A complete set of errors for modeling and simulation

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Motivation

Everyone seems to perform UQ using a different set of uncertainties.

How can you know if they have considered “all” uncertainties?
What errors/uncertainties should be quantified?

**Kennedy & O’Hagan**
- parameter
- model
- residual
- parametric variability
- observation error
- code

**Radaideh et al.,**
- parametric/input
- experimental / measured
- predictive / model discrepancy
- model form
- interpolation / statistical

**D’Auria and Petruzzi**
- code or model
- representation or simulation
- plant data
- “user effect”
Is there an objective way to create a set of errors?

Coleman and Steele

\[ E = D - S \]  \hspace{1cm} (1)

- \[ \delta_S = T - S \] \Rightarrow \[ S = T - \delta_S \]
- \[ \delta_D = T - D \] \Rightarrow \[ D = T - \delta_D \]

\[ E = (T - \delta_D) - (T - \delta_S) \]  \hspace{1cm} (2)

\[ E = \delta_S - \delta_D \]  \hspace{1cm} (3)
Error Decomposition

\[ E = T - X \] (1)

Algebraically introduce a new term, \( Y \)

\[ E = T - Y + Y - X \] (2)

Define new errors, \( \delta_{TY}, \delta_{YX} \)

- \( \delta_{TY} = T - Y \)
- \( \delta_{YX} = Y - X \)

\[ E = \delta_{TY} + \delta_{YX} \] (3)
Total Error Equation

\[ \delta_{Total} = S(I) - C_{\Delta h}(I) \]

- \( \delta_{Total} \) - the total error
- \( S(I) \) - the value of the system at the input of interest
- \( C_{\Delta h}(I) \) - the value of the real computational model at the input of interest

\[ S(I) = C_{\Delta h}(I) + \delta_{Total} \]
What terms can we introduce?

\[ \delta_{Total} = S(I) - C_{\Delta h}(I) \]

Recognize there are two things you can introduce:

1. Different functions (relation), \( f(\cdot) \)
2. Different Inputs, \( I_n \)

These terms \textit{define} how we look at the world.
- Terms should have wide applicability
- More terms = more precise error definitions

ASME 2020 V&V
## Generic Scenario - Functions

<table>
<thead>
<tr>
<th>Functions</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$S(\cdot)$</td>
<td>The behavior of the system</td>
</tr>
<tr>
<td>$C_{\Delta h}(\cdot)$</td>
<td>The results of the real computational model</td>
</tr>
<tr>
<td>$M(\cdot)$</td>
<td>The results of the mathematical model</td>
</tr>
<tr>
<td>$E(\cdot)$</td>
<td>The behavior of the empirical system</td>
</tr>
<tr>
<td>$E^*(\cdot)$</td>
<td>The estimate of the behavior of the empirical system</td>
</tr>
<tr>
<td>$C_\infty(\cdot)$</td>
<td>The results of the ideal computational model</td>
</tr>
</tbody>
</table>
## Generic Scenario - Inputs

<table>
<thead>
<tr>
<th>Inputs</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$I$</td>
<td>Input of interest</td>
</tr>
<tr>
<td>$D$</td>
<td>Input of Empirical data</td>
</tr>
<tr>
<td>$D^*$</td>
<td>Estimate of input of empirical data</td>
</tr>
<tr>
<td>$I^*$</td>
<td>Estimate of the input of interest</td>
</tr>
<tr>
<td>$I_{CV}$</td>
<td>Input of code verification associated with $I$</td>
</tr>
<tr>
<td>$D_{CV}$</td>
<td>Input of code verification associated with $D$</td>
</tr>
<tr>
<td>$I_{SV}$</td>
<td>Input of soln. verification associated with $I$</td>
</tr>
<tr>
<td>$D_{SV}$</td>
<td>Input of soln. verification associated with $D$</td>
</tr>
</tbody>
</table>
## Example Terms

<table>
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<tr>
<th>Terms</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\mathcal{M}(I)$</td>
<td>Mathematical model at the input of interest</td>
</tr>
<tr>
<td>$\mathcal{M}(I_{CV})$</td>
<td>Mathematical model at the input used for code verification associated with $I$</td>
</tr>
<tr>
<td>$C_{\Delta h}(D^*)$</td>
<td>Computational model at the estimate of input of empirical data</td>
</tr>
</tbody>
</table>
Example Derivation: Verification Error

\[
\delta_{\text{Verification}}(I) = \mathcal{M}(I) - C_{\Delta h}(I) \quad (1)
\]

\[
\delta_{\text{Verification}}(I) = \mathcal{M}(I) - C_\infty(I) + C_\infty(I) - C_{\Delta h}(I) \quad (2)
\]

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

- \( \delta_{\text{Code}}(I) = \mathcal{M}(I) - C_\infty(I) \)
- \( \delta_{\text{Solution}}(I) = C_\infty(I) - C_{\Delta h}(I) \)

\[
\mathcal{M}(I) = C_{\Delta h}(I) + \delta_{\text{Code}}(I) + \delta_{\text{Solution}}(I) \quad (3)
\]
Analyzing the Derivation for $\mathcal{M}(I)$

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

This makes sense.

But some things are missing.

- We don’t have $C_{\Delta h}(I)$, we have $C_{\Delta h}(I^*)$
- We don’t have $\delta_{\text{Code}}(I)$, we have $\delta_{\text{Code}}(I_{CV})$
- We don’t have $\delta_{\text{Solution}}(I)$, we have $\delta_{\text{Solution}}(I_{SV})$

Account for these errors… (and others)
\[ \delta_{Total-CM} = \mathbb{S}(I) - C_{\Delta h}(I^*) \]

\[ \delta_{Total-CM} = \delta_{\text{Applicability}}(I, D) + \delta_{\text{Measurement}}(D) + \delta_{\text{Validation}}(D, D^*) + \delta_{\text{Code}}(I_{CV}) + \delta_{\text{Solution}}(I_{SV}) - \delta_{\text{Code}}(D_{CV}) - \delta_{\text{Solution}}(D_{SV}) + \Delta_{C_{\Delta h}}(I, I^*) - \Delta_{C_{\Delta h}}(D, D^*) + \Delta_{\text{Code}}(I, I_{CV}) + \Delta_{\text{Solution}}(I, I_{SV}) - \Delta_{\text{Code}}(D, D_{CV}) - \Delta_{\text{Solution}}(D, D_{SV}) \]
Validation Errors

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

\[ \delta_{\text{Validation}}(D, D^*) = \mathbb{E}^*(D) - C_{\Delta h}(D^*) \]
Verification Errors

\[ \delta_{Code}(I) = M(I) - C_\infty(I) \]

\[ \delta_{Solution}(I) = C_\infty(I) - C_{\Delta h}(I) \]

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

\[ \delta_{\text{Applicability}} (I, D) \]

\[ = [S(I) - M(I)] - [E(D) - M(D)] \]

- Difference is the error in how well \( M \) predicts the system of interest (\( S \)) compared to how well it predicts the empirical system (\( E \))
- Tied to scaling, applicability (V&V 40), predicative capability (V&V 10)
\[
\delta_{Total-CM} = S(I) - C_{\Delta h}(I^*)
\]

\[
\delta_{Total-CM} = \delta_{Applicability}(I, D)
+ \delta_{Measurement}(D) + \delta_{Validation}(D, D^*)
+ \delta_{Code}(I_{CV}) + \delta_{Solution}(I_{SV}) - \delta_{Code}(D_{CV})
- \delta_{Solution}(D_{SV}) + \Delta_{C_{\Delta h}}(I, I^*) - \Delta_{C_{\Delta h}}(D, D^*) + \Delta_{Code}(I, I_{CV})
+ \Delta_{Solution}(I, I_{SV}) - \Delta_{Code}(D, D_{CV}) - \Delta_{Solution}(D, D_{SV})
\]
Summary

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

\[ \delta_{Total-CM} = S(I) - C_{\Delta h}(I^*) \]

- Set is widely applicable to modeling and simulation

- Each error is mathematically defined
Discussion