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Introduction to Uncertainty Quantification Tools for Sensitivity Analysis and Calibration

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Goal of Presentation

- Generation IV and GNEP - modeling and simulation capabilities to reduce the technology development cost
- Uncertainty quantification - plays a significant role
- Sensitivity analysis and calibration – basic UQ tools
- Quantification of Margins and Uncertainties – framework for certification decisions

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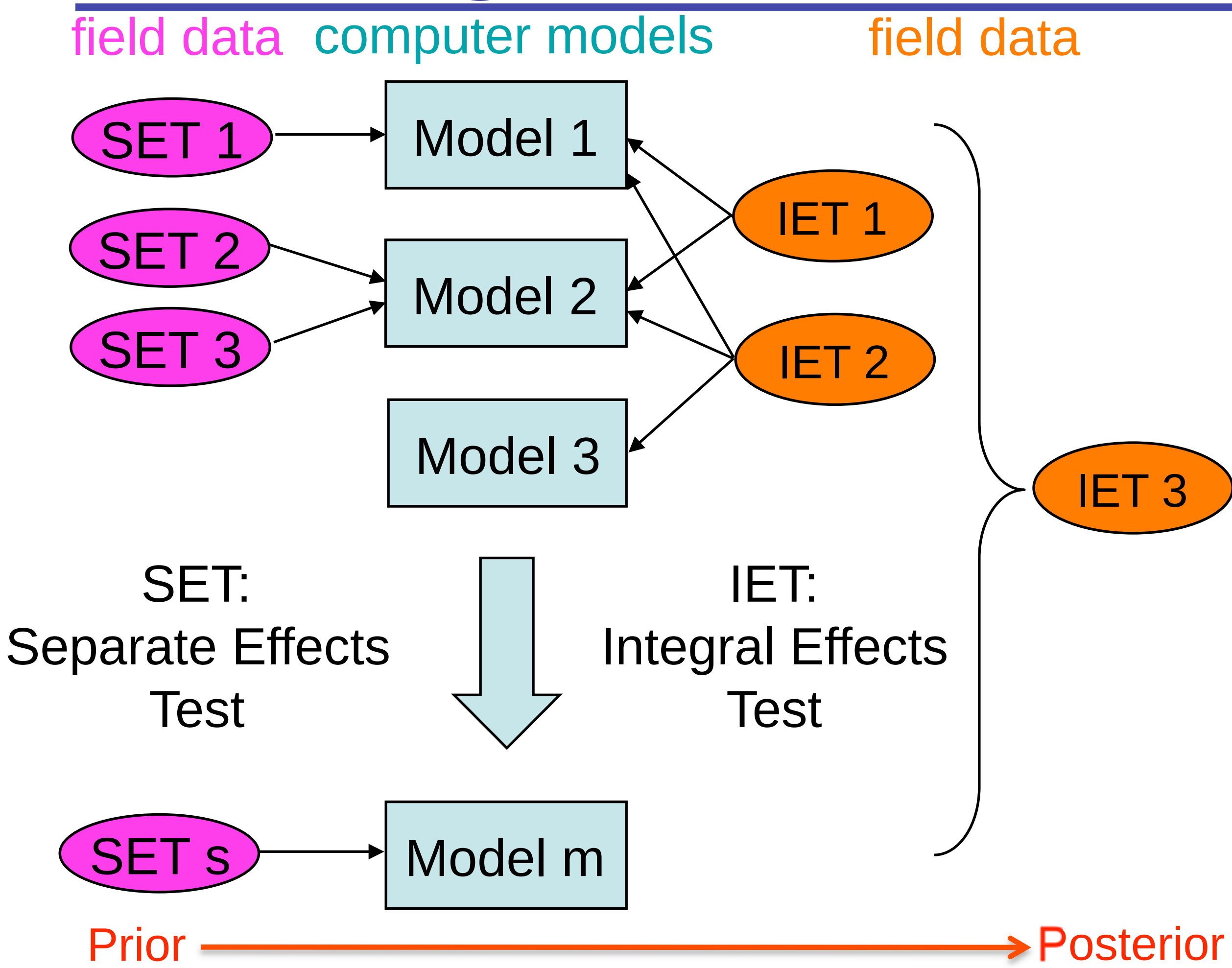
Paradigm for Model Validation



Validation Paradigm

1. Choose level at which validation is to occur
2. Split field data into calibration and validation sets
3. Calibrate uncertain physics parameters to both calibration and calibration + validation sets
4. Compare prediction and discrepancy inference with quantitative criteria for validation sets, using both calibrations
5. Decide on use of model for extrapolation

This approach is being implemented by the UT-Austin PSAAP Center

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Examples of SETs – Local Hydrodynamic and Materials Models are Developed From SETs

- Hopkinson-bar tests – test to obtain stress-strain relations at a given strain rate and temperature
- Diamond anvil tests - to develop EOS
- Reactor Examples
  - Lehigh University post-CHF, Marviken, CREARE, Dartmouth, CCTF, UPTF, W pump, THTF, BCL, CE pump, ORNL, DHIR…

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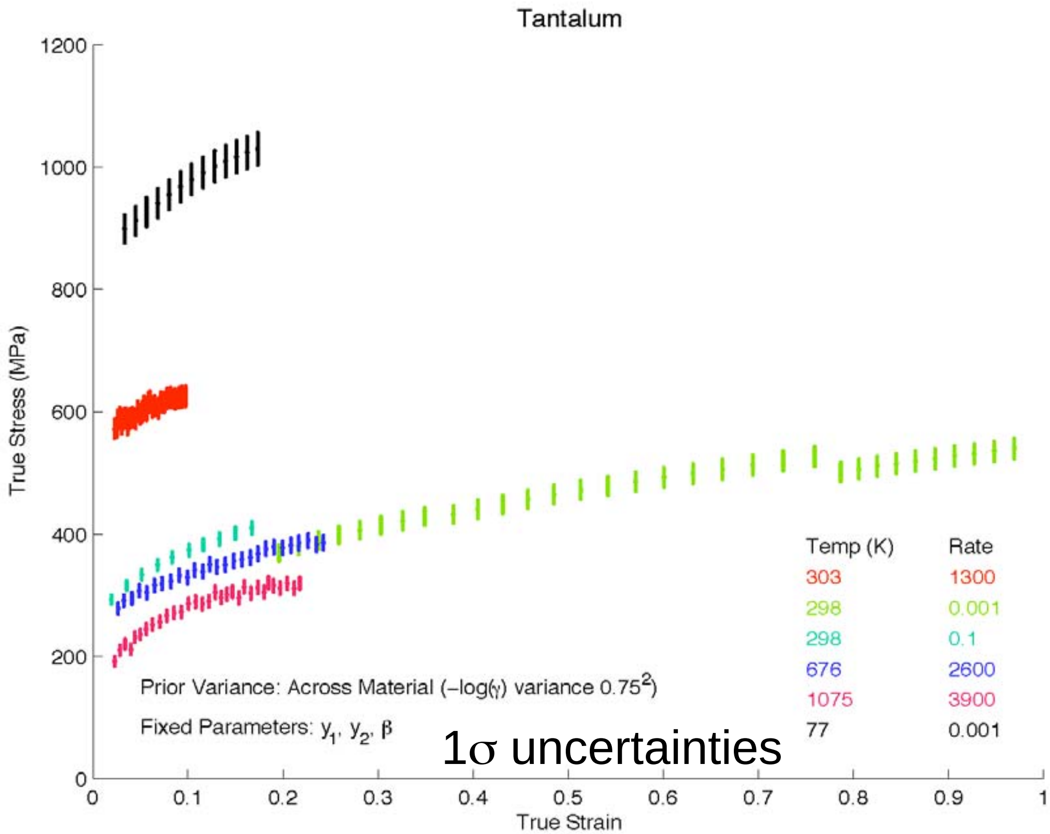
Tantalum Data With Uncertainty

- Data indexed by Temperature and Strain Rate
- Uncertainties estimated by (1) thinning data, fitting a quadratic model and obtaining the residual MSE, and (2) incorporating estimate of replicate variability



PTW Material Strength Model

activation energy   strain rate

$$\hat{\tau}_y = y_0 - (y_0 - y_\infty)\,\mathrm{erf}\left[\kappa \hat{T} \ln\left(\gamma \dot{\xi} / \dot{\psi}\right)\right]$$ yield stress

T/ $T_m(\rho)$

$$\hat{\tau}_s = s_0 - (s_0 - s_\infty)\,\mathrm{erf}\left[\kappa \hat{T} \ln\left(\gamma \dot{\xi} / \dot{\psi}\right)\right]$$ saturation stress

T = temperature

$T_m(\rho)$ = melting temp.

atomic vibration time

strain

$$\hat{\tau} = \hat{\tau}_s + \frac{1}{p}(s_0 - \hat{\tau}_y)\ln\left[1 - \left[1 - \exp\left(-p\frac{\hat{\tau}_s - \hat{\tau}_y}{s_0 - \hat{\tau}_y}\right)\right]\exp\left\{-\frac{p\theta_0 \psi}{(s_0 - \hat{\tau}_y)\left[\exp\left(p\frac{\hat{\tau}_s - \hat{\tau}_y}{s_0 - \hat{\tau}_y}\right) - 1\right]}\right\}\right]$$

$\boxed{\eta = (\theta_0, p, \kappa, \gamma, y_0, y_\infty, s_0, s_\infty)}$ parameters

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Statistical Model

- Parameters “common” to all datasets

stress

strain

dataset-specific parameters (temp., strain rate)

dataset-specific estimated uncertainty

$$y_{ij} = ptw(s_{ij}, \mathbf{x}_i, \boldsymbol{\eta}) + \varepsilon_{ij} ; \boldsymbol{\varepsilon}_i \sim N\left(\mathbf{0}, \frac{\sigma_i^2}{\lambda}\mathbf{I}\right);$$

uncertain model parameters

$$\boldsymbol{\eta} \sim N(\mathbf{b}_0, \mathbf{V}_0^{-1}); \lambda \sim Gamma\ (a, b);$$

adjustment to uncertainty

prior mean (SRC values)

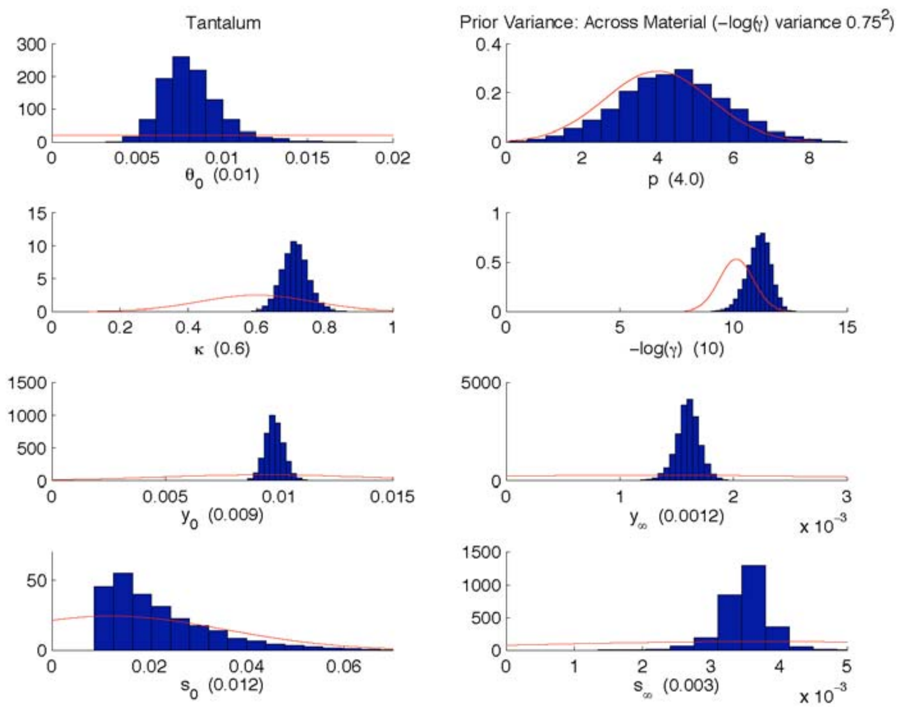
prior covariance (depends on analysis)

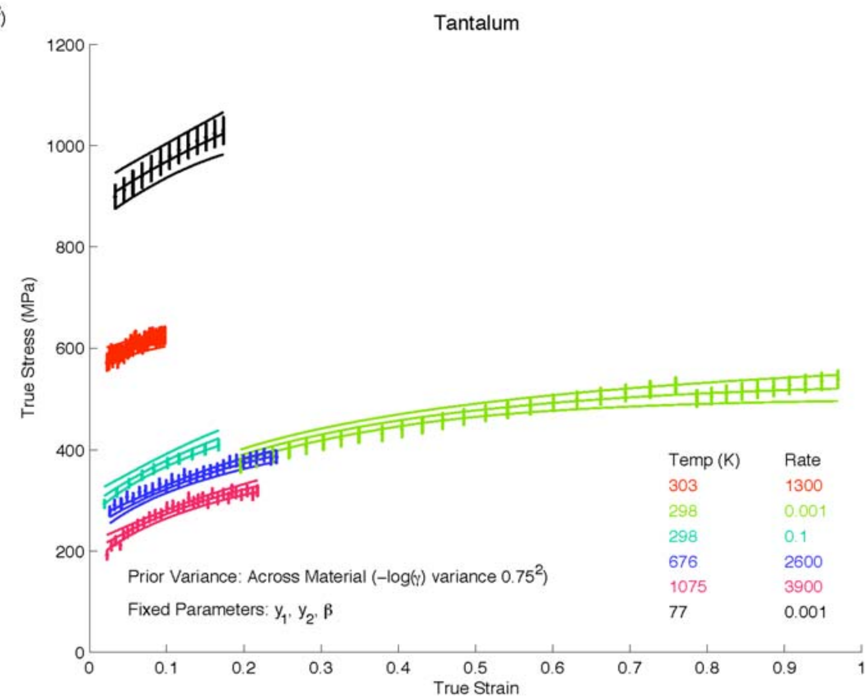
PTW

$$\boxed{\eta = (\theta_0, p, \kappa, -\ln(\gamma), y_0, y_\infty, s_0, s_\infty)}$$

Ta Results

- Prior distribution
  - Mean: SRC values
  - SD: SD of Cu, Ta, Be, DU, U-6Nb, Al and SS nominal values





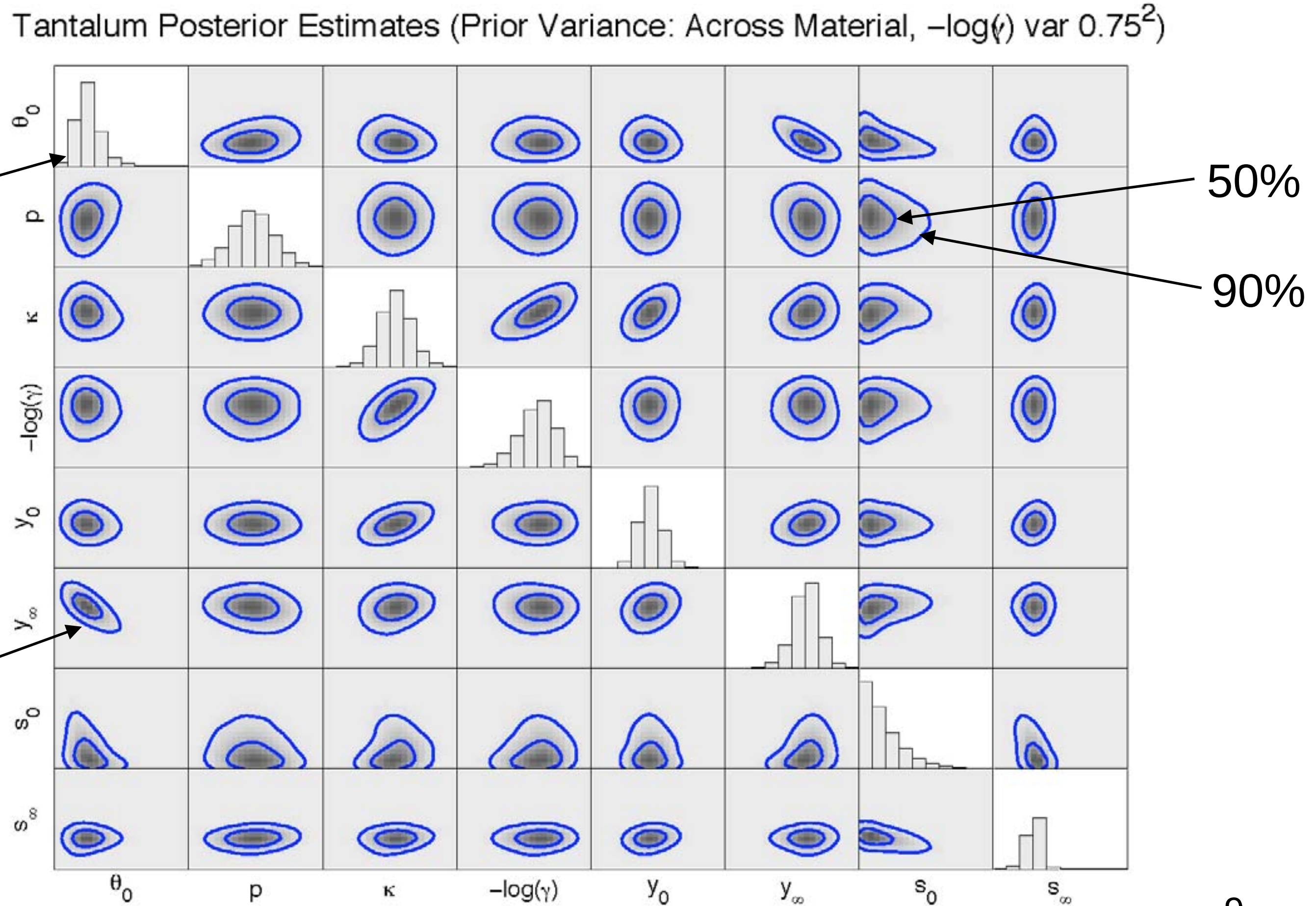
$$\eta = (\theta_0, p, \kappa, -\ln(\gamma), y_0, y_\infty, s_0, s_\infty)$$

Projections of Posterior Distribution

- Calibrated tantalum PTW parameters

Marginal distributions

Bivariate distributions



IET Examples – Integrated Models are Validated

- Flyer plate tests – High explosive driven shock dynamics tests of materials used in EOS development and material strength model assessment
- Hydro tests – Full scale with simulants – model validations
- Reactor Examples
  - LOFT, LOBI, PKL, Semi-scale, Power Burst FAC

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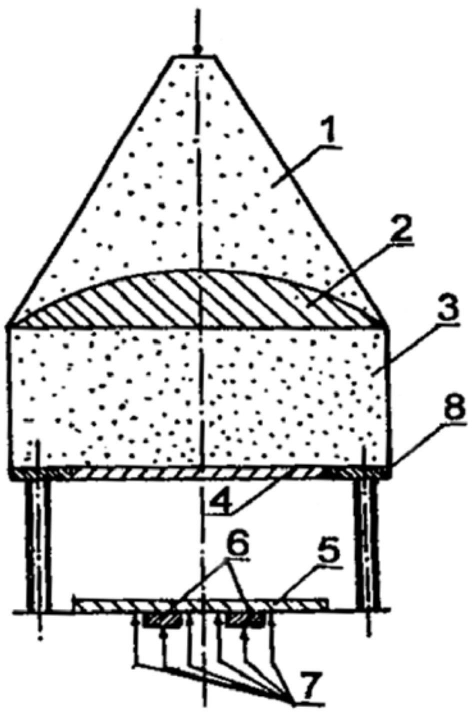
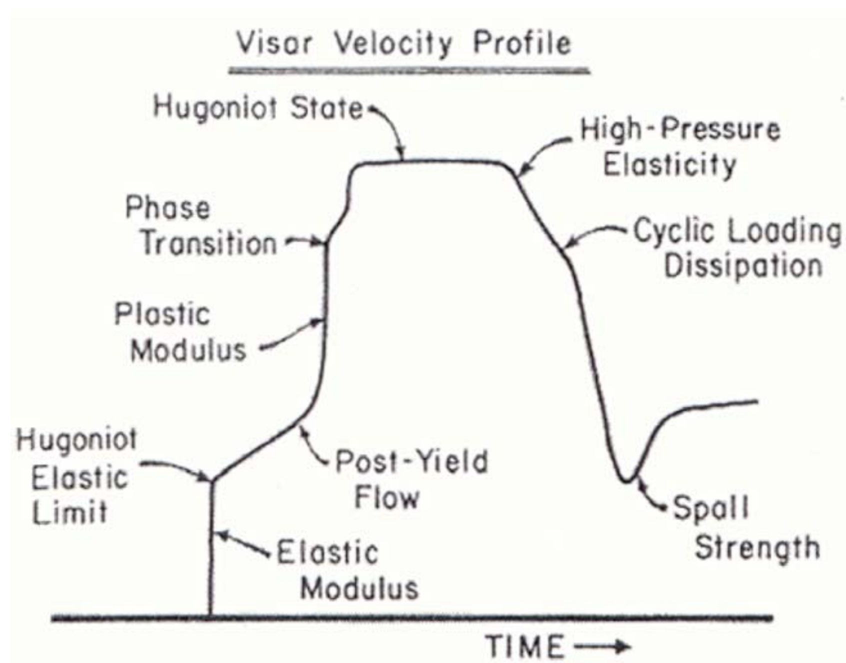
Ta Flyer Plate Experiments

Calibration of Material Properties

- Multiple physics models: Material equation of state (EOS), strength, damage
- Data source: flyer velocity profile

Flyer Plate Experiments





Physics Parameters: Flyer Plate Model

Input	Description	Domain	
		Min	Max
ε	Perturbation of EOS table from nominal	-5%	5%
θ_0	Initial strain hardening rate	2.78×10^{-5}	0.0336
κ	Material constant in thermal activation energy term – relates to the temperature dependence	0.438	1.11
γ	Material constant in thermal activation energy term – relates to the strain rate dependence	6.96×10^{-8}	6.76×10^{-4}
y_0	Maximum yield stress (at 0 K)	0.00686	0.0126
y_∞	Minimum yield stress (~ melting)	7.17×10^{-4}	0.00192
s_0	Maximum saturation stress (at 0 K)	0.0126	0.0564
s_∞	Minimum saturation stress (~ melting)	0.00192	0.00616
P_{min}	Spall strength	-0.055	-0.045
v_s	Flyer plate impact velocity	329.5	338.5

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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

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

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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

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

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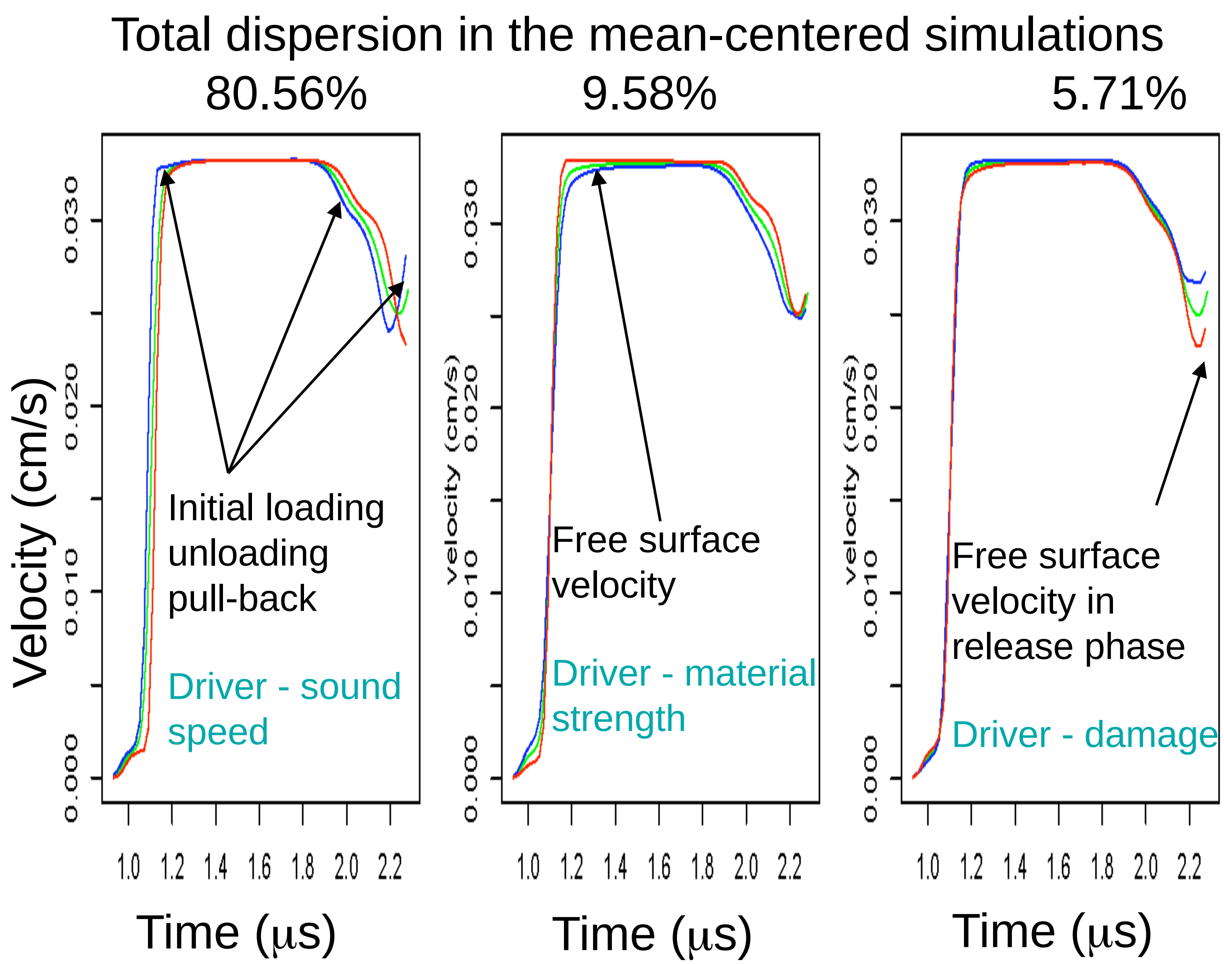
Basis Representation for Tantalum Flyer Plate Experiments

- Mean of simulation runs (green) with basis functions added (red) and subtracted (blue)
- The first through third basis functions are presented from left to right



Main Effect Sensitivity Indices for Main Effect Variation in the Flyer Plate Velocity Profile

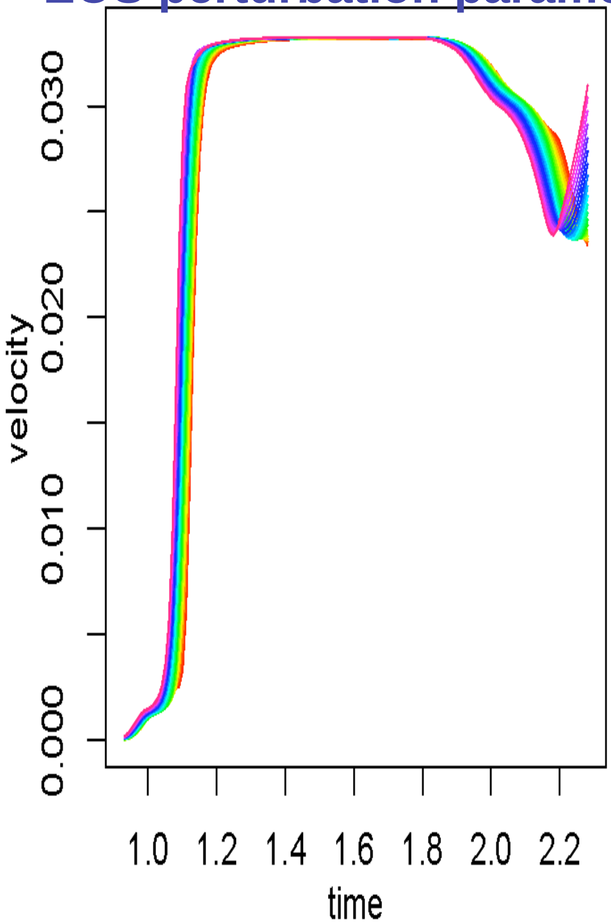
	velocity	pc1	pc2	pc3
s_0	0%	0%	0%	0.1%
s_∞	0%	0%	0%	0.3%
θ_0	0.7%	0.6%	1.2%	0.1%
y_0	0.5%	0%	3.9%	0.5%
v_s	1.2%	0.1%	8.6%	4.6%
y_∞	1.2%	0.7%	5.8%	0.7%
P_{min}	0.9%	0.1%	0.1%	12.3%
γ	1.6%	0.2%	14%	1.5%
κ	4%	0.3%	35%	4.7%
ε	85.7%	96.7%	18.4%	43.9%

Principal component coefficients

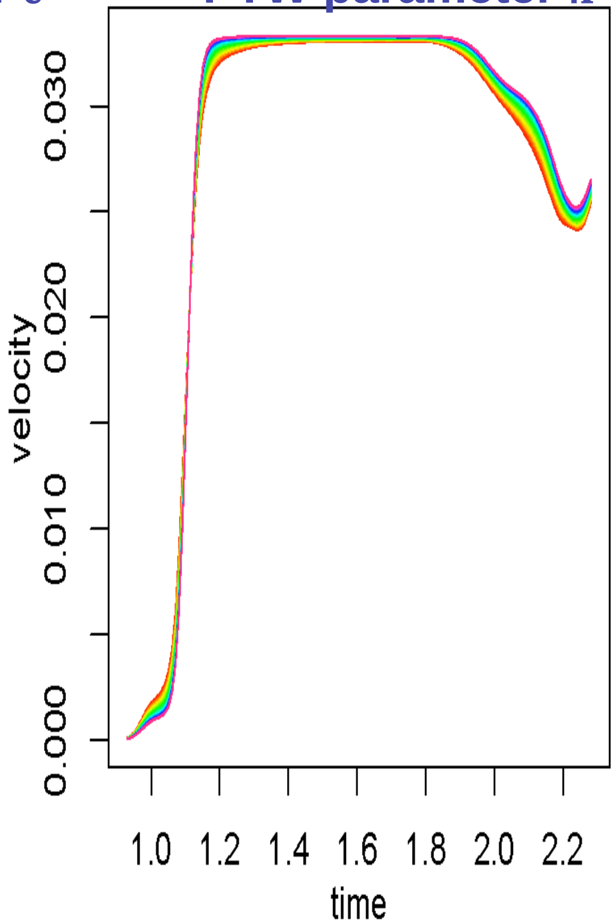
Main Effect Functions for Flyer Plate Velocity Profiles Corresponding to Variations in Tantalum Properties

- The color palate traverses the rainbow colors from red to violet as each parameter varies from its minimum to maximum value

EOS perturbation parameter ε



PTW parameter κ



Calibration and Prediction

<u>Inputs</u>

x controllable

t uncertain physics

θ best, unknown value of **t**

field data · reality · observation error

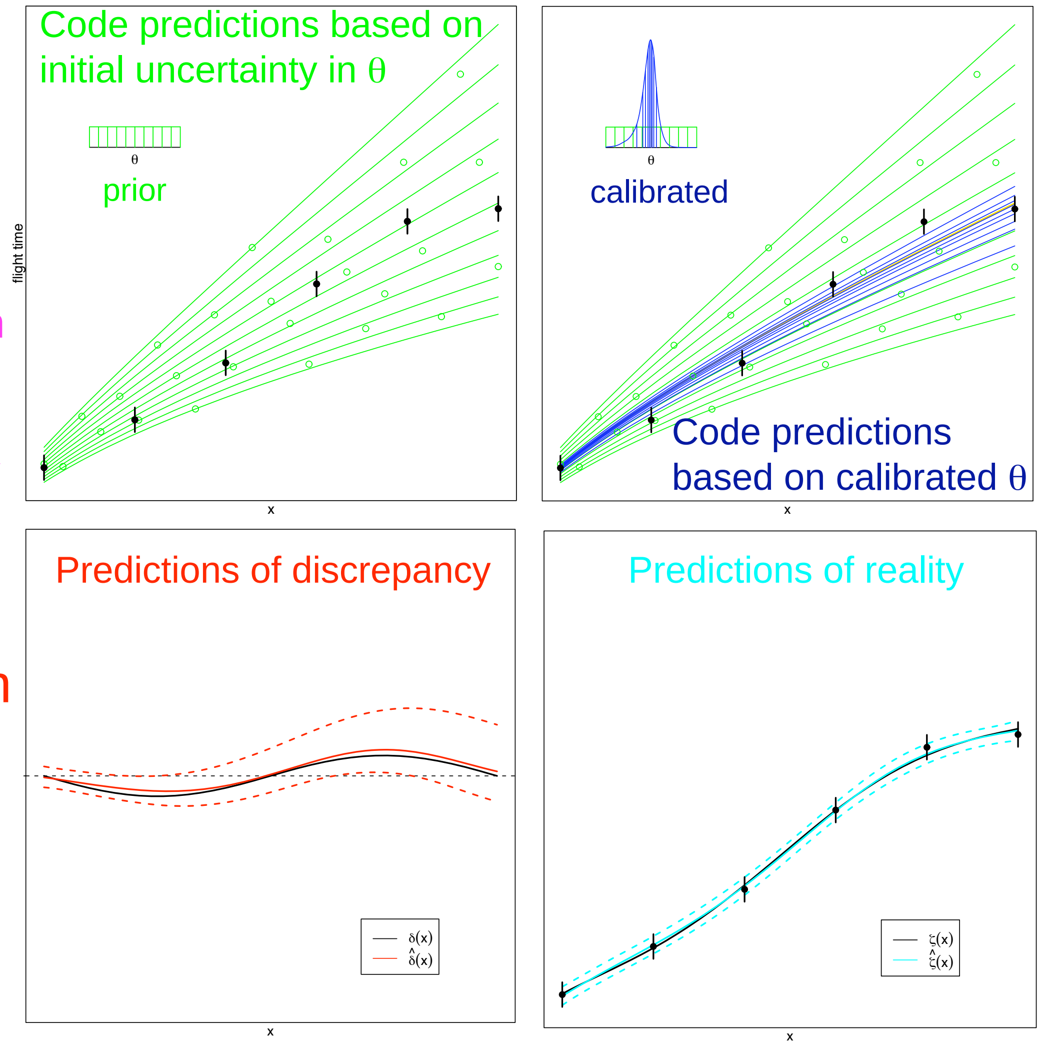
$$y(\mathbf{x}) = \zeta(\mathbf{x}) + \varepsilon(\mathbf{x})$$

computer model · discrepancy

$$\zeta(\mathbf{x}) = \eta(\mathbf{x}, \boldsymbol{\theta}) + \delta(\mathbf{x})$$

Basic steps in calibration analysis:

1. Assume initial probability dist'n for physics uncertainties θ.
2. Calibrate parameters θ to field data and simultaneously infer model discrepancies.



Statistical Analysis

- Basis representation of $\boldsymbol{\eta}(\mathbf{x},\mathbf{t})$ and $\boldsymbol{\delta}(\mathbf{x})$ for the purpose of achieving substantial dimensional reduction

$$\boldsymbol{\eta}(\mathbf{x},\mathbf{t}) = \mathbf{k}_1 w_1(\mathbf{x},\mathbf{t}) + \cdots + \mathbf{k}_{p_\eta} w_{p_\eta}(\mathbf{x},\mathbf{t})$$ Computer model

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

Statistical model $w_i(\mathbf{x},\mathbf{t})$ and $v_i(\mathbf{x})$

Prior distributions θ, stat. model

Sampling algorithm inputs

$\mathbf{k}_1, \ldots, \mathbf{k}_{P\eta}$ – Principal components

$\mathbf{d}_1, \ldots, \mathbf{d}_{P\delta}$ – Gaussian kernels

$w_i(\mathbf{x},\mathbf{t})$ and $v_i(\mathbf{x})$ – Gaussian process models

Statistical analysis → Posterior distributions θ, stat. model → Probabilistic representation of uncertainty

Markov chain Monte Carlo
Single-site parameter scan
Burn-in sets proposal widths

Calibrated prediction
Discrepancy inference
QMU

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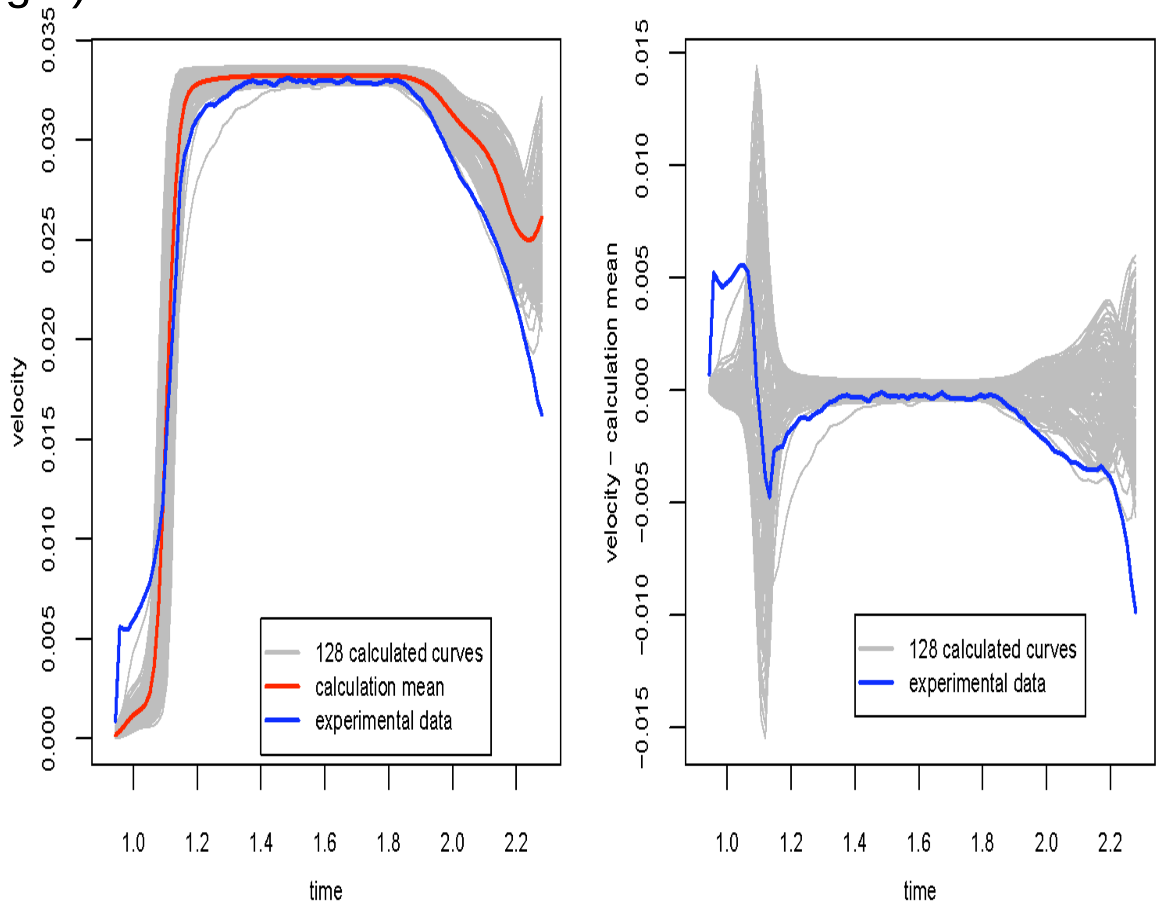
Calibration to Tantalum Flyer Plate Experiments

- Free surface velocity profiles in gray, with the **experimental velocity profile in blue** and the **mean of the calculations in red** (left)
- Mean of the calculations subtracted out of each simulated profile and the experimental data (right)



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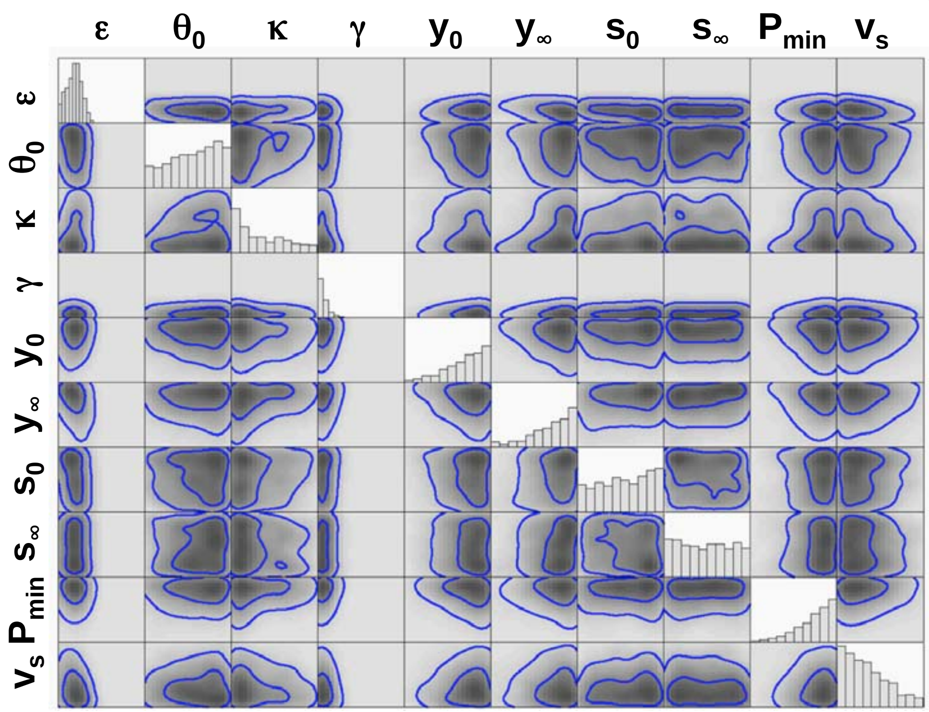
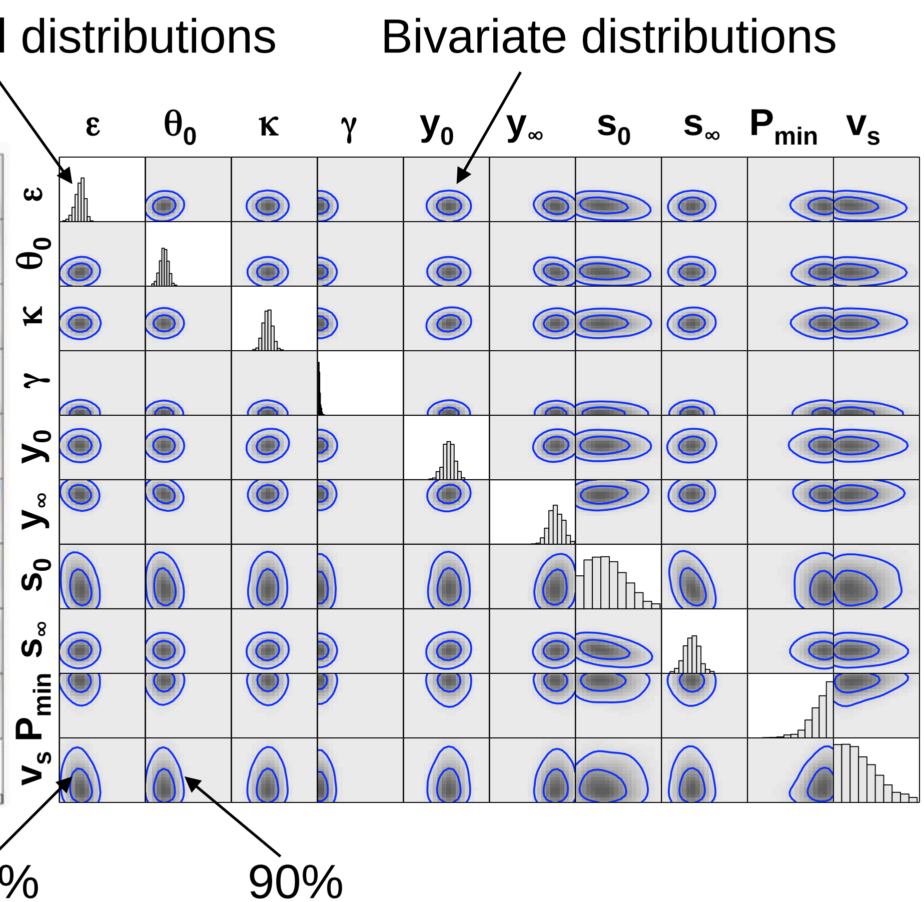
Projections of Posterior Distributions for Calibration Parameters Using Flyer Plate Data

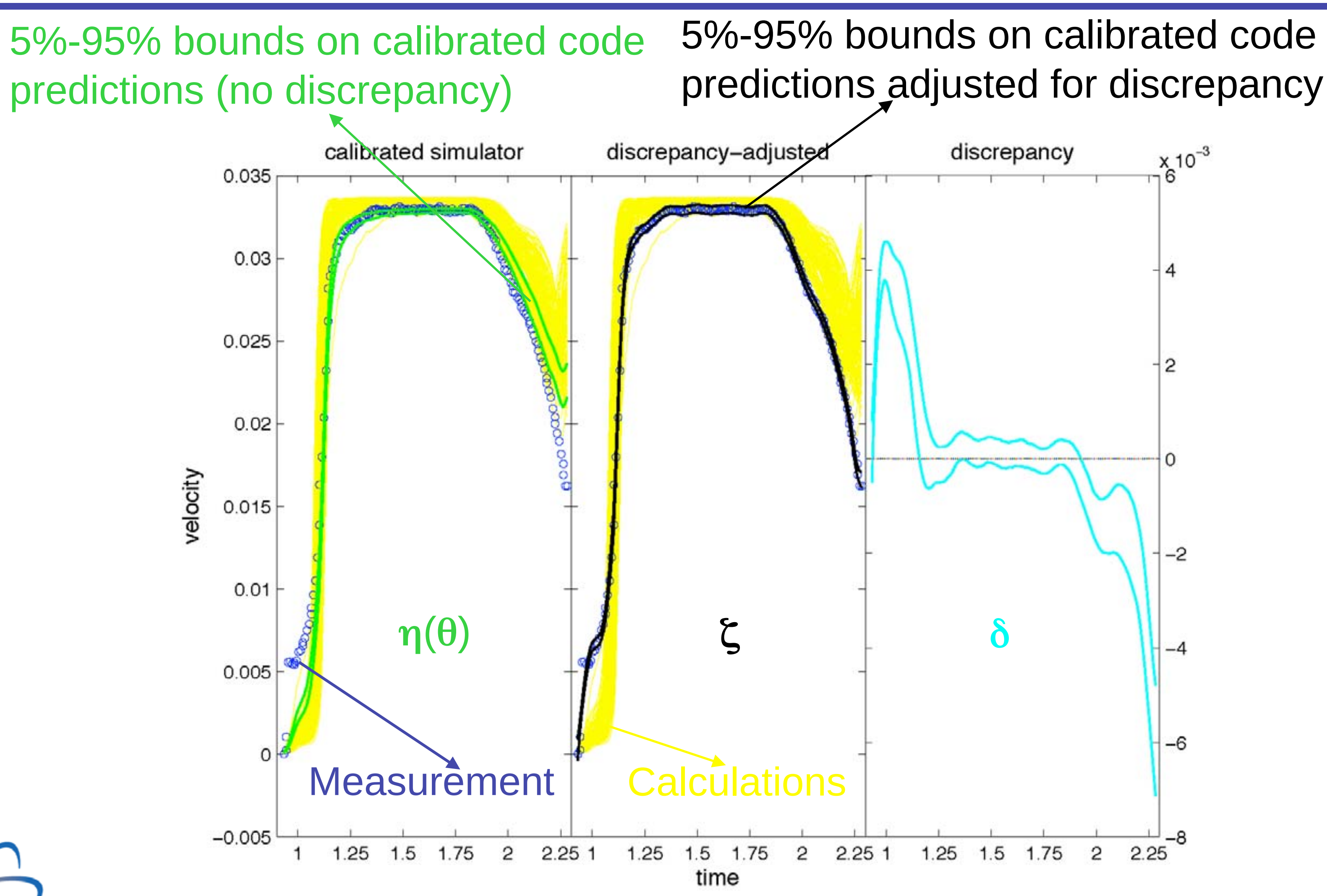
Uniform prior



Prior from SET Analysis



Assessment of Calibrated Code Predictions and Discrepancy



QMU for Certification

- *Margin (M)* is typically defined as the difference between expected performance, $E[\zeta(\mathbf{x})]$, and a threshold level, *a*, required for performance

Lower bound threshold

$$M(\mathbf{x}) = \max\left(E\left[\zeta(\mathbf{x})\right] - a, 0\right)$$

Upper bound threshold

$$M(\mathbf{x}) = \max\left(a - E\left[\zeta(\mathbf{x})\right], 0\right)$$

- *Uncertainty (U)* is defined by some combination of uncertainties in performance, $U_1(\mathbf{x})$, and in the threshold level, U_2. Performance uncertainty $U_1(\mathbf{x})$ is often taken to be the standard deviation of $\zeta(\mathbf{x})$. For example,

$$U(\mathbf{x}) = U_1(\mathbf{x}) + U_2 = SD[\zeta(\mathbf{x})] + U_2.$$

- *Confidence ratio (CR)* is defined as the ratio M/U. Margin *M* and, in particular, uncertainty *U* are chosen so that CR > 1 implies certification.

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Reliability for Certification

- *Reliability (R)* is defined as the probability of successful performance. Assuming random threshold *A*, it is calculated as follows:

Lower bound threshold

$$R(\mathbf{x}) = \Pr[\zeta(\mathbf{x}) > A]$$

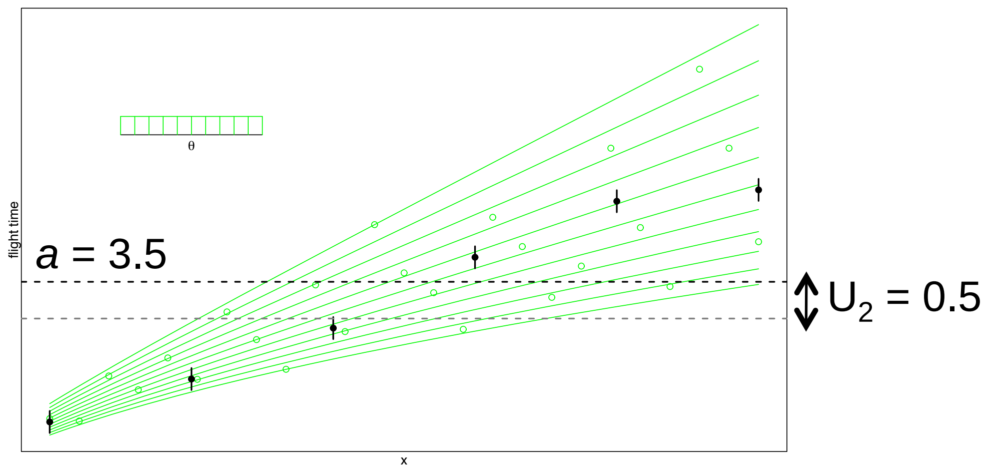
Upper bound threshold

$$R(\mathbf{x}) = \Pr[\zeta(\mathbf{x}) < A]$$

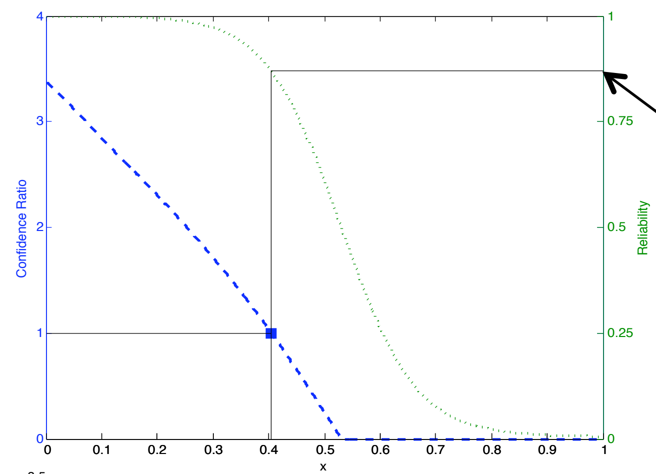
- Reliability exceeding a pre-specified level, e.g. 0.95, implies certification
- In general, no easily specified analytic relationship between *CR* and *R*
- For tower, assume upper bound threshold *A* has mean, $a = 3.5$, and standard deviation, $U_2 = 0.5$.

Confidence ratio and reliability will be calculated and compared.

From statistical analysis, $\zeta(\mathbf{x})$ is a mixture of Gaussian dist'ns. Threshold *A* is assumed to be Gaussian and independent of $\zeta(\mathbf{x})$ for calculating *R*.



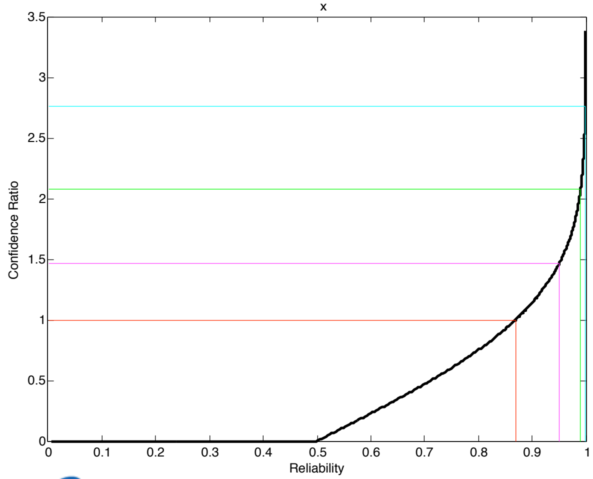
QMU Results



If $x < 0.405$, then CR > 1: Performance is certified for heights up to 0.405.

Reliability at $x = 0.405$ (CR = 1) is only 87%!

Reliability is a more meaningful measure for making certification decisions; however, more assumptions are required (e.g. joint dist'n of $\zeta(\mathbf{x})$ and A).



Confidence Ratio	Reliability
1	0.87
1.46	0.95
2.07	0.99
2.76	0.999

Required confidence for certification increases at higher rate as reliability requirement approaches one.

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Summary and Conclusions

- Generation IV and GNEP - simulation and modeling capabilities to reduce the technology development cost
- Uncertainty quantification - plays a significant role
- Sensitivity analysis provides insight into individual and joint parameter effects on model outputs
- Comprehensive probabilistic approach for calibrating physics uncertainties to data arising from multiple SETs, IETs and full system tests
- Calibrated prediction and discrepancy inferences used in QMU assessments
- We will demonstrate the value of the approach with a computer model of fuel modeling

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