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Role and Impact of Uncertainty Quantification in the Coming Decade

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Definition of Uncertainty Quantification (UQ)

UQ is the end-to-end estimation and analysis of uncertainty in

- models and their parameters
  - – assimilation of experimental/observational data
  - – model fitting and parameter estimation

- model predictions
  - – forward propagation of parametric uncertainty to model outputs
  - – accounting for alternate plausible models

Sources of Uncertainty in computational models

- model structure
  - participating physical processes
  - governing equations
  - constitutive relations
- model parameters
  - transport properties
  - thermodynamic properties
  - constitutive relations
  - rate coefficients
- initial and boundary conditions
- geometry
- numerical errors
- bugs
- faults, data loss, silent errors

The Case for Uncertainty Quantification

UQ enables:

- enhanced scientific understanding from computations
    - exploration of model predictions over range of uncertainty
- Assessment of confidence in computational predictions
- Validation and comparison of scientific/engineering models employing (noisy) data
- Design optimization
- Use of computational predictions for decision-support
- Assimilation of observational data and model construction

Applications of UQ over the past decade

- UQ has been used in a range of physical systems
  - Continuum mechanics; Geophysics; Fluid dynamics
  - Wave phenomena; Electromagnetics; Combustion; Climate
  - Network models; Molecular Dynamics; Multiscale coupling
- UQ has been used for
  - Parameter estimation from data
  - Global sensitivity analysis
  - Estimation of uncertainty in predictions
  - Model validation
- Increased application of UQ methods has been driven by
  - Advances in UQ methods/software
  - Continuing increase in computational science/performance
  - Increased awareness of the need for model validation

UQ Role/Impact over future decade

UQ will:

- be applied to increasingly large-scale computational problems of some relevance – power grids, climate
- enhance understanding of large-scale physical models
- inform observational/experimental campaigns
- drive interdisciplinary math/eng/stats developments
  - Data–UQ–Models
- inform optimal complexity of computational model detail
- require continued expansion in capabilities of computational platforms

Impact on the Computational Scientist

Working with UQ experts:

- Know your model
  - Are there alternate/competing submodels?
  - What's the (experimental/theoretical) evidence for each?
  - Statistical methods for model comparison/selection
  - Model validation
- Know your parameters
  - Identify uncertain parameters
  - Quantify their uncertainties ... joint PDF!
    - Statistical inverse problem – data?
  - Identify important parameters – reduce dimensionality
    - Global sensitivity analysis
- Forward propagation of uncertainty
- Close the loop (again) with data, model validation

UQ Challenges

- Robust statistical methods for stochastic inverse problems
- Characterization of uncertain inputs
- High dimensionality
- Spatiotemporally adaptive order/dimensionality for robust representation of random fields
- Oscillatory/chaotic time dynamics over long time horizons
- Nonlinearity and bifurcations
- Effective sampling strategies in high-D
  - Adaptive sparse quadrature methods
  - Compressive sensing
- Optimized intrusive solvers
- Fault tolerance in UQ algorithms