" symmetric LH design in 30 runs, 3 variables

$\longrightarrow$ Distance criterion: distribute points "evenly" in every 2-d projection

$\longrightarrow$ Select best design from 10 random starts of the CP and SA algorithms

Modeling Simulator Output: R-T Instability

- $n_\eta \times m$ matrix of simulator output ("time" by "space")

$\longrightarrow$ each row mean centered; entire matrix scaled so output has variance 1

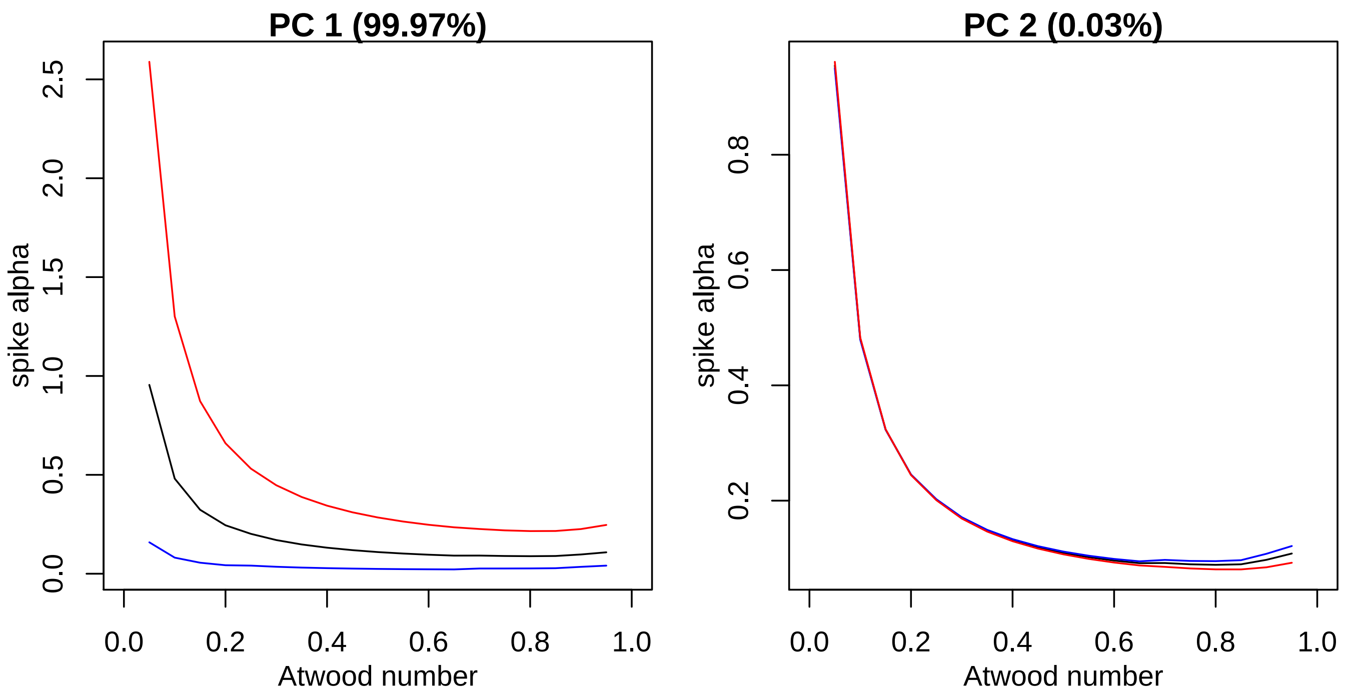
- Statistical model:

$$\boldsymbol{\eta}(\boldsymbol{x}, \boldsymbol{t}) = \sum_{i=1}^{p_\eta} \boldsymbol{k}_i w_i(\boldsymbol{x}, \boldsymbol{t}) + \boldsymbol{\epsilon}$$

$\longrightarrow$ $\boldsymbol{k}_1, \ldots, \boldsymbol{k}_{p_\eta}$ are $n_\eta \times 1$ orthogonal basis vectors (e.g. principal components)

$\longrightarrow$ $w_i(\boldsymbol{x}, \boldsymbol{t})$: basis coefficients; modeled as GP($\boldsymbol{\rho}_{wi}$,λ_{wi}); independent

$\longrightarrow$ $\boldsymbol{\epsilon}$: model error; modeled as GP($\boldsymbol{0}$,λ_η); independent of basis coefficients



Functional Sensitivity Analysis: R-T Instability

→ Sensitivity indices

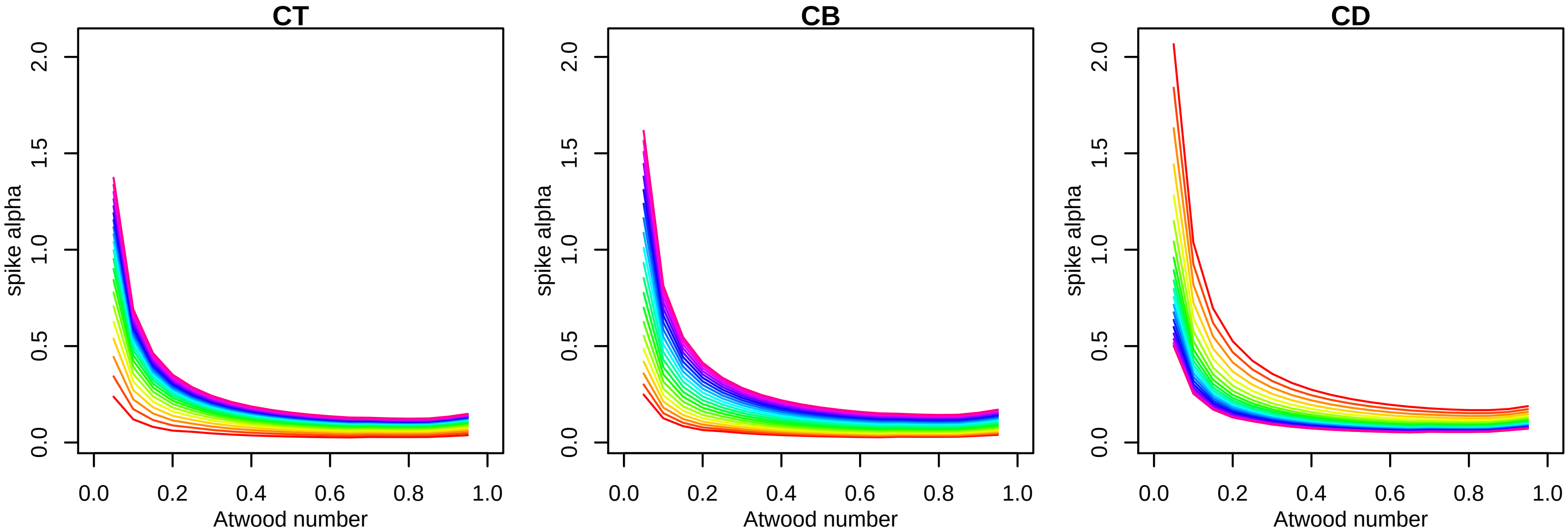
Spike

	C_T	C_B	C_D
C_T	18.82%	3.23%	3.94%
C_B	·	33.99%	6.27%
C_D	·	·	33.38%

total effects

C_T	26.36%
C_B	43.86%
C_D	43.96%

→ Main effect functions



Functional Sensitivity Analysis: R-M Instability

$\longrightarrow$ Sensitivity indices

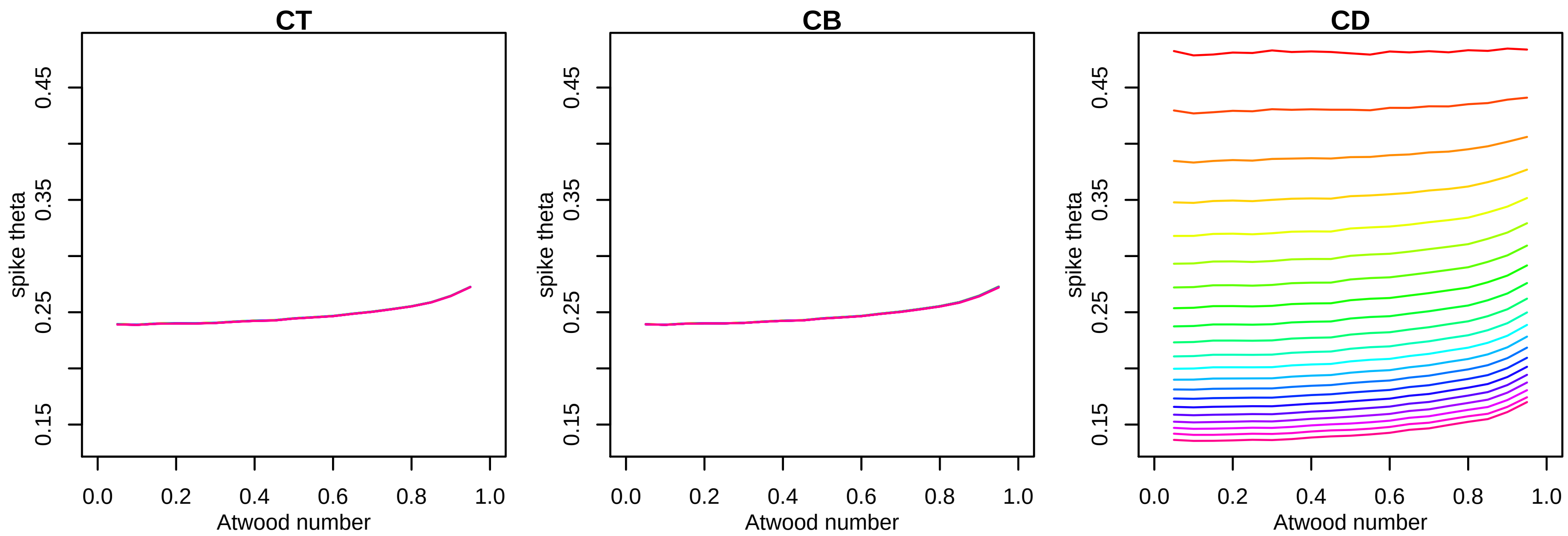
Spike

	C_T	C_B	C_D
C_T	0%	0%	0.001%
C_B	·	0%	0.001%
C_D	·	·	99.998%

total effects

C_T	0.001%
C_B	0.001%
C_D	99.999%

$\longrightarrow$ Main effect functions



Modeling Data: R-T Instability

- $\boldsymbol{y}(\boldsymbol{x}_i)$ is $n_{y_i} \times 1$ vector of centered/scaled experimental data, $i = 1, \ldots, n$
- Statistical model:

$$\boldsymbol{y}(\boldsymbol{x}_i) = \boldsymbol{K}_i \boldsymbol{w}(\boldsymbol{x}_i, \boldsymbol{\theta}) + \boldsymbol{D}_i \boldsymbol{v}(\boldsymbol{x}_i) + \boldsymbol{\epsilon}_i$$

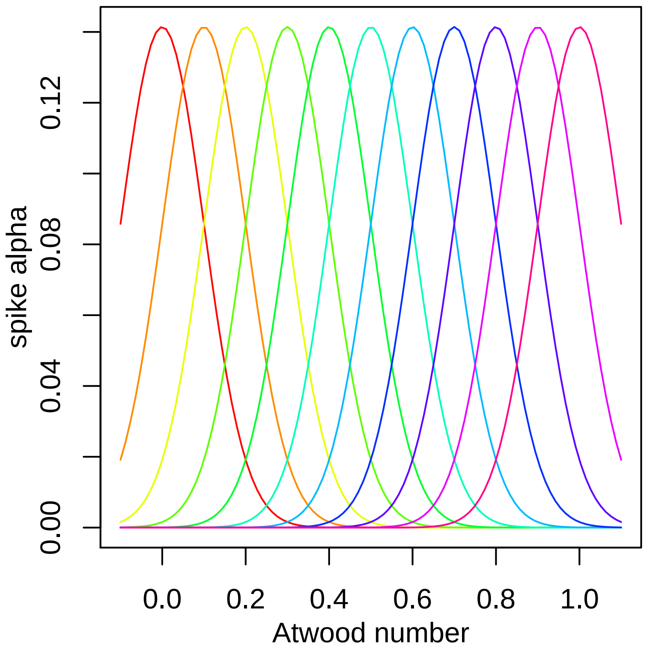
$\longrightarrow$ $\boldsymbol{K}_i$ is $n_{y_i} \times p_\eta$ matrix of simulator basis vectors interpolated onto data grid

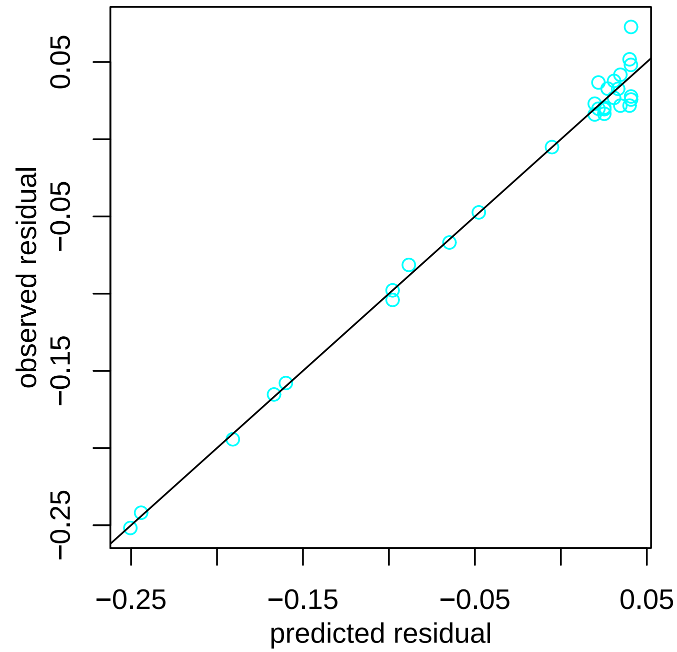
$\longrightarrow$ $\boldsymbol{w}(\boldsymbol{x}_i, \boldsymbol{\theta})$: simulator basis coefficients evaluated at best, unknown $\boldsymbol{\theta}$

$\longrightarrow$ $\boldsymbol{D}_i$ is $n_{y_i} \times p_\delta$ matrix of discrepancy basis vectors

$\longrightarrow$ $\boldsymbol{v}(\boldsymbol{x}_i)$: discrepancy basis coefficients; modeled as GP($\boldsymbol{\rho}_v$,λ_v); independent

$\longrightarrow$ $\boldsymbol{\epsilon}_i$: model error; modeled as GP($\boldsymbol{0}$,λ_y); independent of basis coefficients





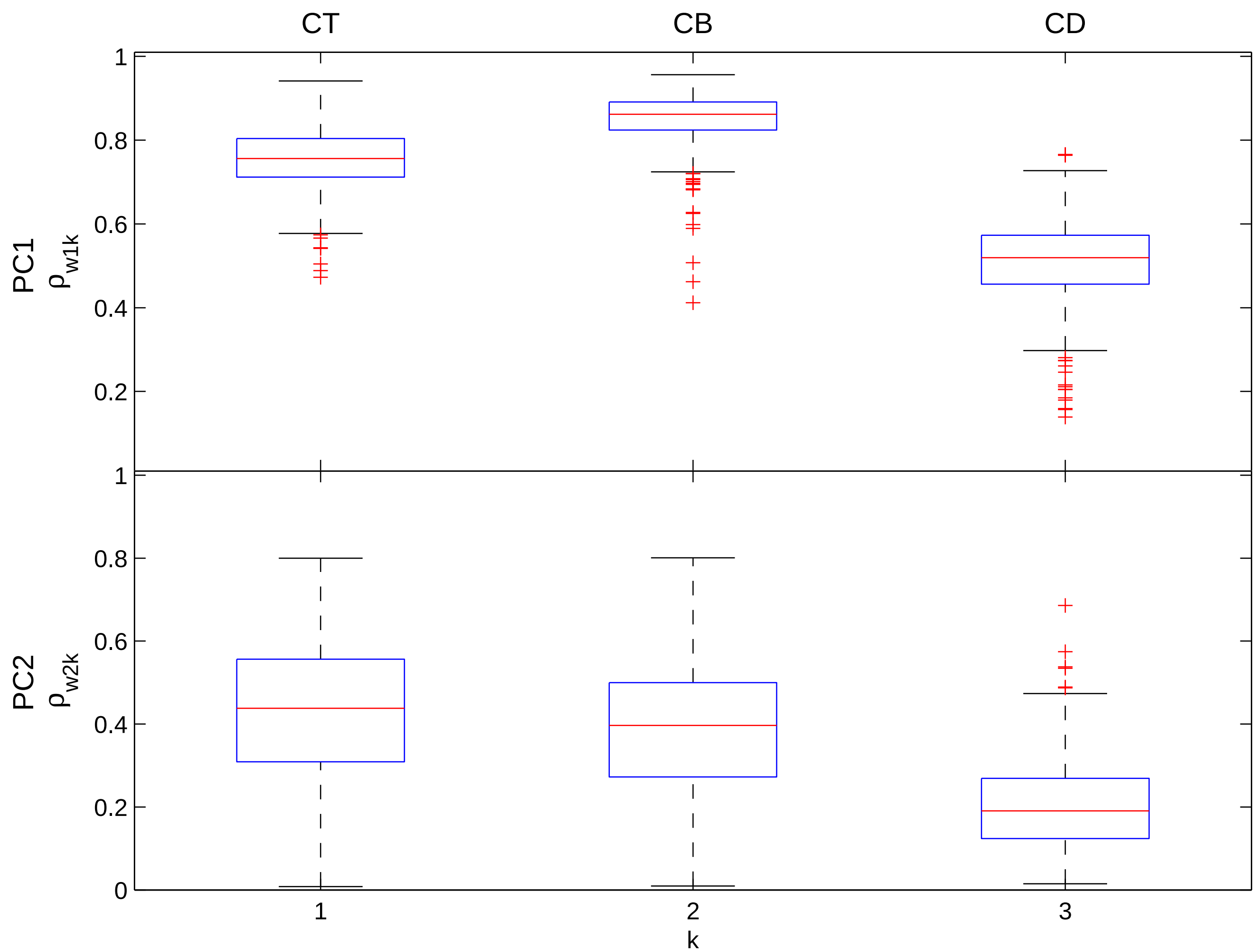
Bayesian Computation for k-L Turbulent Mix Model Calibration

Prior distributions

Parameters	Description	Prior Distribution
$\boldsymbol{\theta}$	k-L calibration parameters	Uniform on hyper–rectangle defined by domains in previous slide
$\boldsymbol{\rho}_{wi}$	Coefficients in simulator correlation models	Beta(1, 0.1)
$\boldsymbol{\rho}_{v}$	Coefficient in discrepancy correlation model	Beta(1, 0.3)
λ_{wi}	Simulator precision	Gamma(5, 5)
λ_{s}	Simulator nugget precision	Gamma(1, 0.0001)
λ_{η}	Simulator model error precision	Gamma(1, 0.0001)
λ_{v}	Discrepancy precision	Gamma(1, 0.0001)
λ_{y}	Measurement precision	Gamma(1, 0.0001)

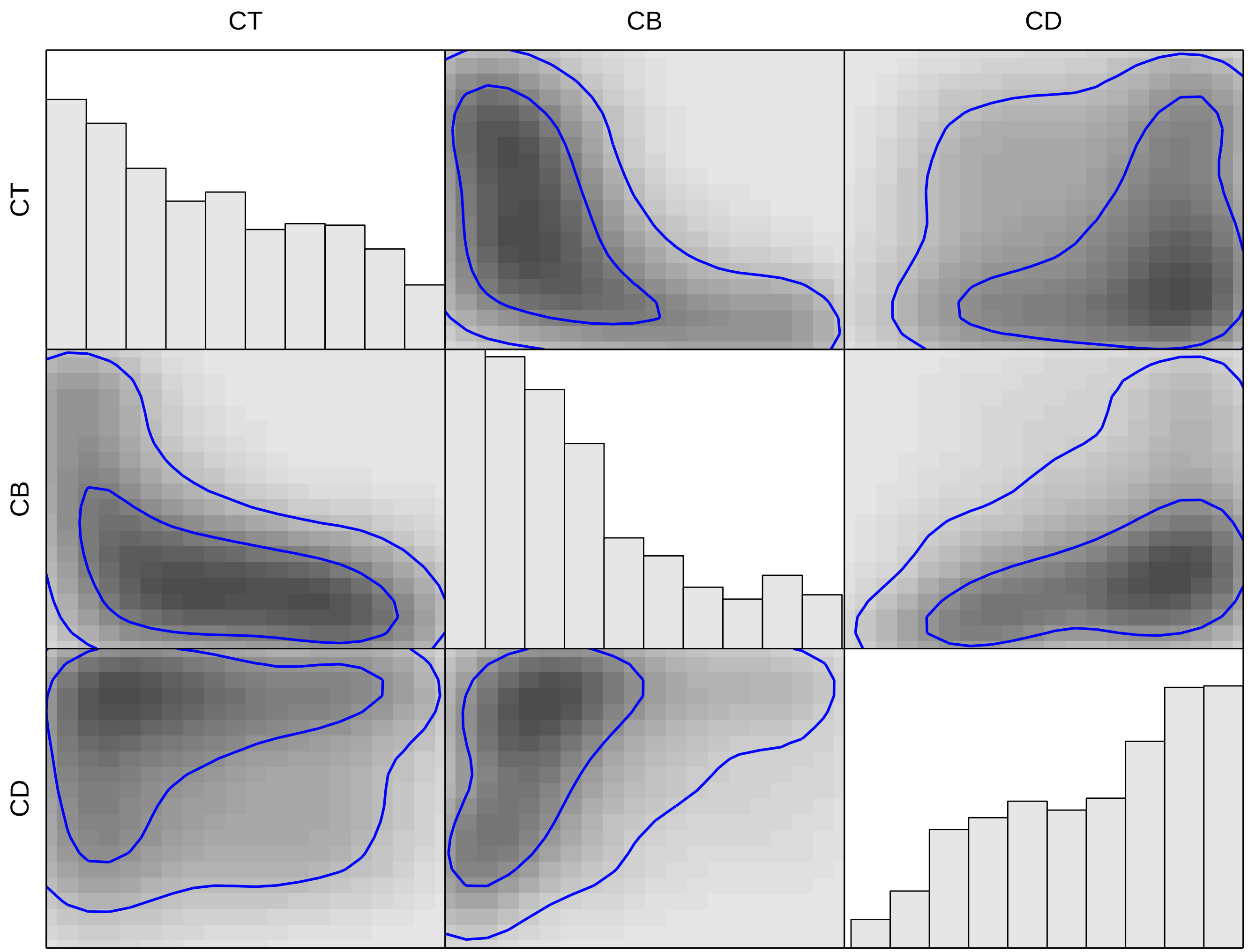
- 10,000 MCMC iterations after 10,500 burn-in

Correlation Parameters: R-T Instability



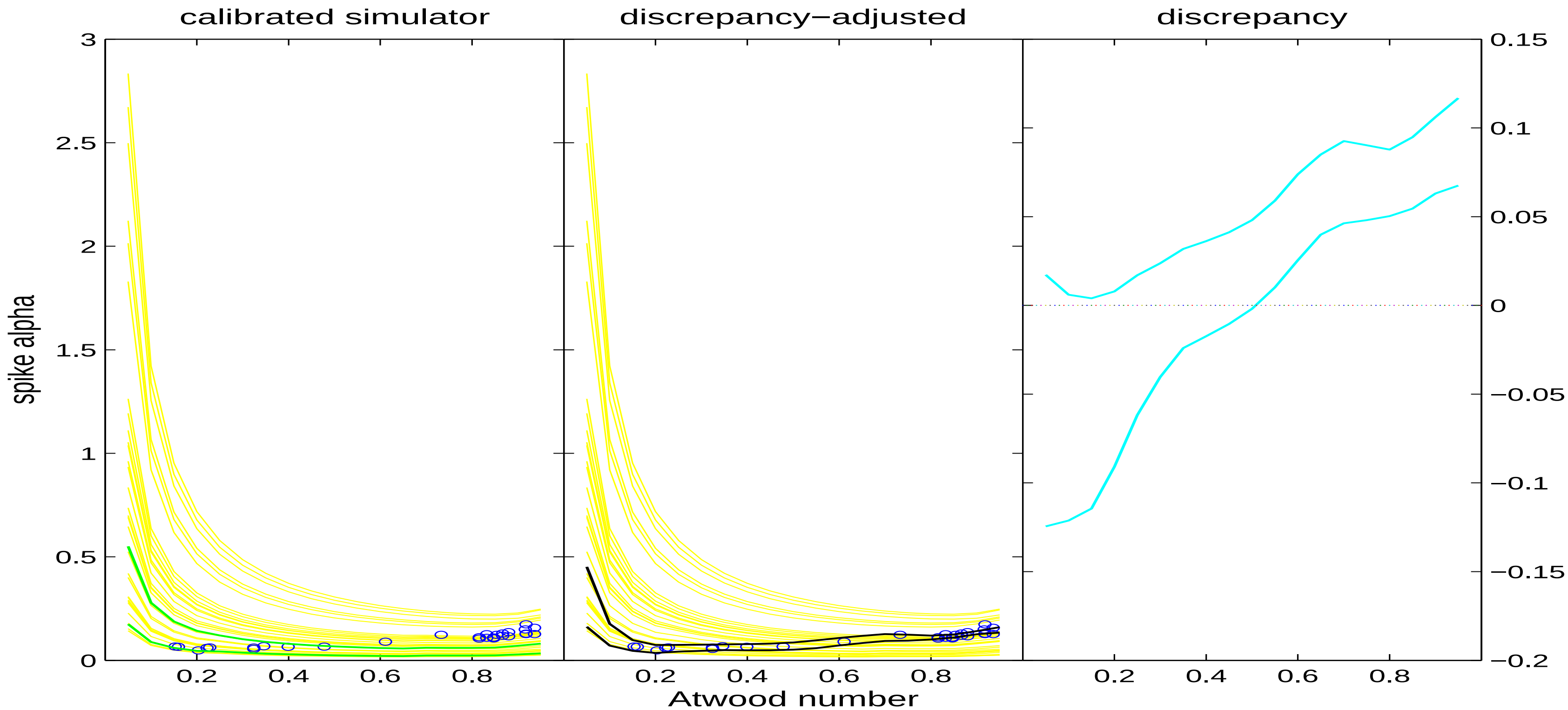
- Based on posterior distribution of $\boldsymbol{\rho}_{wi}$, $[\boldsymbol{\rho}_{wi}|\boldsymbol{y}, \boldsymbol{\Xi}]$

Calibration: R-T Instability



- Based on posterior distribution of $\boldsymbol{\theta}$, $[\boldsymbol{\theta}|\boldsymbol{y}, \boldsymbol{\Xi}]$

Prediction: R-T Instability

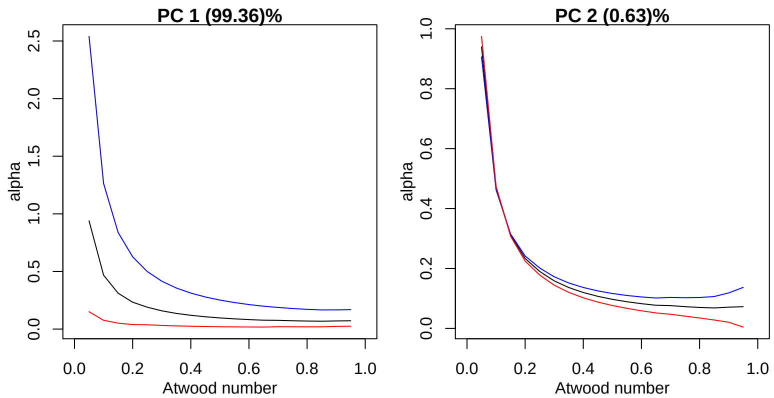


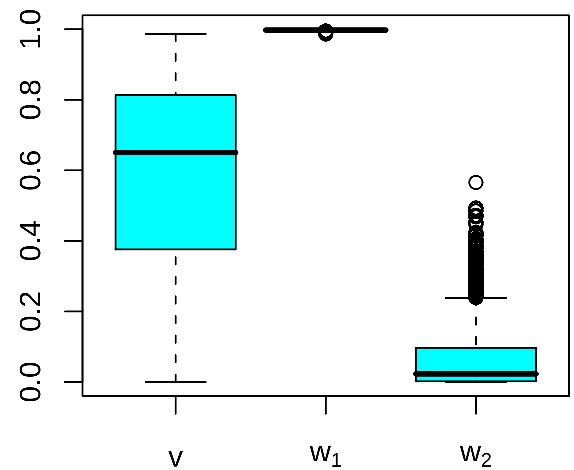
- Calibrated simulator based on realizations of $w_i(\boldsymbol{x}^*, \boldsymbol{\theta})$: $\boldsymbol{\eta}(\boldsymbol{x}^*, \boldsymbol{\theta}) = \sum_{i=1}^{p_\eta} \boldsymbol{k}_i w_i(\boldsymbol{x}^*, \boldsymbol{\theta})$
- Discrepancy based on realizations of $\boldsymbol{v}(\boldsymbol{x}^*)$: $\boldsymbol{\delta}(\boldsymbol{x}^*) = \boldsymbol{D}\boldsymbol{v}(\boldsymbol{x}^*)$
- Discrepancy-adjusted calibrated simulator based on above realizations:
  $\hat{y}(\boldsymbol{x}^*) = \boldsymbol{K}\boldsymbol{w}(\boldsymbol{x}^*, \boldsymbol{\theta}) + \boldsymbol{D}\boldsymbol{v}(\boldsymbol{x}^*)$
- 95/5 pointwise uncertainty bands

Joint Calibration to Spike and Bubble Data: R-T Instability

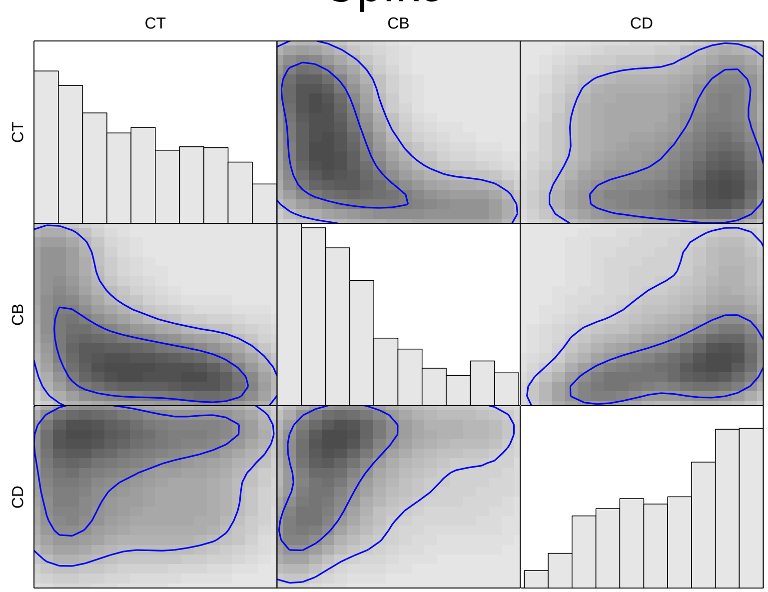
- Dependence introduced through system variable x_1

$\longrightarrow$ spike $(x_1 = 0)$, bubble $(x_1 = 1)$

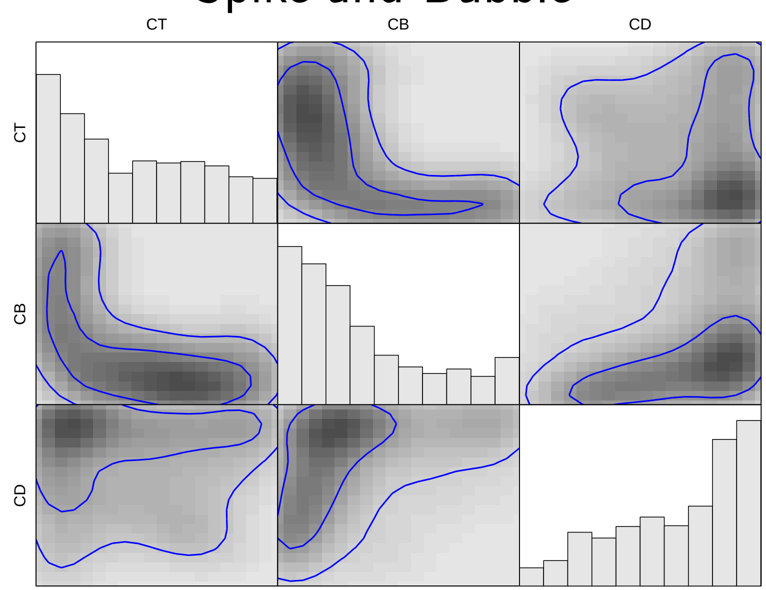




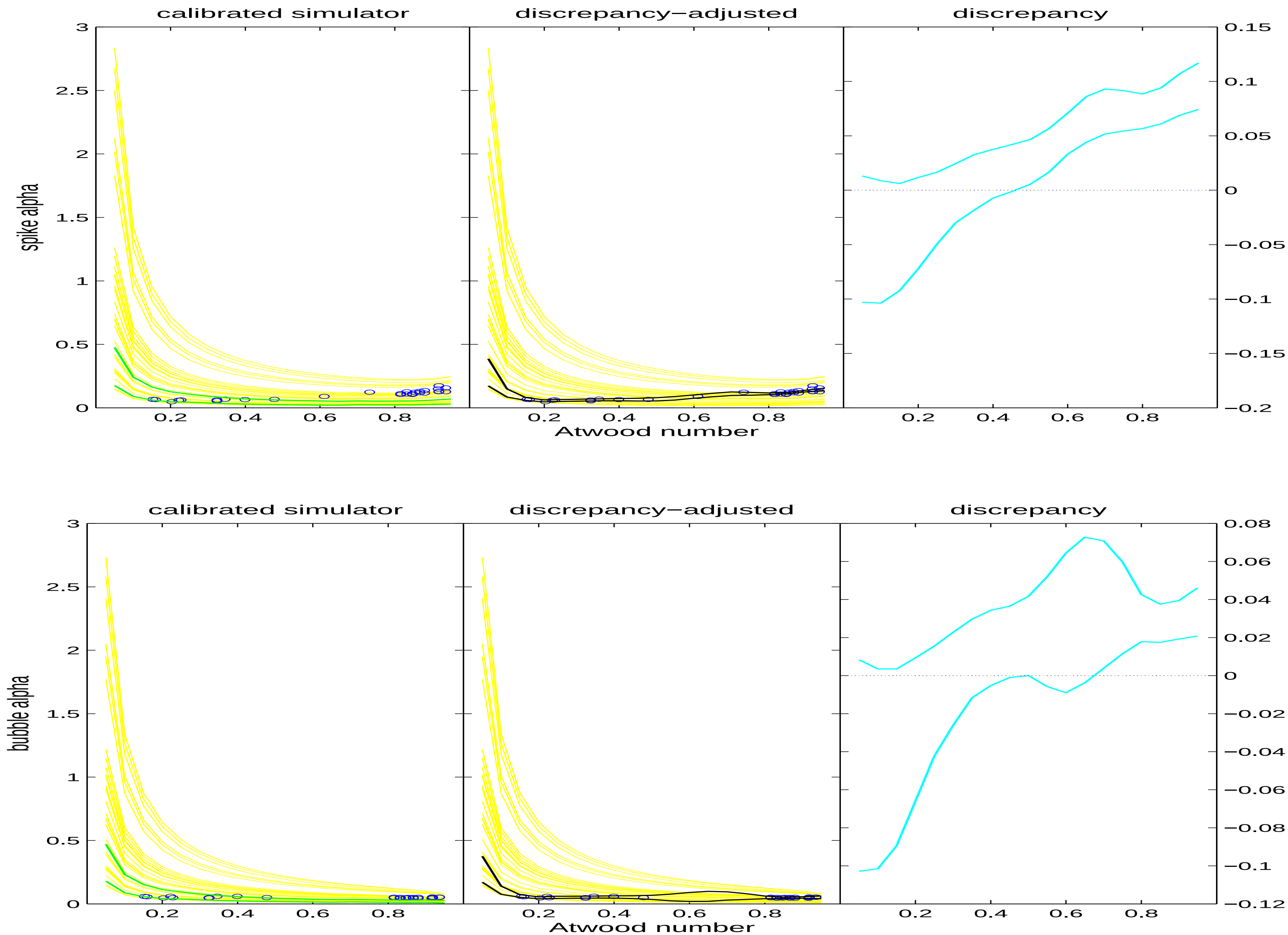
Spike



Spike and Bubble



Prediction Based on Joint Calibration: R-T Instability



Simultaneous Calibration to Multiple Independent Experiments

- Consider E independent experiments

$\longrightarrow$ Experiment-specific subsets $\boldsymbol{\theta}_{[1]}, \ldots, \boldsymbol{\theta}_{[E]}$ of calibration parameter vector $\boldsymbol{\theta}$

$\longrightarrow$ in general, these subsets are *not* mutually exclusive

- Simple modification of likelihood function

$$L\left(\boldsymbol{\theta} \,|\, (\boldsymbol{y}_1, \Xi_1), \ldots, (\boldsymbol{y}_E, \Xi_E)\right) = \prod_{j=1}^{E} L\left(\boldsymbol{\theta}_{[j]} \,|\, (\boldsymbol{y}_j, \Xi_j)\right)$$

- Any parameter in $\boldsymbol{\theta}$ common to multiple experiments is updated simultaneously across experiments

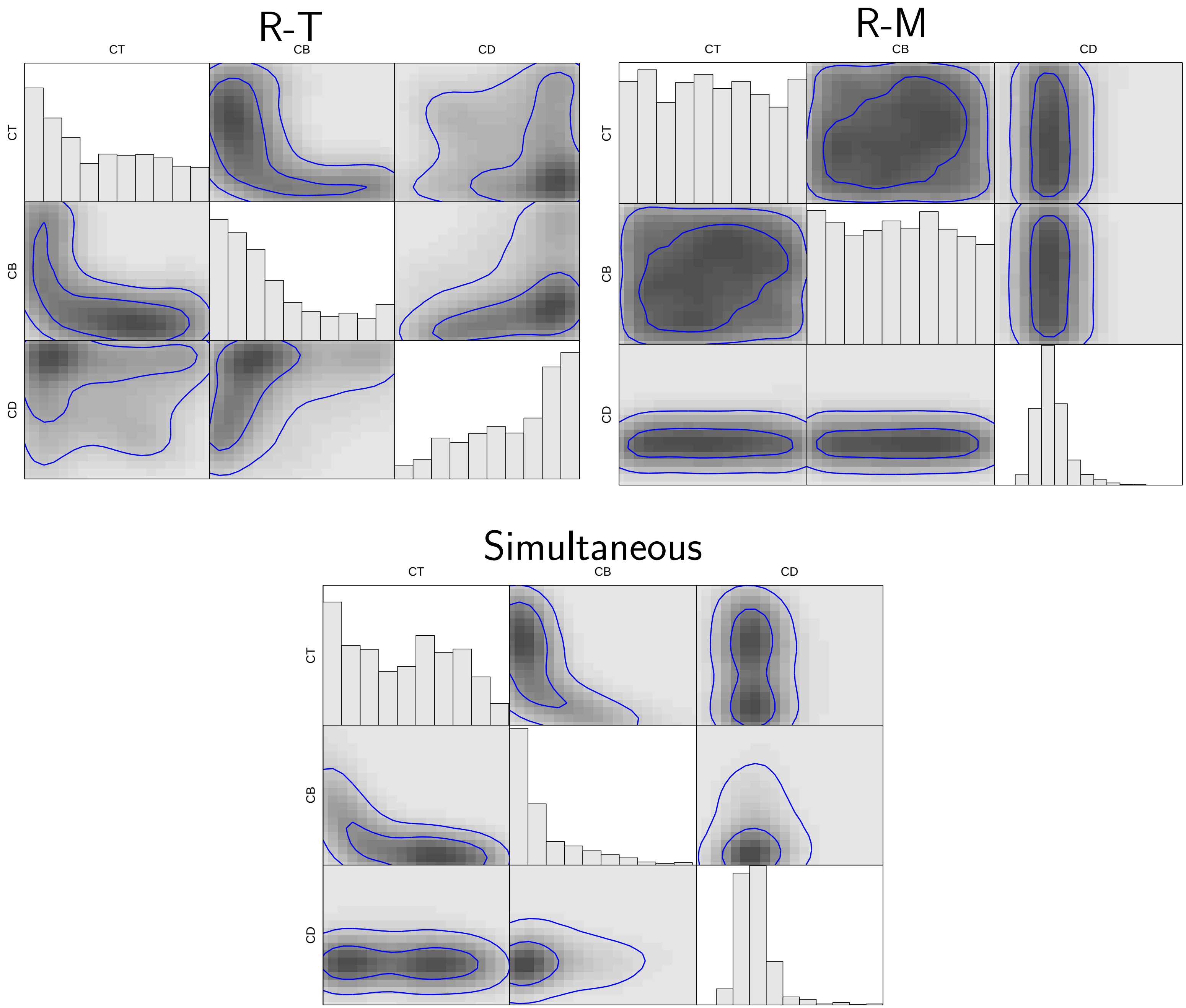
- GP parameters specific to each experiment updated individually in each MCMC iteration

- Extensions relevant to some applications

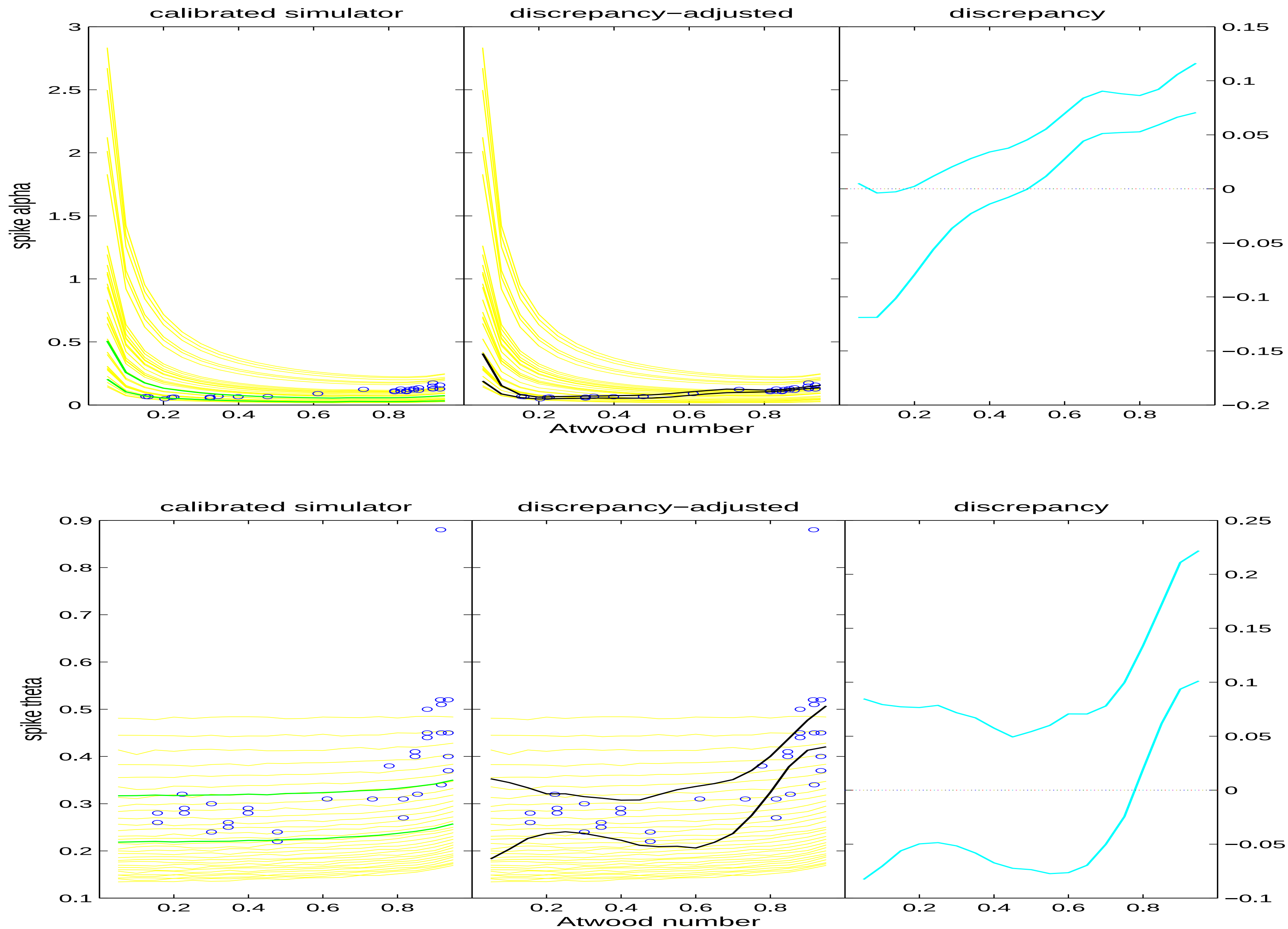
$\longrightarrow$ Hierarchical model for specified calibration parameters common to multiple experiments

$\longrightarrow$ Decomposition of discrepancy for multiple experiments into common and experiment-specific components

Simultaneous Calibration to R-T and R-M Instability Data



Prediction Based on Simultaneous Calibration



Summary

• Framework for calibration of computer models to experimental data

→ accounts for many sources of uncertainty; others could be incorporated

→ provides updated probability distribution for calibration parameters

→ uncertainties in calibration and statistical model propogated through to make predictions of future experiments

• Experimental design considerations central to successful analysis

→ space-filling designs desirable for GP emulation

• Sensitivity analysis aids interpretation of input–output relationships

→ straightforward extension to functional outputs

• Current work focuses on combining calculations/data from multiple relevant sources to perform a joint calibration of physics model parameters

→ parameters common to various components are linked

→ R-M data provided substantial information about k-L drag coefficient C_D