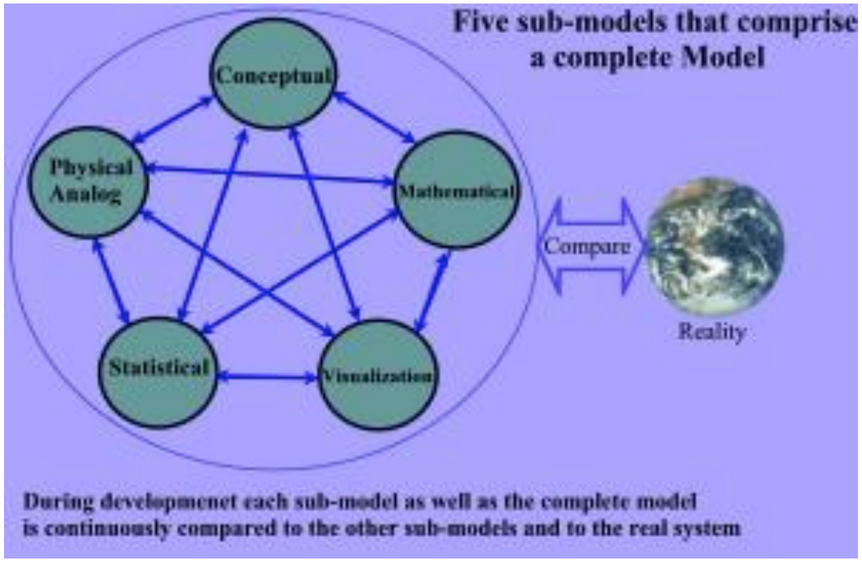
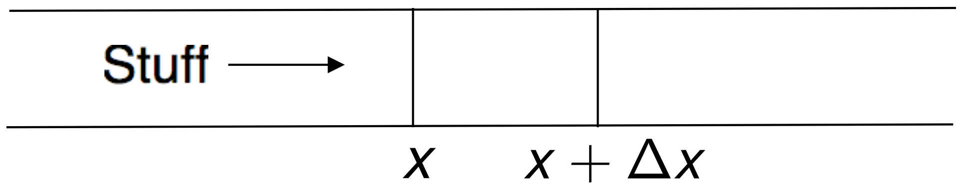
Introduction and Motivation

``Essentially all models are wrong but some are useful,''
George E.P. Box, Industrial Statistician



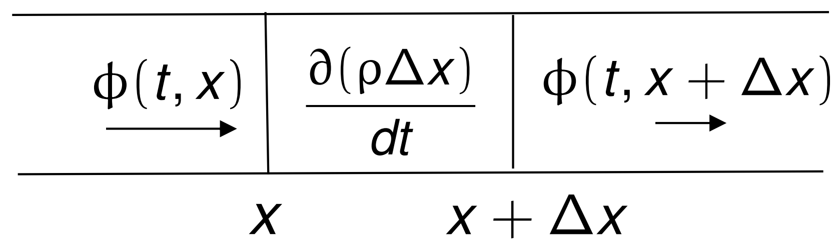
Modeling Strategy

General Strategy: Conservation of stuff



$$\frac{dStuff}{dt} = \text{Stuff in - Stuff out + Stuff created - Stuff destroyed}$$

Continuity Equation:



$$\frac{\partial(\rho\Delta x)}{\partial t} = \phi(t, x) - \phi(t, x + \Delta x)$$

$$\Rightarrow \lim_{\Delta x \to 0} \frac{\partial\rho}{\partial t} = \lim_{\Delta x \to 0} \frac{\phi(t, x) - \phi(t, x + \Delta x)}{\Delta x}$$

$$\Rightarrow \frac{\partial\rho}{\partial t} + \frac{\partial\phi}{\partial x} = 0$$

Density: $\rho(t, x)$ - Stuff per unit length or volume

Rate of Flow: $\phi(t, x)$ - Stuff per second

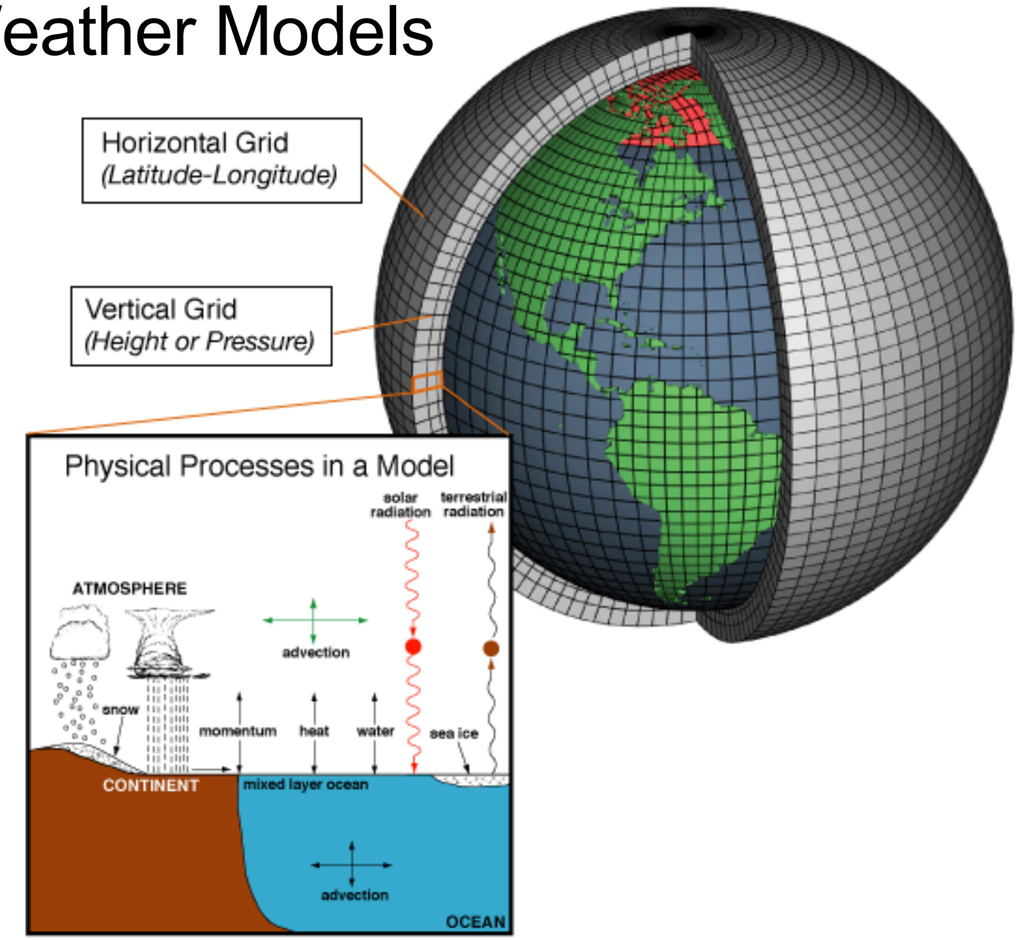
More Generally:

$$\Rightarrow \frac{\partial\rho}{\partial t} + \frac{\partial\phi}{\partial x} = \text{Sources - Sinks}$$

Example 1: Weather Models

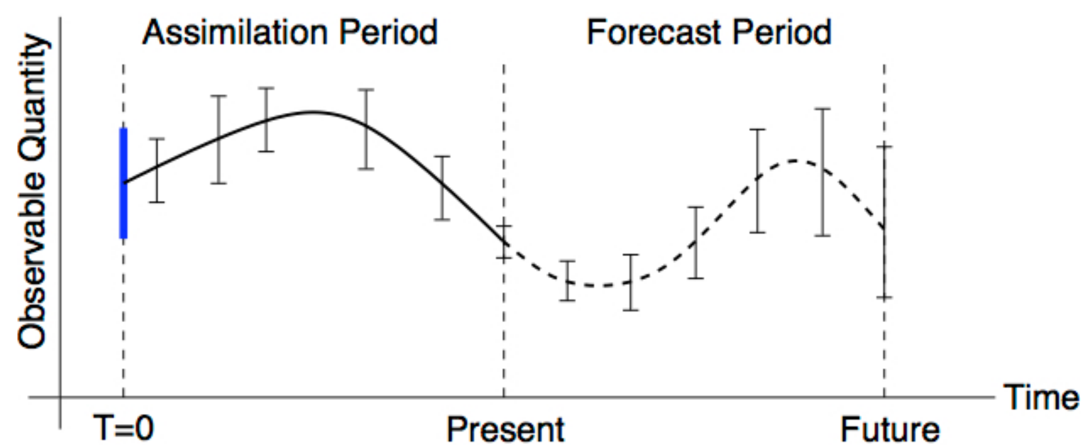
Challenges:

- 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:

$$\frac{\partial \rho}{\partial t} + \frac{\partial \phi}{\partial x} = \text{Sources - Sinks}$$

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

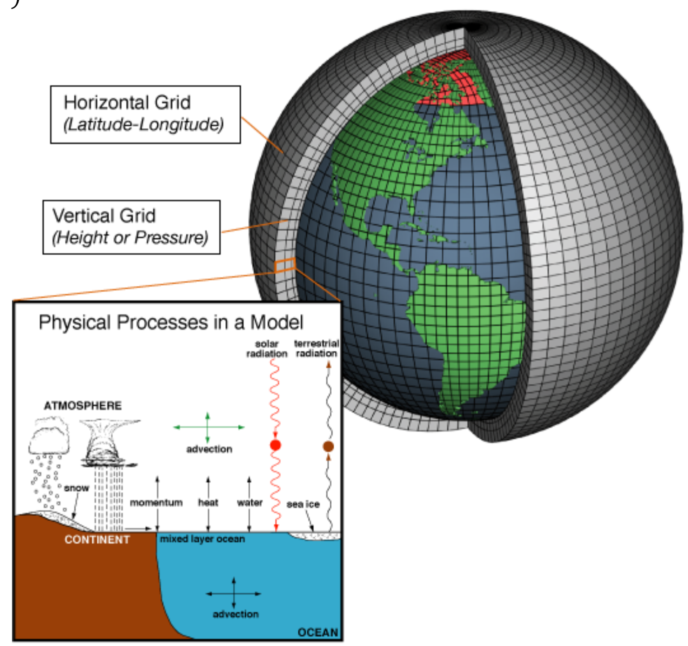
Momentum
$$\frac{\partial v}{\partial t} = -v \cdot \nabla v - \frac{1}{\rho}\nabla p - g\hat{k} - 2\Omega \times v$$

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.,

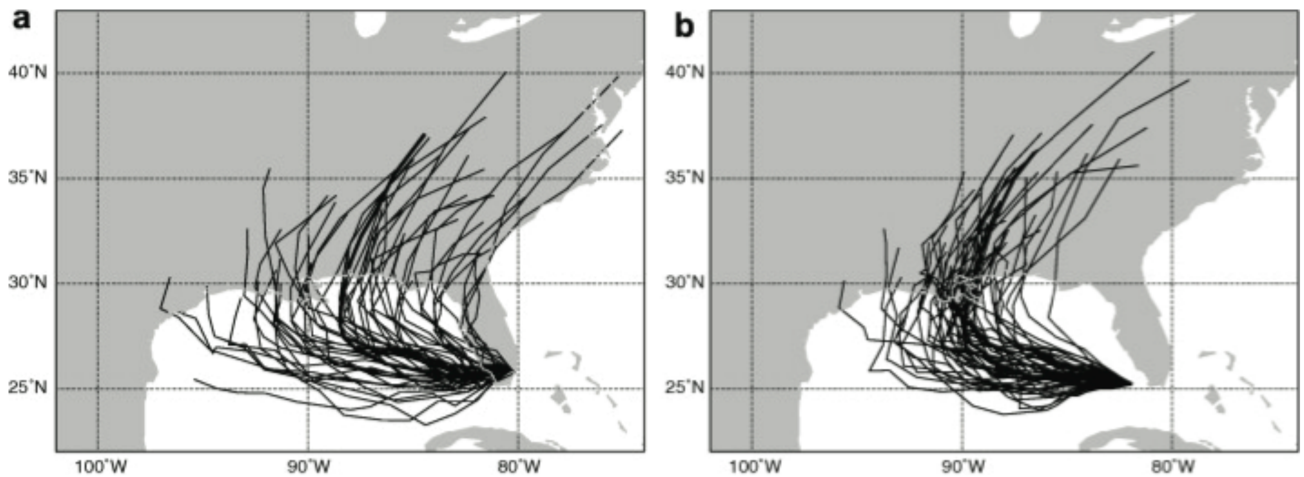
$$S_{m_2} = S_1 + S_2 + S_3 - S_4$$

where

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

Ensemble Predictions

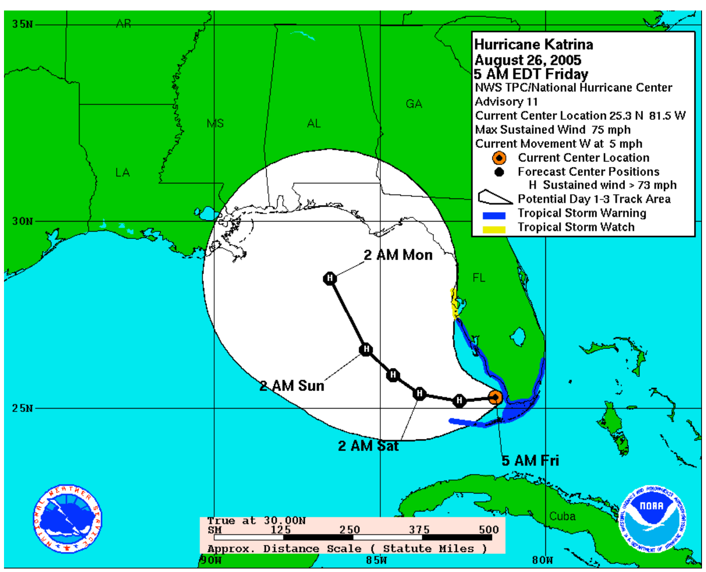
Ensemble Predictions:



00 UTC on August 26, 2005

12 UTC on August 26, 2005

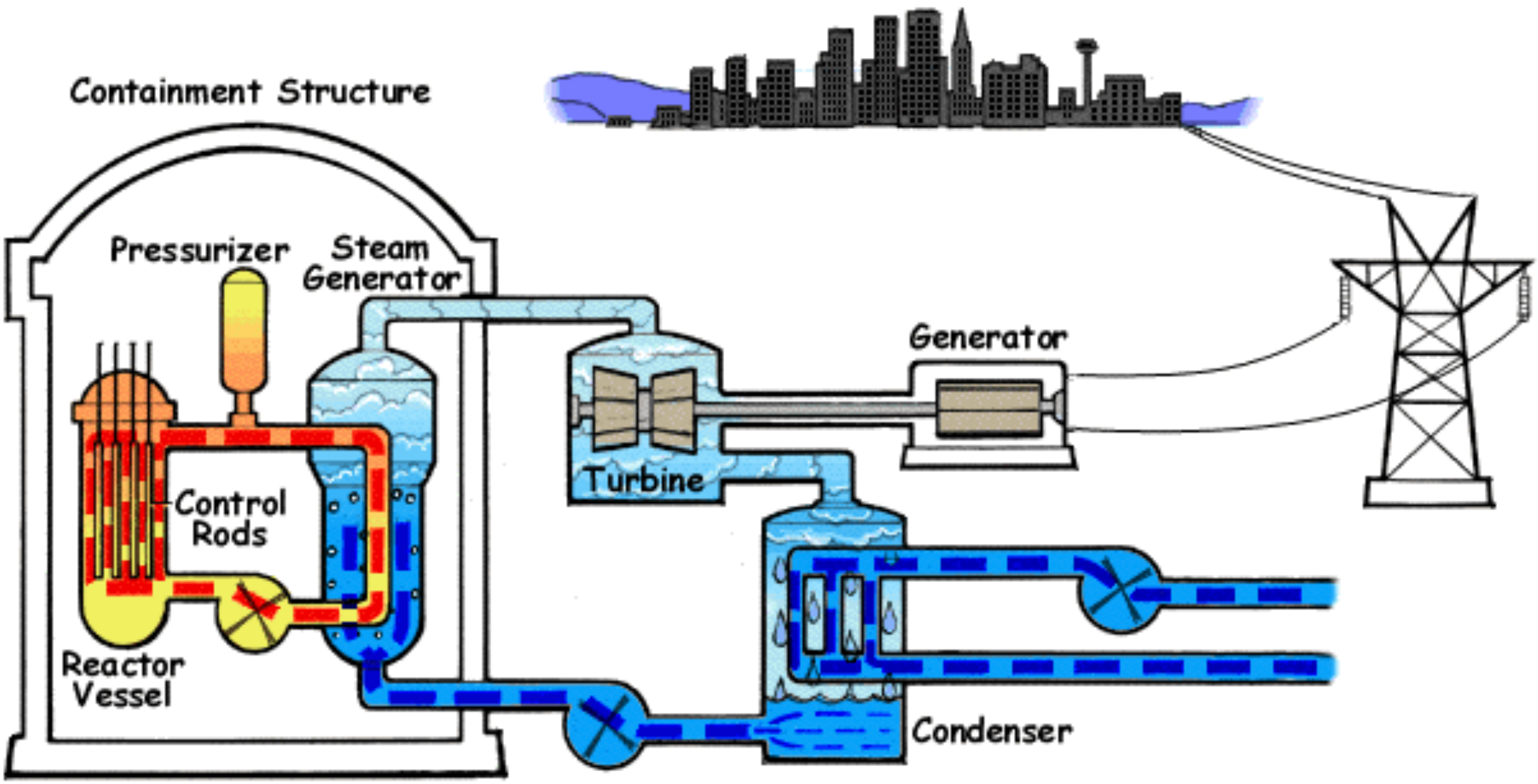
Cone of Uncertainty:



General Questions:

- What is expected rainfall on August 10?
- What are high and low temperatures?
- What is predicted average snow fall?
- Note: Quantities are statistical in nature.

Example 2: Pressurized Water Reactors (PWR)



Models:

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

Objective: Develop Virtual Environment for Reactor Applications (VERA)

Example: Pressurized Water Reactors (PWR)

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

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

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

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

$$\frac{\partial \rho}{\partial t} + \frac{\partial \phi}{\partial x} = \text{Sources - Sinks}$$

Notes:

- Similar relations for gas and bubbly phases
- Models must conserve mass, energy, and momentum

Challenges:

- Codes can have 15-30 closure relations and up to 75 parameters.
- Codes and closure relations often "borrowed" from other physical phenomena; e.g., single phase fluids, airflow over a car (CFD code STAR-CCM+)
- Calibration necessary and closure relations can conflict.
- Inference of random fields requires high- (infinite-) dimensional theory.

Example 3: HIV Model for Characterization and Control Regimes

HIV Model:

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

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

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

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

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

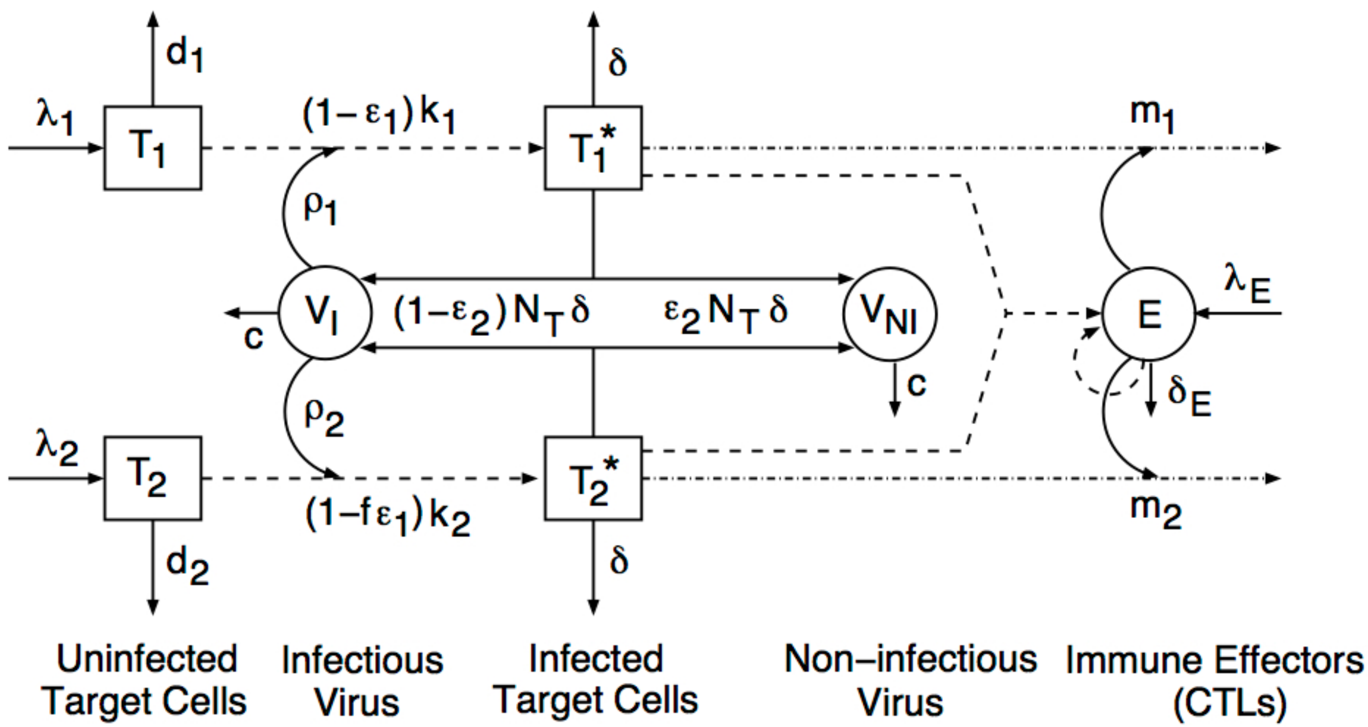
$$\dot{E} = \lambda_E + \frac{b_E(T_1^* + T_2^*)}{T_1^* + T_2^* + K_b}E - \frac{d_E(T_1^* + T_2^*)}{T_1^* + T_2^* + K_d}E - \delta_E E$$

Notes: 21 parameters

[Adams, Banks et al., 2005, 2007]

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

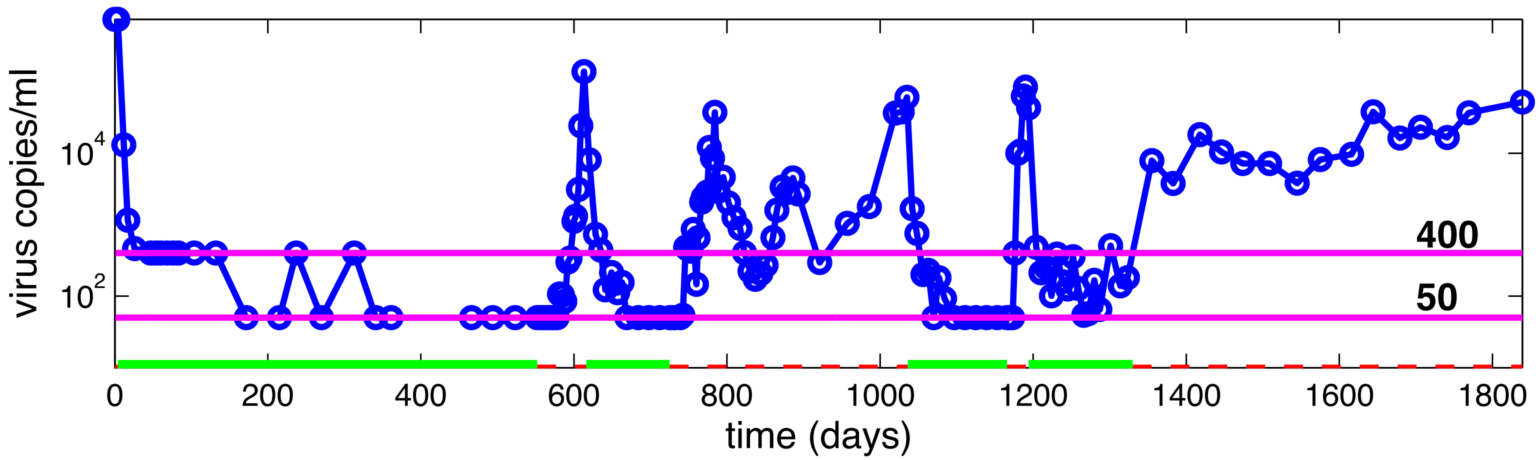
Compartments:



Example: HIV Model for Characterization and Treatment Regimes

HIV Model: Several sources of uncertainty including viral measurement techniques

Example: Upper and lower limits to assay sensitivity



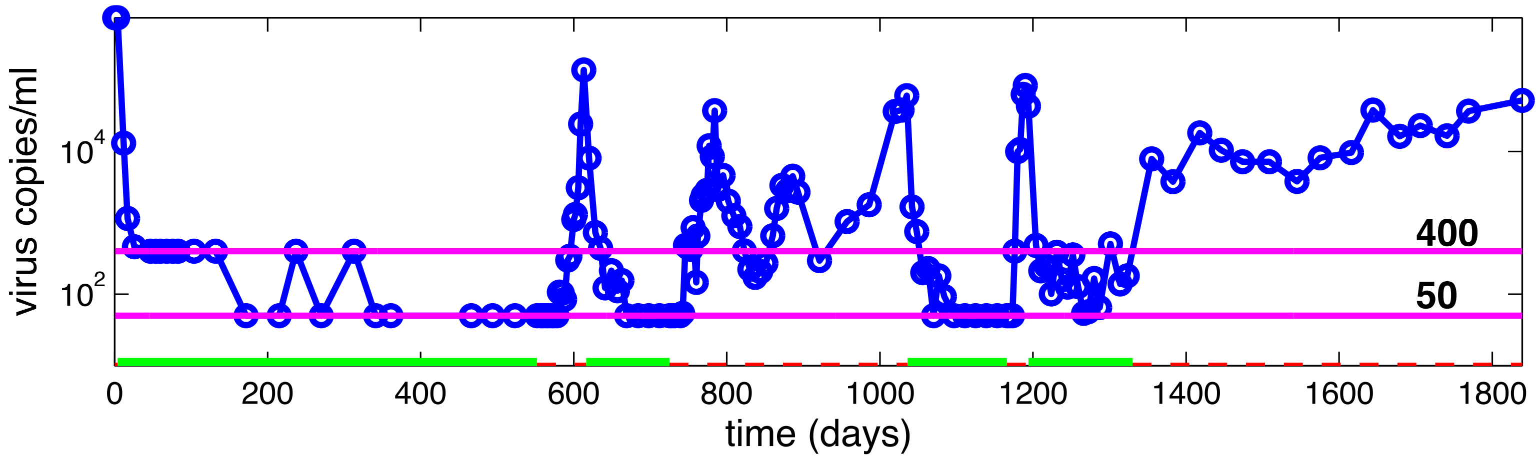
UQ Questions:

- What are the uncertainties in parameters that cannot be directly measured?
- What is optimal treatment regime that is "safe" for patient?
- What is expected viral load? Issue: very often requires high-dimensional integration!
- e.g., $\mathbb{E}[V(t)] = \int_{\mathbb{R}^{21}} V(t,q)\rho(q)dq$

Experimental results are believed by everyone, except for the person who ran the experiment, source anonymous, quoted by Max Gunzburger, Florida State University.

Modeling Process

HIV Model: Several sources of uncertainty including viral measurement techniques



Strategy:

- Use physical understanding to make appropriate assumptions; e.g. uniform longitudinal forces permit use of lumped or spring model.

- Apply physical principles to develop model; e.g., Newtonian (force and moment balancing), Lagrangian (variational principles based on kinetic and potential energy), or Hamiltonian (total energy principles).

- Obtain analytic or numerical solution to model.

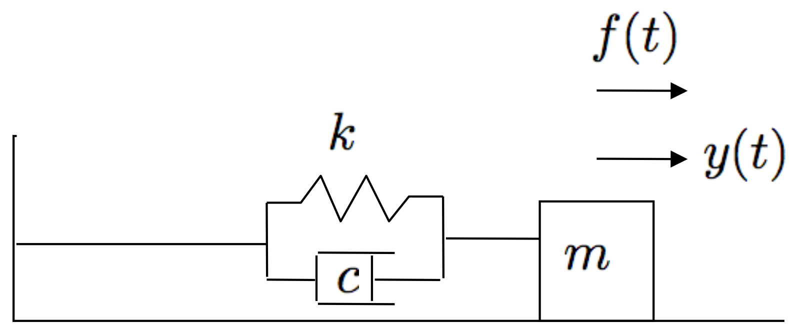
- Compare to experimental data (validate and predict).

- Update model to accommodate missing physics or inappropriate assumptions.

Derivation of Spring Model

Newtonian Principles: Balance forces using Newton's second law

- External Force: $f(t)$
- Spring Force: $F_s(t) = -ky(t)$
- Damping Force: $F_d(t) = -c\frac{dy}{dt}$



Newton's Second Law: $m\frac{d^2y}{dt^2} = F_s(t) + F_d(t) + f(t)$

Spring Model: $m\frac{d^2y}{dt^2} + c\frac{dy}{dt} + ky = f$

Initial Conditions: $y(0) = y_0 \ , \ \frac{dy}{dt}(0) = v_0$

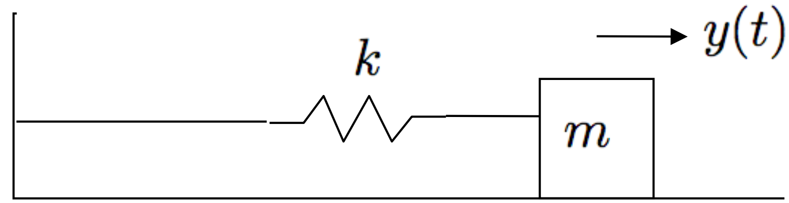
Note: Details regarding classical mechanics can be found in Appendix C of the supplemental material.

Derivation of Spring Model

Lagrangian Principles: Take $c = f = 0$

- Kinetic Energy: $K(\dot{y}) = \frac{1}{2}m\dot{y}^2$

- Potential Energy: $$U(y) = \int_0^y kx\,dx = \frac{1}{2}ky^2$$



- Lagrangian: $$\mathcal{L}(y, \dot{y}, t) = K(\dot{y}) - U(y) = \frac{1}{2}m\dot{y}^2 - \frac{1}{2}ky^2$$

- Euler-Lagrange Equations: $$\frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \dot{y}} - \frac{\partial \mathcal{L}}{dy} = 0$$ $$\Rightarrow m\ddot{y} + ky = 0$$

Note: Details regarding calculus of variation and Lagrangian and Hamiltonian principles can be found in Appendix C of the supplemental material.

Analytic Solution of the Spring Model

Second-Order Model:

$$m\frac{d^2y}{dt^2} + c\frac{dy}{dt} + ky = f$$

$$y(0) = y_0 \ , \ \frac{dy}{dt}(0) = v_0$$

Homogeneous Model: $f(t) = 0$

- Solve characteristic equation to obtain homogeneous solution $y_h(t)$
- Eigenvalue solutions of first-order system

Nonhomogeneous Model:

- Obtain particular solution $y_p(t)$ and general solution $y(t) = y_h(t) + y_p(t)$
  - Method of undetermined coefficients: e.g., $f(t) = \cos(\omega t)$
  - Variation of parameters: e.g., $f(t) = \ln t$
- Laplace transform: e.g., $f(t) = \delta(t - t_0)$

Analytic Solution of the Spring Model

First-Order System: Take $z_1 = y, z_2 = \dot{y}$

$$\Rightarrow \begin{bmatrix} \dot{z}_1 \\ z_2 \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ -k/m & -c/m \end{bmatrix} \begin{bmatrix} z_1 \\ z_2 \end{bmatrix} + \begin{bmatrix} 0 \\ f(t)/m \end{bmatrix}$$

$$\Rightarrow \dot{z}(t) = Az(t) + F(t)$$

Initial Condition: $z(0) = z_0$

Analytic Solution:

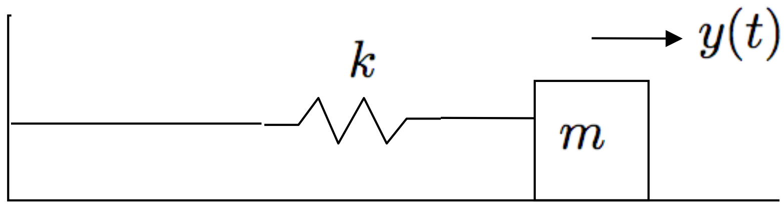
$$z(t) = e^{At} z_0 + \int_0^t e^{A(t-s)} F(s) ds$$

Importance:

- Analytic solution techniques
- Numerical approximation
- Control design

Analytic Solution of the Spring Model

Example: Take $c = f = 0$



$$y(t) = e^{rt} \Rightarrow mr^2 + k = 0$$

$$\Rightarrow r = \pm i\sqrt{k/m}$$

$$\Rightarrow y(t) = A\cos(\omega_0 t) + B\sin(\omega_0 t)\ ,\ \omega_0 = \sqrt{k/m}$$

- Eigenvalues and eigenvectors of A

$$\lambda_{1,2} = \pm i\sqrt{k/m} \qquad v_{1,2} = \begin{bmatrix} \pm 1 \\ i\sqrt{k/m} \end{bmatrix}$$

- Solution

$$z(t) = A\begin{bmatrix} \cos\omega_0 t \\ -\omega_0\sin\omega_0 t \end{bmatrix} + B\begin{bmatrix} \sin\omega_0 t \\ \omega_0\cos\omega_0 t \end{bmatrix}$$

Numerical Solution of the Spring Model

Consider First-Order System:

$$\Rightarrow \begin{bmatrix} \dot{z}_1 \\ z_2 \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ -k/m & -c/m \end{bmatrix} \begin{bmatrix} z_1 \\ z_2 \end{bmatrix} + \begin{bmatrix} 0 \\ f(t)/m \end{bmatrix}$$

$$\Rightarrow \dot{z}(t) = Az(t) + F(t)$$

$$z(0) = z_0$$

Note: See notes for initial value problems (IVP)