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A complete set of errors for modeling and simulation

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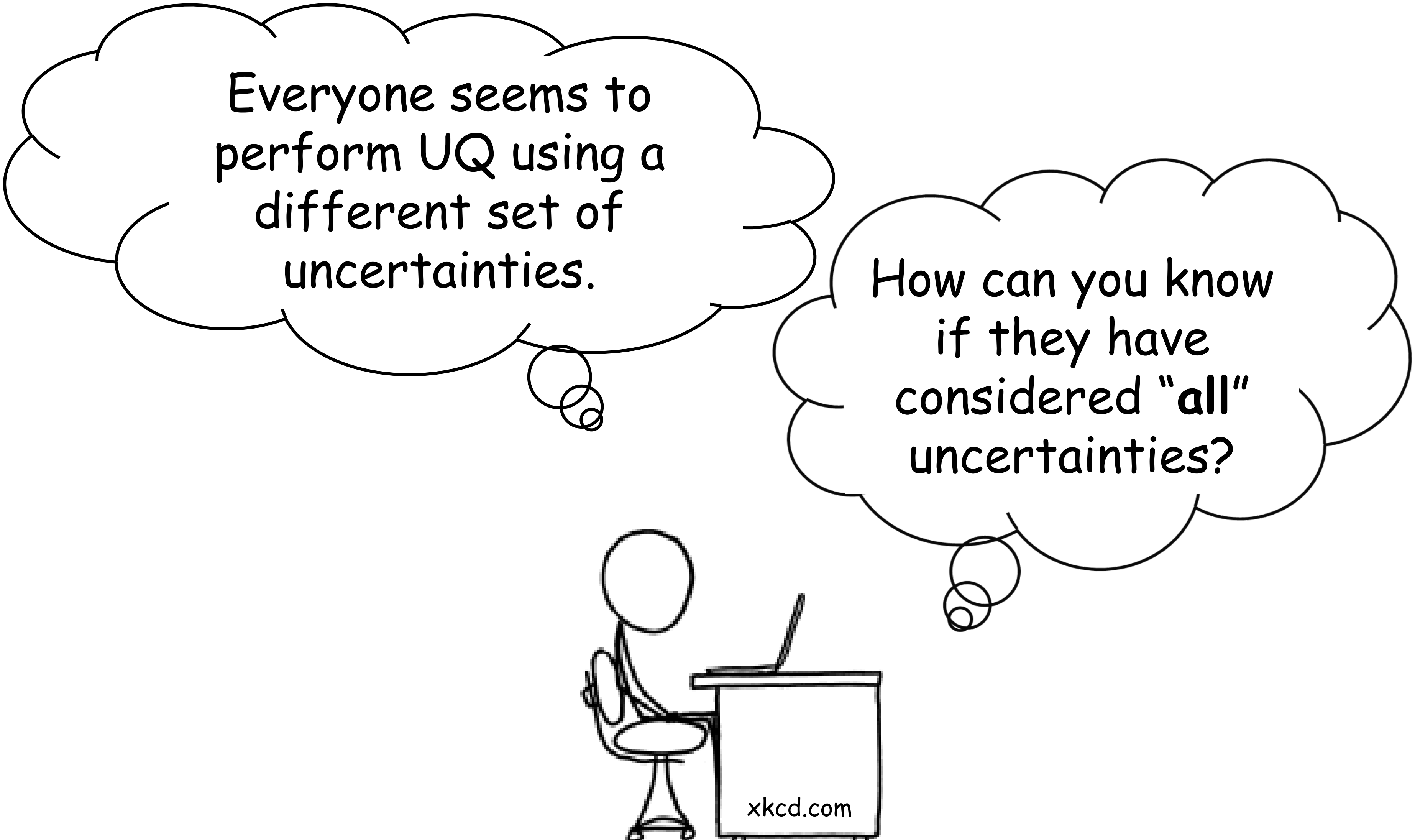
May 20, 2020

Motivation



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What errors/uncertainties should be quantified?

<u>Kennedy & O'Hagan</u>

- parameter
- model
- residual
- parametric variability
- observation error
- code

<u>D'Auria and Petruzzi</u>

- code or model
- representation or simulation
- plant data
- "user effect"

<u>Radaideh et al.,</u>

- parametric/input
- experimental / measured
- predictive / model discrepancy
- model form
- interpolation / statistical

Is there an objective way to create a set of errors?

Coleman and Steele

$$E = D - S \quad (1)$$

- $\delta_S = \boldsymbol{T} - S \quad \Rightarrow \quad S = \boldsymbol{T} - \delta_S$
- $\delta_D = \boldsymbol{T} - D \quad \Rightarrow \quad D = \boldsymbol{T} - \delta_D$

$$E = (\boldsymbol{T} - \delta_D) - (\boldsymbol{T} - \delta_S) \quad (2)$$

$$E = \delta_S - \delta_D \quad (3)$$

Error Decomposition

$$E = \boldsymbol{T} - X \tag{1}$$

Algebraically introduce a new term, Y

$$E = \boldsymbol{T} - Y + Y - X \tag{2}$$

Define new errors, δ_{TY}, δ_{YX}

- $\delta_{TY} = \boldsymbol{T} - Y$
- $\delta_{YX} = Y - X$

$$E = \delta_{TY} + \delta_{YX} \tag{3}$$

Total Error Equation

$$\delta_{Total} = \mathbb{S}(I) - \mathrm{C}_{\Delta h}(I)$$

- δ_{Total} - the total error
- $\mathbb{S}(I)$ - the value of the system at the input of interest
- $\mathrm{C}_{\Delta h}(I)$ - the value of the real computational model at the input of interest

$$\mathbb{S}(I) = \mathrm{C}_{\Delta h}(I) + \delta_{Total}$$

What terms can we introduce?

$$\delta_{Total} = \mathbb{S}(I) - \mathrm{C}_{\Delta h}(I)$$

Recognize there are two things you can introduce:

1. Different functions (relation), $\boldsymbol{f}(\cdot)$
2. Different Inputs, $\boldsymbol{I_n}$

These terms ***define*** how we look at the world.

- Terms should have wide applicability
- More terms = more precise error definitions

Generic Scenario - Functions

Functions	Description
$\mathbb{S}(\cdot)$	The behavior of the system
$C_{\Delta h}(\cdot)$	The results of the real computational model
$\mathcal{M}(\cdot)$	The results of the mathematical model
$\mathbb{E}(\cdot)$	The behavior of the empirical system
$\mathbb{E}^{*}(\cdot)$	The estimate of the behavior of the empirical system
$C_{\infty}(\cdot)$	The results of the ideal computational model

Generic Scenario - Inputs

Inputs	Description
I	Input of interest
D	Input of Empirical data
D^*	Estimate of input of empirical data
I^*	Estimate of the input of interest
I_{CV}	Input of code verification associated with I
D_{CV}	Input of code verification associated with D
I_{SV}	Input of soln. verification associated with I
D_{SV}	Input of soln. verification associated with D

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Example Terms

Terms	Description
$\mathcal{M}(I)$	Mathematical model at the input of interest
$\mathcal{M}(I_{CV})$	Mathematical model at the input used for code verification associated with I
$\mathrm{C}_{\Delta h}(D^*)$	Computational model at the estimate of input of empirical data

Example Derivation: Verification Error

$$\delta_{Verification}(I) = \mathcal{M}(I) - \mathrm{C}_{\Delta h}(I) \tag{1}$$

$$\delta_{Verification}(I) = \mathcal{M}(I) - \mathrm{C}_{\infty}(I) + \mathrm{C}_{\infty}(I) - \mathrm{C}_{\Delta h}(I) \tag{2}$$

Define new errors, $\delta_{Code}(I)$ and $\delta_{Solution}(I)$

- $\delta_{Code}(I) = \mathcal{M}(I) - \mathrm{C}_{\infty}(I)$
- $\delta_{Solution}(I) = \mathrm{C}_{\infty}(I) - \mathrm{C}_{\Delta h}(I)$

$$\mathcal{M}(I) = C_{\Delta h}(I) + \delta_{Code}(I) + \delta_{Solution}(I) \tag{3}$$

Analyzing the Derivation for $\mathcal{M}(I)$

$$\mathcal{M}(I) = \mathrm{C}_{\Delta h}(I) + \delta_{Code}(I) + \delta_{Solution}(I)$$

This makes sense.

But some things are missing.

- We don't have $\mathrm{C}_{\Delta h}(I)$, we have $\mathrm{C}_{\Delta h}(I^*)$
- We don't have $\delta_{Code}(I)$, we have $\delta_{Code}(I_{CV})$
- We don't have $\delta_{Solution}(I)$, we have $\delta_{Solution}(I_{SV})$

Account for these errors… (and others)

$$\delta_{Total-CM} = \mathbb{S}(I) - \mathrm{C}_{\Delta h}(I^*)$$

$$\delta_{Total-CM} = \delta_{\text{Applicability}}(I, D)$$
$$+\delta_{Measurement}(D) + \delta_{Validation}(D, D^*)$$
$$+\delta_{Code}(I_{CV}) + \delta_{Solution}(I_{SV}) - \delta_{Code}(D_{CV})$$
$$-\delta_{Solution}(D_{SV}) + \Delta_{\mathrm{C}_{\Delta h}}(I, I^*) - \Delta_{\mathrm{C}_{\Delta h}}(D, D^*) + \Delta_{Code}(I, I_{CV})$$
$$+\Delta_{Solution}(I, I_{SV}) - \Delta_{Code}(D, D_{CV}) - \Delta_{Solution}(D, D_{SV})$$

Validation Errors

$$\delta_{\text{Measurement}}(D) = \mathbb{E}(D) - \mathbb{E}^*(D)$$

$$\delta_{\text{Validation}}(D, D^*) = \mathbb{E}^*(D) - \mathrm{C}_{\Delta h}(D^*)$$

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Verification Errors

$$\delta_{Code}(I) = \mathcal{M}(I) - \mathrm{C}_{\infty}(I)$$

$$\delta_{Solution}(I) = \mathrm{C}_{\infty}(I) - \mathrm{C}_{\Delta h}(I)$$

These verification errors are at the input I. There are also verification errors at D.

Input Errors

$$\Delta_{C_{\Delta h}}(I, I^*) = C_{\Delta h}(I) - C_{\Delta h}(I^*)$$

$$\Delta_{Code}(I, I_{CV}) = [\mathcal{M}(I) - C_\infty(I)] - [\mathcal{M}(I_{CV}) - C_\infty(I_{CV})]$$

$$\Delta_{Solution}(I, I_{SV}) = [C_\infty(I) - C_{\Delta h}(I)] - [C_\infty(I_{SV}) - C_{\Delta h}(I_{SV})]$$

These input errors are associated with input I. There are also verification errors associated with input D.

Applicability Error

$$\delta_{\text{Applicability}}(I, D)$$

$$= [\mathbb{S}(I) - \mathcal{M}(I)] - [\mathbb{E}(D) - \mathcal{M}(D)]$$

- Difference is the error in how well $\mathcal{M}$ predicts the system of interest ($\mathbb{S}$) compared to how well it predicts the empirical system ($\mathbb{E}$)
- Tied to scaling, applicability (V&V 40), predicative capability (V&V 10)

$$\delta_{Total-CM} = \mathbb{S}(I) - \mathrm{C}_{\Delta h}(I^*)$$

$$\delta_{Total-CM} = \delta_{\text{Applicability}}(I, D) + \delta_{Measurement}(D) + \delta_{Validation}(D, D^*) + \delta_{Code}(I_{CV}) + \delta_{Solution}(I_{SV}) - \delta_{Code}(D_{CV}) - \delta_{Solution}(D_{SV}) + \Delta_{\mathrm{C}_{\Delta h}}(I, I^*) - \Delta_{\mathrm{C}_{\Delta h}}(D, D^*) + \Delta_{Code}(I, I_{CV}) + \Delta_{Solution}(I, I_{SV}) - \Delta_{Code}(D, D_{CV}) - \Delta_{Solution}(D, D_{SV})$$

Summary

- Developed a mathematically ***Complete Set of Errors***

$$\delta_{Total-CM} = \mathbb{S}(I) - \mathrm{C}_{\Delta h}(I^*)$$

- Set is widely applicable to modeling and simulation

- Each error is mathematically defined

Discussion