A Description of a UQ-Predictive Validation Framework for Combustion Applications

\[ C_\mathcal{E} = \max \gamma \text{ subject to constraints:} \]

\[ \begin{align*}
\beta_i & \geq x_i \geq \alpha_i, & \text{for } i = 1, \ldots, n \\
(1 - \gamma)u_e & \geq |y_m(x) - y_e| \geq l_e(1 - \gamma), & \text{for each } e \in \mathcal{E}
\end{align*} \]
expensive data - simulation & experiment

• simulation
  – HPC scaling
  – 1600 cores - 3-5 days

• experiment
  – demonstration scale
  – $1M - 1 year / test
Bayesian probability:
- probability as “a measure of a state of knowledge”
- enables reasoning with uncertain statements
- specifies some prior probability which is updated in light of new data

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“theories are instruments of prediction. From one set of observable data, theories form a bridge over which the investigator can pass to another set of observable data.” (Ernst Mach)

Validation:  
\[ u_e \geq \left[ y_m(x) - y_e \right] \geq l_e, \]

Prediction:  
\[ u \geq \left[ y_m(x) - y_e \right] \geq l \]
UQ - Predictive Validation (V/UQ)

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- Validation: \( u_e \geq \left[ y_m(x) - y_e \right] \geq l_e \),

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1. “All scientifically relevant data have an uncertainty.”
2. “Data without uncertainty cannot be relevant scientifically”  
   Manfred Drosg

$$u_e \geq [y_m(x) - y_e] \geq l_e,$$

- Experimental Uncertainty ($y_e \pm u_e$)
- Verification Error - Numerics ($y_v$ or $x_v \pm u_v$)
- Model Form / Model Parameters ($x_m \pm u_m$)
- Scenario Parameters ($x_s \pm u_s$)
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A Framework for Validation of Computer Models
Technical Report Number 162 April 2005
National Institute of Statistical Sciences 19 T. W. Alexander Drive
PO Box 14006 Research Triangle Park, NC 27709-4006

- create I/U map
- define intended use
- develop DoE
- create surrogate model
- perform consistency analysis
- iterate & predict

\[ C_\varepsilon = \max \gamma \text{ subject to constraints:} \]
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\end{align*} \]
for each \( e \in \mathcal{E} \)

- deterministic solution procedure
- Bayesian (w uniform distributions)
- Inferential (priors to posteriors)
- hierarchical
- iterative
- predictive
V/UQ: heat flux from large pool fires

Incident Heat Flux (kW/m$^2$)

original experimental uncertainty
$u \geq [y_m(x) - y_e] \geq l$

V/UQ: heat flux from large pool fires

original experimental uncertainty
uncertainty after consistency analysis

Incident Heat Flux (kW/m²)
oxy-coal: effect of primary [O₂] on burner stability

P_{O_2(\text{primary})} = 0\%

P_{O_2(\text{primary})} = 21\%

Stand-off distance (cm)

Stand-off distance (cm)
oxy-coal simulation: LES & DQMoM
(7 internal coordinates)

\[ P_{O_2}(\text{primary}) = 0\% \]

\[ P_{O_2}(\text{primary}) = 21\% \]
### traditional validation:

<table>
<thead>
<tr>
<th>$P_{O_2}$ primary</th>
<th>Wall temperature (K)</th>
<th>Measured average stand-off distance</th>
<th>Predicted average stand-off distance</th>
</tr>
</thead>
<tbody>
<tr>
<td>0%</td>
<td>1283K</td>
<td>30 cm</td>
<td>31 cm</td>
</tr>
<tr>
<td>20.9%</td>
<td>1283K</td>
<td>12 cm</td>
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The predicted flame stand-off distance shows no sensitivity to $P_{O_2}$ in the primary.
### V/UQ observations

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The predicted flame stand-off distance shows high sensitivity to wall temperature.
simulation observations:  
Gas Temperature

\[ P_{O_2,\text{primary}} = 0\% \]

\[ P_{O_2,\text{primary}} = 21\% \]
Hierarchical V/UQ

\[
u \geq |y_m(x) - y_e| \geq l
\]

Complete System Case

Overarching Problem
heat flux to container in 10-20m JP-8 fuel pool fire

Benchmark Cases

Buoyancy-Driven Combustion
1m Methane 'Fire'

Buoyant Plumes
1m Helium Plume

Scale-bridging models

Radiation Models
gas & particle participating media

SGS Mixing & Reaction Models
droplet evaporation & gas-phase chemistry, unresolved turbulent mixing

Nonreacting LES Models & Algorithms
turbulent diffusion closure, solution algorithms

Molecular-scale Models

Kinetics & Thermophysical Properties of JP-8 Fuel
chemical kinetics, transport properties, thermodynamic properties, and surrogate fuel formulation

THE INSTITUTE FOR CLEAN AND SECURE ENERGY

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UQ-Predictive Validation Framework for Combustion Applications

V/UQ provides:

- formal hierarchical consistency between experiment and simulation
- reduced uncertainty
- increased physics
- information gain