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Keynote: A Perspective on Model Validation and Validated Models*

SAE paper 2011-01-0238 "Comparison of Several Model Validation Conceptions against a Real Space End-to-End Approach"

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Introduction

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- This talk surveys various conceptions and definitions of
  - models
  - model validation
  - validated models
- A particular philosophy will be presented as the basis for a "*Real Space*" approach to model validation (and model conditioning/calibration)
- Processes and procedures of the Real-Space approach will be sketched
- The pragmatic approach evolved from working many industrial-scale validation problems featuring a broad variety of real-world conditions and constraints
- Among the considerations to be discussed are:
  - the place of model validation within the end-to-end mod./sim. enterprise spanning experiments to prediction
  - relationship and connectivity of model validation to
    - experimental data and its uncertainty
    - basic nature of models
    - extrapolative prediction
    - hierarchical modeling
    - interpretability and practical usability of model validation results and products

MOTIVATION for model validation

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As an example, consider a finite-element model of a device or system

- **Let all model inputs like material properties and boundary conditions be crisp values**
- **All these crisp inputs will have some amount of error**
  - even if all model inputs are actually measured, measurement error will exist
  - typically, the majority of inputs for material properties and model parameters will come from catalogued values determined somewhere else, under different conditions
- **Model-form error will also exist** – *all model conceptions are simplified abstractions of reality; no conception is exact*
- **The numerous errors in the model (each hopefully "small") add to an unknown discrepancy between model predictions and "reality"**

Model Validation

- **How well do model results match reality for relevant quantities of interest?**
- **Is the model "*good enough*" for defined use purposes of the model? (e.g., specific design, analysis, or decision-making purposes)**

Two ELEMENTS of model validation

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- **<u>Accuracy</u> assessment – quantify the discrepancy between model predictions and reality**
  - **discrepancy is measured via relevant norms or "validation metrics"**
  - **these norms or metrics must be <u>meaningful</u>, <u>interpretable</u>, <u>usable</u>**

- **<u>Adequacy</u> assessment – is the discrepancy small enough for stated uses of the model?**
  - **various approaches and criteria for determining adequacy are proposed in the literature**
    - *an area of present difficulty and debate*…to be elaborated later
    - *not all validation frameworks address model adequacy*
  - **adequacy can only be determined at validation points in the modeling space, not at other points where the model is to be used**
  - **thus, the stated *<u>objective</u>* of model adequacy determination for intended uses of the model (beyond the validation conditions) is impossible to achieve fully, but the Real Space approach enables partial achievement**

The Contemporary "Standard" Definition of Model Validation

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Definition used by the recognizing bodies below:

"*Model Validation is the process of determining the degree to which a computer model is an accurate representation of the real world from the perspective of an intended use of the model*."

- **originated by U.S. Dept. of Defense (DoD) – 1996**
- **adopted essentially without change by**:
  - American Institute of Astronautics and Aeronautics (AIAA) – 1998
    - Guide on V&V in Computational Fluid Dynamics
  - U.S. Dept. of Energy (DoE) – 2000
    - various program documents
  - American Society of Mechanical Engineers (ASME)
    - V&V 10 Guide for V&V in Computational Solid Mechanics – 2006
    - V&V 20 Standard for V&V in Computational Fluids & Heat Transfer – 2009
  - NASA
    - Standard for Models and Simulations – 2008
- **<u>NOTE</u> – standard definition does <u>not</u> mention <u>*model adequacy*</u>**

Different Interpretations of the Standard Definition by its Adopters

Ambiguities regarding model-adequacy element of validation

- **DoD** (**originators**)
  - *Accuracy*
  - *Adequacy* for Extrapolative Predictions (compile evidence & arguments for or against)
- **AIAA V&V Guide; Oberkampf & Roy – *V&V in Scientific Computing* (2010)**
  - *Accuracy*
- **ASME V&V20 Standard; Roache – *Fundamentals of V&V* (2010)**
  - *Accuracy*
  - *Adequacy* at Validation Conditions *in asymptotic cases* (order of magnitude determin.)
    - Adequacy in Extrapolation considered to be a different part of the M&S process, e.g. Accreditation
- **DoE; NASA; ASME V&V10 Guide**
  - *Accuracy*
  - *Adequacy,* but unclear how to determine adequacy requirements at Validation Conditions, much less how to address adequacy in Extrapolation
- **Real-Space Framework**
  - *Accuracy*
  - *Adequacy* at Validation Conditions and *Zeroth-order adequacy* for Extrapolative prediction

Earlier Consensus Definitions of model validation, and the Need for an Operational Defn.

- **The following respected definitions specifically include *<u>adequacy</u>* determination**
  - Technical Committee on Model Credibility of the Society for Modeling and Simulation Intrnt'l. (1979) DoD, U.S. Dept. of Agriculture; Europe, Canada, Engrg., Natural & Social Sciences

    "*Model Validation is the substantiation that a computerized model within its domain of applicability possesses a <u>satisfactory range of accuracy</u> consistent with the intended application of the model*."

  - Miser & Quade – 1988, Validation chapter in *Handbook of Systems Analysis*

    "*Validation is the process by which the analyst assures himself and others that a model is a representation of the phenomena being modeled that is <u>adequate</u> for the purposes of the study of which it is a part.*"

- **The 3 defns. have various differences and shortcomings, but one major difficulty in common**
  - **determine accuracy and/or adequacy of model <u>for intended uses</u> *beyond the validation conditions* (*extrapolation performance*)**
  - **A laudable objective, but how to do? Full determination is impossible in principle.**

- **Therefore, all three defns. are seen as <u>Objective Statements</u> for model validation:**
  - THE OBJECTIVE OF model validation is.....*this is what to shoot for as an **<u>idealized objective</u>***

- **An <u>Operational Definition</u> is needed**….*what validation is from an <u>operational perspective</u>* — pragmatically executable and achievable

A Proposed <u>Operational Definition</u> of model validation (for computational phys. engr. models)

<u>Model Validation</u> is the compilation of useful indicators of the accuracy and adequacy of a model's predictive capability for particular output quantities (possibly filtered and transformed) that are important to predict for some purpose, where meaningful comparison of experiment and simulation results is conducted at points in the modeling space that present significant prediction tests for the model use purpose.

- It is important to make a distinction between <u>objective statements</u> and <u>operational definitions</u> of model validation.

- Nonetheless, I agree with Patrick Roache (***Fundamentals of V&V*, 2010)** that definition of specific procedures and processes for model validation is vastly more important and meaningful than definitions in the abstract (like the one above).

De Marsily et al. Concept of "Strongly" and "Weakly" Defined Models (from the groundwater flow literature)

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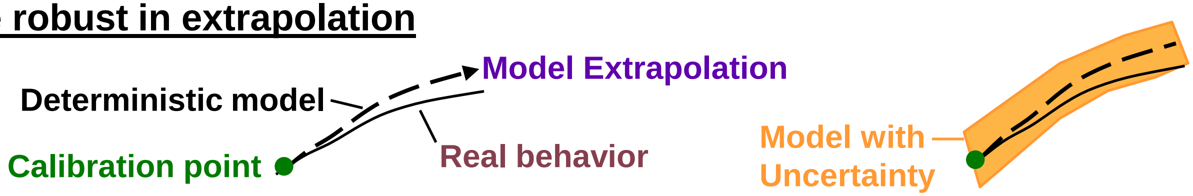
- Fully “strongly” defined models have crisp, <u>determined</u> values for parameters, boundary conditions, etc.
  - e.g. a FE model of a device, with crisp parameter values
- Fully “weakly” defined models’ parameters are <u>free variables</u>
  - e.g. partial differential equation sets (PDEs) like Fourier’s Law and the Navier-Stokes Equations
- Models exist over the spectrum from fully weak to fully strong

Intersection of Validation and Strong and Weak Models

- **Fully strong "deterministic" models generally do not match reality (non-zero error) and are *<u>non-robust in extrapolation</u>***
    - **Calibrated strong models, even if they match experimental data, are <u>fragile</u> in extrapolation beyond the calibration conditions**
        - *no margin for model accuracy degradation*
    - **<u>Weaker models</u> having uncertainty can provide margin against accuracy degradation ➡ <u>more robust in extrapolation</u>**



- Therefore, not necessarily true that the model with less uncertainty is better
- Downside of weaker models is that they predict with greater uncertainty
- This tradeoff is a subject for further research re. optimized modeling approaches

☞ **Some weakness in model parameters and/or model-form representation is required for model predictions to bound or capture reality**

- **<u>Analogy</u> – more productive to pursue weak solutions of PDEs than strong solns.**

Intersection of Validation and Strong and Weak Models (cont'd)

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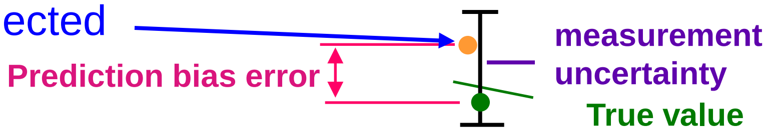
- **Fully weak models like PDEs are exceedingly difficult to validate because they require an essentially infinite number of validation tests over diverse instantiations of the equations**
  - ***How do I validate Fourier's Law*?**

    ☞ Test it in a huge number of circumstances and see if it holds up.

  - **Each individual validation test can hide model bias (*Type II and Type X error*)**
    - e.g., this model result <u>not</u> rejected



    - **The greater the uncertainty in a validation activity, the more bias a model can have before being rejected.**

  - **If a model is <u>not rejected</u> over a <u>large number</u> of <u>diverse validation tests</u> then the assembly of evidence could statistically average-out individual validation bias-error parallaxes and thereby support the model as true or unbiased**
  - **Ultimately, though, trueness of a law or theory is <u>not provable</u>, just "*not disproved so far*" (Karl Popper and others)**
    - Always subject to being overturned by new evidence that may come along

- **Continual testing in new circumstances is part of this "<u>*anti-invalidation*</u>" paradigm**

Anti-Invalidation approach to validation <u>does not</u> apply for most Engineering Application Models

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Some validation conceptions apply this line of thinking to strong or semi-strong application models:

"*We can't validate models, we can only show that they are <u>not</u> <u>in</u>valid*."

- **Paradigm <u>does not</u> legitimately transfer to application models**
  - **Validation of application models is almost always limited to <u>one or a few validation tests</u>**
    - non-rejection in one or a small number of validation tests is not enough to statistically dismiss Type II or Type X validation error and thereby support the model as un-biased
  - **Modelers usually don't propose their application models to be unflawed anyway; just strive for "good enough" (acceptable error) for the modeling job at hand**
    - Foregone conclusion is that model results **<u>are</u>** different from the data
  - **Hypothesis tests for whether the model is different from the data are improperly posed**
    - skewed toward not rejecting the null HO that model is different from the data, even though that HO is known beforehand to be less reasonable than alternative HO that a diff. exists
  - **"<u>Interval Null</u>" HO tests for whether the model is different from the data by > some specified amount Δ are properly posed, but**
    - so far in the literature these only consider error Δ between <u>means</u> of data and model results**—not adequate**, as next slide shows

A Model that is “Consistent” with the Data is Not Necessarily Accurate or Adequate

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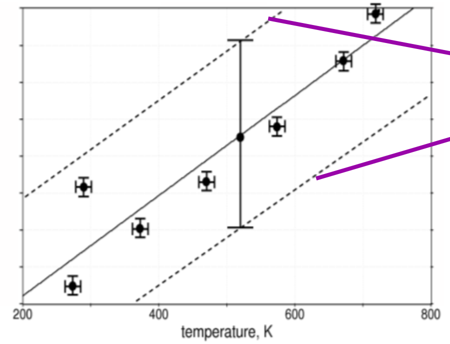
<u>Example</u>:
measured material property data as a function of temperature

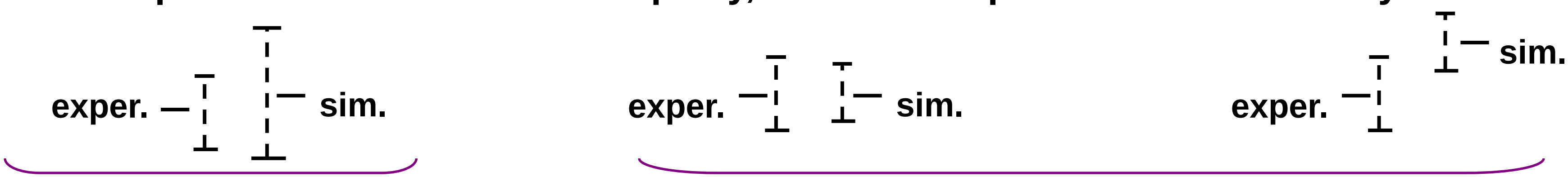


Total uncertainty associated with set of measurements (our best perception of where reality lies)

- The solid black line is a Least-Squares best-fit regression line through the data
- Regression line not an accurate model for material prop. value vs. temperature
  - Some validation paradigms would categorize the model as “<u>consistent</u>” with the data and therefore would <u>accept</u> it (➡ poses “Model User’s Risk”)
  - model too precise, not representative of real property variability
    - Under-predicted uncertainty could lead to trouble in downstream uses of model
  - model better characterized as: “<u>not fully consistent</u>” or “<u>not inconsistent</u>” with data
- Also demonstrates why popular validation criterion of “<u>means matching</u>” (does mean of sim. = mean of data?) is not an effective test for model accuracy

A Simple "Real Space" Accuracy/Discrepancy measure and Criterion for Model Adequacy

- **Real Space – involves no subtractive difference of results from simulation and experiment, or other "validation metric" discrepancy measures**
- **Simple criterion for model adequacy, scaled to experimental uncertainty**



This case meets "Zeroth-order" conditions for model adequacy

- **model prediction bounds experimental uncertainty bar** (as the best available evidence of where "reality" lies)
- **If the data/model relationship remains consistent in extrapolation (*the hope in all modeling*), the predictions will bound reality in the extrapolation conditions**

☑**Reality lying w/in the predictions is what a designer or decision maker wants***
*assuming non-excessive sim. uncer. bar extents beyond experim. uncer. bar

Greater prediction risk

- **much of reality lies outside the model predictions**
- **If data/model relationship remains consistent in extrapolation then the predictions will not contain reality**

Adequacy criterion can be relaxed if auxiliary information is available, e.g.

- OK if reality lies outside predictions by X% above and/or Y% below
- However, very difficult to rigorously quantify such allowables (next slide)

Difficulty of Pre-Specified Accuracy Requirements for Model Adequacy

- **In hierarchical modeling projects a non-uniqueness problem exists with Top-Down parsing of acceptable error tolerances down to the various submodeling activities**

- **In “isolated” phenominological model development & validation work, e.g. turbulence or constitutive model development at a university, there is no ‘project’-level accuracy requirement in the first place**

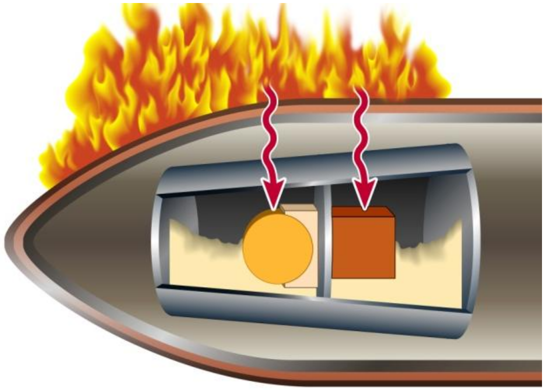
- **Potential constraint violation of a-priori accuracy requirement:**

  ➡ Experimental uncer. is lower limit on validation accuracy requirement that can be placed on a model.

  —not known until after the experims. performed and processed

Bottom Line: not a viable approach

System-Level risk analysis — Weapon in a Fire



Multiple underlying submodels:

Fire model for heat load BCs

\+

Heat Transfer models (mult. modes)

\+

Mtl. behavior & transformation models

\+

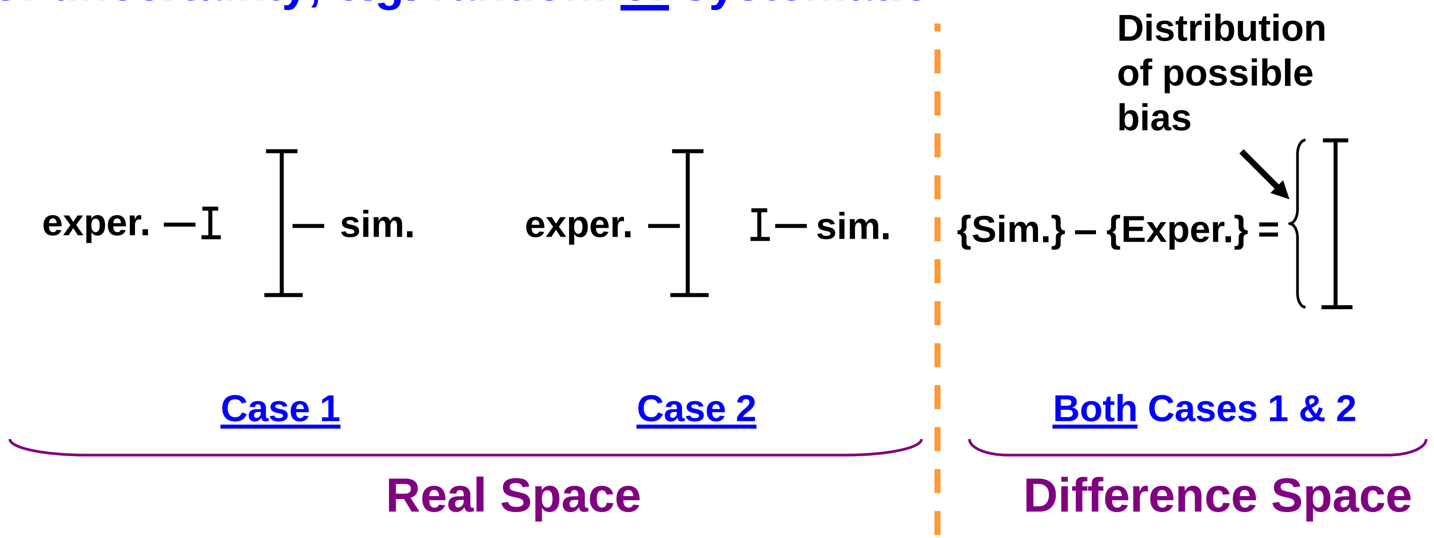
Component response & failure models

+…+…+…

Real Space vs. Transform Space Representation of Model Discrepancy

- E.g., subtractive difference is a popular way of comparing data against model predictions for model validation assessments
- The subtractive difference transform yields a less definitive validation result vs. staying in real space – see example below
- **Subtr. Diff. has non-unique mapping from real space to transform space, as do other (perhaps all?) validation metric discrepancy transforms**
- **Some transform discrepancy metrics (perhaps all?) are geared toward one type of uncertainty, e.g. random or systematic**

Example:



Real-Space Framework handles Random and Systematic Uncertainties represented in Interval, Distributional, and Discrete (non-parametric) forms

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- Most Validation Frameworks in the literature are built exclusively on a probabilistic representation of uncertainty.

- Most uncertainties in validation projects do not have well-defined probability distributions
  ➡ other representations of uncertainty are necessary, as accommodated by the Real-Space framework.

- The Framework ultimately represents combined uncertainties of disparate type as an uncertainty interval.

Equations for Constructing Net Experimental & Simulation Uncertainty Bars for Real-Space Comparisons

(I don't expect you to read these!)

Model | **Experiment**

Experiment

$$Intvl\_d\left\{\hat{r}_{e\_adjusted_{(1)}},\cdots,\hat{r}_{e\_adjusted_{(k)}},\cdots,\hat{r}_{e\_adjusted_{(K)}}\right\}$$

$$;\ \hat{r}_{e\_adjusted_{(k)}} =$$

$$\hat{r}_{e\_observed_{(k)}} \qquad \text{(A)}$$

$$-\left[\sum_{j}^{\#rand\_correlMeas\_I.A} \Delta\hat{r}_{e\_j(k)}\right] \qquad \text{(B)}$$

$$-\left[\sum_{i}^{\#rand\_correlMeas\_II.2,\,NonTrav\ II.1.a} \Delta\hat{r}_{e_{i(k)}}\big|_{\Delta\hat{x}_{i(k)}}\right] \qquad \text{(C)}$$

$$+$$

$$\bigcup_{j}^{\#syst\_I.B} U[r_e]_{I.B_j} \qquad \text{(D)}$$

$$+$$

$$\bigcup_{i}^{\#syst\_nonTrav IV} U[(r_e^L, r_e^U)\big|_{U[X_i\ \ nonTrav]}] \qquad \text{(E)}$$

$$= \boxed{\Delta r_{e\_net}}$$

—Experimental uncertainty bar (net)

Model

$$\text{(F)} \qquad Intvl\_d\left\{\hat{r}_{m_{(1)}},\cdots,\hat{r}_{m_{(k)}},\cdots,\hat{r}_{m_{(K)}}\right\}$$

$$;\ \hat{r}_{m_{(k)}} = \overline{r}_m + \sum_{n}^{\#rand\_correlMeas\_Trav\ II.1.a} \Delta\hat{r}_{n(k)}\big|_{\Delta\hat{x}_{n(k)}}$$

$$+$$

$$\text{(G)} \qquad \bigcup_{i}^{\#syst\_nonTrav\ IV} U[r_m\big|_{U[X_i\ \ nonTrav]}]$$

$$+$$

$$\text{(H)} \qquad \bigcup_{i}^{\#syst\_Trav\ IV} U[r_m\big|_{U[X_i\ \ Trav]}]$$

$$+$$

$$\text{(I)} \qquad \bigcup_{k}^{\#model\_intrinsic\_Trav} U[r_m\big|_{U[\theta_k\_Trav]}] - \bigcup_{k}^{\#model\_intrinsic\_nonTrav} U[r_m\big|_{U[\theta_k\_nonTrav]}]$$

$$+$$

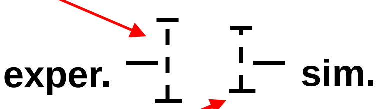
$$\text{(J)} \qquad \bigcup_{k}^{\#postprocessing\ \ Trav} \Delta r_{m\_postproc\_Trav_k} - \bigcup_{k}^{\#postprocessing\ \ nonTrav} \Delta r_{m\_postproc\_nonTrav_k}$$

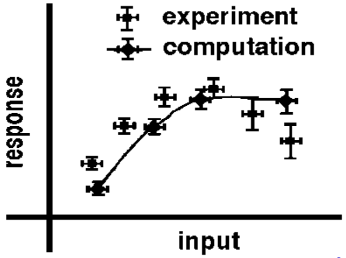
$$+$$

$$\text{(K)} \qquad \bigcup_{k}^{\#discretization\ \ Trav} \Delta r_{m\_discr\_Trav_k} - \bigcup_{k}^{\#discretization\ \ nonTrav} \Delta r_{m\_discr\_nonTrav_k}$$

$$= \boxed{\Delta r_{m\_net}}$$

—Simulation uncertainty bar (net)





— Vertical Uncertainty Bars

— Horizontal Uncertainty Bars

Model

(F)
$$Intvl\_d\left\{\hat{r}_{m_{(1)}},\cdots,\hat{r}_{m_{(k)}},\cdots,\hat{r}_{m_{(K)}}\right\}$$
$$;\ \hat{r}_{m_{(k)}} = \bar{r}_m + \sum_{n}^{\#rand\_correlMeas\_Trav\ II.1.a} \Delta\hat{r}_{n(k)}\,|_{\Delta\hat{x}_{n(k)}}$$

\+

(G)
$$\bigcup_{i}^{\#syst\_nonTrav\ IV} U[r_m\,|_{U[X_i\_nonTrav]}]$$

\+

(H)
$$\bigcup_{i}^{\#syst\_Trav\ IV} U[r_m\,|_{U[X_i\_Trav]}]$$

\+

(I)
$$\bigcup_{k}^{\#model\_intrinsic\_Trav} U[r_m\,|_{U[\theta_k\_Trav]}] - \bigcup_{k}^{\#model\_intrinsic\_nonTrav} U[r_m\,|_{U[\theta_k\_nonTrav]}]$$

\+

(J)
$$\bigcup_{k}^{\#postprocessing\_Trav} \Delta r_{m\_postproc\_Trav\ k} - \bigcup_{k}^{\#postprocessing\_nonTrav} \Delta r_{m\_postproc\_nonTrav\ k}$$

\+

(K)
$$\bigcup_{k}^{\#discretization\_Trav} \Delta r_{m\_discr\_Trav_k} - \bigcup_{k}^{\#discretization\_nonTrav} \Delta r_{m\_discr\_nonTrav_k}$$

$_{m\_net}$

Experiment

$$Intvl\_d\left\{\hat{r}_{e\_adjusted_{(1)}},\cdots,\hat{r}_{e\_adjusted_{(k)}},\cdots,\hat{r}_{e\_adjusted_{(K)}}\right\}$$
$$;\ \hat{r}_{e\_adjusted_{(k)}} =$$

(A)
$$\hat{r}_{e\_observed_{(k)}}$$

(B)
$$-\left[\sum_{j}^{\#rand\_correlMeas\_I.A} \Delta\hat{r}_{e\ j(k)}\right]$$

(C)
$$-\left[\sum_{i}^{\#rand\_correlMeas\_II.2,\ NonTrav\ II.1.a} \Delta\hat{r}_{e_{i(k)}}\,|_{\Delta\hat{x}_{i(k)}}\right]$$

\+

(D)
$$\bigcup_{j}^{\#syst\_I.B} U[r_e]_{I.B_j}$$

\+

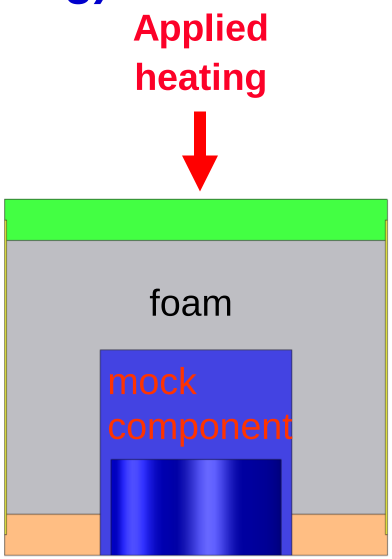
(E)
$$\bigcup_{i}^{\#syst\_nonTrav\ IV} U[(r_e^L, r_e^U)\,|_{U[X_i\_nonTrav]}]$$

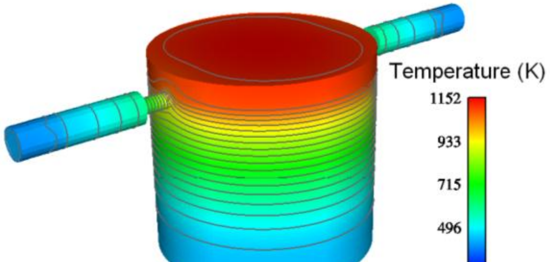
$$= \Delta r_{e\_net}$$

Concept of “Traveling” and “Non-Traveling” portions of the Experiment Model (E Model)

☞ **connectivity to Downstream predictions (extrapolation, incl. hierarchical modeling)**

- **E.g., E model (at right) is the model that participates in the val. or calibration activity**
- **Foam behavioral model (vaporization & altered heat transfer) is object of val. or cal.:**
  - **is the only traveling portion of E model**
- **Everything else in E model does not travel to downstream use:**
  - canister, vents, and slug
  - BC models of heating loads and radiative and convective cooling





Uncertainties are treated in the Framework according to whether they are affiliated with traveling or non-traveling aspects of E model

Model | **Experiment**

— Traveling Uncertainty

— Non-Traveling Uncertainty

Experiment

(A)
$$Intvl\_d\left\{\hat{r}_{e\_adjusted_{(1)}},\cdots,\hat{r}_{e\_adjusted_{(k)}},\cdots,\hat{r}_{e\_adjusted_{(K)}}\right\}\; ;\; \hat{r}_{e\_adjusted_{(k)}} = \hat{r}_{e\_observed_{(k)}}$$

(B)
$$-\left[\sum_{j}^{\#rand\_correlMeas\_I.A} \Delta\hat{r}_{e\;j(k)}\right]$$

(C)
$$-\left[\sum_{i}^{\#rand\_correlMeas\_II.2,\,NonTrav\;II.1.a} \Delta\hat{r}_{e_{i(k)}}\,|_{\Delta\hat{x}_{i(k)}}\right]$$

$+$

(D)
$$\bigcup_{j}^{\#syst\_I.B} U[r_e]_{I.B\;j}$$

$+$

(E)
$$\bigcup_{i}^{\#syst\_nonTrav\,IV} U[(r_e^L, r_e^U)\,|_{U[X_i\_nonTrav]}]$$

$= \Delta r_{e\_net}$

Model

(F)
$$Intvl\_d\left\{\hat{r}_{m_{(1)}},\cdots,\hat{r}_{m_{(k)}},\cdots,\hat{r}_{m_{(K)}}\right\}\; ;\; \hat{r}_{m_{(k)}} = \overline{r}_m + \sum_{n}^{\#rand\_correlMeas\_Trav\;II.1.a} \Delta\hat{r}_{n(k)}\,|_{\Delta\hat{x}_{n(k)}}$$

$+$

(G)
$$\bigcup_{i}^{\#syst\_nonTrav\;IV} U[r_m\,|_{U[X_i\_nonTrav]}]$$

$+$

(H)
$$\bigcup_{i}^{\#syst\_Trav\;IV} U[r_m\,|_{U[X_i\_Trav]}]$$

$+$

(I)
$$\bigcup_{k}^{\#model\_intrinsic\_Trav} U[r_m\,|_{U[\theta_k\_Trav]}] - \bigcup_{k}^{\#model\_intrinsic\_nonTrav} U[r_m\,|_{U[\theta_k\_nonTrav]}]$$

$+$

(J)
$$\bigcup_{k}^{\#postprocessing\_Trav} \Delta r_{m\_postproc\_Trav\;k} - \bigcup_{k}^{\#postprocessing\_nonTrav} \Delta r_{m\_postproc\_nonTrav\;k}$$

$+$

(K)
$$\bigcup_{k}^{\#discretization\_Trav} \Delta r_{m\_discr\_Trav_k} - \bigcup_{k}^{\#discretization\_nonTrav} \Delta r_{m\_discr\_nonTrav_k}$$

$= \Delta r_{m\_net}$

Model | **Experiment**

$$Intvl\_d\left\{\hat{r}_{e\_adjusted_{(1)}},\cdots,\hat{r}_{e\_adjusted_{(k)}},\cdots,\hat{r}_{e\_adjusted_{(K)}}\right\}$$

$$;\ \hat{r}_{e\_adjusted_{(k)}} =$$

(A) $$\hat{r}_{e\_observed_{(k)}}$$

(B) $$-\left[\sum_{j}^{\#rand\_correlMeas\_I.A} \Delta\hat{r}_{e\ j(k)}\right]$$

(C) $$-\left[\sum_{i}^{\#rand\_correlMeas\_II.2,\,NonTrav\ II.1.a} \Delta\hat{r}_{e_{i(k)}}\Big|_{\Delta\hat{x}_{i(k)}}\right]$$

Deal with <u>random</u> uncertainty (aleatory, variability) over multiple repeat experiments

(F) $$Intvl\_d\left\{\hat{r}_{m_{(1)}},\cdots,\hat{r}_{m_{(k)}},\cdots,\hat{r}_{m_{(K)}}\right\}$$
$$;\ \hat{r}_{m_{(k)}} = \overline{r}_m + \sum_{n}^{\#rand\_correlMeas\_Trav\ II.1.a} \Delta\hat{r}_{n(k)}\Big|_{\Delta\hat{x}_{n(k)}}$$

+

+

(D) $$\bigcup_{j}^{\#syst\_I.B} U[r_e]_{I.B_j}$$

+

(E) $$\bigcup_{i}^{\#syst\_nonTrav\,IV} U[(r_e^L, r_e^U)|_{U[X_i\_nonTrav]}]$$

$$= \Delta r_{e\_net}$$

(G) $$\bigcup_{i}^{\#syst\_nonTrav\ IV} U[r_m|_{U[X_i\_nonTrav]}]$$

+

(H) $$\bigcup_{i}^{\#syst\_Trav\ IV} U[r_m|_{U[X_i\_Trav]}]$$

+

(I) $$\bigcup_{k}^{\#model\_intrinsic\_Trav} U[r_m|_{U[\theta_k\_Trav]}] - \bigcup_{k}^{\#model\_intrinsic\_nonTrav} U[r_m|_{U[\theta_k\_nonTrav]}]$$

+

(J) $$\bigcup_{k}^{\#postprocessing\_Trav} \Delta r_{m\_postproc\_Trav\ k} - \bigcup_{k}^{\#postprocessing\_nonTrav} \Delta r_{m\_postproc\_nonTrav\ k}$$

+

(K) $$\bigcup_{k}^{\#discretization\_Trav} \Delta r_{m\_discr\_Trav_k} - \bigcup_{k}^{\#discretization\_nonTrav} \Delta r_{m\_discr\_nonTrav_k}$$

$$= \Delta r_{m\_net}$$

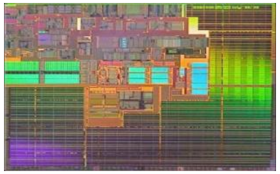
Deal with <u>systematic</u> uncertainty (epistemic: interval & probabilistic) over one or multiple experiments

The Framework has evolved from working many varied applications

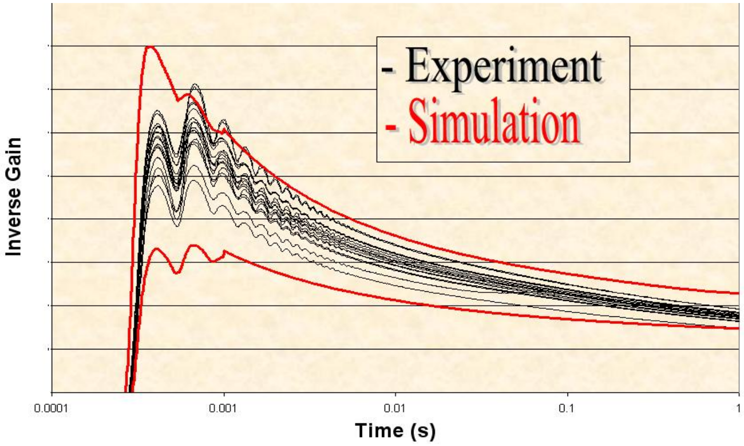
- **Radiation-damaged electronics response & recovery/annealing**
  - **model conditioning & validation**

neutrons
x-rays
γ-rays

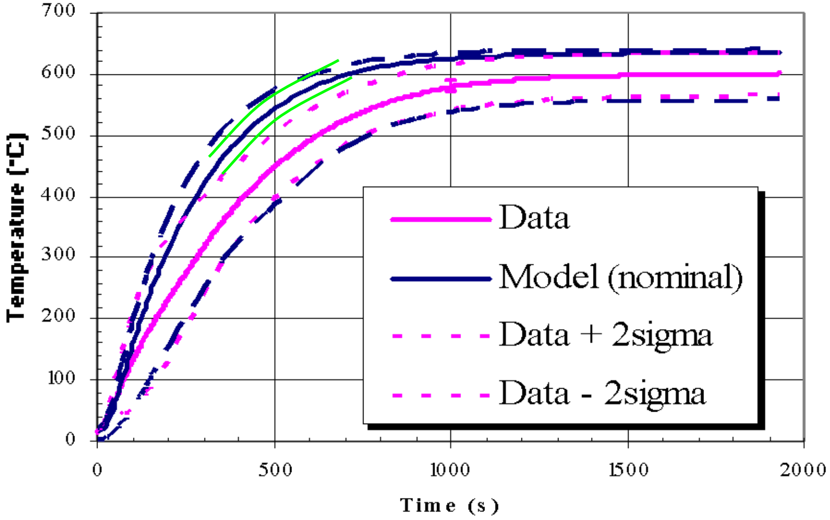
radiation damage



Device effects (transistor, diode, etc.) and circuit effects



- **Electro-mechanical component internal temperature response**
  - **Validation refuted the model**
  - **mapped bias & uncertainty to traveling parameters of the model ("model conditioning")**



The Framework has evolved from working many and varied applications

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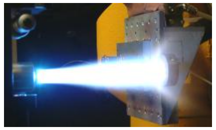
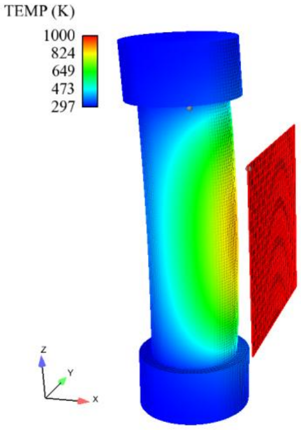
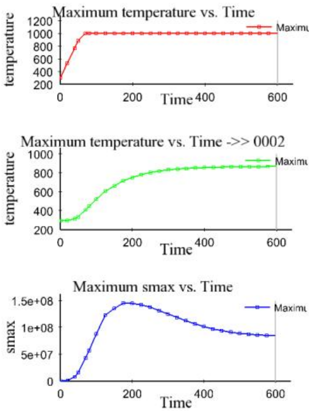
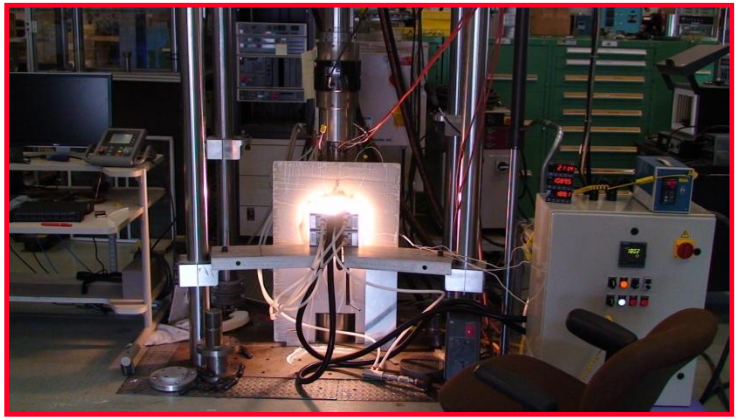
- **Validation of Propellant Fire Models**



- <u>**Response/Failure of Steel Pressure Vessels at high temperatures**</u>
  - – <u>**Conditioning**</u> of high-temperature material constitutive model for elastic-plastic response and failure of steel
  - – <u>**Validation**</u> of mechanical failure of steel pressure vessel (ultimately foam-filled sealed compartments in weapons)







Validation/Conditioning of Foam Thermal Property Model at Elevated Temperatures
(thermal conductivity with radiation enhancement term)

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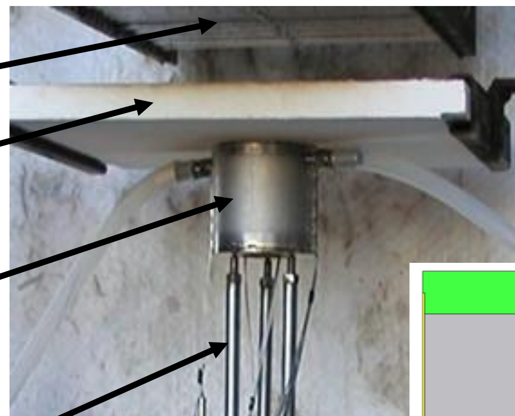
Experiments

quartz heating lamps

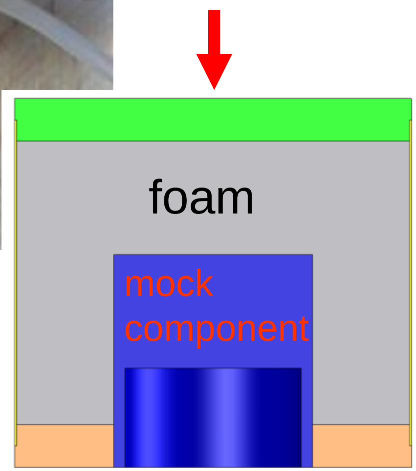
insulation board

24 thermocouples on and inside canister

pointed low-thermal-contact holding posts

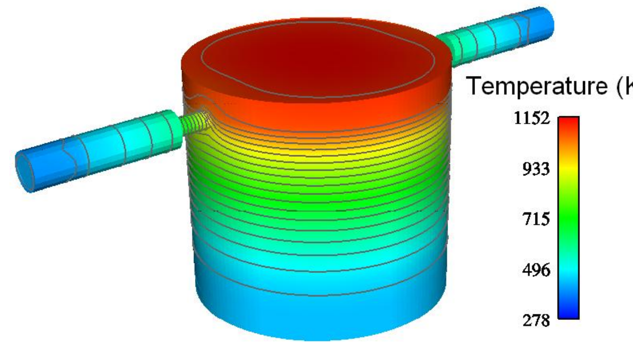


Applied heating



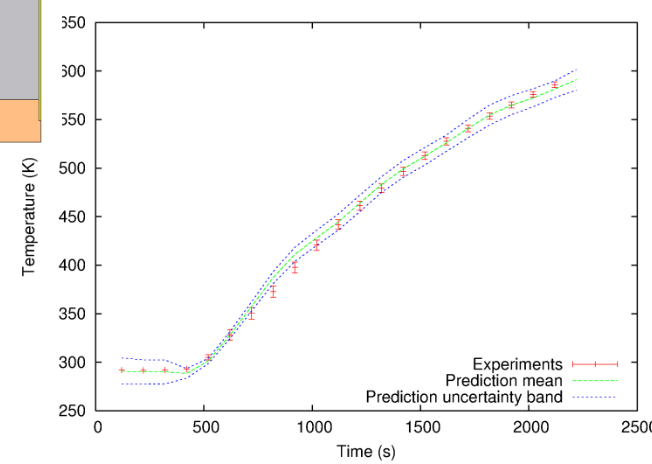
decomposed foam char matrix

Simulations



FE Thermal Model:

- **Conduction,**
- **Convection**
- **Radiation**

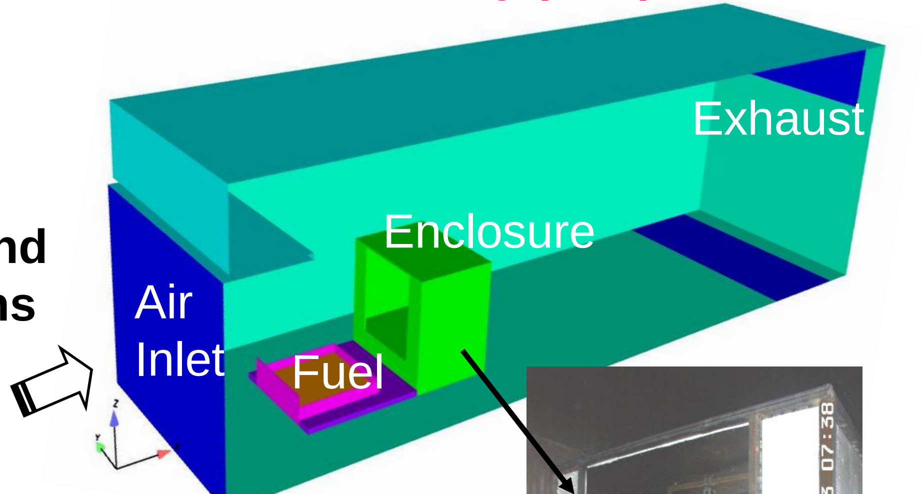


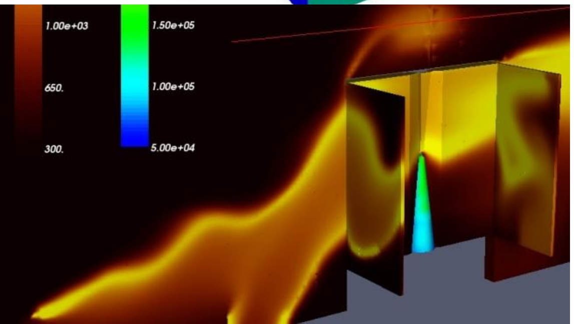
Sandia Thermal Test Complex

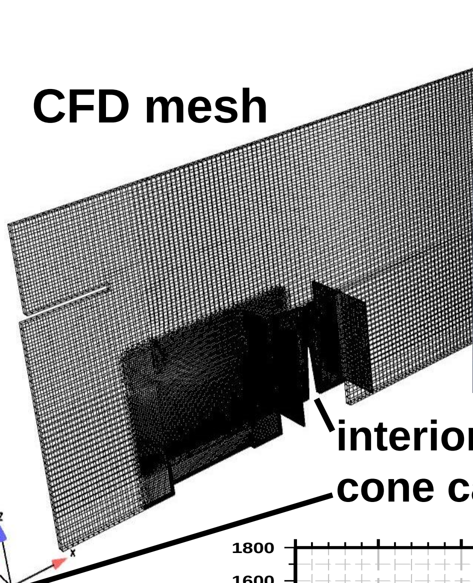
Validation of Fire CFD sims.

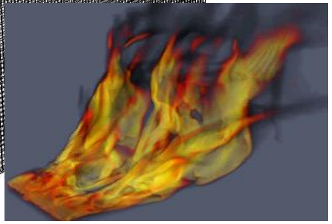
- **Validate fire CFD simulations of radiative and convective heating of a weapon-like calorimeter in wind-driven fire.**

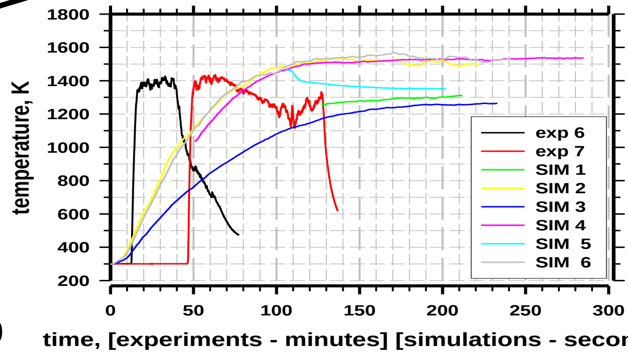
Cross-Wind Test Facility (XTF)











Calorimeter Response at location 10

Closing

- Various parties are still working out the details of model validation — many different conceptions, approaches, and frameworks exist in the literature.
- Therefore, beware the ambiguity involved when one expresses that they have "validated" their model, or have a "validated" model.
- The rationale behind the Real Space approach to model validation has been sketched here, much more development in the paper.
- The Real Space methodology has been successfully implemented on a variety of industrial-scale validation problems.
- Prediction Science requires development of effective and robust methodologies for data and model conditioning, verification, validation, and risk-mitigated extrapolation for "best estimate" predictions. Progress in prediction will depend on advancing these methodologies as well as physics models and math/computing.