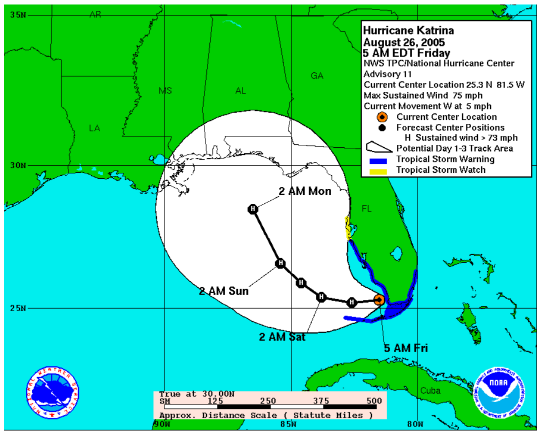
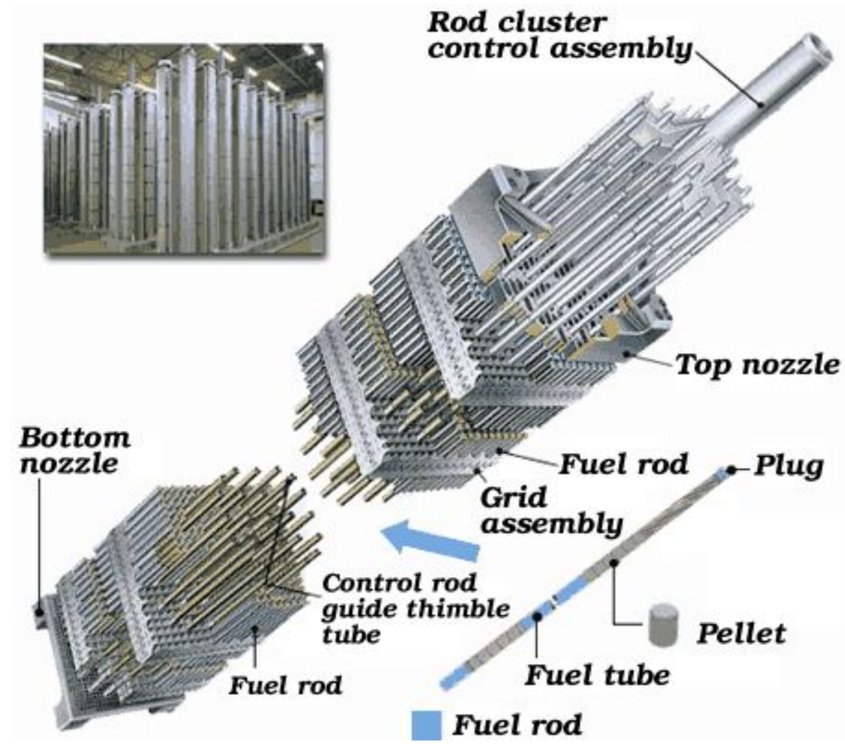
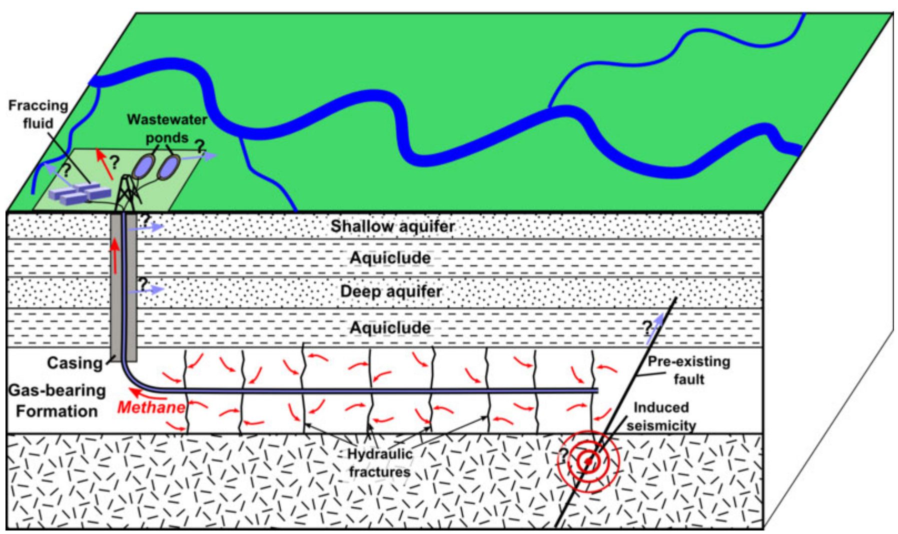
Lecture 1: Motivation and Prototypical Examples

“Essentially all models are wrong, but some are useful,”

George E.P. Box, Industrial Statistician



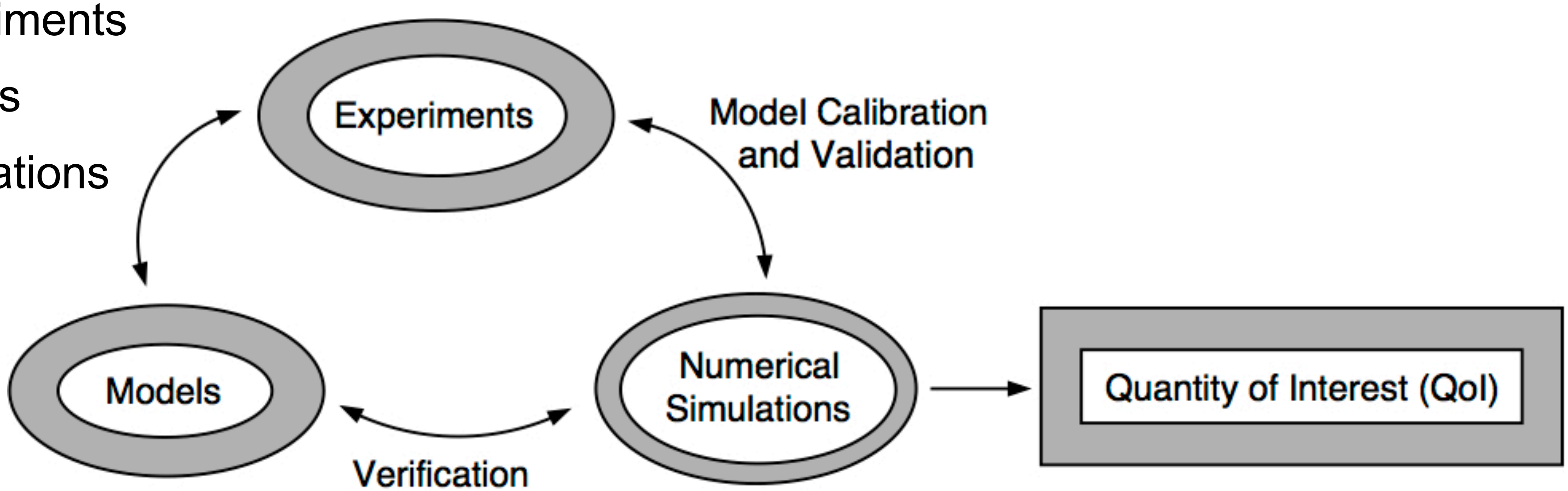




Predictive Science

Components: All involve uncertainty

- Experiments
- Models
- Simulations

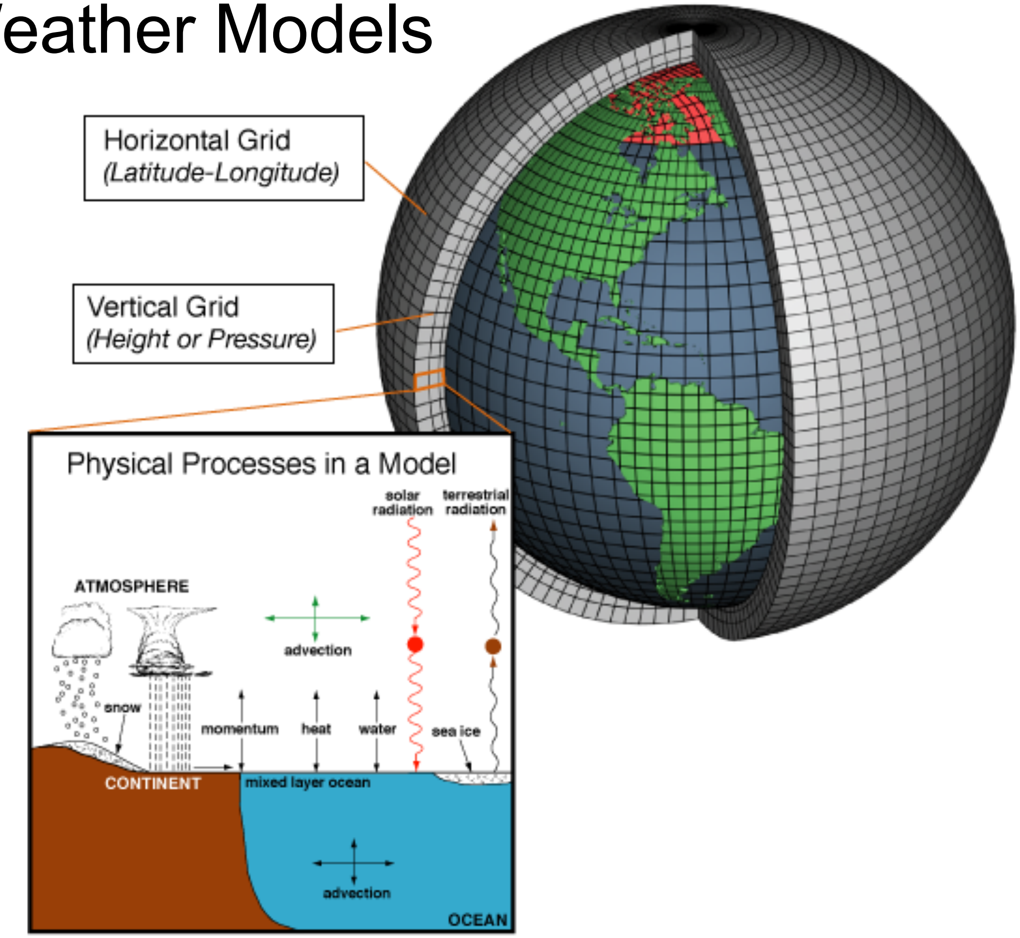


- *Essentially, all models are wrong, but some are useful,* George E.P. Box, Industrial Statistician.
- *Computational results are believed by no one, except the person who wrote the code*, source anonymous, quoted by Max Gunzburger, Florida State University.
- *Experimental results are believed by everyone, except for the person who ran the experiment,* source anonymous, quoted by Max Gunzburger, Florida State University.
- *I have always done uncertainty quantification. The difference now is that it is capitalized.* Bill Browning, Applied Mathematics Incorporated.

Example 1: Weather Models

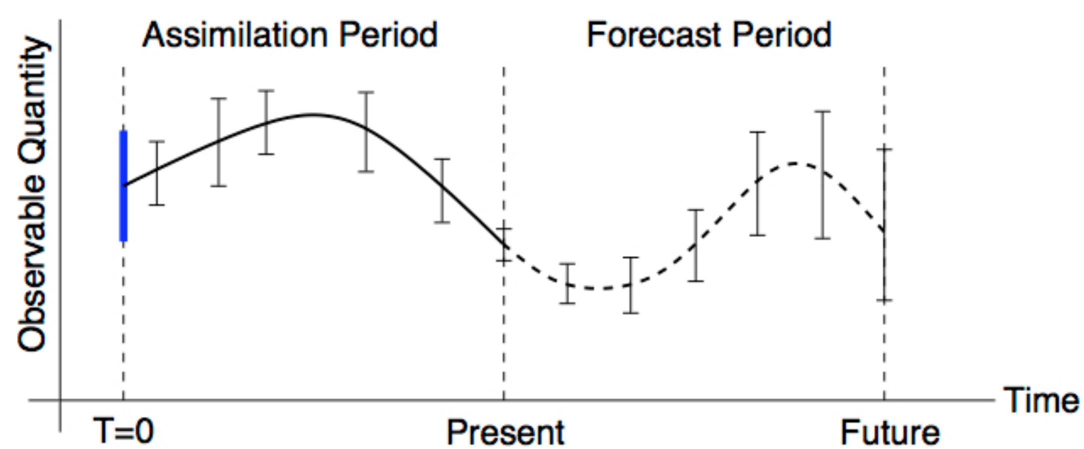
Challenges:

- Coupling between temperature, pressure gradients, precipitation, aerosol, etc.;
- Models and inputs contain uncertainties;
- Numerical grids necessarily larger than many phenomena; e.g., clouds
- Sensors positions may be uncertain; e.g., weather balloons, ocean buoys.



Goal:

- Assimilate data to quantify uncertain initial conditions and parameters;
- Make predictions with quantified uncertainties.



Equations of Atmospheric Physics

Conservation Relations:

Mass
$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho v) = 0$$

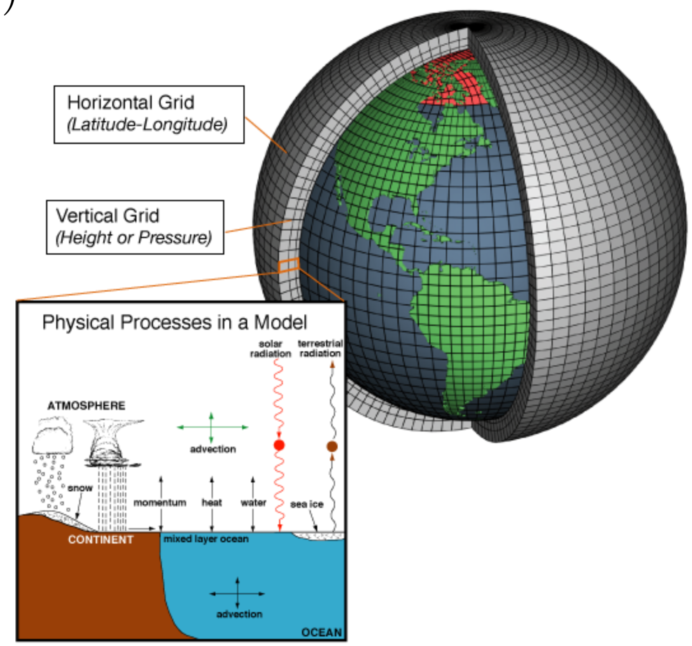
Momentum
$$\frac{\partial v}{\partial t} = -v \cdot \nabla v - \frac{1}{\rho}\nabla p - g\hat{k} - 2\Omega \times v$$

Energy
$$\rho c_V \frac{\partial T}{\partial t} + p\nabla \cdot v = -\nabla \cdot F + \nabla \cdot (k\nabla T) + \rho \dot{q}(T, p, \rho)$$

$$p = \rho R T$$

Water
$$\frac{\partial m_j}{\partial t} = -v \cdot \nabla m_j + S_{m_j}(T, m_j, \chi_j, \rho)\ ,\ j = 1, 2, 3,$$

Aerosol
$$\frac{\partial \chi_j}{\partial t} = -v \cdot \nabla \chi_j + S_{\chi_j}(T, \chi_j, \rho)\ ,\ j = 1, \cdots, J,$$



Constitutive Closure Relations: e.g.,

$$S_{m_2} = S_1 + S_2 + S_3 - S_4$$

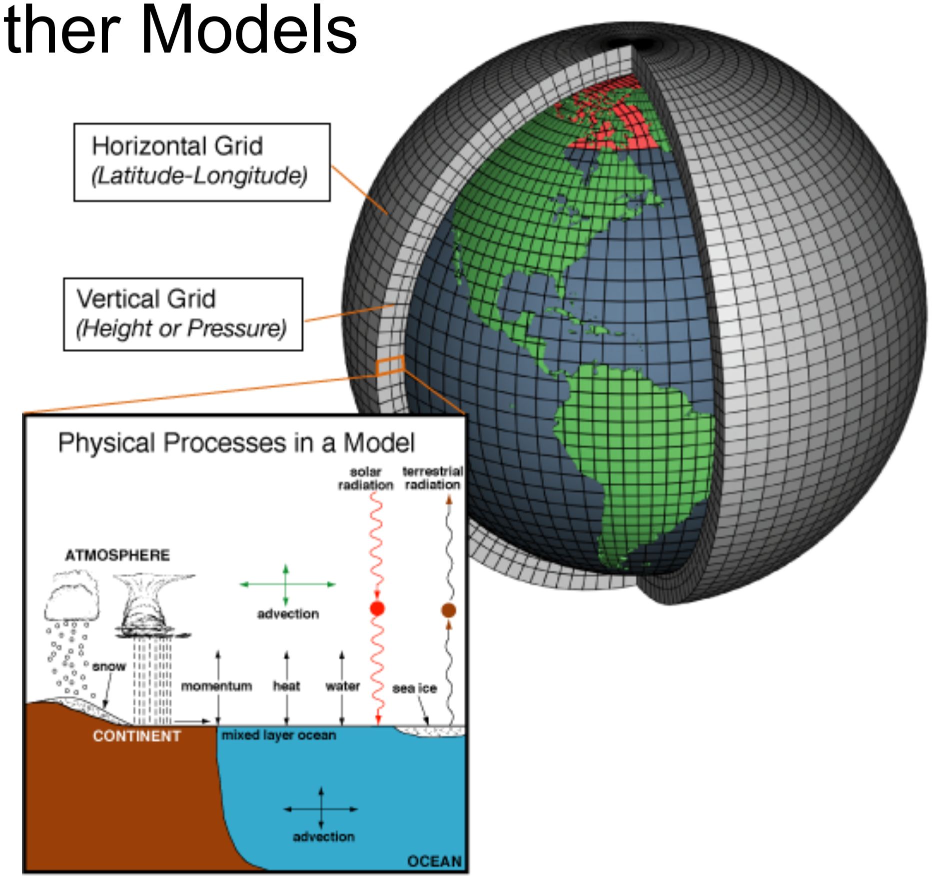
where

$$S_1 = \bar{\rho}(m_2 - m_2^*)^2 \left[\underline{1.2 \times 10^{-4}} + \left(\underline{1.569 \times 10^{-12}} \frac{n_r}{d_0(m_2 - m_2^*)} \right) \right]^{-1}$$

Example 1: Weather Models

Sources of Uncertainty:

- Model errors or discrepancies
- Input uncertainties
- Numerical errors and uncertainties
- Measurement errors and uncertainties

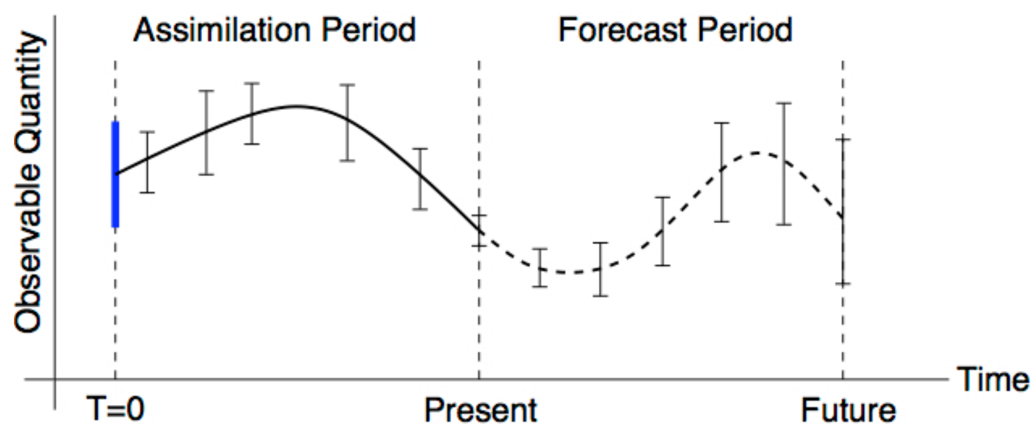


Steps:

• Model Calibration: Involves the assimilation or integration of data to quantify and update input uncertainties.

• Model Prediction: Here one computes the response along with statistics, error bounds, or PDF; extrapolation is important and difficult.

• Estimation of the Validation Regime:

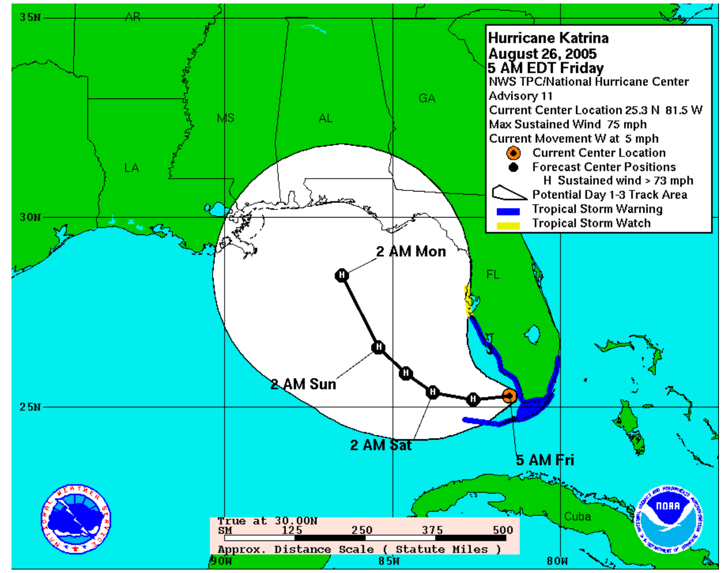


• **Goal:** Construct best estimate parameters and responses or quantities of interest with best estimate reduced uncertainties.

Example 1: Weather Models

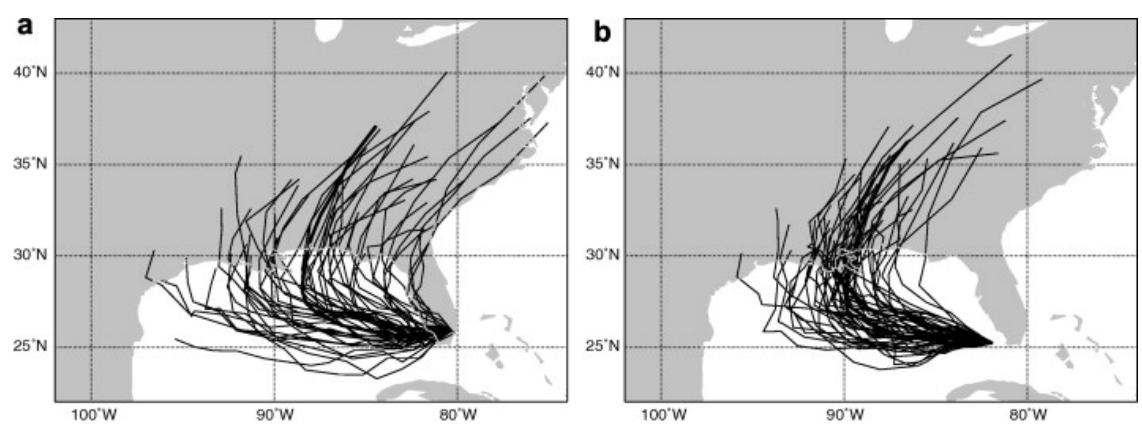
Sources of Uncertainty:

- Model errors or discrepancies
- Input uncertainties
- Numerical errors and uncertainties
- Measurement errors and uncertainties

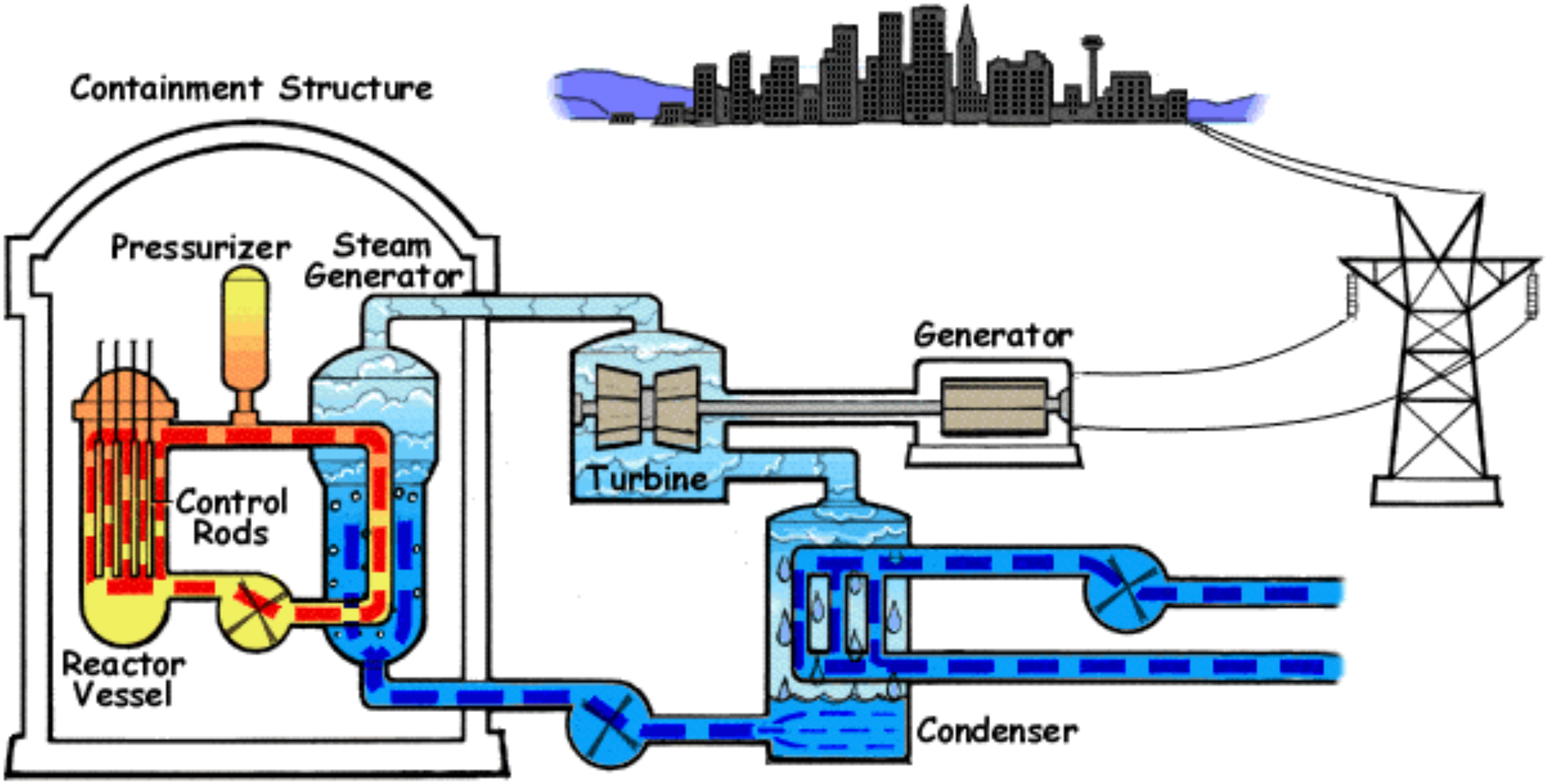


Ensemble Forecasts:

- Run multiple simulations with differing parameter values or initial conditions drawn from appropriate pdf.
- A 50% chance of rain means that given present atmospheric conditions, half of simulations predict measurable rain amount at random point in specified area.



Example 2: Pressurized Water Reactors (PWR)



Models:

- Involve neutron transport, thermal-hydraulics, chemistry.
- Inherently multi-scale, multi-physics.

CRUD Measurements: Consist of low resolution images at limited number of locations.

Example 2: Pressurized Water Reactors (PWR)

3-D Neutron Transport Equations:

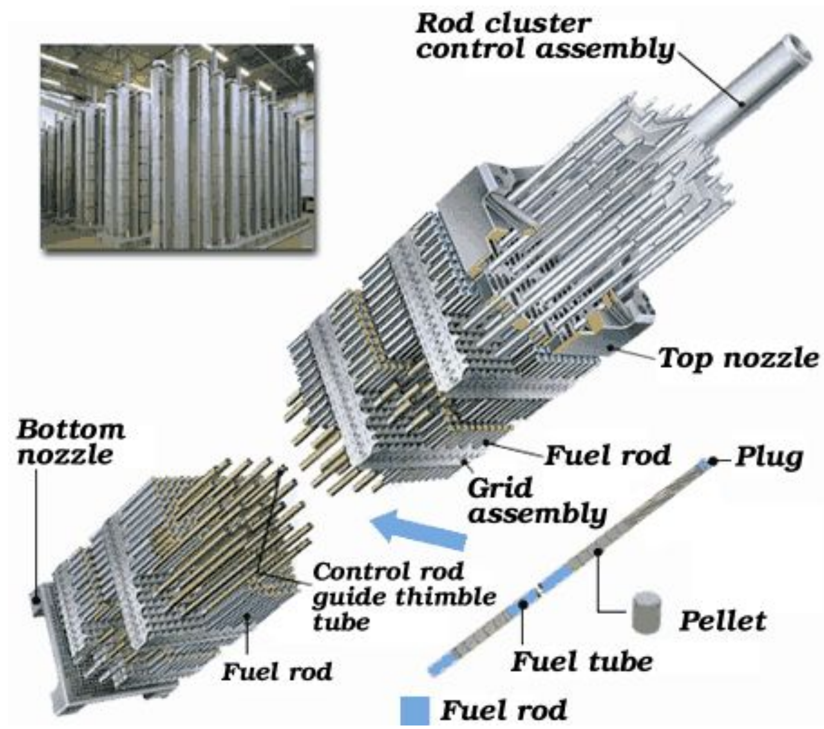
$$\frac{1}{|v|}\frac{\partial\varphi}{\partial t} + \Omega\cdot\nabla\varphi + \Sigma_t(r,E)\varphi(r,E,\Omega,t)$$
$$= \int_{4\pi} d\Omega' \int_0^\infty dE'\Sigma_s(E'\to E,\Omega'\to\Omega)\varphi(r,E',\Omega',t)$$
$$+ \frac{\chi(E)}{4\pi}\int_{4\pi} d\Omega' \int_0^\infty dE'\nu(E')\Sigma_f(E')\varphi(r,E',\Omega',t)$$

Challenges:

- Linear in the state but function of 7 independent variables:

$$r = x,y,z; E; \Omega = \theta,\phi; t$$

- Very large number of inputs; e.g., 100,000; Active subspace construction is critical.
- ORNL Code SCALE: can take minutes to hours to run.



- SCALE TRITON has adjoint capabilities via TSUNAMI-2D and NEWT.

Example 2: Pressurized Water Reactors (PWR)

Thermo-Hydraulic Equations: Mass, momentum and energy balance for fluid

$$\frac{\partial}{\partial t}(\alpha_f \rho_f) + \nabla \cdot (\alpha_f \rho_f v_f) = -\Gamma$$

$$\alpha_f \rho_f \frac{\partial v_f}{\partial t} + \alpha_f \rho_f v_f \cdot \nabla v_f + \nabla \cdot \sigma_f^R + \alpha_f \nabla \cdot \sigma + \alpha_f \nabla p_f$$
$$= -F^R - F + \Gamma(v_f - v_g)/2 + \alpha_f \rho_f g$$

$$\frac{\partial}{\partial t}(\alpha_f \rho_f e_f) + \nabla \cdot (\alpha_f \rho_f e_f v_f + Th) = (T_g - T_f)H + T_f \Delta_f$$
$$-T_g(H - \alpha_g \nabla \cdot h) + h \cdot \nabla T - \Gamma[e_f + T_f(s^* - s_f)]$$
$$-p_f \left(\frac{\partial \alpha_f}{\partial t} + \nabla \cdot (\alpha_f v_f) + \frac{\Gamma}{\rho_f} \right)$$

Note: Similar equations for gas

Codes:

- Low-Fidelity Code: COBRA-TF: Takes minutes to run
  - Sub-channel code -- cannot resolve between pins; no adjoint capabilities
- High-Fidelity Code: HYDRA: Takes hours to run
  - 3-D CFD code; no adjoint capabilities

Example 2: Pressurized Water Reactors (PWR)

Thermo-Hydraulic Equations: Mass, momentum and energy balance for fluid

$$\frac{\partial}{\partial t}(\alpha_f \rho_f) + \nabla \cdot (\alpha_f \rho_f v_f) = -\Gamma$$

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$$-p_f \left(\frac{\partial \alpha_f}{\partial t} + \nabla \cdot (\alpha_f v_f) + \frac{\Gamma}{\rho_f} \right)$$

Example: Shearon Harris outside Raleigh

UQ Questions:

- What is peak operating temperature?
- What is expected level of CRUD buildup?
- What is risk associated with operating regime?
- What is expected profit for new design?

Example 3: HIV Model for Characterization/Treatment Regimes

HIV Model:

$$\dot{T}_1 = \lambda_1 - d_1 T_1 - (1-\varepsilon)k_1 V T_1$$

$$\dot{T}_2 = \lambda_2 - d_2 T_2 - (1-f\varepsilon)k_2 V T_2$$

$$\dot{T}_1^* = (1-\varepsilon)k_1 V T_1 - \delta T_1^* - m_1 E T_1^*$$

$$\dot{T}_2^* = (1-f\varepsilon)k_2 V T_2 - \delta T_2^* - m_2 E T_2^*$$

$$\dot{V} = N_T \delta (T_1^* + T_2^*) - cV - [(1-\varepsilon)\rho_1 k_1 T_1 + (1-f\varepsilon)\rho_2 k_2 T_2]V$$

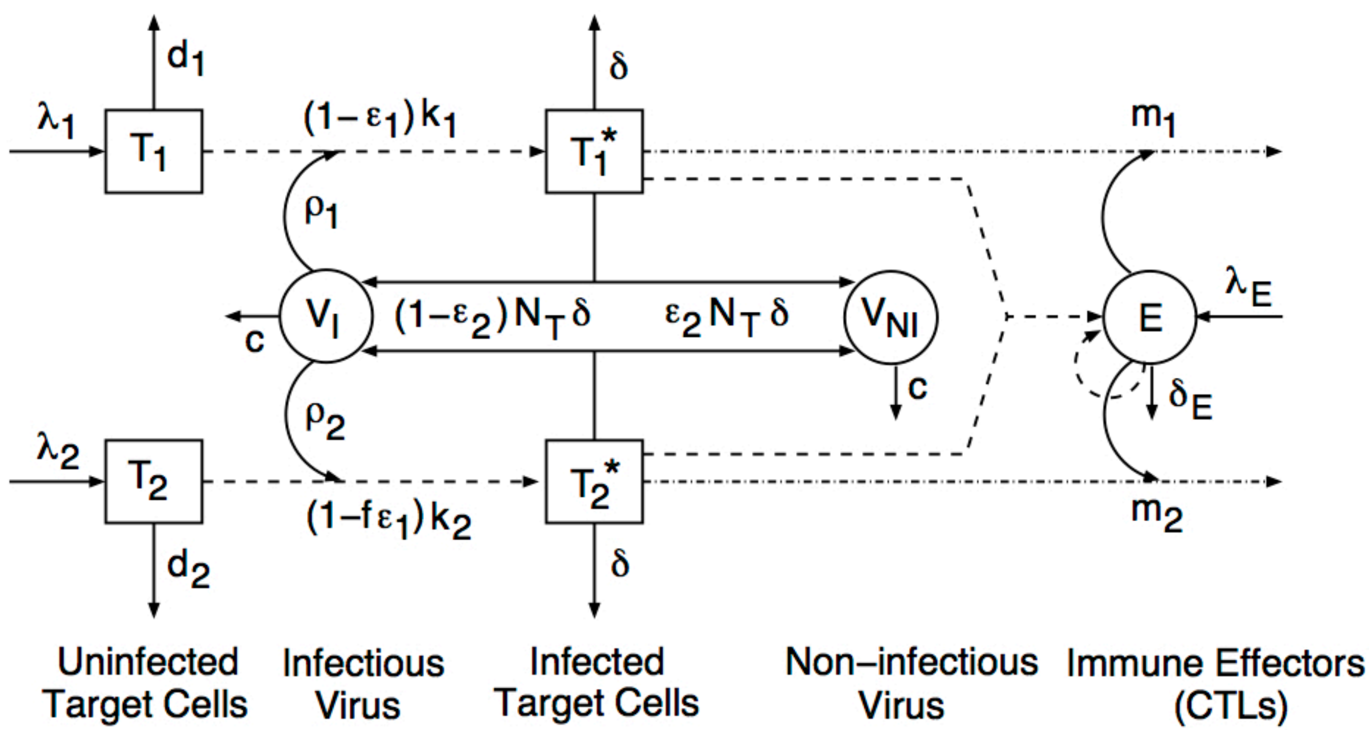
$$\dot{E} = \lambda_E + \frac{b_E(T_1^* + T_2^*)}{T_1^* + T_2^* + K_b}E - \frac{d_E(T_1^* + T_2^*)}{T_1^* + T_2^* + K_d}E - \delta_E E$$

Notes: 21 parameters

[Adams, Banks et al., 2005]

Notation: $\dot{E} \equiv \dfrac{dE}{dt}$

Compartments:



Example 3: HIV Model for Characterization and Control Regimes

HIV Model: Used for characterization and control treatment regimes.

$$\dot{T}_1 = \lambda_1 - d_1 T_1 - (1-\varepsilon) k_1 V T_1$$

$$\dot{T}_2 = \lambda_2 - d_2 T_2 - (1-f\varepsilon) k_2 V T_2$$

$$\dot{T}_1^* = (1-\varepsilon) k_1 V T_1 - \delta T_1^* - m_1 E T_1^*$$

$$\dot{T}_2^* = (1-f\varepsilon) k_2 V T_2 - \delta T_2^* - m_2 E T_2^*$$

$$\dot{V} = N_T \delta (T_1^* + T_2^*) - cV - [(1-\varepsilon)\rho_1 k_1 T_1 + (1-f\varepsilon)\rho_2 k_2 T_2] V$$

$$\dot{E} = \lambda_E + \frac{b_E (T_1^* + T_2^*)}{T_1^* + T_2^* + K_b} E - \frac{d_E (T_1^* + T_2^*)}{T_1^* + T_2^* + K_d} E - \delta_E E$$

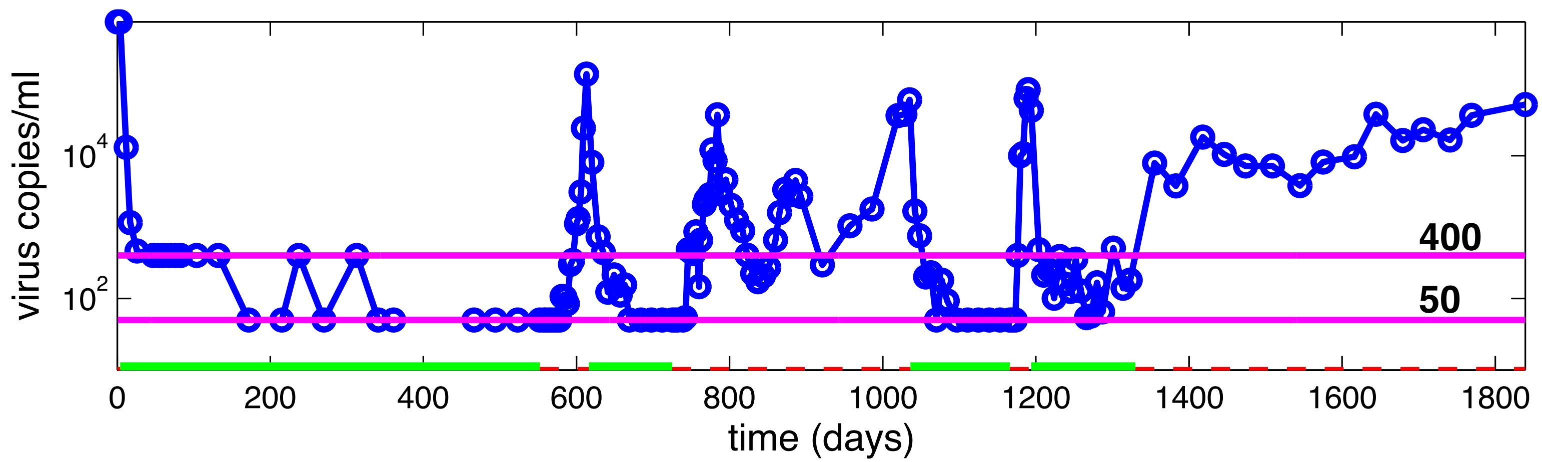
Parameters: Most are unknown and must be estimated from data

λ_1	Target cell 1 production rate	ρ_1	Ave. virions infecting type 1 cell
λ_2	Target cell 2 production rate	ρ_2	Ave. virions infecting type 2 cell
d_1	Target cell 1 death rate	b_E	Max. birth rate immune effectors
d_2	Target cell 2 death rate	d_E	Max. death rate immune effectors
k_1	Population 1 infection rate	K_b	Birth constant, immune effectors
k_2	Population 2 infection rate	K_d	Death constant, immune effectors
c	Virus natural death rate	λ_E	Immune effector production rate
δ	Infected cell death rate	δ_E	Natural death rate, immune effectors
ε	Population 1 treatment efficacy	N_T	Virions produced per infected cell
m_1	Population 1 clearance rate	f	Treatment efficacy reduction
m_2	Population 2 clearance rate		

Example 3: HIV Model for Characterization and Control Regimes

HIV Model: Several sources of uncertainty including viral measurement techniques

Example: Upper and lower limits to assay sensitivity



UQ Questions:

- What are the uncertainties in parameters that cannot be directly measured?
- What is expected viral load?
- What is optimal treatment regime that is “safe” for patient?

Example 4: Portfolio Model

Example: Portfolio model

$$Y = c_1 Q_1 + c_2 Q_2$$

Note:

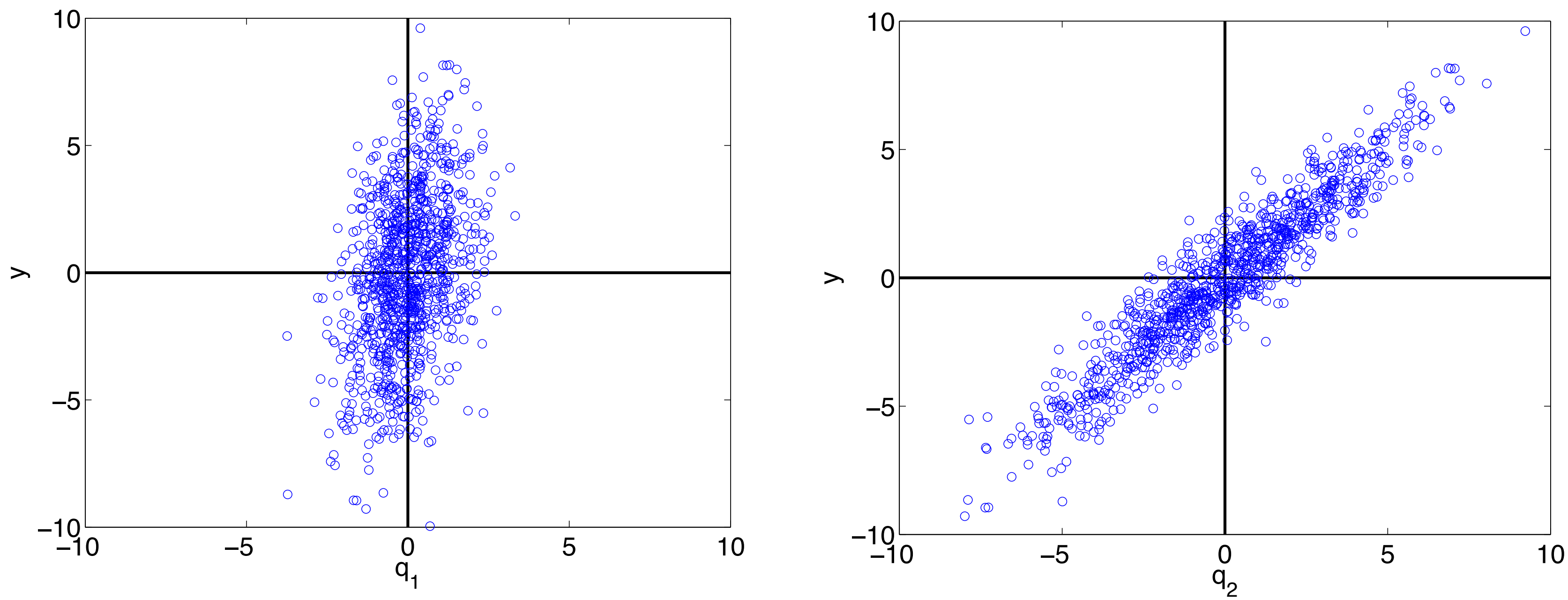
- Q_1 and Q_2 represent hedged portfolios
- c_1 and c_2 amounts invested in each portfolio

Take

$$c_1 = 2 \; , \; c_2 = 1$$

$Q_1 \sim N(0, \sigma_1^2)$ with $\sigma_1 = 1$

$Q_2 \sim N(0, \sigma_2^2)$ with $\sigma_2 = 3$



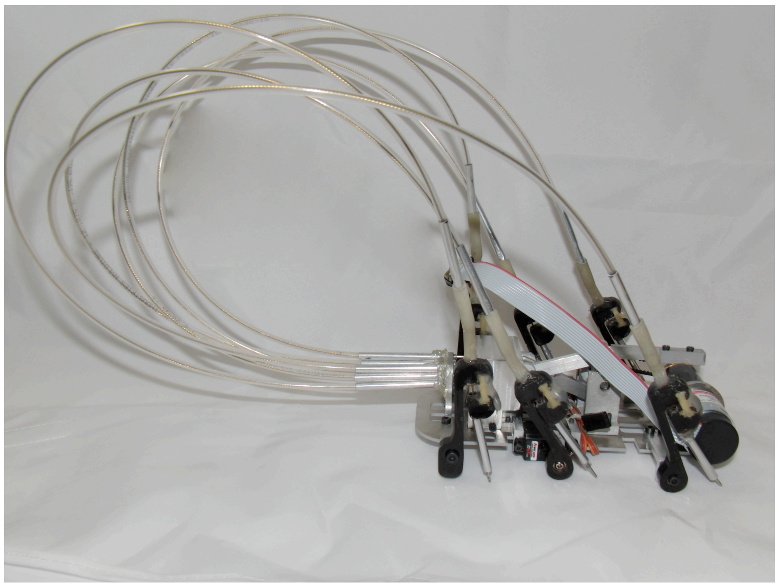
UQ Questions:

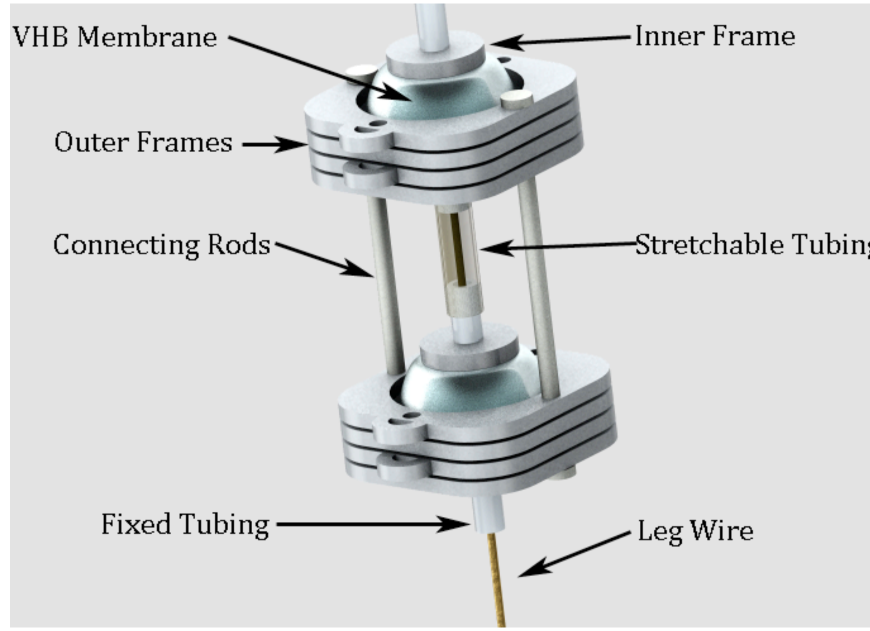
- What is expected investment return?
- What is impact of market uncertainty on investment return?

Example 5: Viscoelastic Material Models

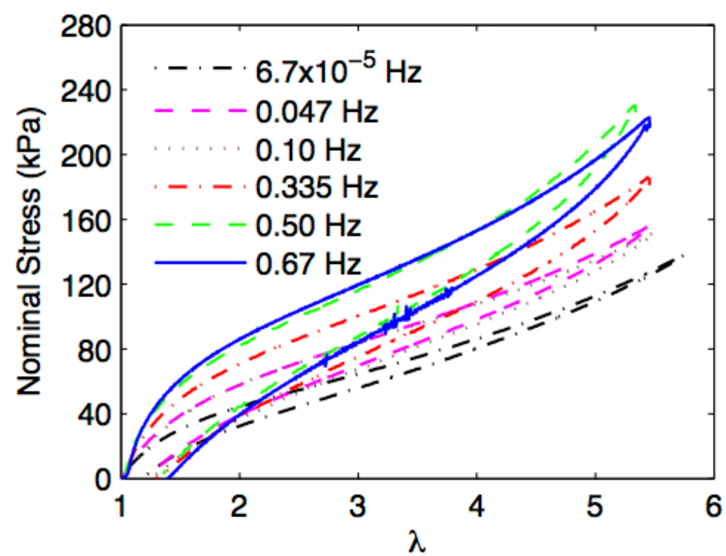
Application: Adaptive materials for legged robotics

- Figure: Billy Oates



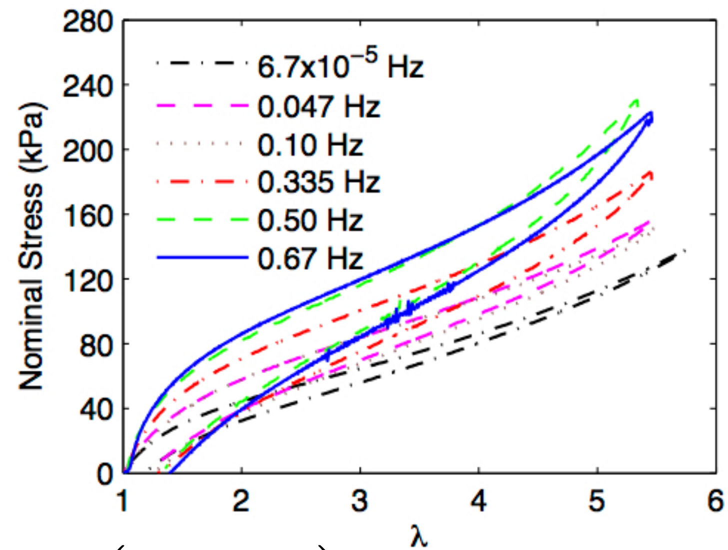


Material Behavior: Significant rate dependence



Example 5: Viscoelastic Material Models

Material Behavior: Significant rate dependence



Finite-Deformation Model:

- Nonlinear non-affine
- Hyperelastic energy function

$$\psi_{\infty}^{N} = \frac{1}{6}G_c I_1 - G_c \lambda_{\max}^2 \ln\left(3\lambda_{\max}^2 - I_1\right) + G_e \sum_j \left(\lambda_j + \frac{1}{\lambda_j}\right)$$

Parameters:

$q = [G_e, G_c, \lambda_{\max}, \eta, \beta, \gamma]$

$q = [\eta, \beta, \gamma]$: Viscoelastic parameters

G_c: Crosslink network modulus

G_e: Plateau modulus

$\lambda_{\max}$: Max stretch effective affine tube

Uncertainty Quantification Goals:

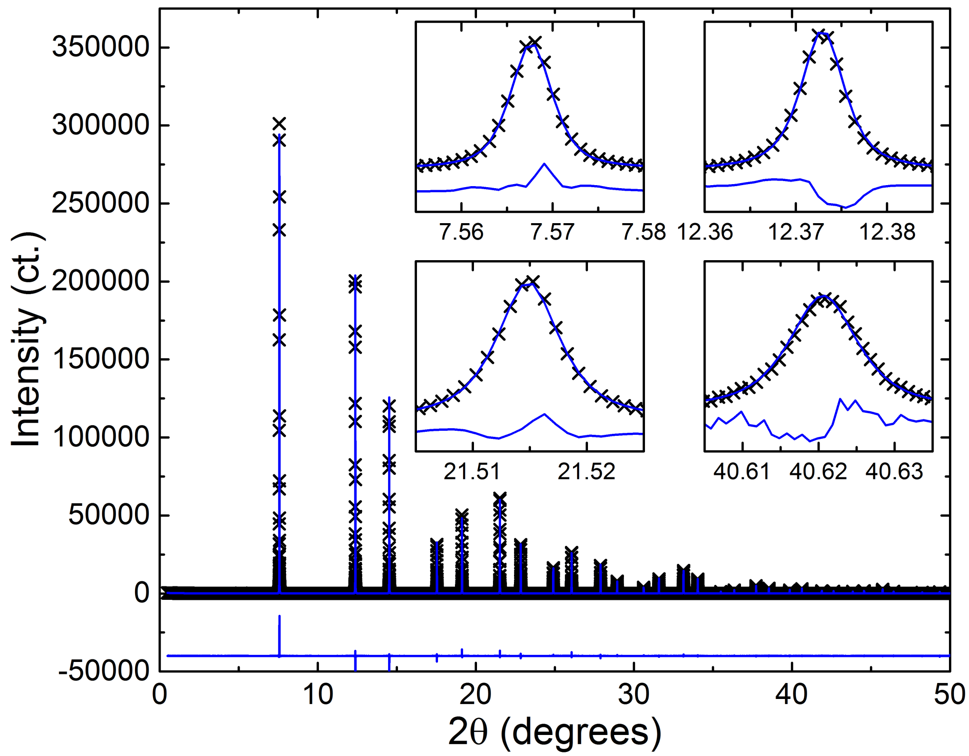
- Quantify measurement errors.
- Quantify uncertainty in parameters.
- Use statistics to quantify accuracy of considered models.

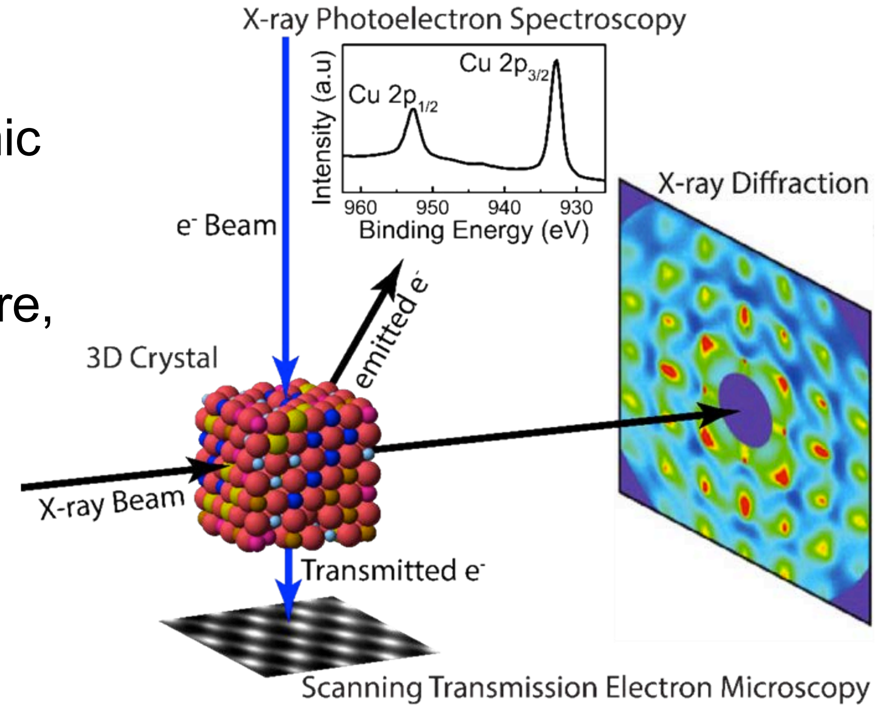
Example 6: X-Ray Crystallography

Properties:

- Reveal relative positions of atoms, their atomic number, types of chemical bonds, etc.

- Applications: determination of of DNA structure, design of pharmaceuticals, etc..





Uncertainty Quantification Goals:

- Use Bayesian analysis to quantify uncertainty associated with Rietveld model and background.

- Quantify heteroskedasticity and correlation of error structure.

Collaborators: Chris Fancher, Zhen Han, Igor Levin, Katherine Page, Brian Reich, Alyson Wilson, Jacob Jones

Example 7: Quantum-Informed Continuum Models

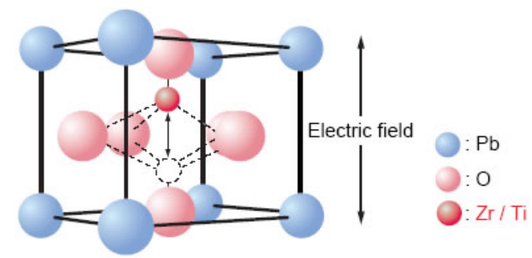
Objectives:

- Compute energy about different strain states using density functional theory (DFT).
- Use DFT energy to calibrate Landau energy-based continuum models.

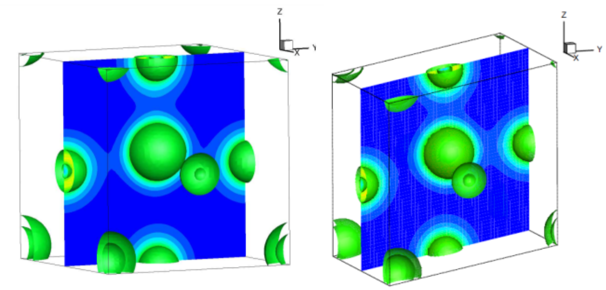
$$\Sigma = \Sigma(E_{IJ}, E_{IJ,K}, P_I, Q_{IJ}, \ldots)$$

UQ and Sensitivity Analysis Goals:

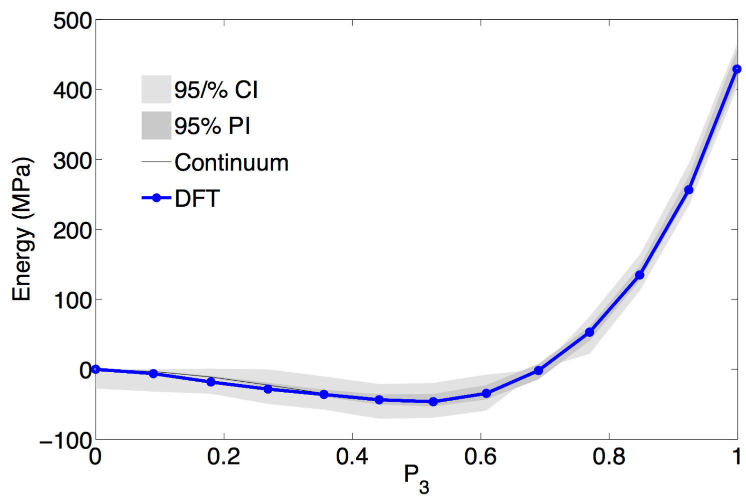
- Quantify uncertainty introduced when internal atomic and electronic degrees of freedom are neglected.
- Construct credible and prediction intervals to quantify accuracy of continuum models.
- Employ sensitivity analysis to determine influential model parameters.



Lead titanate



DFT electronic structure simulation



Landau energy

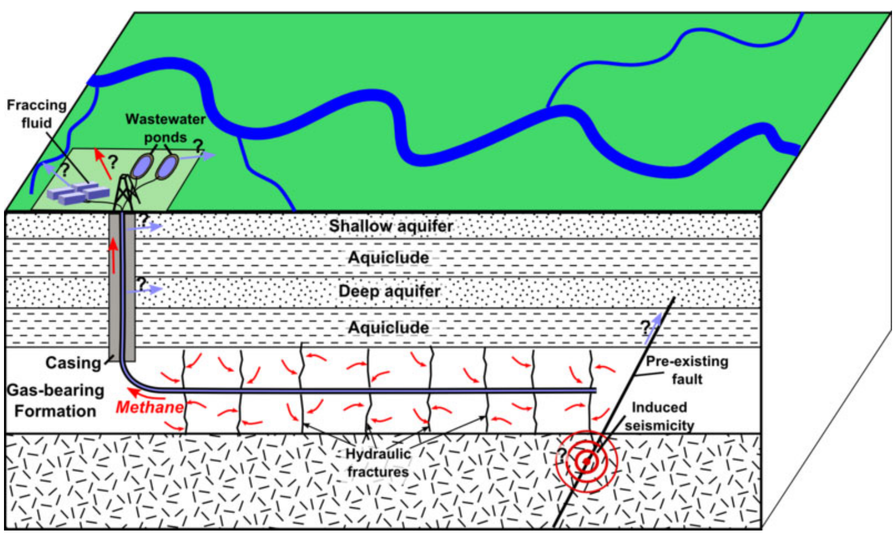
Experimental Uncertainties and Limitations

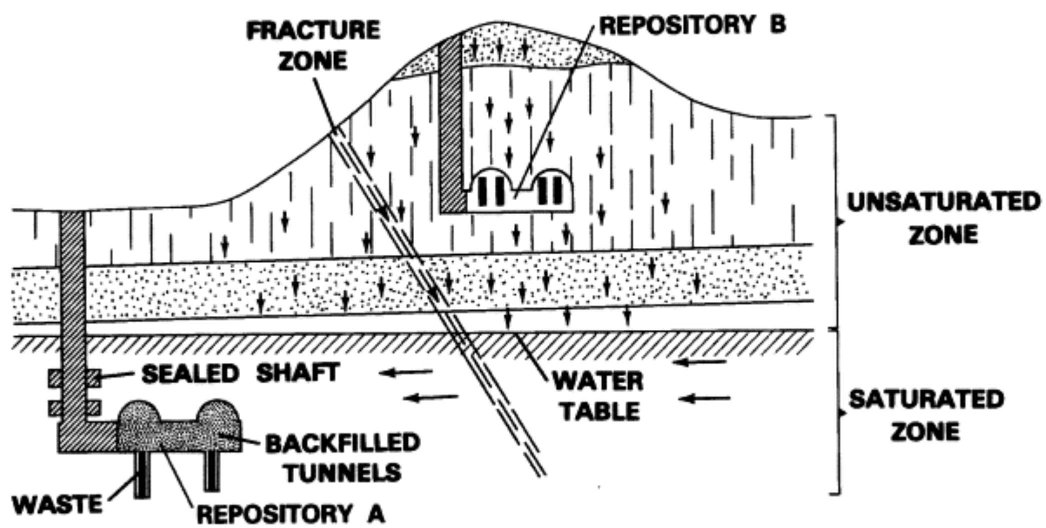
Examples: *Experimental results are believed by everyone, except for the person who ran the experiment*, Max Gunzburger, Florida State University.

• Pharmaceutical and disease treatment strategies often too dangerous or expensive for human tests or large segments of the population.

• Climate scenarios cannot be experimentally tested at the planet scale. Instead, components such as volcanic forcing tested using measurements such as the 1991 Mount Pinatubo data.

• Subsurface hydrology data very limited due to infeasibility of drilling large numbers of wells. Result: significant uncertainty regarding subsurface structures.



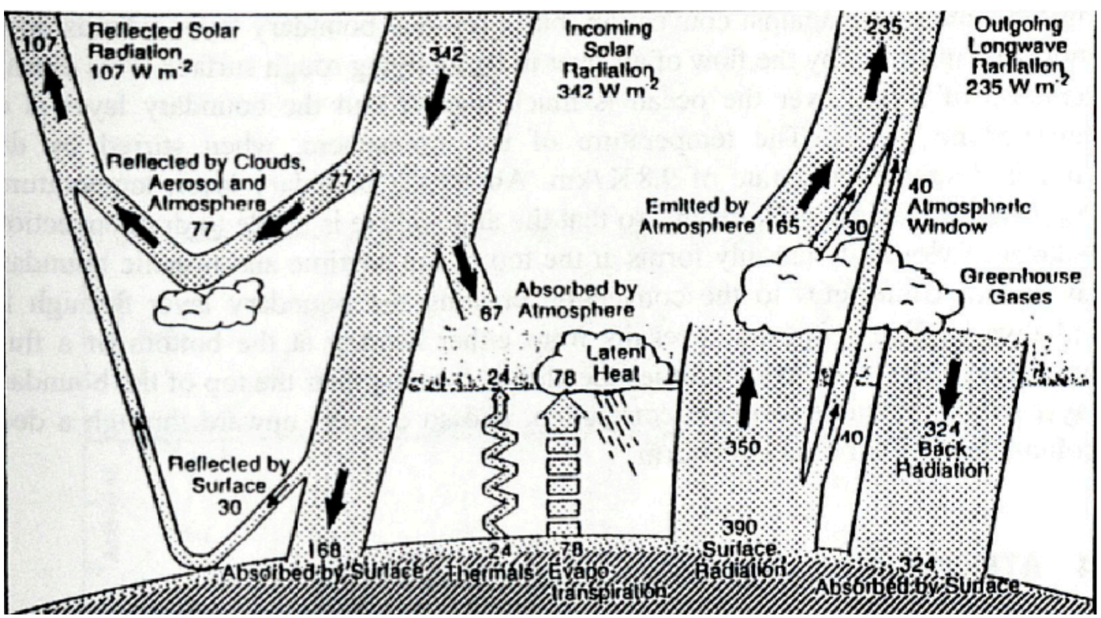


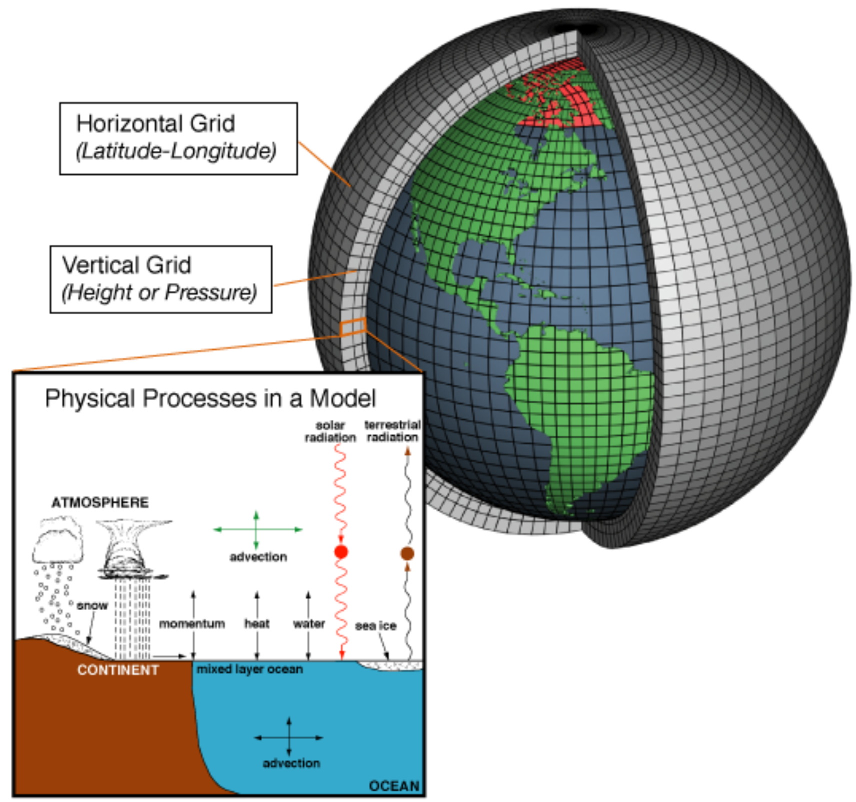
Model Errors

Examples: *Essentially, all models are wrong, but some are useful,* George E.P. Box, Industrial Statistician

• Numerous components of weather and climate models --- e.g., aerosol-induced cloud formation, greenhouse gas processes --- occur on scales that are much smaller than numerical grids used to solve the atmospheric equations of physics. These processes represent highly complex physics that is only partially understood.

• Many biological applications are coupled, complex, highly nonlinear, and driven by poorly understood or stochastic processes.



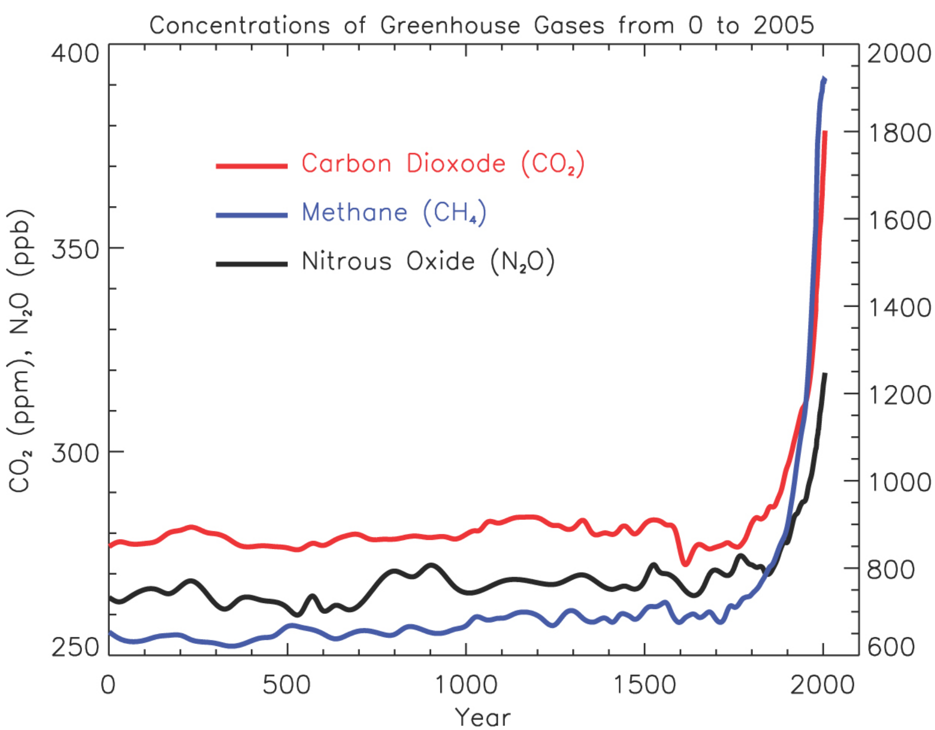


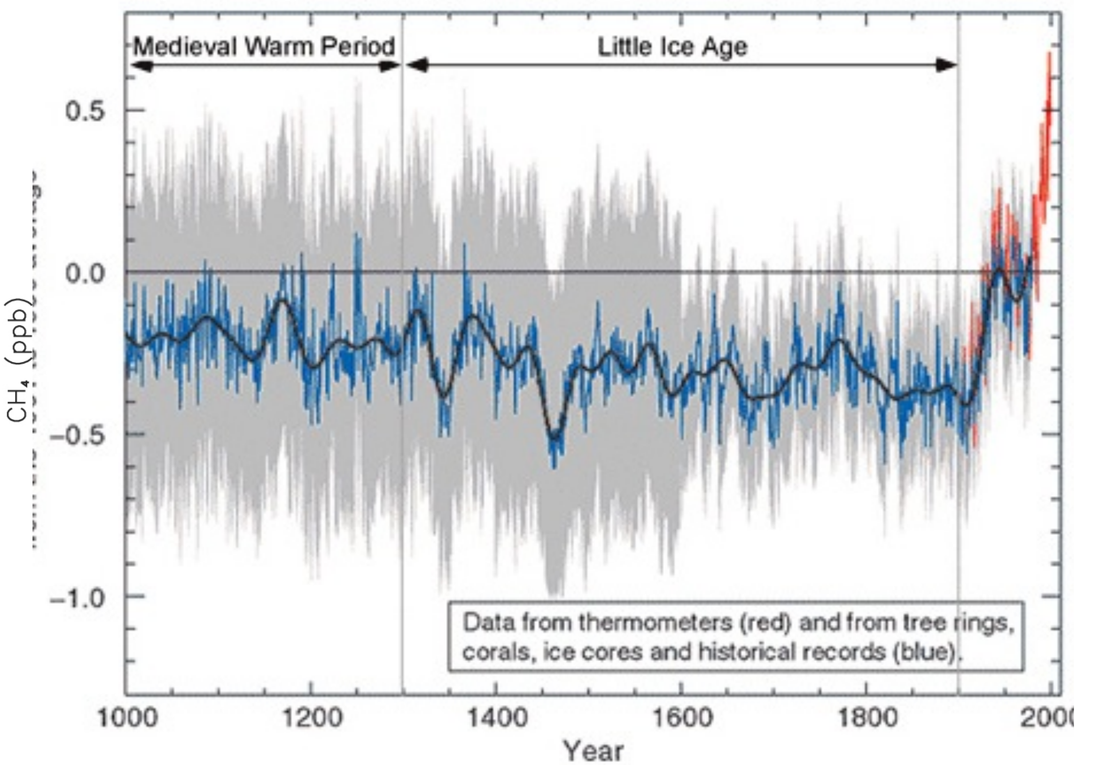
Input Uncertainties

Note: *Essentially, all models are wrong, but some are useful,* George E.P. Box, Industrial Statistician

• Phenomenological models used to represent processes such as turbulence in weather, climate and nuclear reactor models have nonphysical parameters whose values and uncertainties must be determined using measured data.

• Forcing and feedback mechanisms in climate models serve as boundary inputs. These parameterized phenomenological relations introduce both model and parameter uncertainties.





Numerical Errors

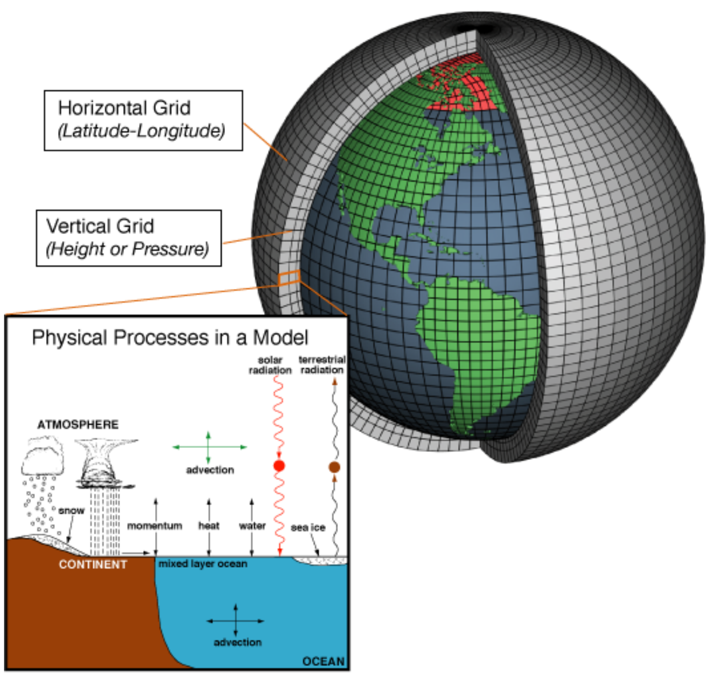
Note: *Computational results are believed by no one, except the person who wrote the code*, Max Gunzburger, Florida State University.

• Roundoff, discretization or approximation errors; e.g., mesh for nuclear subchannel code COBRA-TF is on the order of subchannel between rods.

• Bugs or coding errors;

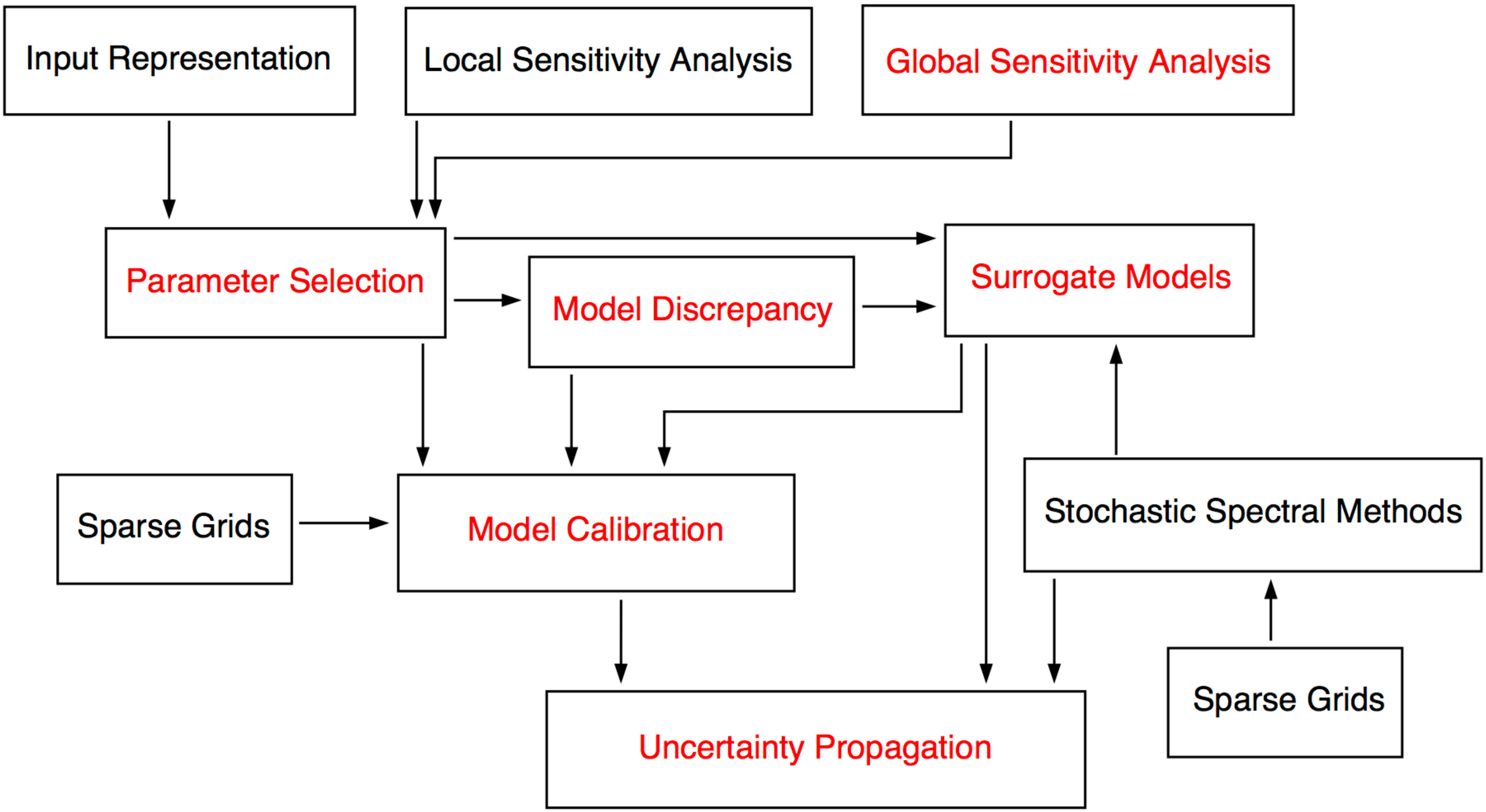
• Bit-flipping, hardware failures and uncertainty associated with future exascale and quantum computing;

• Grids required for numerical solutions of field equations in applications such as weather or climate models (e.g., 50~km) are much larger than the scale of physics being modeled (e.g., turbulence or greenhouse gases).

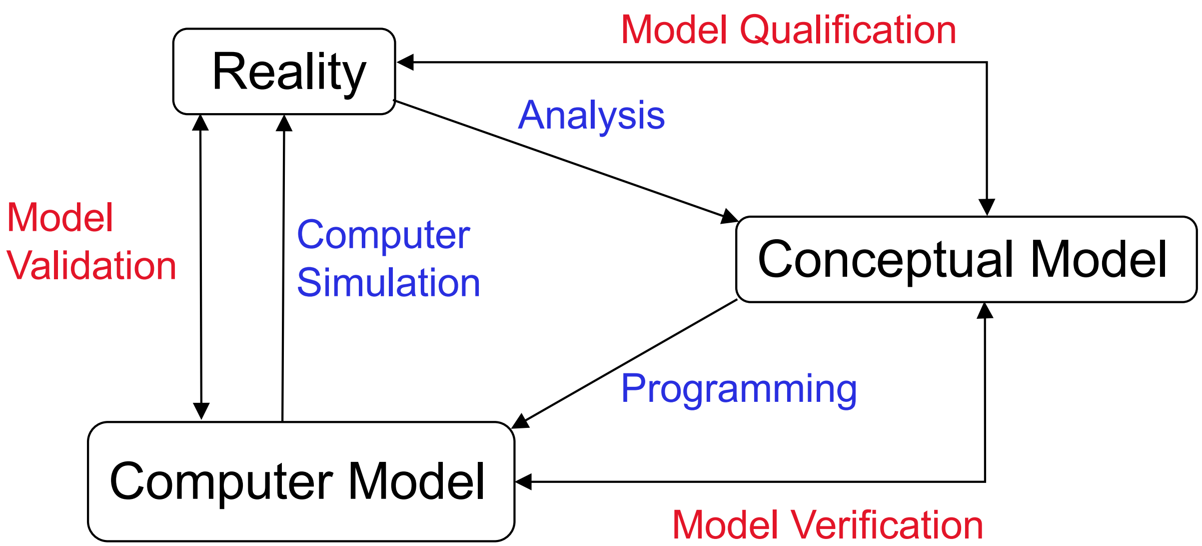


Steps in Uncertainty Quantification

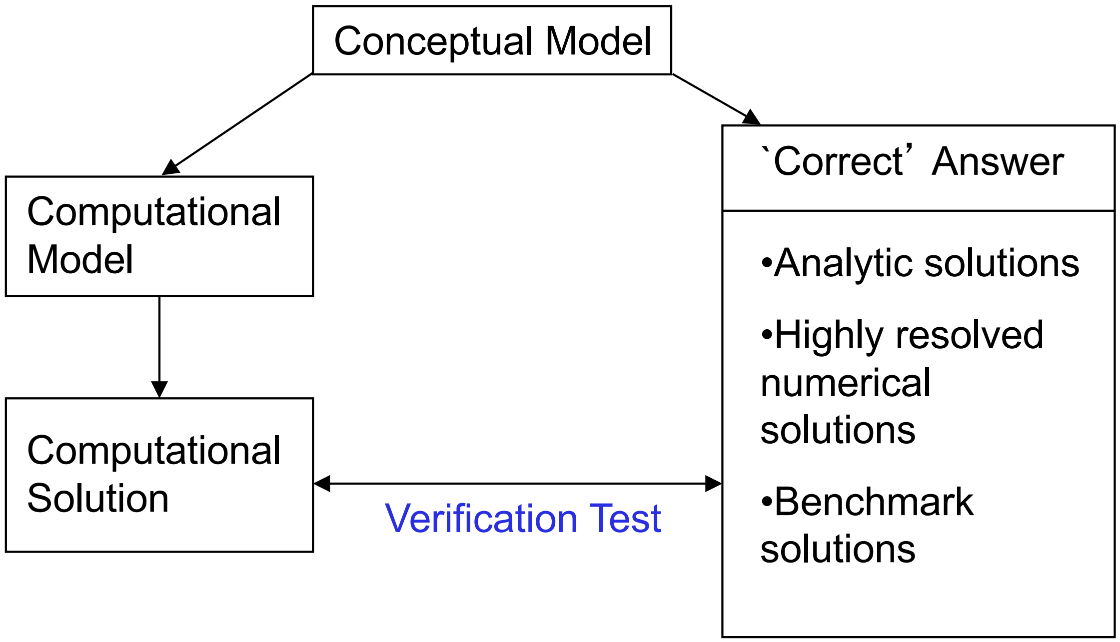
Note: Uncertainty quantification requires synergy between statistics, mathematics and application area.



Modeling Issues



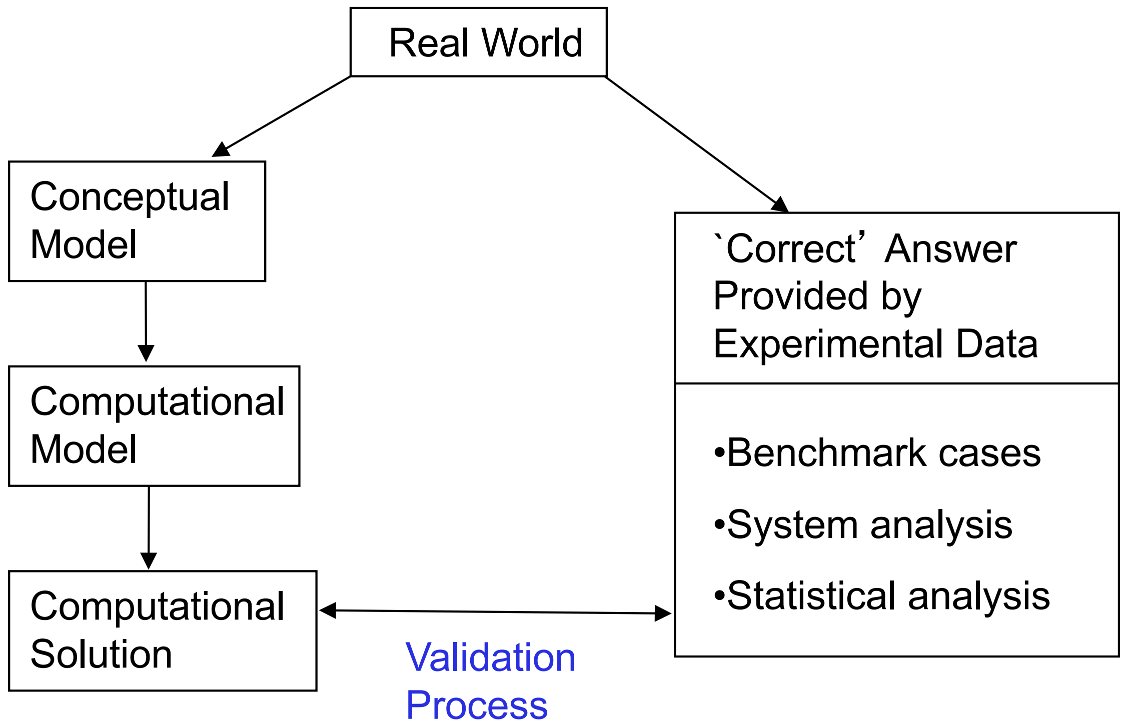
Verification Process



Verification: The process of determining that a model implementation accurately represents the developer's conceptual description of the model and the solution to the model.

Note: Verification deals with mathematics

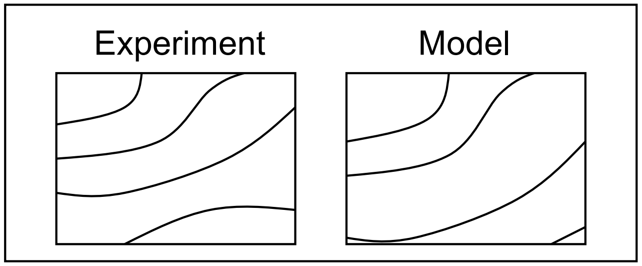
Validation Process



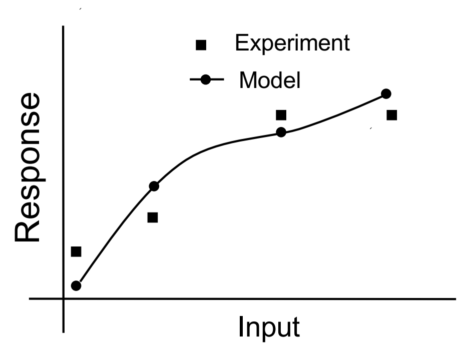
Validation: The process of determining the degree to which a model is an accurate representation of the real world from the perspective of the intended model users.

Note: Validation deals with physics and statistics

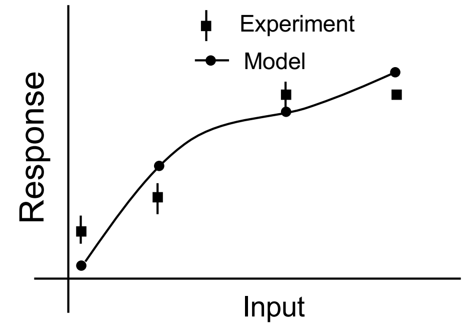
Validation Metrics



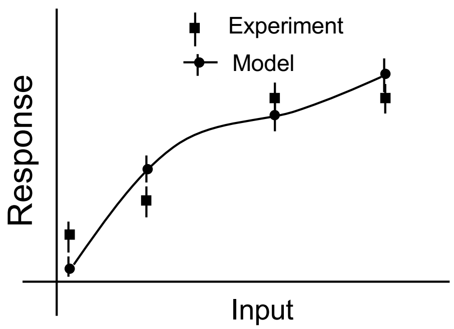
`Viewgraph' Norm



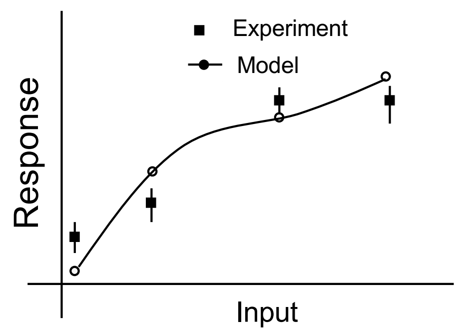
Deterministic



Experimental Uncertainty



Numerical Error



Nondeterministic Computation