PECOS

Predictive Engineering and Computational Sciences

Model Validation and Uncertainty Quantification

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Outline

- Introduction and definitions
- A validation process
- Planning of validation processes
- Examples
- Verification of validation processes
- Conclusions

Introduction

Questions pertaining to validation

Is the model any good?
Is the model a good model?
How good is the model?

If one wants to be philosophical...

What is a good model?

Before answering those questions, one must have an objective in mind.

Quantities of interest:

Specific objectives that can be expressed as the target outputs of a model (mathematically, they are often defined by functionals of the solutions).

Examples:

$$\boxed{\begin{aligned} Q(u) &= u(x) \\ Q(u) &= \int u(x)dx \end{aligned}}$$

Some Definitions:

Verification:

The process of determining the accuracy with which a computational model can produce results deliverable by the mathematical model on which it is based.
$\Rightarrow$ **Code and Solution Verification**

Validation:

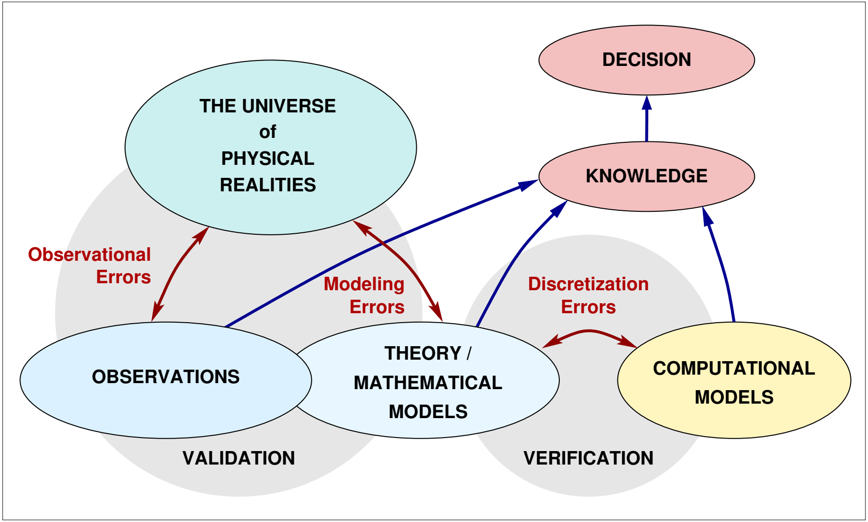
The process of determining the accuracy with which a model can predict observed physical events (or the important features of a physical reality).

P. Roache (2009): "The process of determining the degree to which a model (and its associated data) is an accurate representation of the real world from the perspective of the intended uses of the model".

Uncertainty Quantification:

The process of determining the degree of uncertainty in the prediction of the QoI. Typically, the degree of uncertainty is related to the probability distribution for the QoI.

Paths to Knowledge



Published in SIAM News, Oden, Moser, and Ghattas (Nov. 2010)

Control of Errors

Errors are all a matter of comparison!

- Code Verification: Using the method of “manufactured solutions”, for example, we can easily compare the computed solution with the manufactured solution.
- Solution Verification: In this case, the solution of the problem is unknown and one can use convergence (uniform or adaptive methods) to assess the accuracy of the approximate solutions.
- Calibration Process: Comparison of observable data with model estimates of the observables.
- Validation Process: The main idea behind validation is to know whether a model can be used for prediction purposes.

$\Rightarrow$ What should we compare in this case?

Validation Process

1. Calibration:

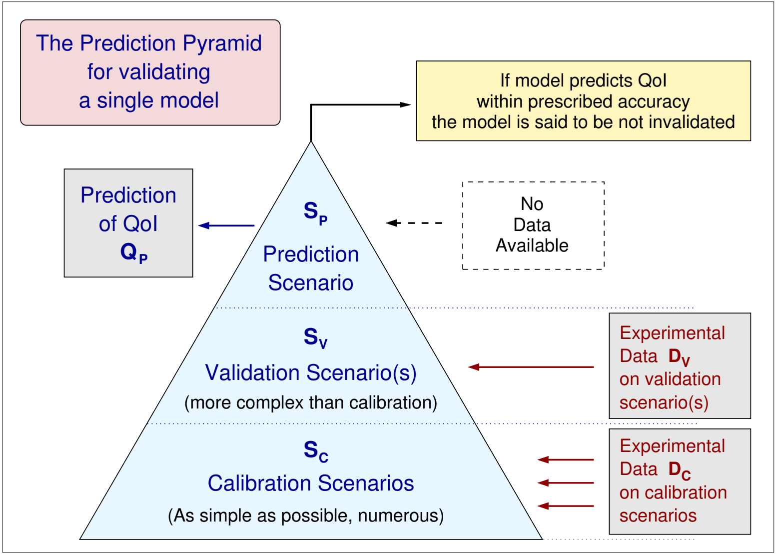
   Identification of values of parameters of a model designed to bring model results into agreement with measurements.

2. Validation:

   The process of determining the accuracy with which a model can predict observed physical events (or the important features of a physical reality).

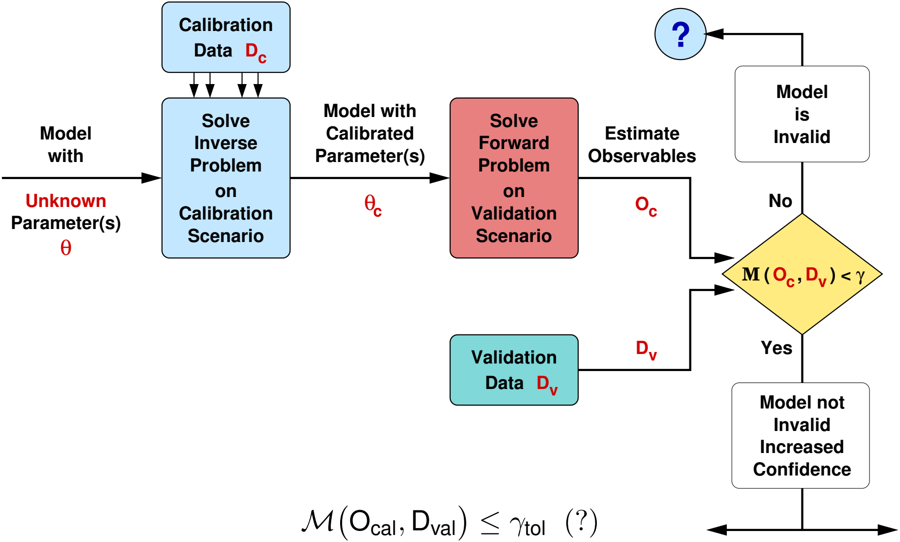
3. Prediction:

   The forecast of an event (a predicted event cannot be measured or observed, for then it ceases to be a prediction).



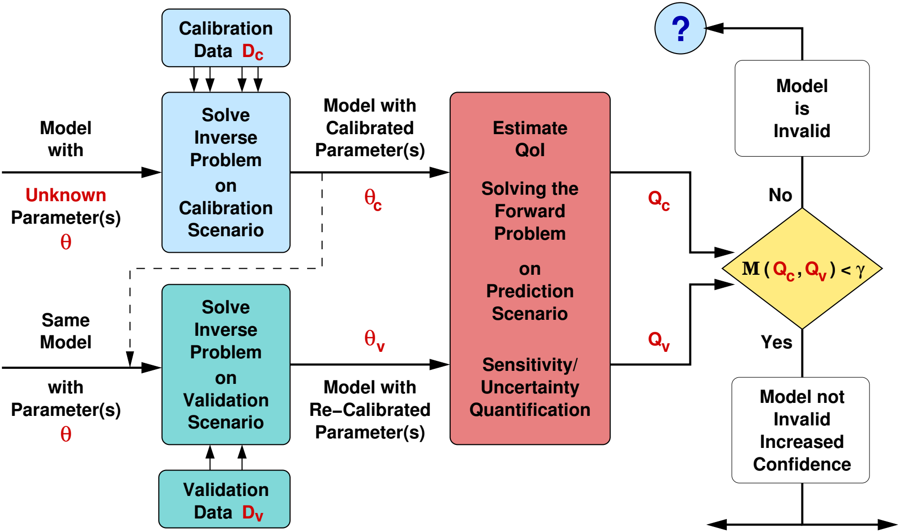
The Validation Pyramid

Classical Approach for Validation



$$\mathcal{M}\left(\mathrm{O_{cal}}, \mathrm{D_{val}}\right) \leq \gamma_{\mathrm{tol}} \quad (?)$$

Proposed Validation Process (2009)

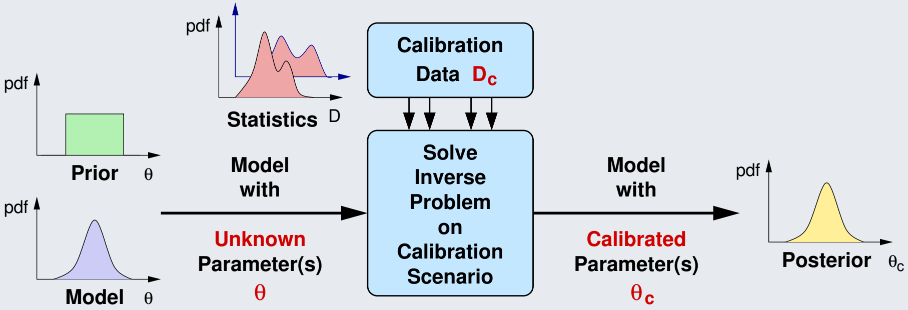


$$\mathcal{M}\left(Q_{cal}, Q_{val}\right) \leq \gamma_{tol} \quad (?)$$

Objective of Calibration Phase

To identify the model parameters on scenarios that are as simple as possible. Parameters are in general associated with constitutive equations and are material dependent.

Calibration Phase



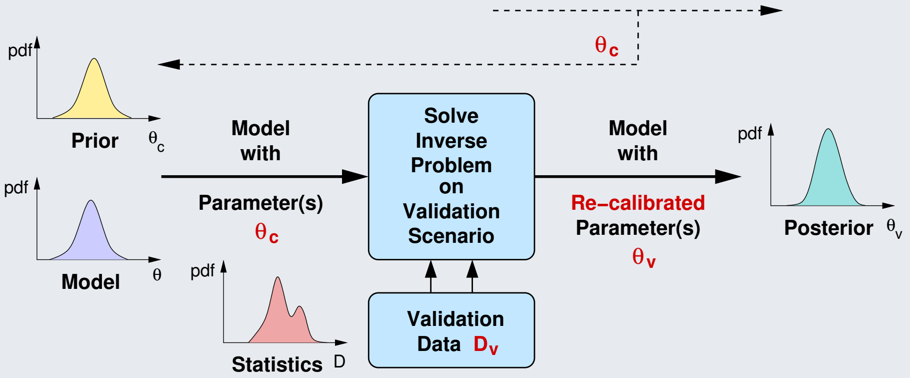
Objective of Validation Phase

To test the mathematical model on scenarios that are different from those of the calibration phase. $\Rightarrow$ **Two-stage process:**

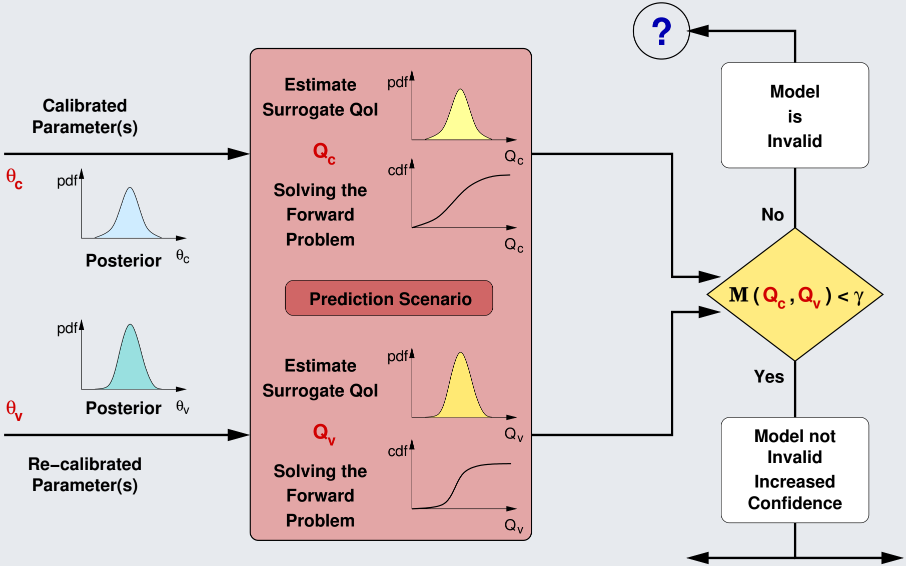
1) Re-calibrate the parameters θ.

2) Verify the sensitivity of Q with respect to variations in θ.

Recalibration Phase



Prediction Phase



Validation process requires detailed planning:

1. **Description of goals:** Describe background and goals of the predictions. Clearly define the quantity (or quantities) of interest.
2. **Modeling:** Write mathematical equations of selected model(s), list all parameters that are necessary to solve the problem, as well as assumptions and limitations of the model(s),
3. **Data collection:** Collect as many data as possible from literature or available sources (data should include, if available, the statistics).
4. **Sensitivity analysis:** Quantify the sensitivity of QoI with respect to parameters of the model. Rank parameters according to their influence.
5. **Calibration experiments:** Provide description of scenario (as precisely as possible), observables and statistics, prior and likelihood of the parameters to be calibrated.
6. **Validation experiments:** Provide same as above + clearly state assumption to be validated.

Morgan & Henrion's "Ten Commandements" (1990)*

In relation to quantitative risk and policy analysis

1. Do your homework with literature, experts and users.
2. Let the problem drive the analysis.
3. Make the analysis as simple as possible, but no simpler.
4. Identify all significant assumptions.
5. Be explicit about decision criteria and policy strategies.
6. Be explicit about uncertainties.
7. Perform systematic sensitivity and uncertainty analysis.
8. Iteratively refine the problem statement and the analysis.
9. Document clearly and completely.
10. Expose to peer review.

* Extracted from D. Vose, "Risk Analysis: A Quantitative Guide" (2008)

A systematic approach to the planning and implementation of experiments (Chapter 1 - Section 2)

In Wu & Hamada “Experiments, Analysis, and Optimization” (2009)

1. State objective.
2. Choose response.
3. Choose factors and levels.
4. Choose experimental plan.
5. Perform the experiment.
6. Analyze the data.
7. Draw conclusions and make recommendations:

   . . . the conclusions should refer back to the stated objectives of the experiment. A confirmation experiment is worthwhile for example, to confirm the recommended settings. Recommendations for further experimentation in a follow-up experiment may also be given. For example, a follow-up experiment is needed if two models explain the experimental data equally well and one must be chosen for optimization.

Planning

- Planning is a cumbersome and time-consuming process.
- Planning of validation processes involves many choices that eventually need to be carefully checked.

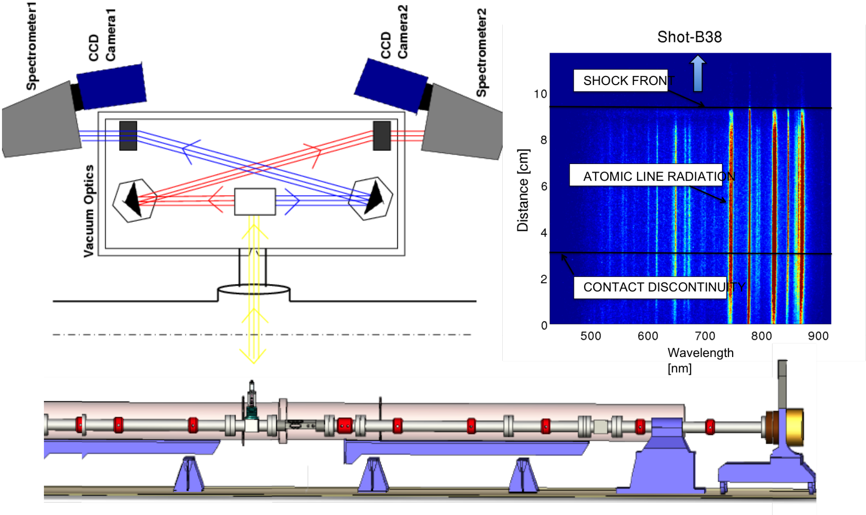
Choices are made about:

- Physical models
- Quantities of interest and surrogate quantities of interest
- Experiments for calibration and validation purposes
- Data sets to be used in calibration and validation
- Prior pdf and likelihood function
- Probabilistic models . . .

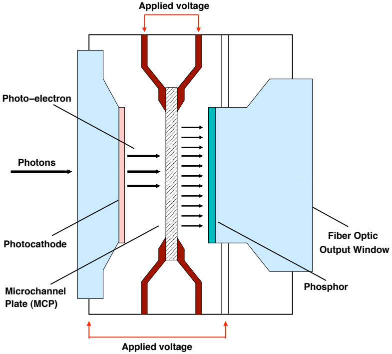
Our preliminary experiences with validation has revealed that many “sanity checks” need to be added within the proposed validation process.

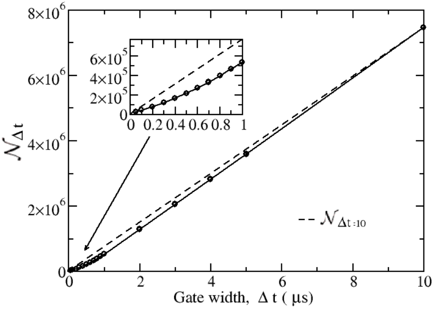
Our objective is to develop a suite of tools to systematically verify the correctness of each stage of the validation process.

EAST Shock-Tube Experiments

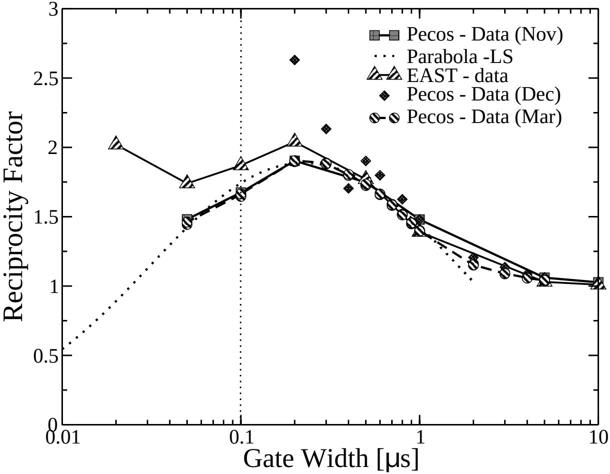


Example:
Data reduction model for ICCD Camera



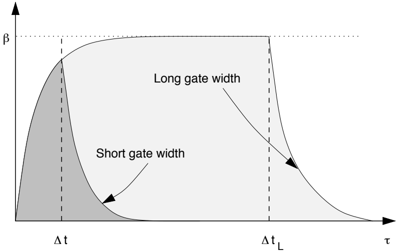


Example:
Data reduction model for ICCD Camera



Validation Planning

Proposed physical models and corresponding model parameters.



	α_1	α_2	β	δ	ν	Photon counts $\mathcal{N}_{\Delta t}$
M_1	✗	✗	✓	✗	✗	$\beta\Delta t$
M_2	✓	✓	✓	✗	✗	$\beta\Delta t - \Lambda(\Delta t, \alpha_1, \alpha_2, \beta)$
M_3	✓	✓	✓	✓	✗	$\beta(\Delta t + \delta) - \Lambda(\Delta t + \delta, \alpha_1, \alpha_2, \beta)$
M_4	✓	✓	✓	✗	✓	$(\beta + \nu)\Delta t - \Lambda(\Delta t, \alpha_1, \alpha_2 \beta)$
M_5	✓	✓	✓	✓	✓	$(\beta + \nu)(\Delta t + \delta) - \Lambda(\Delta t + \delta, \alpha_1, \alpha_2 \beta)$

Symbols ✓ or ✗ indicate that the parameter is or is not part of the model, respectively.

Validation Planning

QoI

- Reciprocity $\rho(\Delta t)$ at $\Delta t = 0.1$ [μs]

Hypothesis to be validated

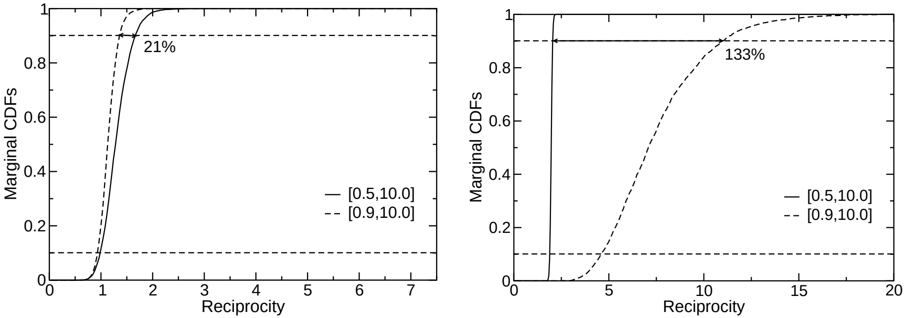
- Is the model predictive at the low gate width?

Calibration/Validation data

- Calibration data: Exp. data between 0.9 [μs] to 10.0 [μs]
- Validation data: Exp. data between 0.5 [μs] to 0.8 [μs]

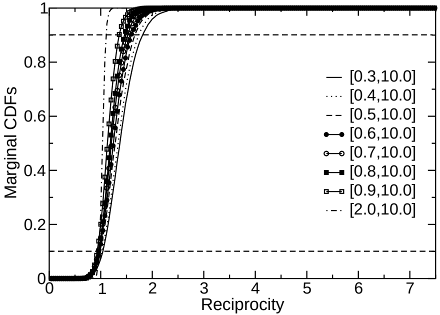
Results

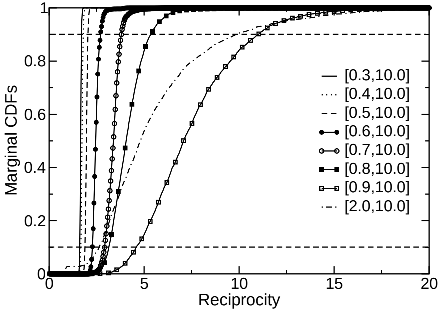
CDF of QoI for model M1 (left) and model M5 (right):



Convergence of calibration process with respect to number of data points

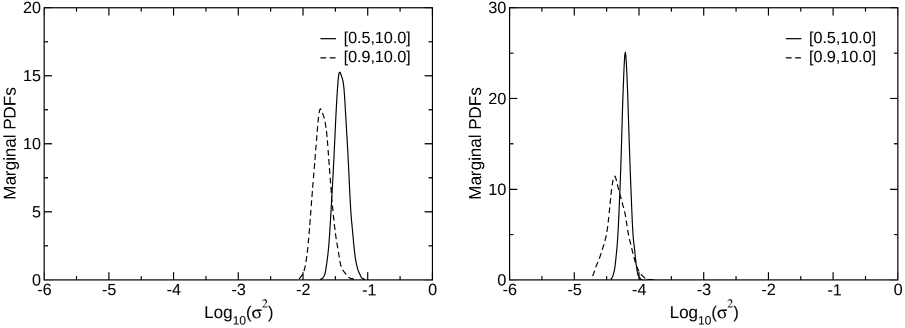
CDF of QoI for model M1 (left) and model M5 (right) for different data sets:





Analysis of calibrated variance

PDF of calibrated variance σ for model M1 (left) and model 5 (right):



The validation process presupposes that the models can accurately predict observable data.

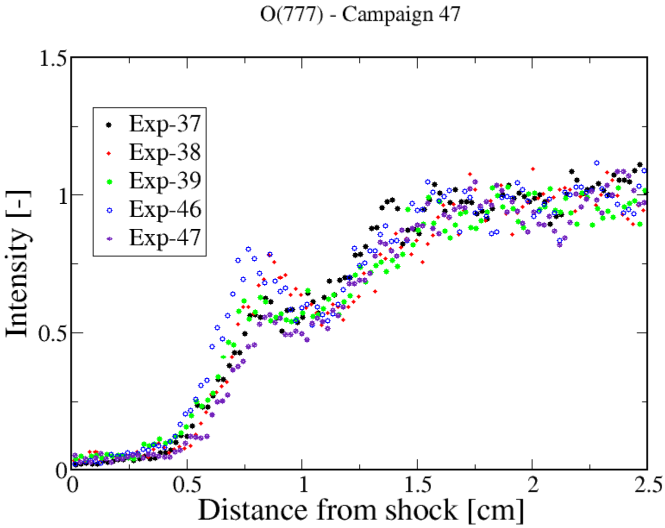
Verification of validation process

Our objective is to develop a suite of computational tools to systematically verify the correctness of each stage of the validation process.

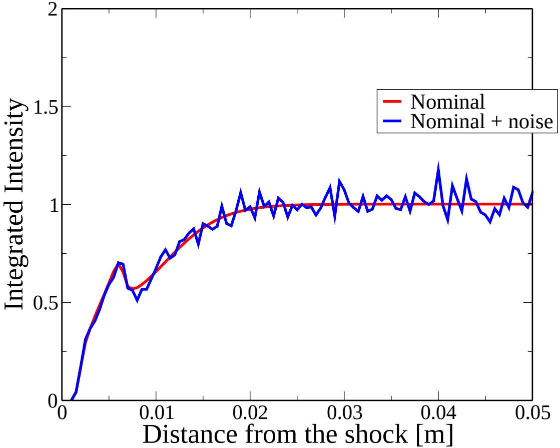
Examples of approaches:

- Method of manufactured (synthetic) data
- Sensitivity of observables w.r.t. parameters
- Mutual information
- Evidence and plausibility
- ...

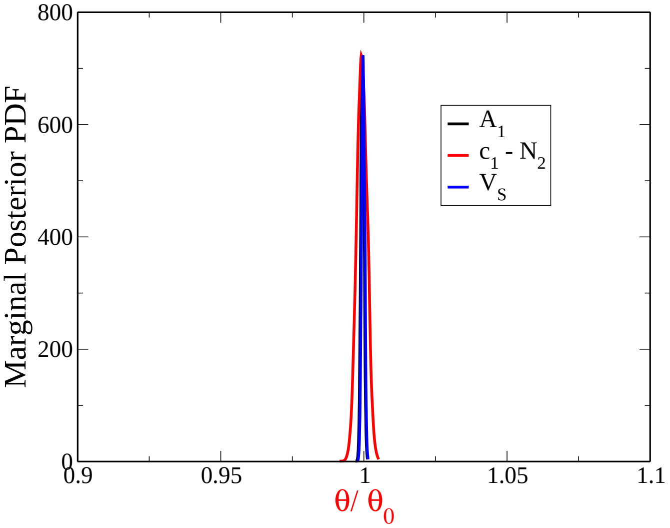
Thermal & Chemical Non-equilibrium Models Using EAST data



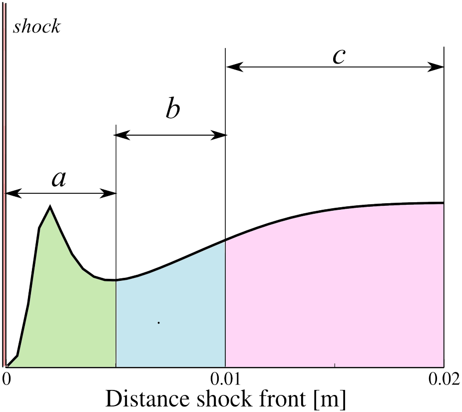
Verification of inverse problem: manufactured data



Verification of inverse problem: manufactured data

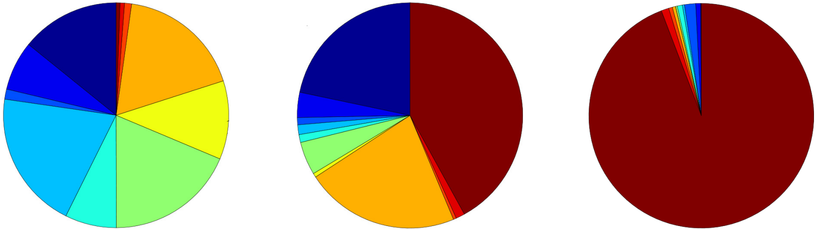


Sensitivity of observables w.r.t. parameters



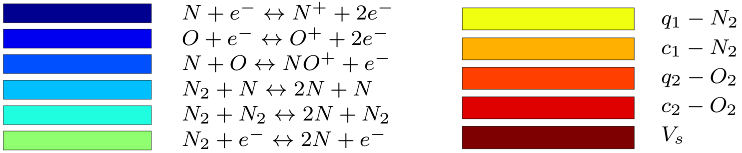
$$\mathcal{Q}_k = \sum_{i \in \mathcal{G}_k} I_i^2 \quad \text{where} \quad k \in [a, b, c]$$

Sensitivity of observables w.r.t. parameters (cont'd)

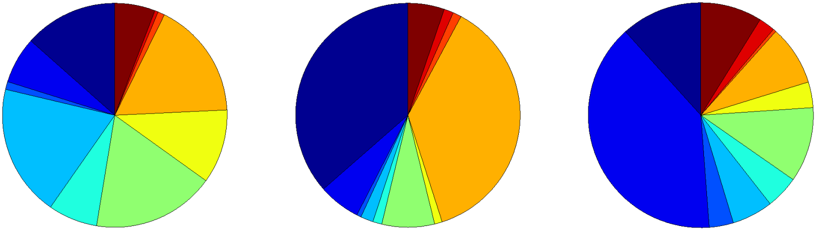


(a) (b) (c)

Is shock speed an issue?

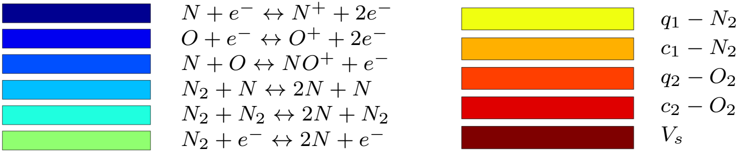


Sensitivity to the shock speed



(a) (b) (c)

Normalized intensity profiles are insensitive to the shock speed!



Model Selection

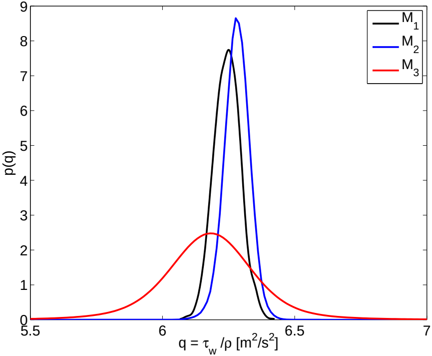
General Ideas and Approach

- Goal: Capture effect of data misfit on QoI
- Equip physical model with multiple stochastic model inadequacy models
- Enables representation of uncertainty due to misfit remaining after parameter calibration
- Multiple model framework gives opportunity for model rejection after initial calibration

Example: Spalart-Allmaras turbulence model

- Calibrate model using boundary layer data
- Three competing model inadequacy models
  - Denial (M_1): No model inadequacy, only parameter uncertainty
  - Independent (M_2): Calibrated variance
  - Correlated (M_3): Calibrated variance and length scale

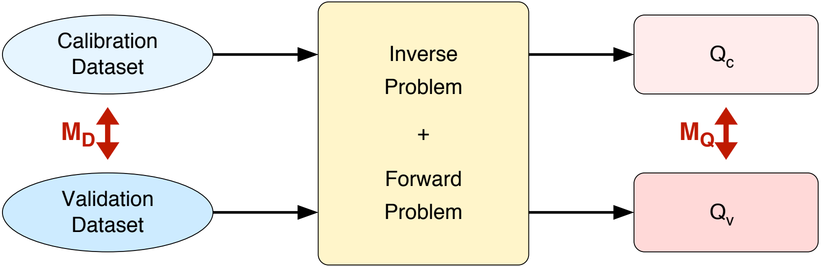
Spalart-Allmaras Results



M_i	N	$P(M_i \mid \mathbf{d}, \mathcal{M})$
M_1	7	1.6×10^{-10}
M_2	8	1.4×10^{-10}
M_3	9	≈ 1

- M_3 dramatically preferred by the data
- May allow rejection of M_1 and M_2 depending on QoI tolerance
- M_3 requires additional validation challenges

One last word



Assuming everything has been correctly done:

- If $\mathcal{M}_Q$ is large, the model should be rejected.
- If $\mathcal{M}_Q$ is small, we cannot conclude unless we can estimate $\mathcal{M}_D$.

Conclusions

1. Model validation is a complex process.
   - Model is never validated. It is at best not invalidated.
   - Validation is performed with respect to given QoI's.
   - Quantification of uncertainties in QoI's is useful for comparison purposes.
2. Validation planning requires insight and creativity.
   - Documentation
   - Data selection and analysis, etc.
3. Verification tools are needed to test correctness of processes.
   - Manufactured data to test calibration process
   - Sensitivity analysis to partially test the quality of the data
   - Evidence/plausibility to select best model among class of models
   - Tools to test selection of calibration and validation data sets
   - Tools to test various probabilistic models: prior pdf, likelihood