Model Validation: Unit to System

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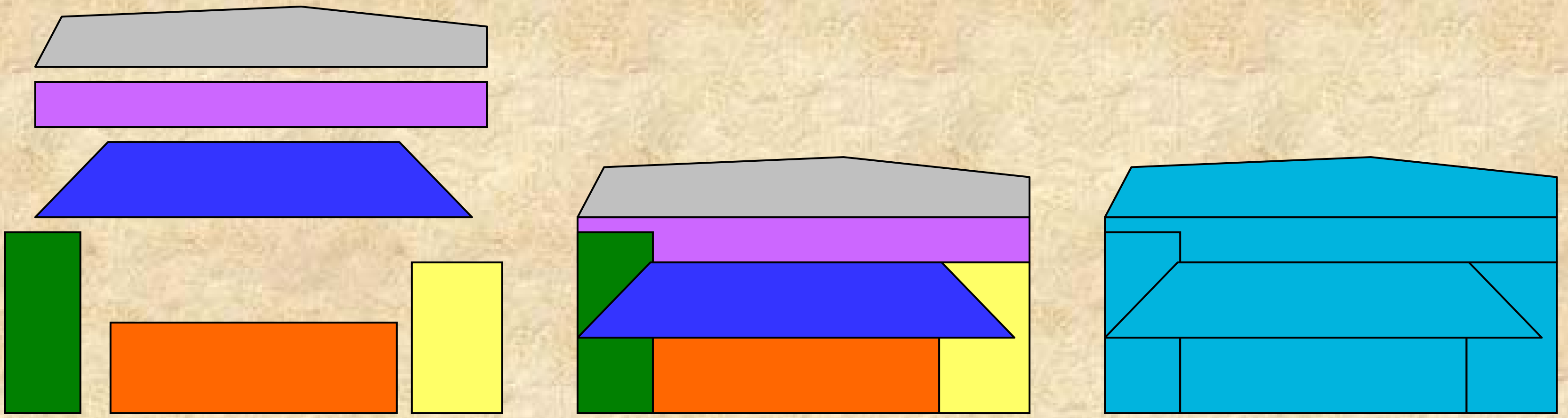
Unit to System

- Suites of validation experiments are often performed at the unit (component) level whereas we are interested in applying a model at the system level.

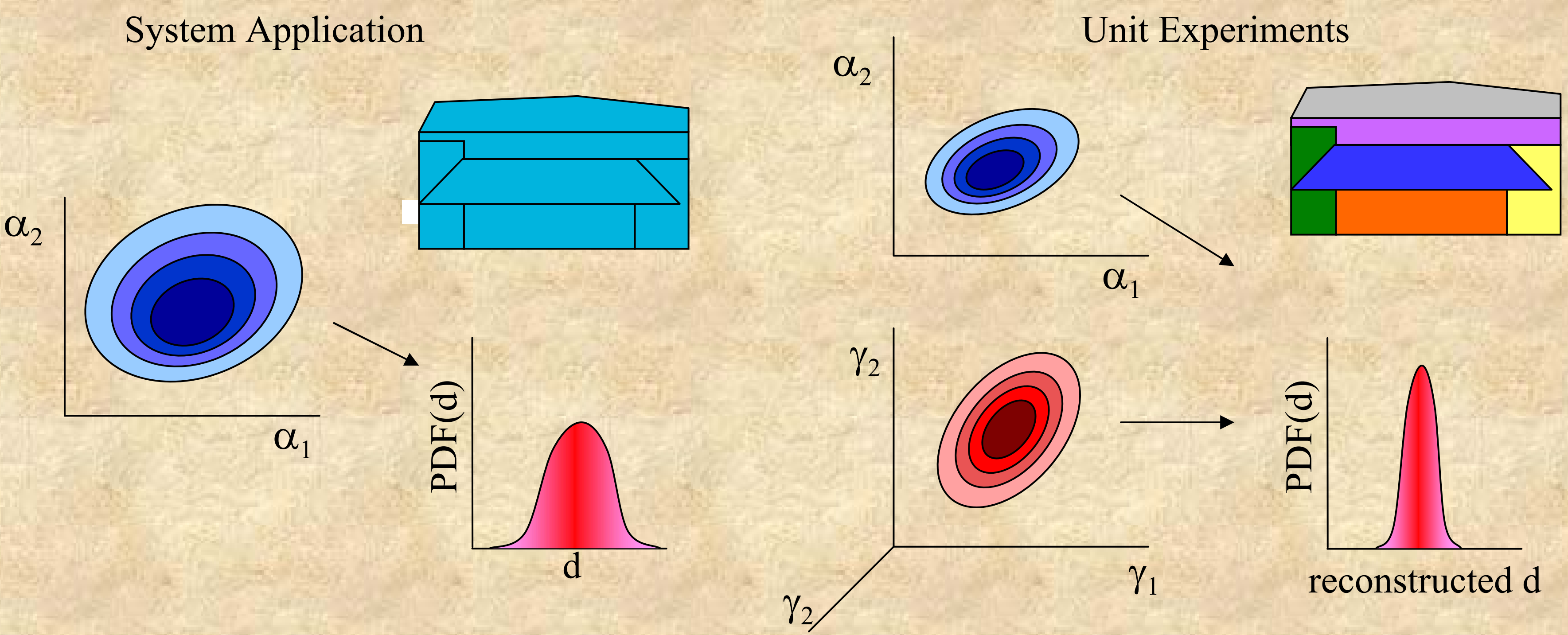


Unit Experiments　　Combined Results　　System

Definitions

- Target Application (System)
  - Anticipated application of the model
  - Can be different from the validation experiments
- Decision Variables
  - Important predictions of target application model
  - Can be different from the validation experiment measurement variables
- Reconstructed Decision Variables
  - Weighted combination of the validation experimental measurements to approximate the sensitivity of the decision variables to the important parameters

Uncertainties Modeled



- Model parameter uncertainty for validation (component level) experiment
- Measurement uncertainty at unit level
- Model parameter uncertainty for target application

Questions

- How do we combine data at the unit level to represent the target application at the system level?
- How do we evaluate whether the combined data can resolve the system level model with sufficient accuracy?
- How do we define validation metrics that represent the system level?

Our Approach

- Some measurements are more important than others!
- Some model parameters (represent physics) are more important than others!
- We will weight the measurements at the unit level so that they best represent the sensitivities of the system level predictions (decision variables) to these important parameters.

- Practical to perform first order uncertainty analysis of
  - systems level application
  - each of the unit level validation experiments
- The results are valid only to first order (can be extended to higher order)

Theory

Application (system level):

$$\mathbf{d} = \mathbf{G}(\mathbf{x},\alpha_a)$$

where

d – vector of decision variables – note that these are not necessarily the same as those quantities measured at the unit level

G – model for target application decision variables

x – important model parameters

α_a – perturbations from expected values representing uncertainty in important model parameters for the system

Validation Experiments (unit level):

$$\gamma = \mathbf{F}(\mathbf{x},\alpha_v)$$

where

γ – vector of predicted measurements for the suite of unit level experiments

F – model for validation experiments

x – important model parameters

α_v – perturbations from expected values representing uncertainty in important model parameters for the validation experiments

First Order Uncertainty Analysis

Validation Experiments (unit):

$$\Delta\gamma = \nabla_{\mathbf{x}} \mathbf{F}(\mathbf{x},\alpha_{\mathbf{v}})\, \Delta\mathbf{x} + \nabla_{\alpha\mathbf{v}} \mathbf{F}(\mathbf{x},\alpha_{\mathbf{v}})\, \Delta\alpha_{\mathrm{v}}$$

Application (system):

$$\Delta\mathbf{d} = \nabla_{\mathbf{x}} \mathbf{G}(\mathbf{x},\alpha_{\mathbf{a}})\, \Delta\mathbf{x} + \nabla_{\alpha\mathrm{a}} \mathbf{G}(\mathbf{x},\alpha_{\mathbf{a}})\, \Delta\alpha_{\mathrm{a}}$$

We weight the suite of measurement perturbations to best represent the sensitivities at the application level.

$$\mathbf{A}^{\mathrm{T}}\, \Delta\gamma = \Delta\mathbf{d}$$

so

$$\mathbf{A}^{\mathrm{T}}\, \nabla_{\mathbf{x}} \mathbf{F}(\mathbf{x},\alpha_{\mathbf{v}})\, \Delta\mathbf{x} + \mathbf{A}^{\mathrm{T}}\, \nabla_{\alpha\mathbf{v}} \mathbf{F}(\mathbf{x},\alpha_{\mathbf{v}})\, \Delta\alpha_{\mathrm{v}} = \nabla_{\mathbf{x}} \mathbf{G}(\mathbf{x},\alpha_{\mathbf{a}})\, \Delta\mathbf{x} + \nabla_{\alpha\mathrm{a}} \mathbf{G}(\mathbf{x},\alpha_{\mathbf{a}})\, \Delta\alpha_{\mathrm{a}}$$

Uncertainty Analysis, continued

For the present application, we define α_v and α_a such that their expected values are zero. Taking the expected value of the previous equation leads to

$$(\nabla_{\mathbf{x}} \mathbf{F}(\mathbf{x},\alpha_{\mathbf{v}}))^T \mathbf{A} = (\nabla_{\mathbf{x}} \mathbf{G}(\mathbf{x},\alpha_{\mathbf{a}}))^T$$

This equation relates sensitivities at the unit level to sensitivities at the system level. Solve for the weighting matrix **A**.

Case 1: The columns of $(\nabla_{\mathbf{x}} \mathbf{F}(\mathbf{x},\alpha_{\mathbf{v}}))^T$ do not span the columns of $(\nabla_{\mathbf{x}} \mathbf{G}(\mathbf{x},\alpha_{\mathbf{a}}))^T$

No solution – there is no combination of the experimental data sensitivities that can represent the target application - the validation experiments do not span or "cover" the target application

Uncertainty Analysis, continued 2

Case 2: $(\nabla_{\mathbf{x}} \mathbf{F}(\mathbf{x},\alpha_{\mathbf{v}}))^T$ is square and full rank and thus spans $(\nabla_{\mathbf{x}} \mathbf{G}(\mathbf{x},\alpha_{\mathbf{a}}))^T$

$$\mathbf{A} = ((\nabla_{\mathbf{x}} \mathbf{F}(\mathbf{x},\alpha_{\mathbf{v}}))^T)^{-1} (\nabla_{\mathbf{x}} \mathbf{G}(\mathbf{x},\alpha_{\mathbf{a}}))^T$$

Case 3: $(\nabla_{\mathbf{x}} \mathbf{F}(\mathbf{x},\alpha_{\mathbf{v}}))^T$ spans $(\nabla_{\mathbf{x}} \mathbf{G}(\mathbf{x},\alpha_{\mathbf{a}}))^T$, but we have more measurements than model parameters. We choose that solution which minimizes the sensitivity of the weighted combination of data to the measurement uncertainty (use Lagrange multipliers):

$$\min L = \min [\, \mathbf{A}^T \mathrm{cov}(\mathbf{F}\text{-}\gamma)\, \mathbf{A} + \lambda^T ((\nabla_x \mathbf{F}(\mathbf{x},\alpha_{\mathbf{v}}))^T \mathbf{A} - (\nabla_x \mathbf{G}(\mathbf{x},\alpha_{\mathbf{a}}))^T]$$

which gives

$$\mathbf{A} = (\mathrm{cov}(\mathbf{F}\text{-}\gamma))^{-1} (\nabla_{\mathbf{x}} \mathbf{F}(\mathbf{x},\alpha_{\mathbf{v}})) [(\nabla_{\mathbf{x}} \mathbf{F}(\mathbf{x},\alpha_{\mathbf{v}}))^T (\mathrm{cov}(\mathbf{F}\text{-}\gamma))^{-1} (\nabla_{\mathbf{x}} \mathbf{F}(\mathbf{x},\alpha_{\mathbf{v}}))]^{-1} (\nabla_{\mathbf{x}} \mathbf{G}(\mathbf{x},\alpha_{\mathbf{a}}))^T$$

Uncertainty Analysis, continued 3

Cases 2 and 3:

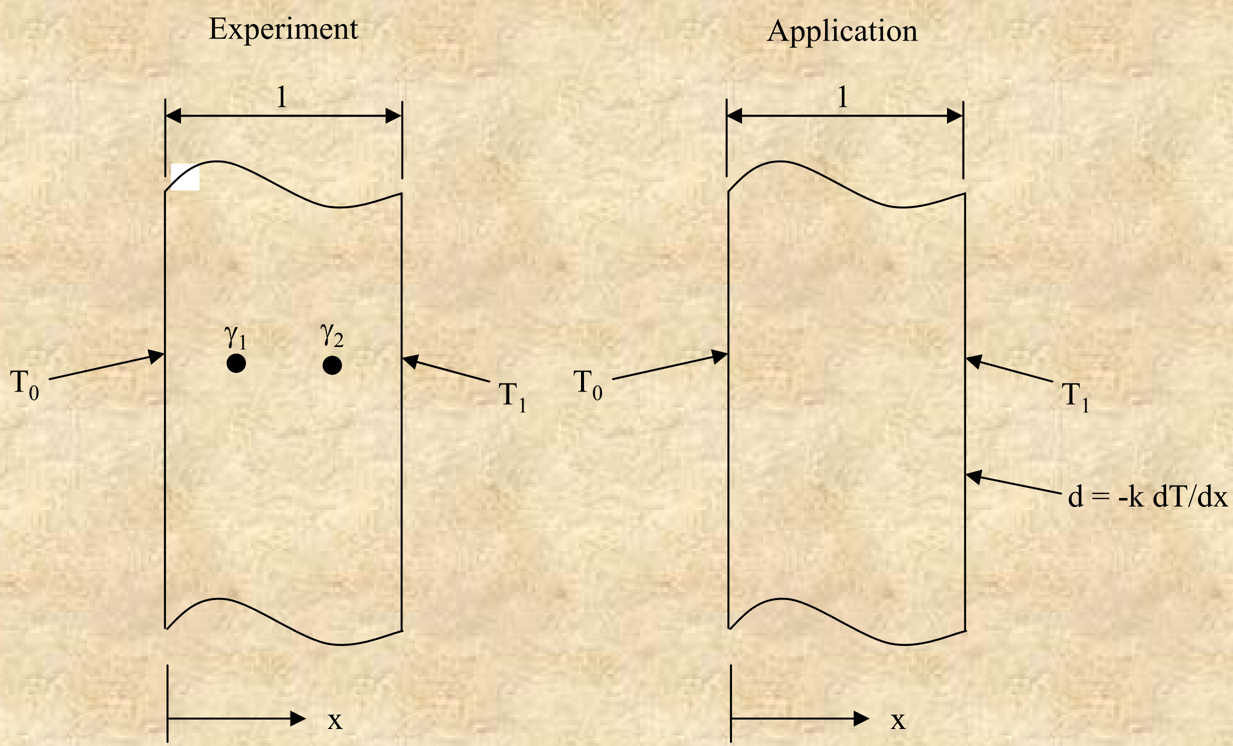
Once we know the weights $\mathbf{A}$, we can evaluate the covariance matrix for the reconstructed decision variable. Our reconstructed decision variable is

$$\Delta\mathbf{d} = \mathbf{A}^T \Delta\gamma - \mathbf{A}^T \nabla_{\alpha v} \mathbf{F}(\mathbf{x},\alpha_{\mathbf{v}}) \Delta\alpha_v + \nabla_{\alpha a} \mathbf{G}(\mathbf{x},\alpha_{\mathbf{a}}) \Delta\alpha_a$$

and

$$\mathrm{cov}(\mathbf{d}) = \mathbf{A}^T \mathrm{cov}(\gamma)\, \mathbf{A} + \mathbf{A}^T \nabla_{\alpha \mathbf{v}} \mathbf{F}(\mathbf{x},\alpha_v)\, \mathrm{cov}(\alpha_v)\, (\mathbf{A}^T \nabla_{\alpha \mathbf{v}} \mathbf{F}(\mathbf{x},\alpha_v))^T + \nabla_{\alpha a} \mathbf{G}(\mathbf{x},\alpha_{\mathbf{a}})\, \mathrm{cov}(\alpha_{\mathbf{a}})\, (\nabla_{\alpha a} \mathbf{G}(\mathbf{x},\alpha_{\mathbf{a}}))^T$$

Example 1: One validation experiment with 2 measurements (steady state)



Important model parameters: T_0, T_1

Example 1: One validation experiment with 2 measurements

Experiment:

Model

$d^2T/dx^2 = 0$

$T(0) = T_0 = \alpha_1$

$T(1) = T_1 = \alpha_2$

Measurements

$\gamma_1 = T(0.25)$

$\gamma_2 = T(0.75)$

Application:

Model

$d^2T/dx^2 = 0$

$T(0) = T_0 = \alpha_1$

$T(1) = T_1 = \alpha_2$

Decision Variable

$d = -k\ dT(1)/dx$

Example 1, continued

$$\left(\nabla_{x}\mathbf{F}(\mathbf{x},\boldsymbol{\alpha}_{v})\right)^{T}=\begin{bmatrix}0.75 & 0.25\\0.25 & 0.75\end{bmatrix}; \qquad \left(\nabla_{x}\mathbf{G}(\mathbf{x},\boldsymbol{\alpha}_{a})\right)^{T}=\begin{bmatrix}k\\-k\end{bmatrix}$$

$$\begin{bmatrix}0.75 & 0.25\\0.25 & 0.75\end{bmatrix}\mathbf{a}=\begin{bmatrix}k\\-k\end{bmatrix}$$

$$\mathbf{a}=\begin{bmatrix}2k\\-2k\end{bmatrix} \quad\Rightarrow\quad \Delta d=-k\frac{\Delta T(0.75)-\Delta T(0.25)}{0.5}$$

- Columns of matrix span the RHS – validation experiments resolve target application decision variable
- Weighted measurements give the finite difference approximation to the decision variable!

Corresponding Decision Variable Uncertainty

- $\operatorname{cov}(\Delta\mathbf{d}) = \mathbf{a}^{T}\operatorname{cov}(\Delta\boldsymbol{\gamma})\mathbf{a}$

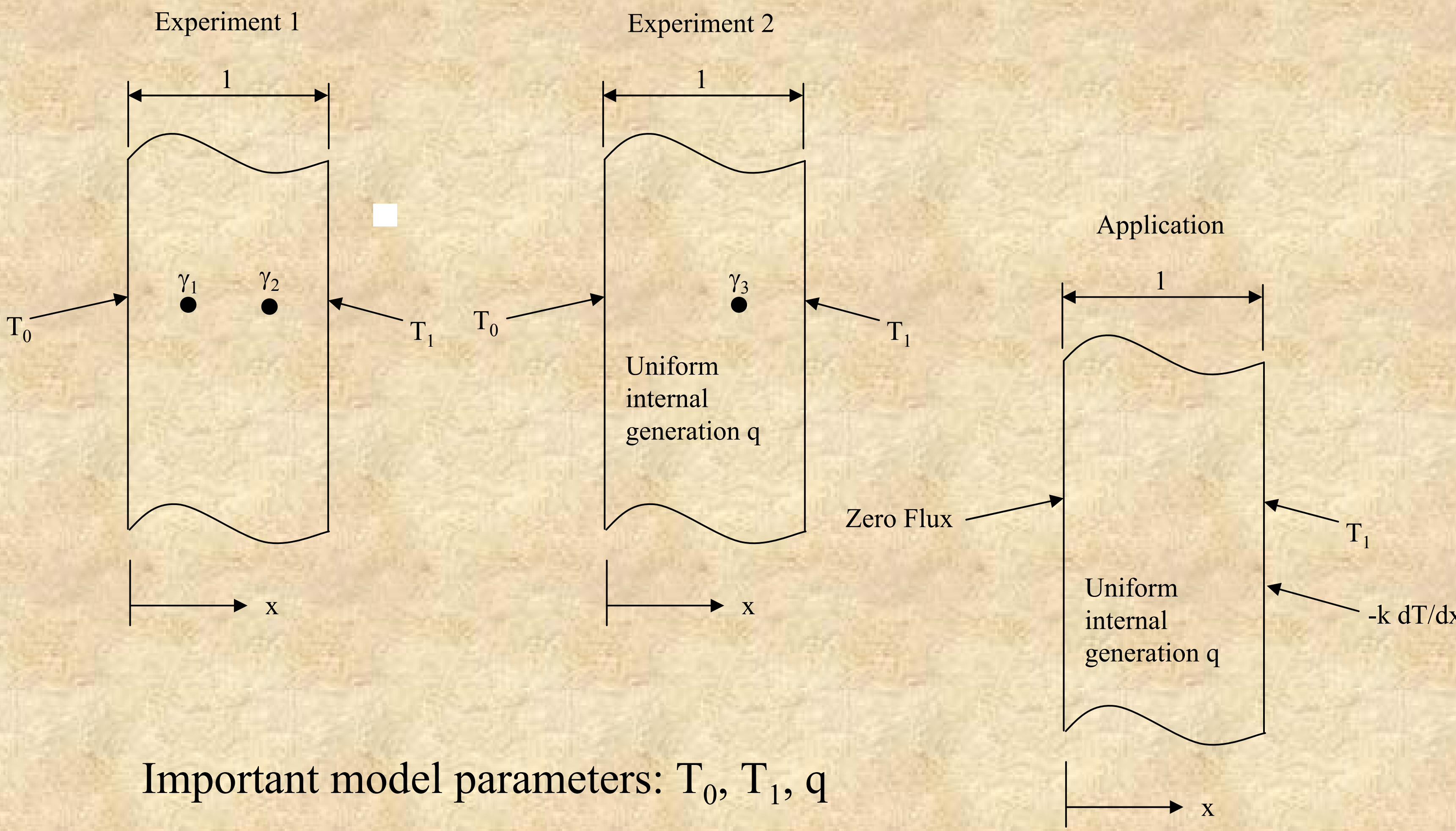
If $\operatorname{cov}(\Delta\boldsymbol{\gamma}) = \sigma_m^{\ 2}\mathbf{I}; \quad \operatorname{cov}(\Delta\mathbf{d}) = 8\sigma_m^{\ 2}k^2$

- Is this uncertainty acceptable for the application?

- If not, then validation experiments do not resolve the application!

(assume independent measurements with uniform variance)

Example 2: Two Validation Experiments



Important model parameters: T_0, T_1, q

Example 2: Two Validation Experiments

Experiment and Model 1:

$d^2T/dx^2 = 0$

$T(0) = T_0 = \alpha_1$

$T(1) = T_1 = \alpha_2$

Measurements

$\gamma_1 = T(0.25)$

$\gamma_2 = T(0.75)$

Experiment and Model 2:

$d^2T/dx^2 = q = \alpha_3$

$T(0) = T_0 = \alpha_1$

$T(1) = T_1 = \alpha_2$

Measurement

$\gamma_3 = T(x_v)$

Application Model:

$d^2T/dx^2 = q = \alpha_3$

$dT(0)/dx = 0$

$T(1) = T_1 = \alpha_2$

Decision Variable

$d = -k\, dT(1)/dx$

Example 2, continued

Experiment 1: Measurements at x=0.25, 0.75

$$\left(\nabla_{\mathbf{x}}\mathbf{F}(\mathbf{x},\boldsymbol{\alpha}_{\mathbf{v}})\right)^{T} = \begin{bmatrix} 0.75 & 0.25 \\ 0.25 & 0.75 \\ 0 & 0 \end{bmatrix}$$

Application:

$$\left(\nabla_{\mathbf{x}}\mathbf{G}(\mathbf{x},\boldsymbol{\alpha}_{\mathbf{a}})\right)^{T} = \begin{bmatrix} 0 \\ 0 \\ -k \end{bmatrix}$$

Experiment 2: Measurement at $\mathbf{x=x_v}$

$$\left(\nabla_{\mathbf{x}}\mathbf{F}(\mathbf{x},\boldsymbol{\alpha}_{\mathbf{v}})\right)^{T} = \begin{bmatrix} 1-x_v \\ x_v \\ \dfrac{x_v^{\,2}-x_v}{2} \end{bmatrix}$$

Experiments 1 and 2:

$$\left(\nabla_{\mathbf{x}}\mathbf{F}(\mathbf{x},\boldsymbol{\alpha}_{\mathbf{v}})\right)^{T} = \begin{bmatrix} 0.75 & 0.25 & 1-x_v \\ 0.25 & 0.75 & x_v \\ 0 & 0 & \dfrac{x_v^{\,2}-x_v}{2} \end{bmatrix}$$

Do experiments span (represent) the application?

Experiment 1: Measurements at 0.25, 0.75

$$\begin{bmatrix} 0.75 & 0.25 \\ 0.25 & 0.75 \\ 0 & 0 \end{bmatrix} \mathbf{a} = \begin{bmatrix} 0 \\ 0 \\ -k \end{bmatrix}$$

Does not span the application
- no sensitivity to q

Experiment 1 and Experiment 2 with measurement at x=0

$$\begin{bmatrix} 0.75 & 0.25 & 1 \\ 0.25 & 0.75 & 0 \\ 0 & 0 & 0 \end{bmatrix} \mathbf{a} = \begin{bmatrix} 0 \\ 0 \\ -k \end{bmatrix}$$

Does not span the application
- no sensitivity to q

Experiment 1 and Experiment 2 with measurement at x=0.5

$$\begin{bmatrix} 0.75 & 0.25 & 0.5 \\ 0.25 & 0.75 & 0.5 \\ 0 & 0 & -0.125 \end{bmatrix} \mathbf{a} = \begin{bmatrix} 0 \\ 0 \\ -k \end{bmatrix}$$

Does span the application

Coefficients

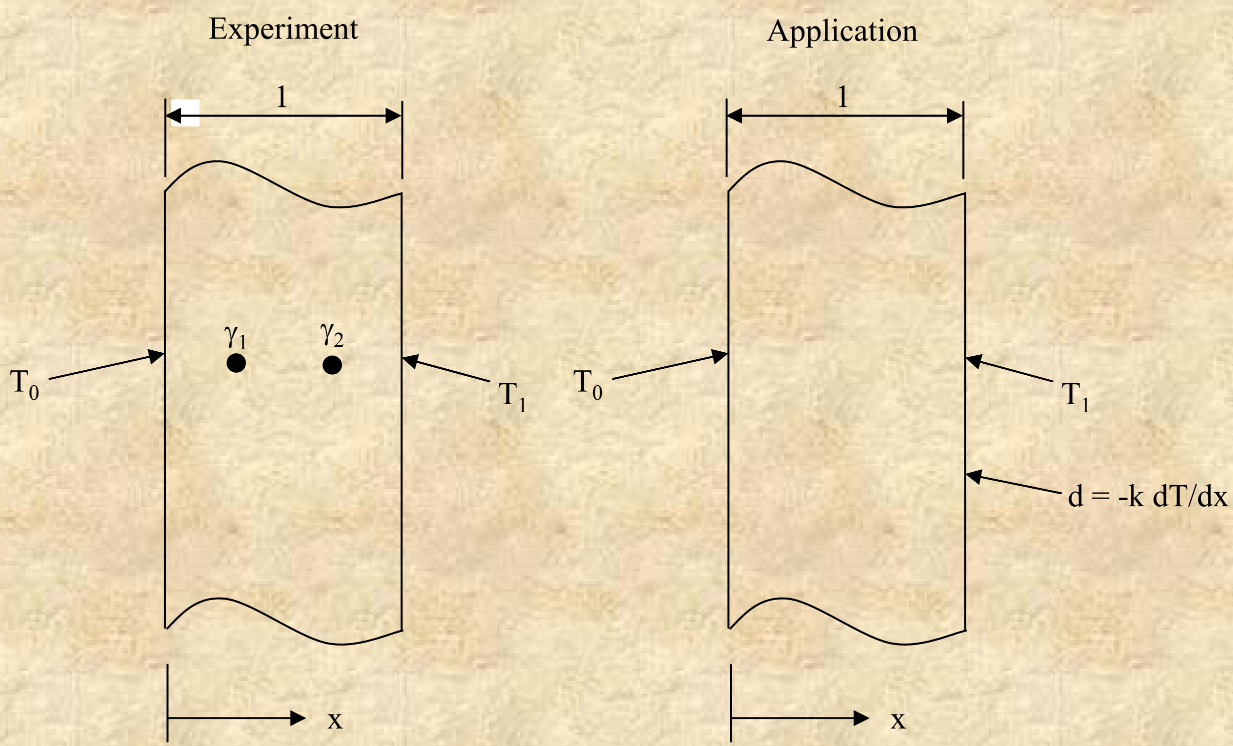
Experiment 1 and Experiment 2 with Exp. 2 measurement at x=0.5

$$\mathbf{a} = k\begin{bmatrix} -4 \\ -4 \\ 8 \end{bmatrix}$$

$$\sigma_d^{\,2} = \sigma_m^{\,2}\,\mathbf{a}^T\,\mathbf{I}\,\mathbf{a} = 96\,\sigma_m^{\,2}\,k^2$$ ouch!

(assume independent measurements with uniform variance)

Example 3: Transient Heat Conduction with 2 Measurements



Example 3: Transient Heat Conduction

Experiment:

$$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2}$$

$T(x,0)=0$
$T(0,t) = T_0$
$T(1,t) = T_1$

$\gamma_1 = T(0.25,t_j), \quad j=1,n$
$\gamma_2 = T(0.75,t_j), \quad j=1,n$

Application:

$$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2}$$

$T(x,0)=0$
$T(0,t) = T_0$
$T(1,t) = T_1$

$d = -k\, \partial T(1,t_a)/\partial x$

Parameters

Experiment:
Important: T_0, T_1, α
Uncertain: α

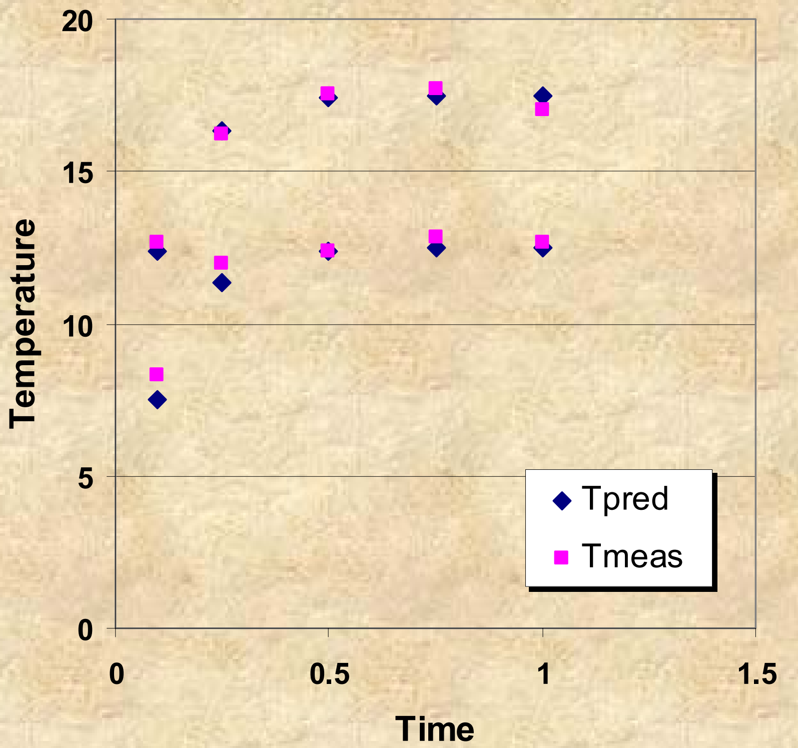
Application:
Important: T_0, T_1, α
Uncertain: T_0, T_1, α

Parameter Uncertainty

Parameter	Mean Value	Standard Deviation
Validation Experiment		
α	1.0	0.05
γ		0.25
Application		
T_1	10.0	2.0
T_2	20.0	2.0
k	1.0	0.1
α	1.0	0.1

Distribution of Uncertainty in Decision Variable

Time	$\sigma_{d\text{-meas}}$	$\sigma_{d\text{-v}}$	$\sigma_{d\text{-a}}$	σ_d
0.125	0.949	1.106	4.84	5.06
0.250	0.579	0.621	3.47	3.57
0.375	0.381	0.269	3.10	3.14
0.500	0.329	0.104	3.02	3.04
0.625	0.320	0.038	3.01	3.02
0.750	0.318	0.013	3.00	3.02
0.875	0.318	0.004	3.00	3.02
1.000	0.318	0.001	3.00	3.02
10.00	0.318	0.000	3.00	3.02



Given σ_d, we can define a validation metric (see paper)

Discussion

While this approach is first order – it does provide significant insight.

- Tells us how to weight the measurements to best represent the sensitivity of the application decision variables to the important model parameters.
- Provides methodology to test whether a suite of validation experiments spans the application to first order (experimental design!)
- Provides an estimate of the uncertainty of the reconstructed decision variables given the uncertainty in the validation variables and measurements. Should be small compared to the acceptable level of uncertainty in the decision variable (experimental design)!
- Can be used to define a validation metric (see paper) if we can develop an adequate model for the PDFs of the differences between measurements and predictions

Four Most Important Ideas

1. We should test models based on an anticipated target application
2. We should not do model validation in a vacuum – models should be used to design validation experiments
   – Models for the validation experiments
   – Models for the application
3. Effect of uncertainty must be considered in this design
4. First order sensitivity analysis provides a first order approach to the above.