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1 Dynamic systems modeling

System: a potential source o data

- boundary
- inputs / outputs

Experiments: Extracting data from a system

- apply condition to input and observe outputs (Obeservability / Controlability)

Model: of a system and an experiment is anything to which exp can be applied. This is results in an experimental frame of the model. A model in the general case doesn't need to be mathematical or computational. No model is valid for all experiments but the system itself. The purpose of modeling is to simply. "All models are wrong but some of them are useful"

Simulation: Perform the experiment on the model.

Continuity:

- Discrete and Deterministic (Molecular Dynamics)
- Continuous and Deterministic (Partial differential equations)
- Discrete and Stochastic (Agent based models)
- Continuous and Stochastic (Stochastic differential equations)

The continuum limit assumes the changes of a single molecular does not matter for the overall concentration in the region of the length scale λ. The length scale L field gradients are established

$$\mathrm{Kn} := \frac{\lambda}{L} \tag{1.1}$$

If $\mathrm{Kn} << 1$ the continuum assumption is justified.

Extensive quantities: depend on the system size.(Mass, Volume, molecules ...)
Intensive quantities: do not depend on the system size (Temperature, concentration ...).

Differential equations are always expressed in terms of intensive quantities in simulation needs to use extensive quantities. This is not necessary but helpful to design the simulation experiment properly.

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Dimensional Analysis:

- dependence of variables (Which are the important variables?)
- orders of magnitude
- Model - System similitude (Where show model and system same dynamics?)

Dim: Mass, length, time, force, ...
Units: kg, lb ...

Theorem:
All dimensions are power series of 6 basic dimensions.

- mass M
- length L
- time T
- temperature θ
- charge C
- resistance R

Example: $force = M^1 L^1 T^{-1}$

Buckingham Theorem:
If n is the number of basic dimensions and p variables of a system. The system is completely described by p-n dimensionless groupings.
Example:
A force acting on a point mass in vacuum:
$n = 3(\mathrm{M, L, T})$
$p = 4(\mathrm{m, F, t, v})$
Therefore, the system is described by a single dimensionless quantity.

All physical equations are dimensionally homogeneous: $A + B = C$. The dimensions of A, B and C needs to be the same.

Taylor (1979) proposed and algorithm to find the dimensionless groupings of a system.
Example:
Shear stress on red blood cell traveling with a velocity u though an artery. If the shear stress τ is to hight the blood cell would be destroyed. The shear stress then depends on the distance from the wall h, the viscosity η, the density ρ and the velocity u.

$n = 3(M, L, T)$
$p = 4(\eta, \rho, h, \tau, u)$

$$
\begin{array}{c|ccc}
 & M & L & T \\ \hline
h & 0 & 1 & 0 \\
u & 0 & 1 & -1 \\
\eta & 1 & -1 & -1 \\
\rho & 1 & -3 & 0 \\
\tau & 1 & -1 & -2
\end{array}
\rightarrow
\begin{array}{c|ccc}
 & M & L & T \\ \hline
h & 0 & 1 & 0 \\
u & 0 & 1 & -1 \\
\eta & 0 & 2 & -1 \\
\rho & 1 & -3 & 0 \\
\tau & 0 & 2 & -2
\end{array}
\rightarrow
\begin{array}{c|cc}
 & L & T \\ \hline
h & 1 & 0 \\
u & 1 & -1 \\
\eta/\rho u & 1 & 0 \\
\tau/\rho u^2 & 0 & 0
\end{array}
\rightarrow
\begin{array}{c|c}
 & L \\ \hline
\eta/\rho u h & 0 \\
\tau/\rho u^2 & 0
\end{array}
\tag{1.2}
$$

The dimensionless numbers are then $\Pi_1 = \frac{\eta}{\rho u h}$ and $\Pi_1 = \frac{\tau}{\rho u^2}$.
We also know that: $\Pi_1 = f(\Pi_2)$ this helps us to design an experiment because only the dimensionless numbers need to be varied to understand the function the relates Π_1 and Π_2

Modeling Dynamics:

1) Define the system boundaries and the input and outputs
2) Identify reservoirs (for any quantity) of relevant time scales
3) Formulate equations for the flows to the reservoirs.
All flows have the form $flow = f(activatinglevel - inhibitinglevel)$.
4) Formulate the balance equations for the reservoirs. $\frac{d}{dt}level = \sum inflows - \sum outflows$ 5) Simplify the system of equations
6) Solving the systems will give $level(t)$
7) Identify unknown parameters based on the given data
8) Validate the model. Prove that the model can predict another experiment!

2 Recap of vector calculus

3 Spatiotemporal models

Control volumes:
Discretization of space into finite small volumes. Considering that the control volumes can vary with time the rate of change of the intensive variable f. For being the density $f = m/V$:

$$\frac{df}{dt} = \frac{1}{V}\frac{dm}{dt} + \frac{m}{V}\frac{1}{V}\left(-\frac{dV}{dt}\right) \tag{3.1}$$

Fixes control volumes / Eulerian :
When using fixed control volumes the flow between the control volumes V_i is define by the field derivative:

$$\frac{\partial f(x,t)}{\partial t}|_{x=const} = D\nabla^2 f - \nabla \cdot (f \cdot \mathbf{v}(\mathbf{r}, t)) + k(f) \tag{3.2}$$

Co-moving control volume / Lagrangian:
When considering moving volumes the flow of the intensive quantity is given by the material

derivative:

$$\frac{\mathrm{d}f}{\mathrm{d}t} = \frac{\partial}{\partial t}\left[f(\mathbf{r}(r), t)\right] = \nabla f \cdot \frac{\partial \mathbf{r}(t)}{\partial t} + \frac{\partial f}{\partial t} \tag{3.3}$$

For considering mass conservation:

$$m = \int f \mathrm{d}V \tag{3.4}$$

$$\frac{\mathrm{d}m}{\mathrm{d}t} = 0 \tag{3.5}$$

Inserting the derivative above leads to the Reynolds transport theorem:

$$\frac{\mathrm{d}m}{\mathrm{d}t} = \int_V \frac{\partial f}{\partial t}\mathrm{d}V + \int_V f\mathbf{v} \cdot \mathbf{n} dS \tag{3.6}$$

Infinitesimal control volumes: For $V \to 0$ the Conservation:

$$\frac{\mathrm{d}m}{\mathrm{d}t} = 0 \tag{3.7}$$

translate Lagrange to Eulerian:

$$\frac{\mathrm{d}m}{\mathrm{d}t} = \int_V \frac{\partial f}{\partial t}\mathrm{d}V + \int_V f\mathbf{v} \cdot \mathbf{n} dS \tag{3.8}$$

With the field $\mathbf{v}$ Fick's law is defined as:

$$f \cdot \mathbf{v} = -D\nabla f \tag{3.9}$$

Where D is Diffusion tensor with the elements $D_{ij}, [i, j]\{x, y, z\}$ Insertion of the the relations derived above gives:

$$\frac{\mathrm{d}m}{\mathrm{d}t} = \int_V \left[\frac{\partial f}{\partial t} - \nabla(D\nabla f)\right] \mathrm{d}V = 0 \tag{3.10}$$

This relation recovers Fick's second law:

$$\frac{\partial f}{\partial t} = D\Delta f \tag{3.11}$$

Conclusion:
In an Eulerian description the formulation of the advective transport needs to be addressed with the term $-\nabla \cdot (f \cdot \mathbf{v}(\mathbf{r}, t))$. This can be avoided using a Largangian formalism as the convective transport is described by the movement of the control volumes