Lecture 7 (Modeling), Outline

- **Model building**
- **Constitutive and conservation equations**
- **Examples from biology, epidemiology, physics, chemistry and electrical engineering**

SUGGESTED READING:

M. Tenenbaum and H. Pollard, Ordinary Differential Equations

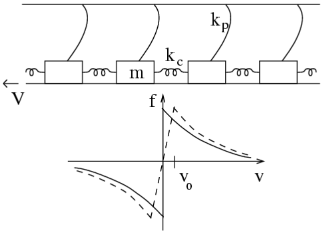
A **mathematical model** is a complete and consistent set of mathematical equations used to represent a physical process.
The steps involved in a mathematical simulation of a physical process are:

1. formulation of the mathematical model,
2. scaling and simplification of the model equations,
3. solution of the mathematical equations by analytical, approximate or numerical methods,
4. interpretation of the solution and its empirical verification.

When **building a model**, start with the simplest approach that captures the essential physics, rather than trying to reproduce detailed nature.

Introductory example

Example from geophysics: EARTHQUAKES



Empirically observed power law: $P(M) = am^{-b}$, where $M \equiv \log m$ is the magnitude of the quake, m is its moment (proportional to energy released), a and b are constants and $P(M)$ is the probability of the quake of magnitude M occurring.
This simple mechanical model captures the observed power law.

Definitions

Dependent variables are properties of the system that are of interest, they can be functions of the independent variables — e.g the mass of the system or concentration of reactant or the temperature.

Idependent variables are the variables that describe the evolution or extent of the system under investigation – e.g. time or spatial coordinate variables.

The decision ultimately lies within the discretion of the individual; the choice will usually be determined by convenience.

Classification

Ordinary Differential Equations: only one independent variable

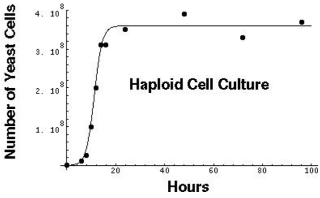
- **Initial-Value Problem:** State of system is specified at some initial time
- **Boundary-Value Problem:** State of system is specified at system boundaries

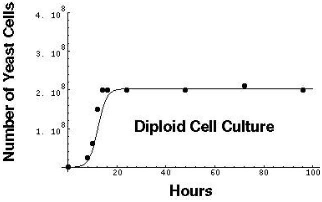
Partial Differential Equations: more than one independent variable

Algebraic Equations: no independent variable; involve only relations between dependent variables

Population Growth: Malthusian vs Logistic eqns

The growth pattern of a bacterial culture follows a regular pattern: there is an initial lag phase, followed by a period of exponential growth. However, as the population of bacteria increases, beyond a certain point, nutrients become limiting (or waste products that limit growth increase) and the culture enters a stationary growth phase.





- Malthusian law:
  $\frac{dN}{dt} = rN \Rightarrow N = N_0 e^{rt}$ (isolated, no competition for resources)
- Logistic equation:
  $\frac{dN}{dt} = rN(1 - N) \Rightarrow N = \frac{N_0 e^{rt}}{1+N_0(e^{rt}-1)}$ (number of encounters $\propto N^2$)

Radioactive Decay

In the atmosphere and living organisms, the ratio of radioactive carbon $_6C^{14}$ to ordinary carbon $_6C^{12}$ is constant.After an organism's death, $_6C^{14}$ begins to decay according to first-order kinetics (**assumption!**), whereas the amount of stable $_6C^{12}$ remains constant. If this carbon ratio $y(t)$ is found to be 10% of its initial value in a fossilized bone, how old is it (half-life of $_6C^{14}$ is 5,715 years)?

$$\begin{aligned} \frac{dy}{dt} &= ky \\ \Rightarrow y(t) &= y_0 e^{kt} \\ \Rightarrow t &= \frac{1}{k} \ln \frac{y(t)}{y_0} \end{aligned}$$

For carbon-14: $y(t_{1/2})/y_0 = 1/2$ at $t = t_{1/2} = 5715$ years

$$\Rightarrow k = -\frac{\ln 2}{5715} = -1.213 \times 10^{-4} \text{year}^{-1}$$

$$\text{Age of fossil } t = -(1.213 \times 10^{-4})^{-1} \cdot \ln 0.1 = 19000 \text{ years}$$

Newton's law of cooling (an interfacial BC)

The rate at which the temperature of a body changes is proportional to the difference between the temperature of the body and the temperature of the surrounding medium (ambient temperature).If T(t) represents the temperature of the body at time t and T_a the ambient temperature:

$$\frac{dT}{dt} = -k(T - T_a)$$

where k is a constant of proportionality

Problem: How long will it take a cup of coffee at 185^0F to cool to a drinkable temperature of 143^0 F, if it's temperature after 50 s is 181.2^0F, and the ambient T is 68^0F.

Solution: $k = 6.603 \times 10^{-4}$ s^{-1} and t=674 s.

A simple model for the rate of spread of an infectious disease is that it is proportional to the number of encounters between infected and non-infected people.If y(t) is the number of infected people, and x(t) is the number of people who have not yet been exposed, then:

$$\frac{dy}{dt} = kxy$$

k is a proportionality constant that reflects the contagiousness of the diseases and safety measures practiced.

Problem: If ten students returning from the winter break to an isolated college of 1000 students have a flu virus, how long before half the students have been infected, for k=10^{-4} day^{-1}.

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$$\frac{dy}{dt} = 10^{-4} y(1000 - y) \qquad y(0) = 10$$

$$\Rightarrow \int dt = 10^4 \int \frac{dy}{y(1000-y)} = 10 \left[\int \frac{dy}{y} + \int \frac{dy}{1000-y} \right]$$

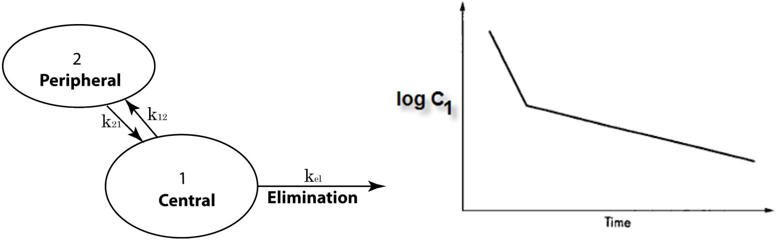
$$\Rightarrow t = 10 \ln \frac{y}{1000-y} + c$$

$$t = 10 \ln \frac{99y}{1000-y} \qquad \text{using } y(t=0) = 10$$

About 46 days for 50% infection.

Two-compartment Pharmacokinetic models

- a lumped parameters model



Compartment 1 (central) blood and well perfused organs, e.g. liver, kidney, etc. ("plasma")

Compartment 2 (peripheral) poorly perfused tissues, e.g. muscle, lean tissue, fat ("tissue")

$$\left.\begin{aligned} \frac{dC_1}{dt} &= k_{21}C_2 - k_{12}C_1 - k_{el}C_1 \\ \frac{dC_2}{dt} &= k_{12}C_1 - k_{21}C_2 \end{aligned}\right\} \dot{C} = KC$$

Conservation equations (fundamental):

$$\underbrace{\textbf{Accumulation}}_{\frac{db}{dt}} = \underbrace{\textbf{Input - Output}}_{-\nabla \cdot F} + \underbrace{\textbf{Generation- Consumption}}_{S},$$

where b is the concentration of some quantity, F is the flux (rate of transport of that quantity per unit area), and S is the generation/consumption term.

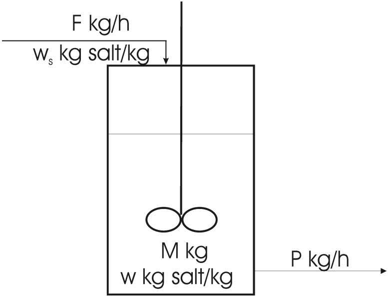
Constitutive equations (empirical) relate fluxes to local material properties, e.g.:

$$q = -k\nabla T \text{ (Fourier Law)}$$
$$J = -D\nabla C \text{ (Fick's Law)},$$

where q and J are heat flux and molar flux, constants k and D are conductivity and diffusivity, T and C are temperature and molar concentration.

Initial-Value ODE Problem—Filling of a tank

A well stirred tank is being filled with a salt solution of weight fraction w_s at a rate of F kg/h and product is being removed at a rate of P kg/h. If the tank initially contains M_0 kg of water with salt concentration w_0, obtain a mathematical model of the process that describes the rate of change of the mass of solution M and salt concentration w in the tank.



The dependent variables of interest are the total mass and salt concentration of liquid in the tank. Hence, conservation balances are written for the total mass of liquid and mass of salt:

$$\underbrace{\frac{dM}{dt}}_{\text{Accumulation}} = \underbrace{F}_{\text{Input}} - \underbrace{P}_{\text{Output}}$$

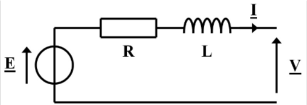
$$\frac{d(Mw)}{dt} = Fw_s - Pw$$

$$M(t=0) = M_0 \qquad w(t=0) = w_0$$

We have two differential equations in seven variables: M, F, P, w, w_s, w_0, M_0. This can be solved if five of the variables are specified,e.g. F=10 kg/h, P=5 kg/h, w_s=0.1 kg salt/kg, as well as the initial conditions for the differential equations: M_0=100 kg, w(t=0)=w_0=0 (pure water).

Linear electric circuit

- RL circuit



2nd Kirchhoff's Law:

$$L\frac{di}{dt} + Ri = E,$$

where R is the resistance of resistor, L is the inductance of inductor and E is the emf of the energy source. Using the relationship between current i and charge $q, i = \frac{dq}{dt}$, we have

$$L\frac{d^2q}{dt^2} + R\frac{dq}{dt} = E$$