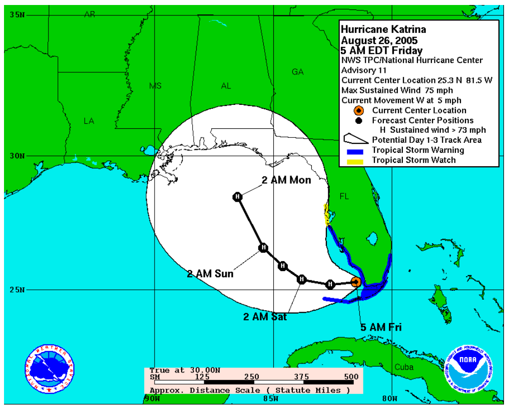
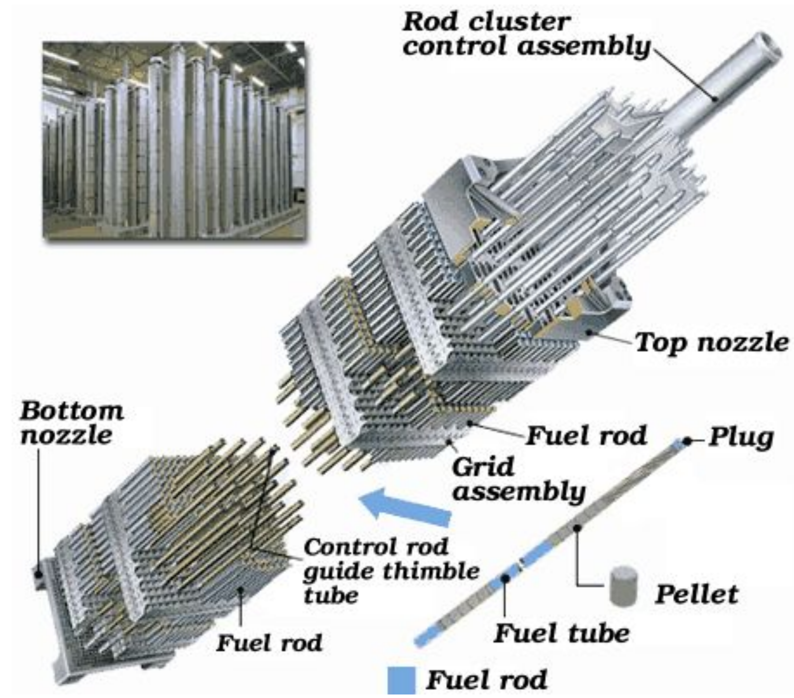
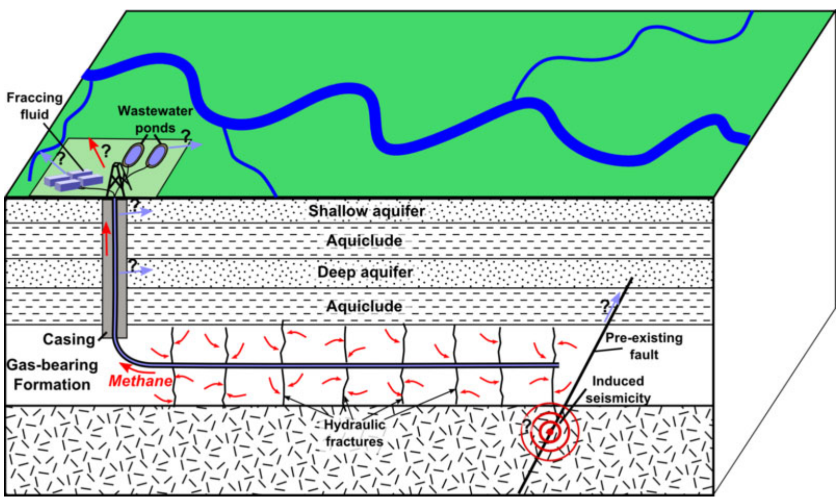
Lecture 1: Motivation and Prototypical Examples

"Essentially all models are wrong, but some are useful,"

George E.P. Box, Industrial Statistician



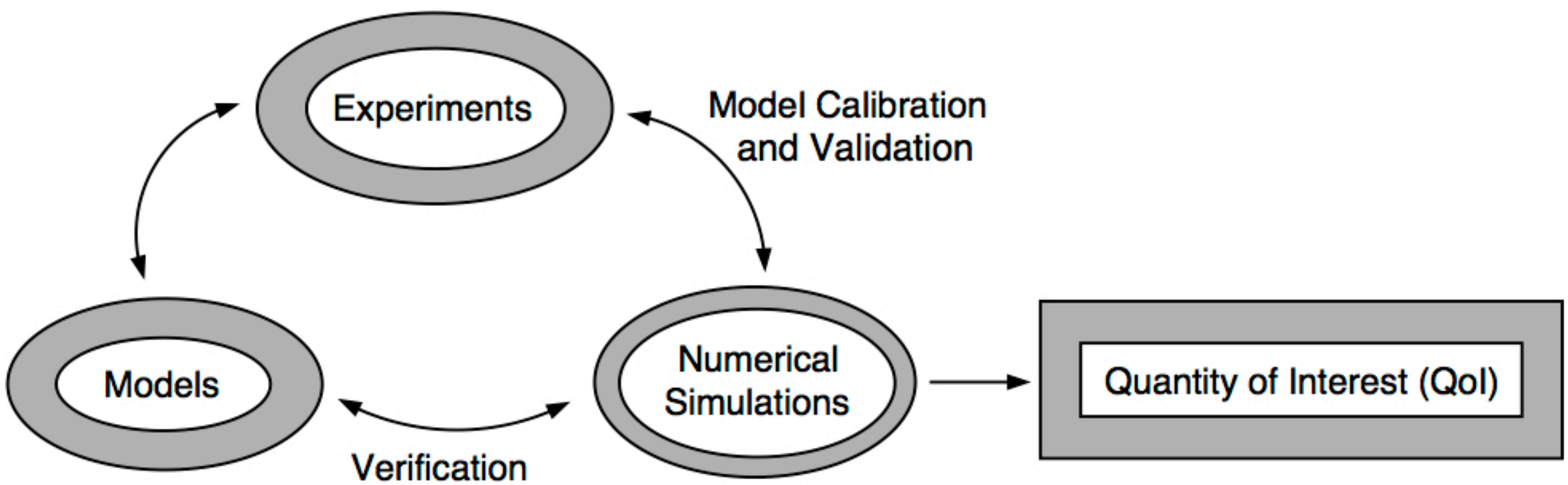




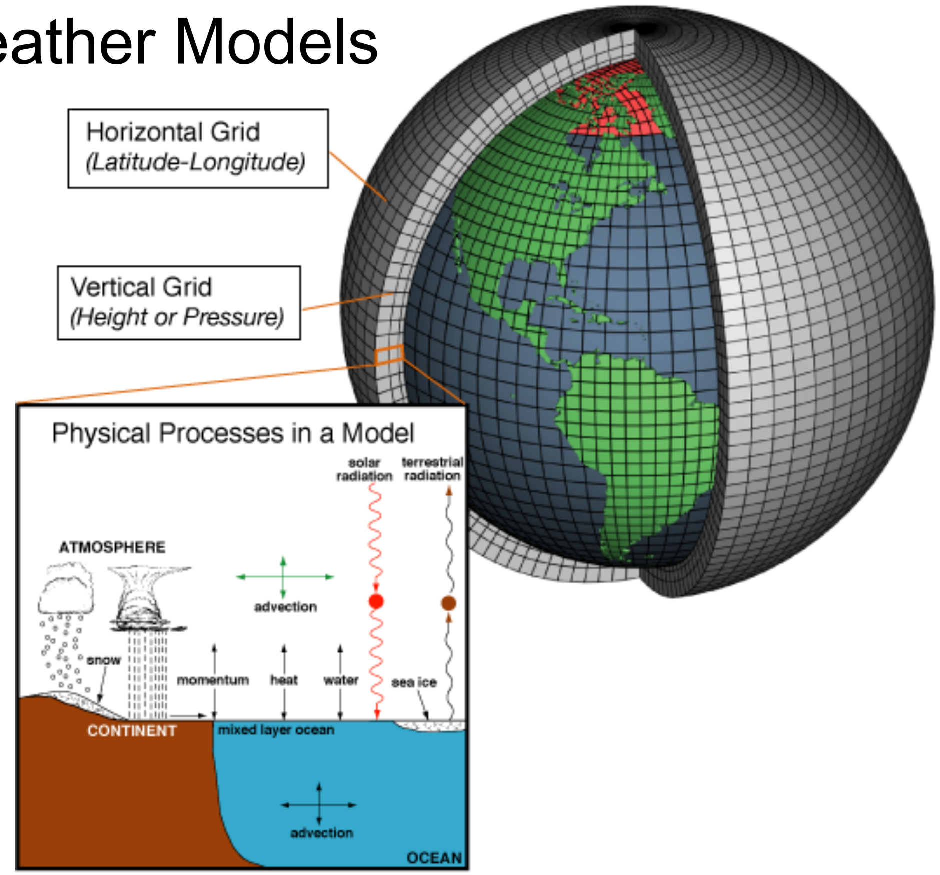
Predictive Science

Components: All involve uncertainty

- Experiments
- Models
- Numerical Simulation
- Quantity of Interest: usually a statistical quantity; e.g., mean



Example: Weather Models



Physical Processes:

- Temperature
- Precipitation
- Winds
- Chemistry of aerosol species

Equations of Atmospheric Physics:

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

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

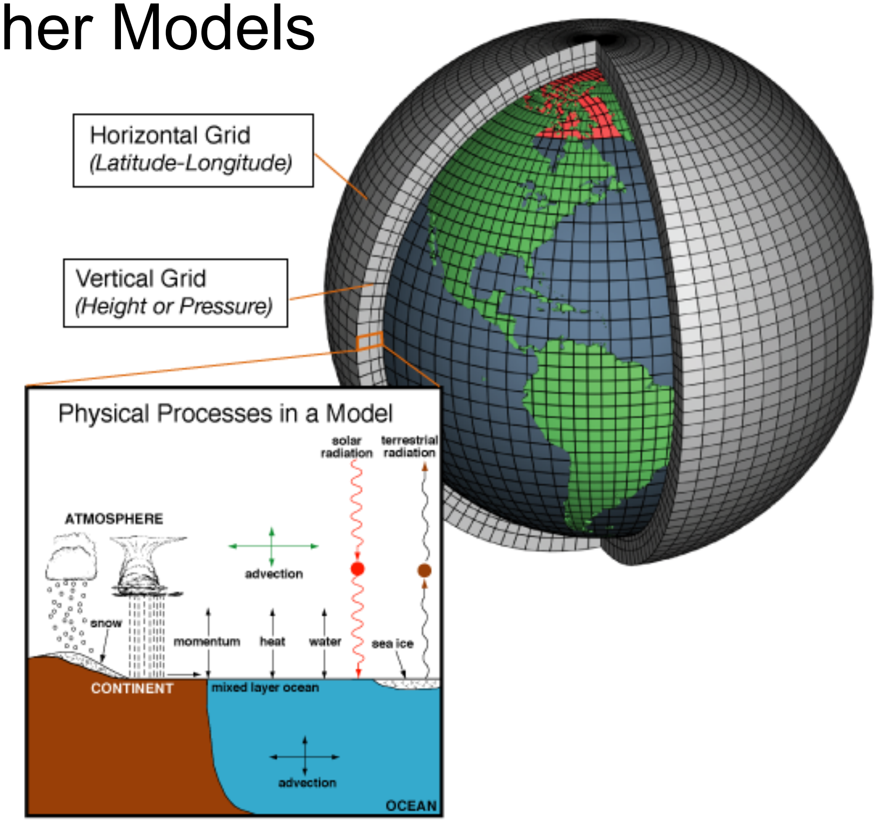
$$\rho c_V \frac{\partial T}{\partial t} + p\nabla \cdot v = -\nabla \cdot F + \nabla \cdot (k\nabla T) + \rho \dot{q}(T, p, \rho)$$

$$p = \rho R T$$

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

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

Example: Weather Models



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Phenomenological Model for Sources:

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

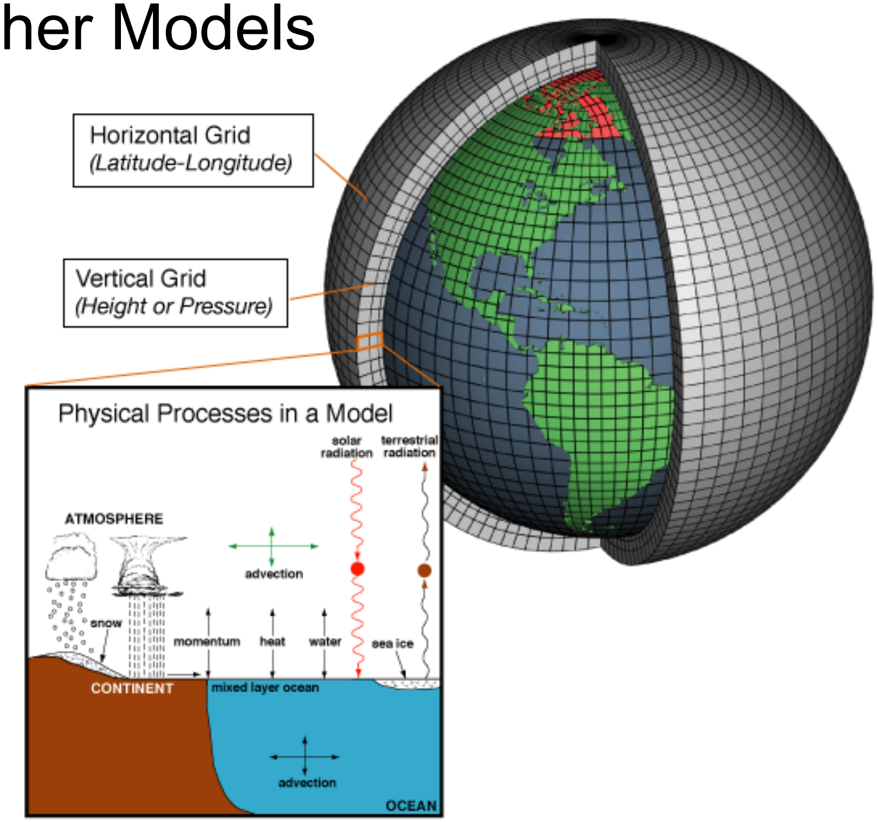
where

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

Example: Weather Models

Sources of Uncertainty:

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

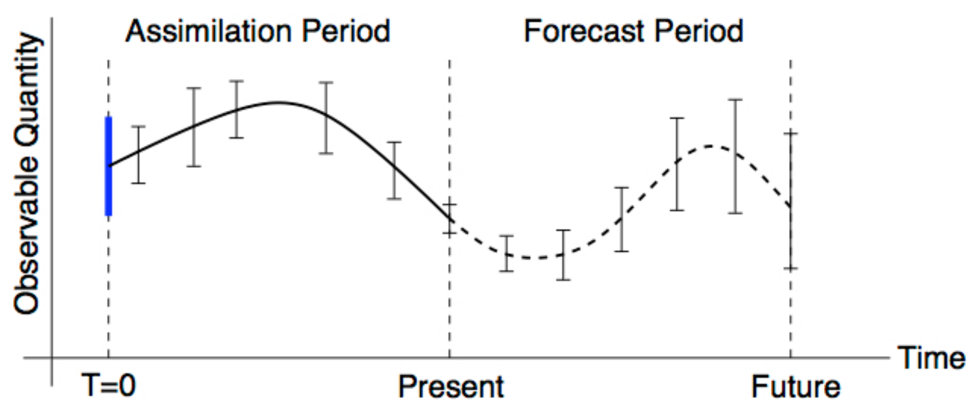


Steps:

• 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: Weather Models

Sources of Uncertainty:

- Model errors or discrepancies
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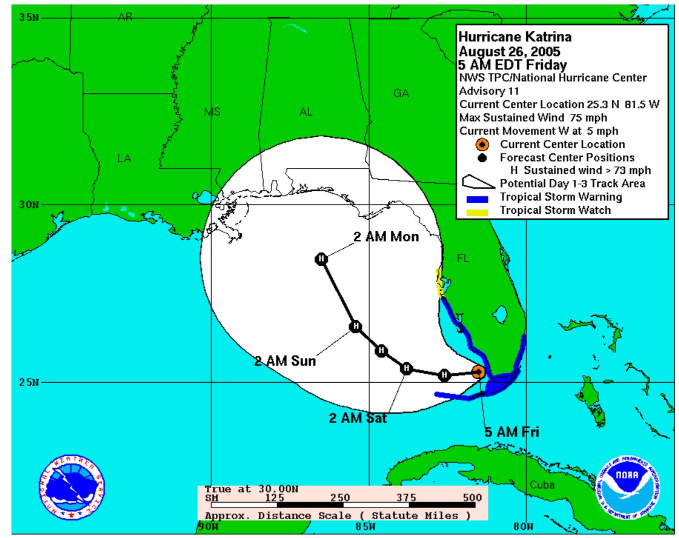
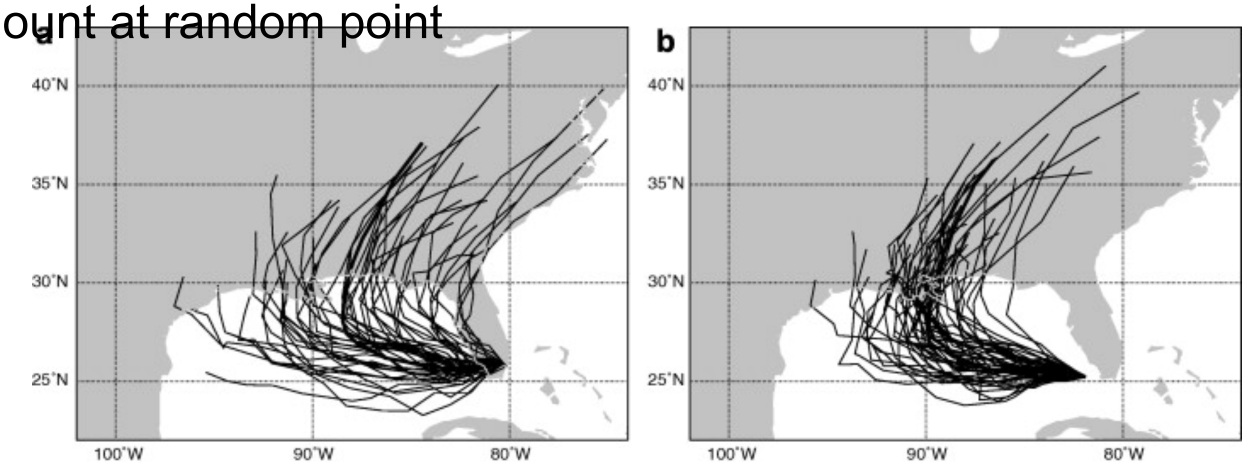
- Measurement errors and uncertainties

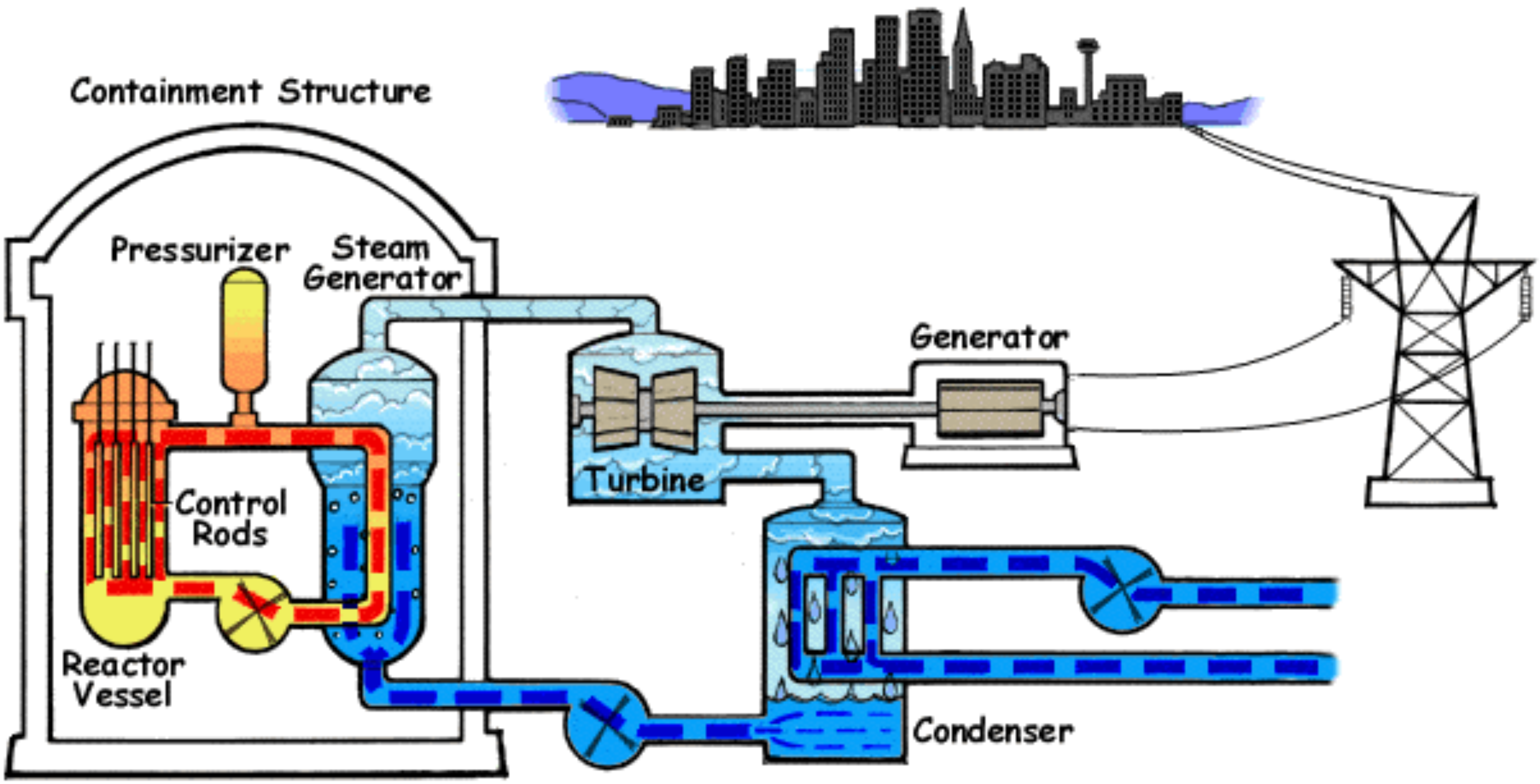


Ensemble Forecasts:

- 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

Example 2: Pressurized Water Reactors (PWR)

3-D Neutron Transport Equations:

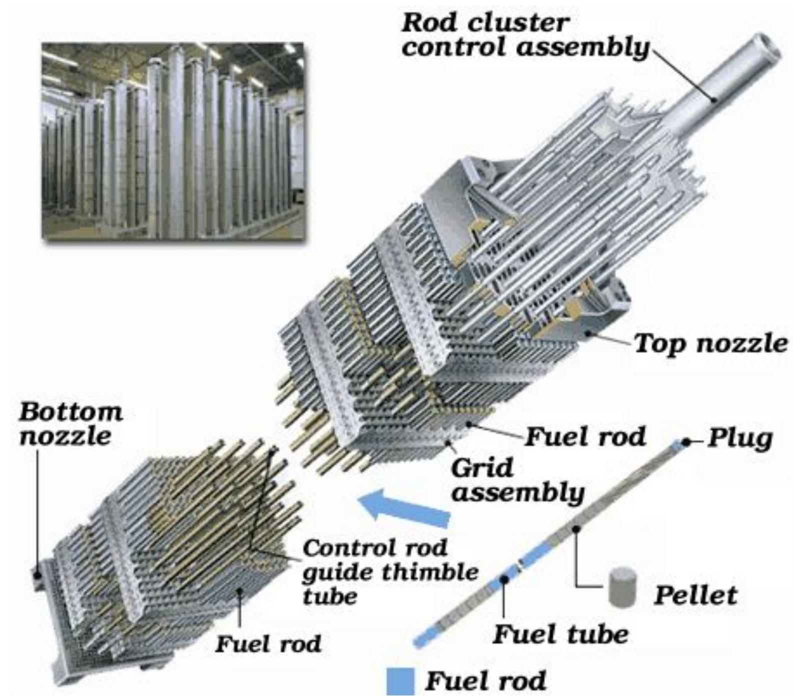
$$\frac{1}{|v|}\frac{\partial\varphi}{\partial t} + \Omega\cdot\nabla\varphi + \Sigma_t(r,E)\varphi(r,E,\Omega,t)$$
$$= \int_{4\pi} d\Omega' \int_0^\infty dE'\Sigma_s(E'\to E,\Omega'\to\Omega)\varphi(r,E',\Omega',t)$$
$$+\frac{\chi(E)}{4\pi}\int_{4\pi} d\Omega' \int_0^\infty dE'\nu(E')\Sigma_f(E')\varphi(r,E',\Omega',t)$$

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 or parameters; e.g., 100,000
- ORNL Code: Denovo;
- Codes can take hours to days to run.



Example 2: Pressurized Water Reactors (PWR)

Thermo-Hydraulic Model: 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

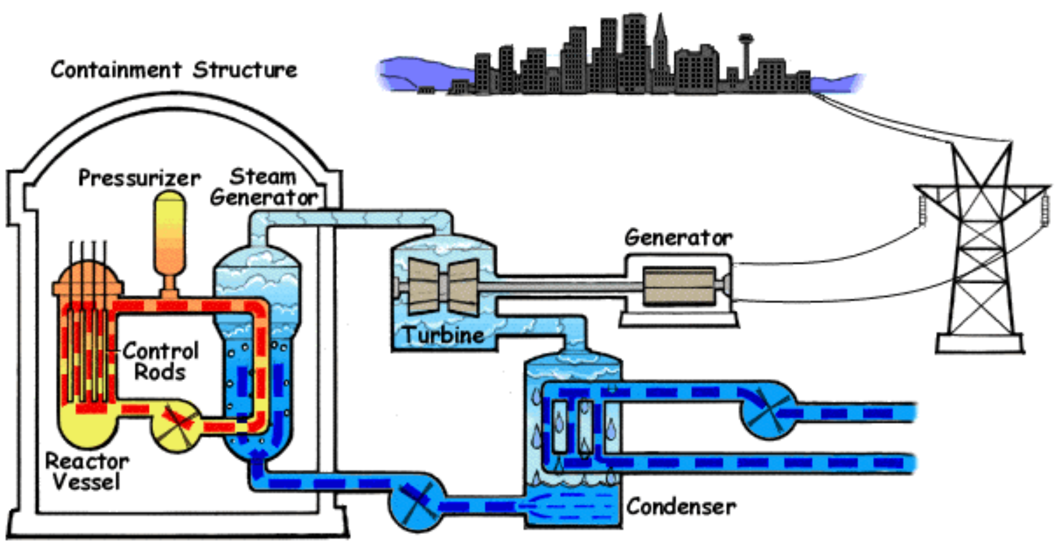
Challenges:

- Nonlinear coupled PDE with nonphysical parameters due to closure relations;
- CASL code: COBRA-TF – Difficult to access primary parameters and inputs.
- Codes can take minutes to days to run.

Example 2: Pressurized Water Reactors (PWR)

UQ Challenges:

- Specify bounds on void fraction distributions and boiling transitions that guarantee specified performance levels and safety margins.
- Specify conditions that limit CRUD on the outside of fuel cladding to within prescribed levels.
- Determine new cladding materials, fuel materials, and fuel pin geometries that provide an average specified improvement in performance and increased resistance to damage.
- Determine conditions that produce specified levels of radiation damage, mechanical thermal fatigue, and corrosion.



Example 3: HIV Model for Characterization and Control Regimes

HIV Model:

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

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

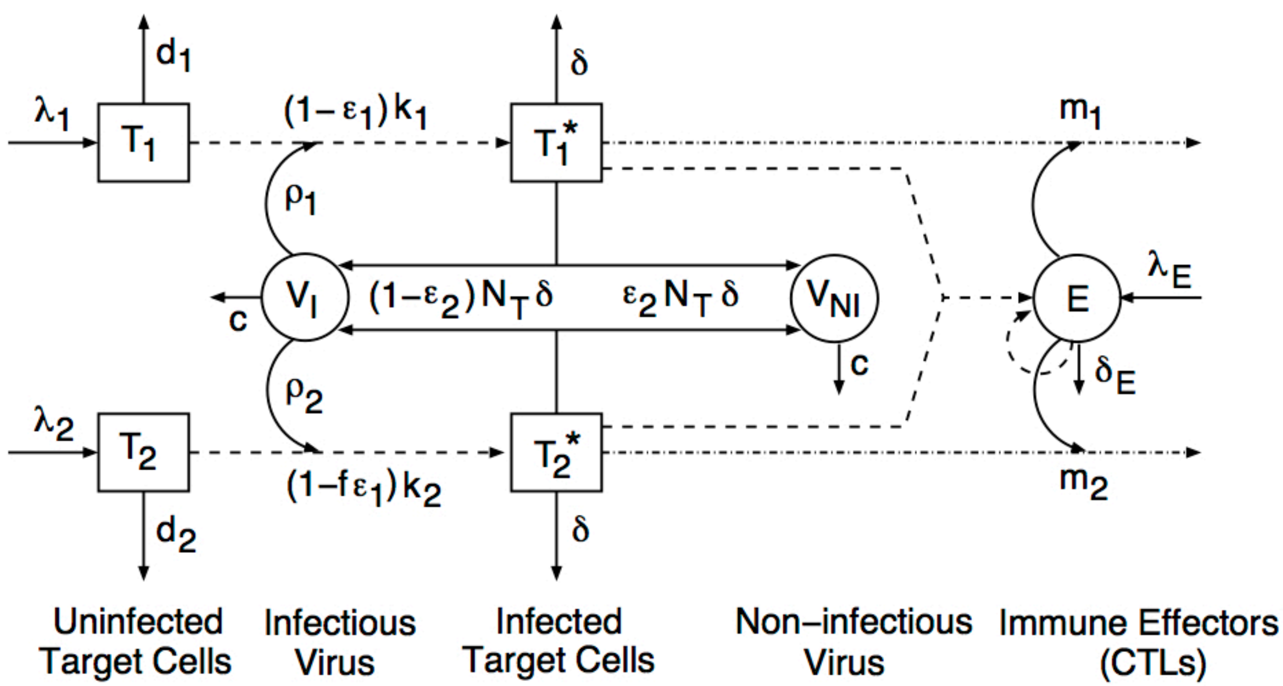
$$\dot{T}_1^* = (1-\varepsilon) k_1 V T_1 - \delta T_1^* - m_1 E T_1^*$$

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

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

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

Compartments:



Example 3: HIV Model for Characterization and Control Regimes

HIV Model: Used for characterization and control treatment regimes.

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

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

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

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

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

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

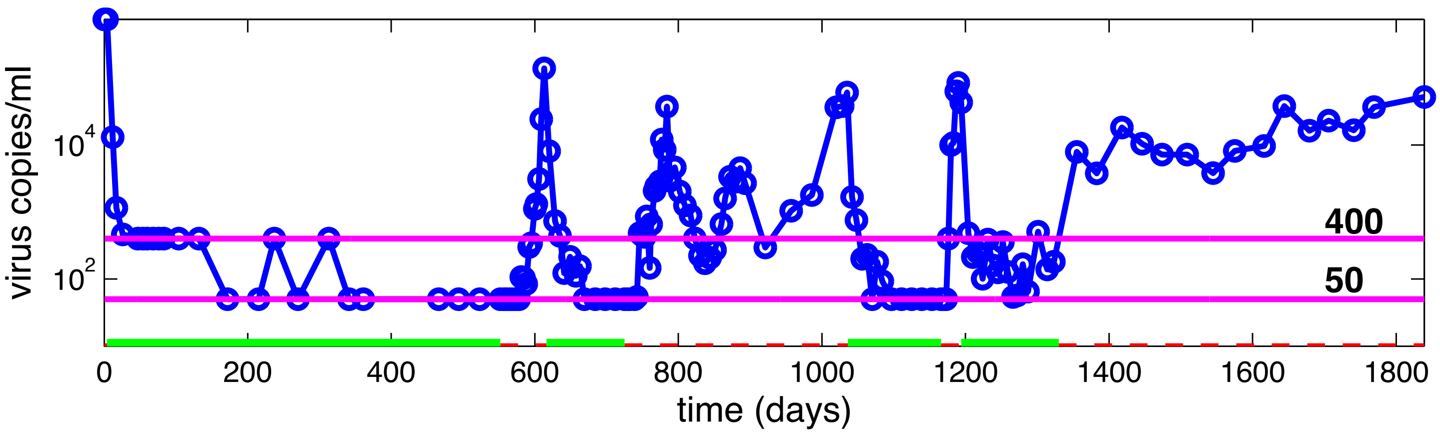
Parameters: Most are unknown and must be estimated from data

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



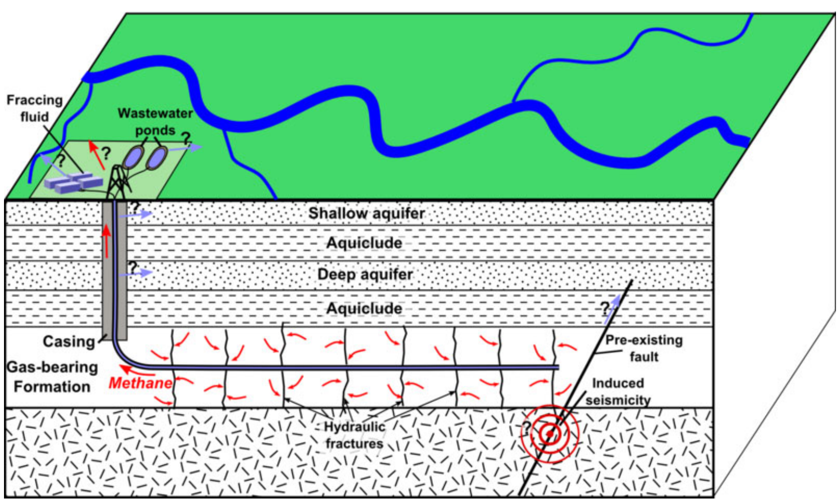
Experimental Uncertainties and Limitations

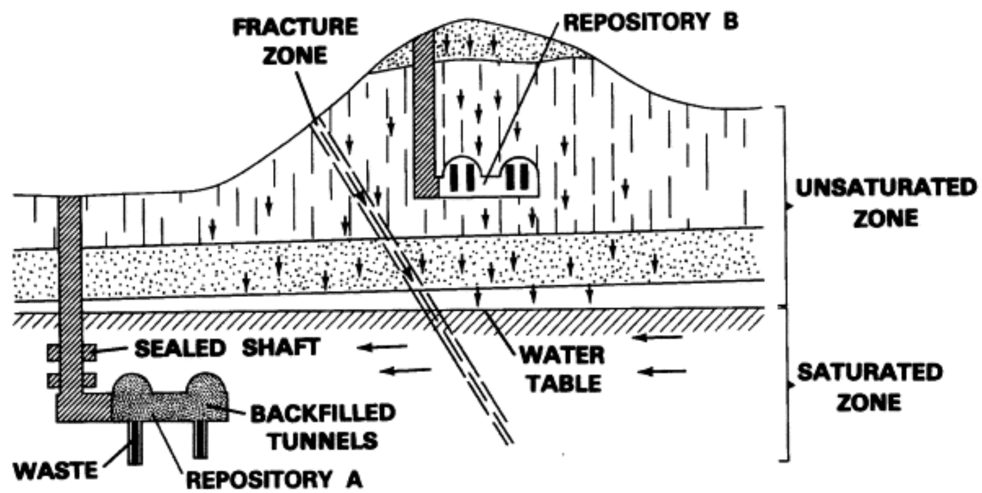
Examples: *Experimental results are believed by everyone, except for the person who ran the experiment*, Max Gunzburger, Florida State University.

• 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.



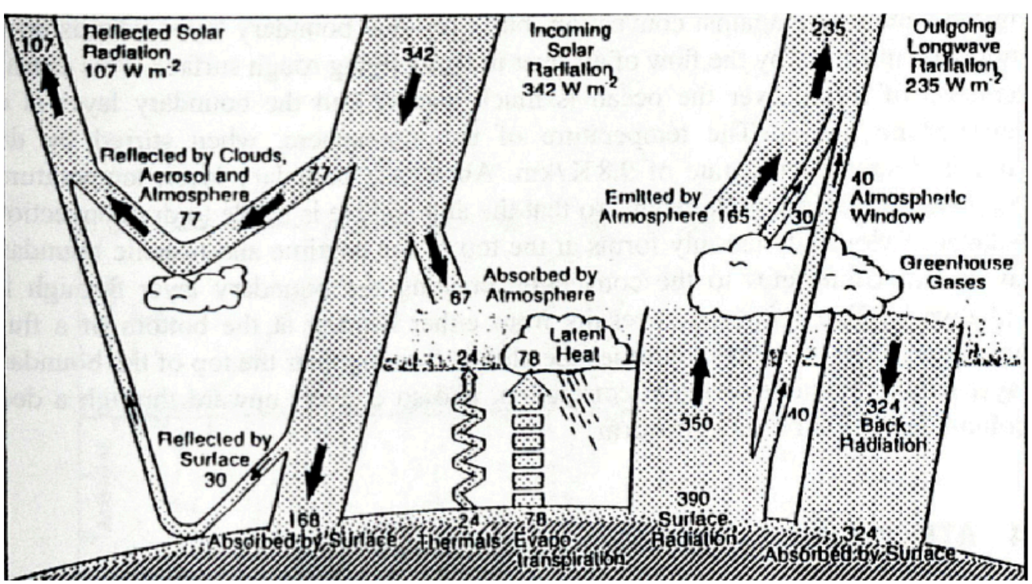


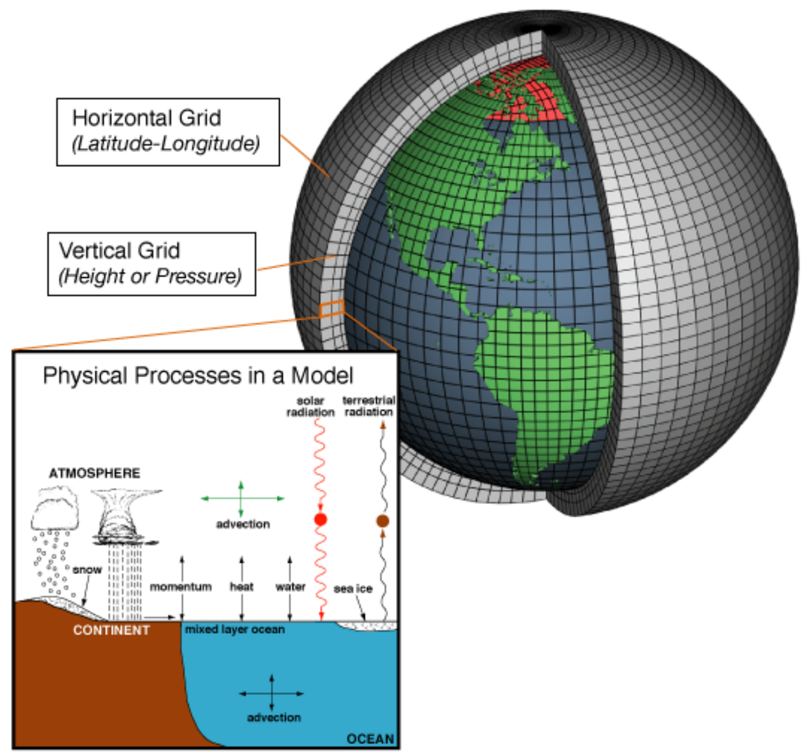
Model Errors

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.



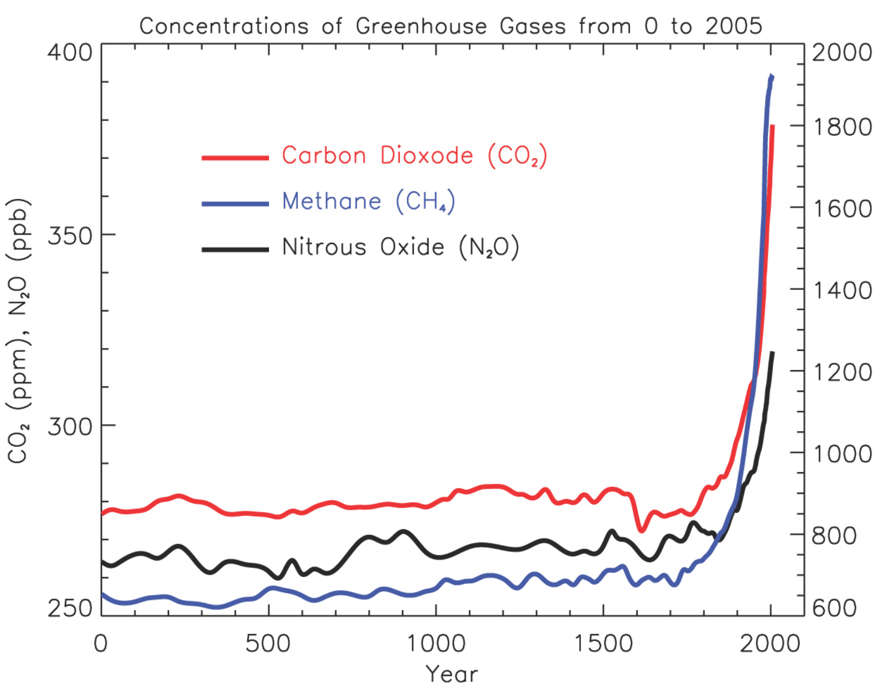


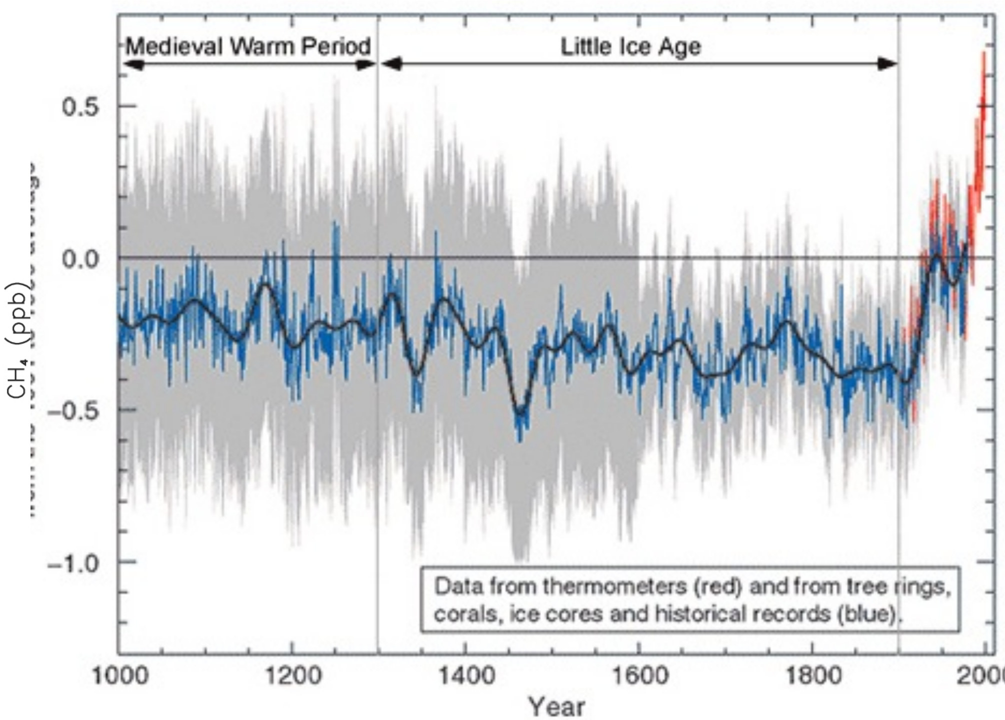
Input Uncertainties

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

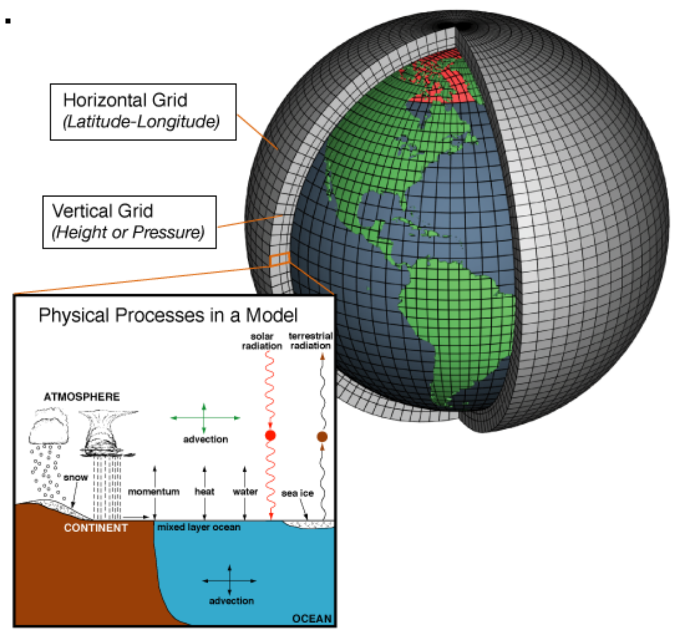
Note: *Computational results are believed by no one, except the person who wrote the code*, Max Gunzburger, Florida State University.

• 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;

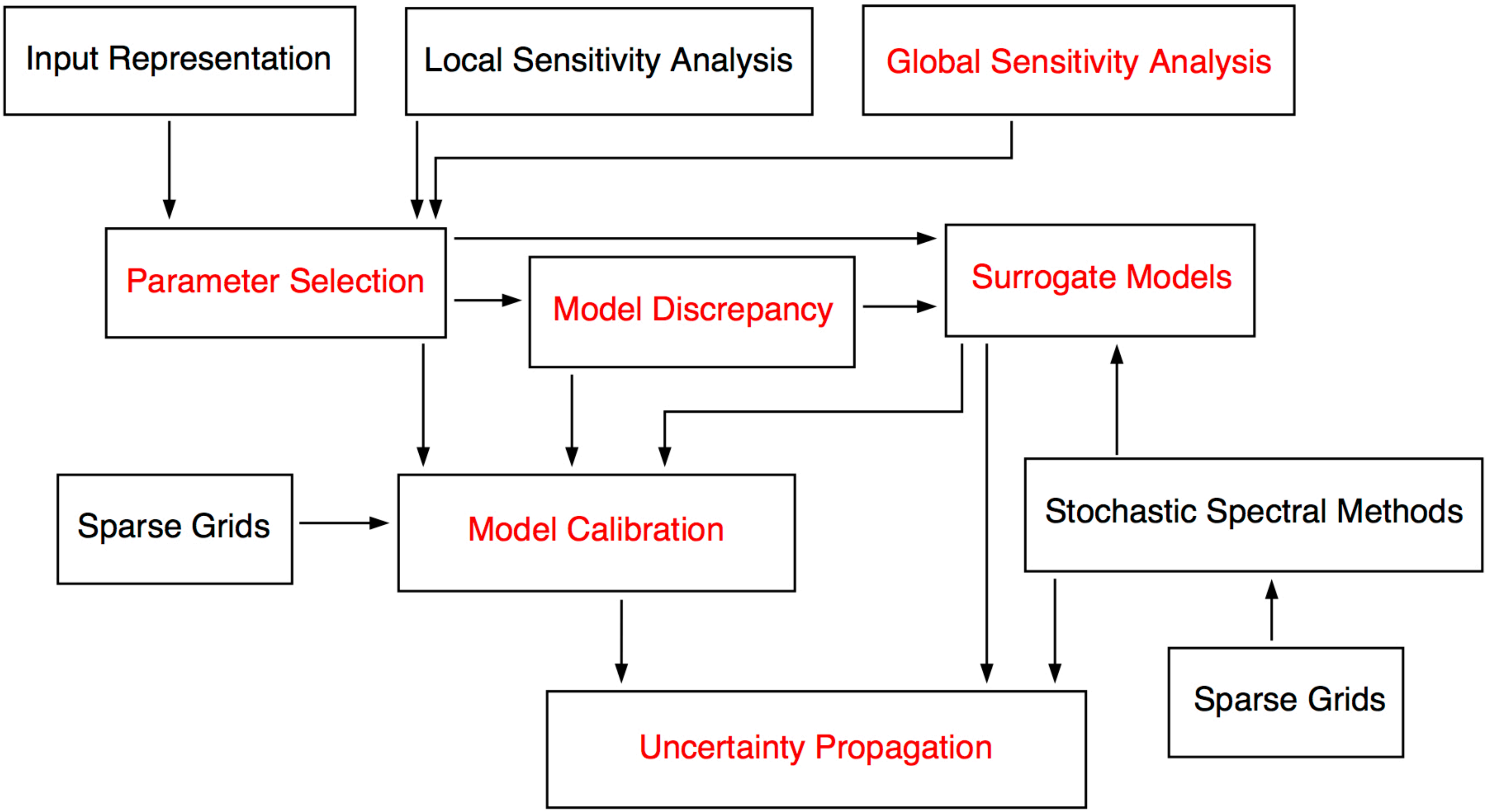
• Bit-flipping, hardware failures and uncertainty associated with future exascale and quantum computing;

• 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).

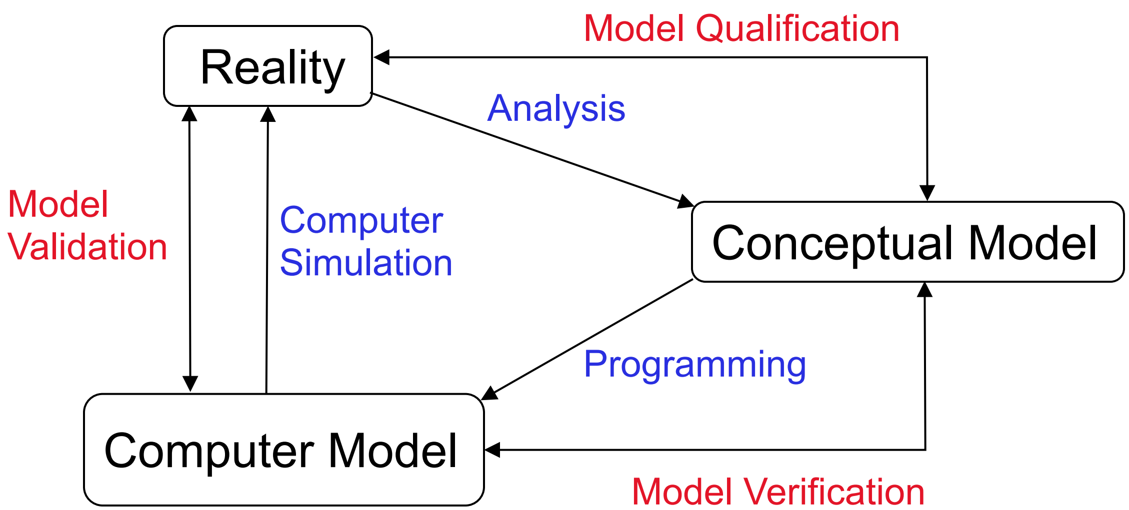


Steps in Uncertainty Quantification

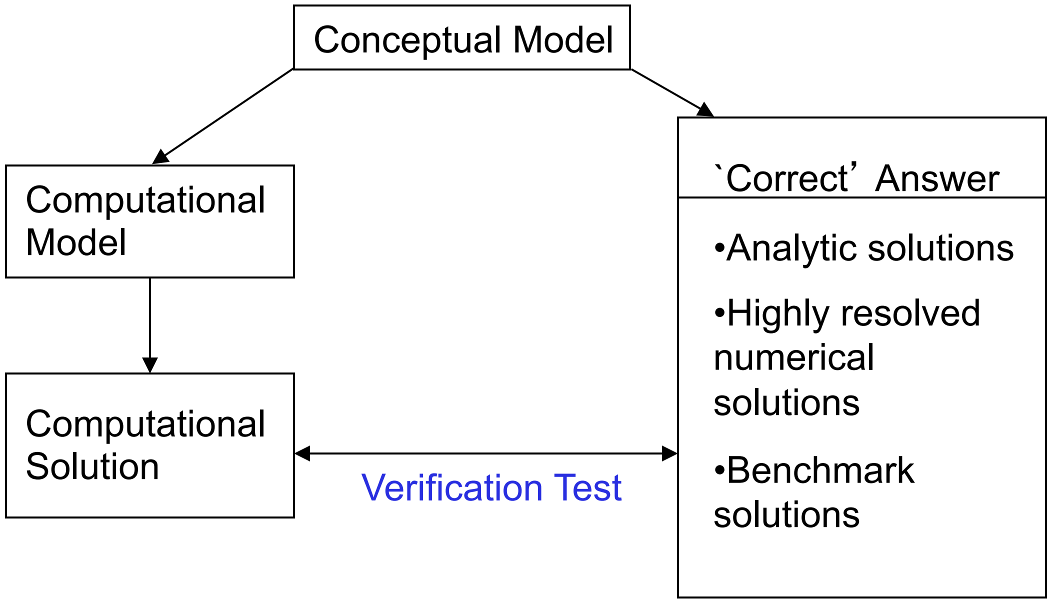
Note: Uncertainty quantification requires synergy between statistics, mathematics and application area.



Modeling Issues



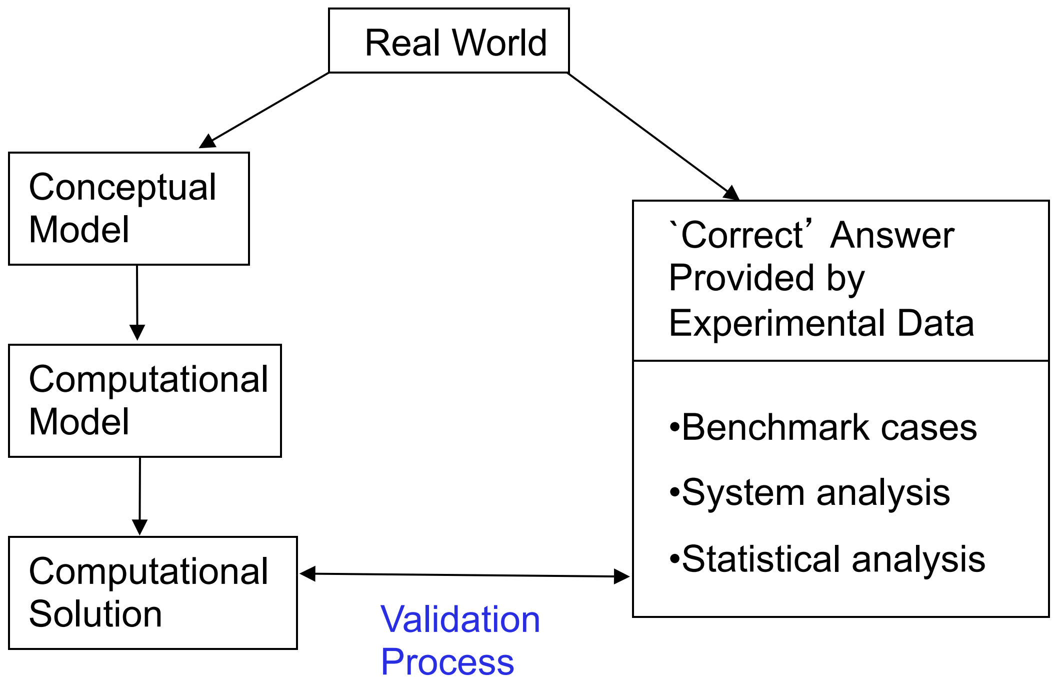
Verification Process



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

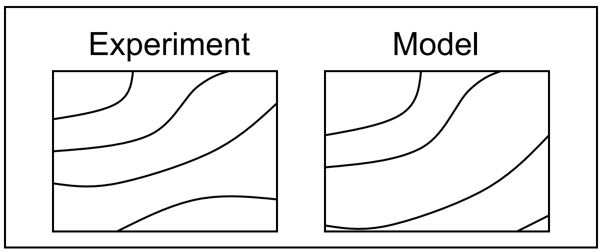
Validation Process



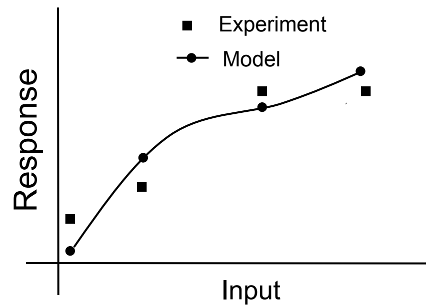
Validation: The process of determining the degree to which a model is an accurate representation of the real world from the perspective of the intended model users.

Note: Validation deals with physics and statistics

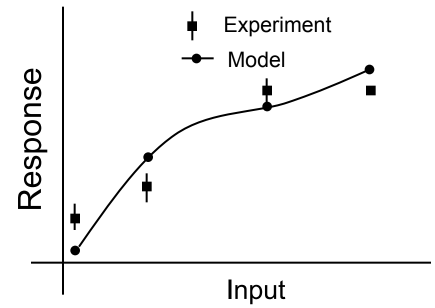
Validation Metrics



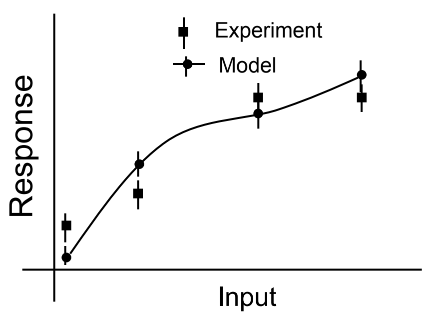
`Viewgraph’ Norm



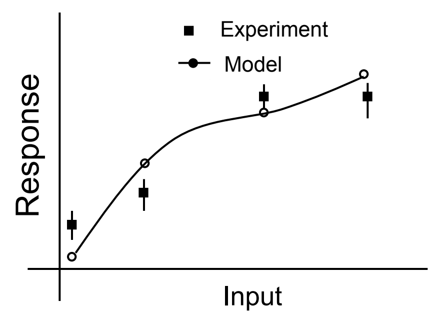
Deterministic



Experimental Uncertainty



Numerical Error



Nondeterministic Computation