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Challenges in Uncertainty Quantification and Model Validation

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The Scope of UQ and Model Validation

Uncertainty Quantification:

- Global sensitivity analysis
- Model calibration, parameter estimation
- Forward uncertainty propagation

Validation:

- Interpolation – prediction within calibration region
- Extrapolation – prediction outside calibration region
- Statistical evaluation of model performance
  - against data
  - compared to other models
- A model is “valid" if it predicts a Quantity of Interest (QoI) with desired accuracy, under conditions of interest

State of the Art

UQ:

- Probabilistic UQ framework
- Functional representation of random variables
  - Polynomial Chaos (PC) expansion
- Inverse: Statistical inference
- Forward: Adaptive sparse quadrature sampling methods

Validation:

- Cross validation
- Posterior predictive
- Model discrepancy
- Model plausibility and model comparison

Challenges in UQ – 1 – Model Calibration

Published information is frequently inadequate

- Calibration not at conditions of interest
- At best: nominal parameter values and error bars
  - Correlations can be crucial to predictive uncertainty

Insufficient measurements

- Time and expense of experimental studies
- Need to constrain a large number of parameters

Many cases where measurements are simply not possible

- Expert elicitation
- Physical constraints, maximum entropy

Challenges in PC UQ – 2 – High-Dimensionality

- # degrees-of-freedom, PCE dimension, determined by
  - Number of uncertain parameters
  - Correlation structure of random fields
- Impacts:
  - # sparse quadrature samples – high-D integrals
  - Computational feasibility
- Reduction of # degrees of freedom
  - Sensitivity analysis
  - Dependencies/correlations among parameters
  - Dominant eigenmodes of random fields
  - Manifold learning: Isomap, Diffusion maps
  - Sparsification: Compressed Sensing, LASSO

Challenges in PC UQ – 3 – Non-Linearity

- Bifurcative response at critical parameter values
  - Rayleigh-Bénard convection
  - Transition to turbulence
  - Chemical ignition
- Discontinuous dependence on parameter space
  - Failure of global PCEs in terms of smooth basis
  - $\Leftrightarrow$ failure of Fourier series in representing a step function
- Local PC methods
  - Subdivide parametric space: regions of smooth behavior
  - Local PC, with compact support basis, on each region
  - A spectral-element vs. spectral construction
  - Meshing; Domain mapping

Challenges in PC UQ – 4 – Time Dynamics

- Systems with limit-cycle or chaotic dynamics
- Large amplification of phase errors over long time horizon
- PC order needs to be increased in time to retain accuracy
- Time shifting/scaling remedies

- *e.g.*: Futile to attempt representation of detailed turbulent velocity field $\boldsymbol{v}(\boldsymbol{x}, t; \omega))$ as a PCE
  - Fast loss of correlation due to energy cascade
  - Problem studied in 60's and 70's
- Focus on flow statistics, *e.g.* Mean/RMS quantities
  - Well behaved
  - Frequently of more practical relevance

Challenges — Model Validation

- Data is under conditions outside regime of interest
- Quantities of interest not observable
- Identifying the observable to calibrate to accurately constrain prediction of a given QoI
  - *e.g.* in climate modeling
- Cross validation combinatorial choices
- Cost of evaluation of marginal likelihoods
  - Bayes Factors; Model plausibility
- Quantifying model discrepancy, or model bias
  - Error modeling choices
  - Confounding of bias and precision errors

Closure

- Increasing practical relevance of computational predictions
  - Need for effective VVUQ in large scale computing
- Difficult to constrain complex physical model parameters
  - Too many knobs
- Multimodel ensembles
  - Model averaging does not address correlated models
- Calibration versus predictive skill
  - Observables versus QoIs
- VVUQ technical challenges
  - Math
  - Algorithmic
  - Computational