Conservation Laws

Let $u(\vec{x}, t)$ be the concentration of something at position $\vec{x} \in \Omega$ and time t. For instance

$u \quad = \quad$ mass density of a fluid (gas)

$u \quad = \quad$ chemical concentration

$u \quad = \quad$ population density of an organism

$u \quad = \quad$ ionic concentration

Then at any given instant

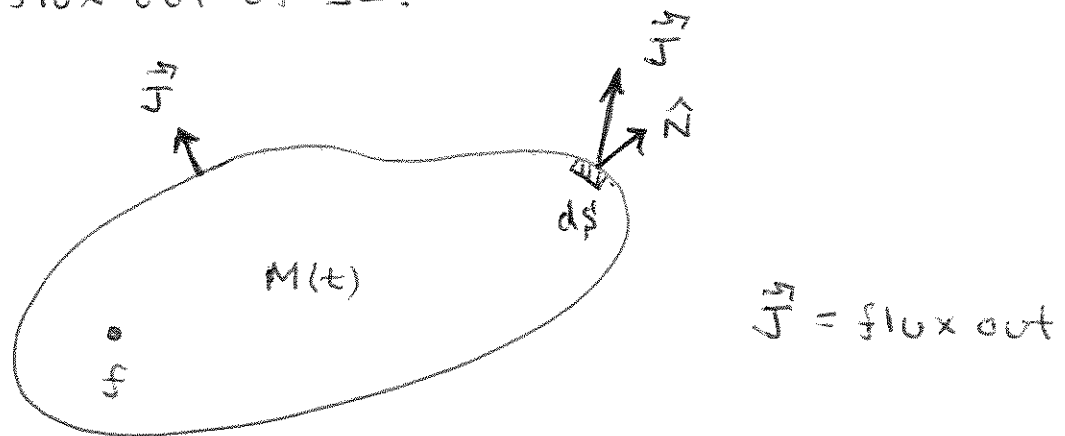$$M(t) \quad = \quad \int_\Omega u(\vec{x}, t) \, d\vec{x}$$

is the total amount at time t. Here M could be total mass, population or net charge

Let

$\vec{J} \quad = \quad$ flux of u at $\vec{x} \in \Omega$

$f \quad = \quad$ internal sources or sinks of u at $\vec{x}$. For instance if u is a chemical concentration $f(\vec{x}, t, u)$ is the local production rate per unit volume

If u is conserved the rate of change of M must balance the rate of production and flux out of Ω.

For <u>any domain</u> Ω

$$\frac{d}{dt} \int_\Omega u(\vec{x},t)\,d\vec{x} = - \int_{\partial\Omega} \vec{J}\cdot\hat{N}\,dS + \int_\Omega f(\vec{x},t,u)\,d\vec{x}$$

where the minus sign indicates a flux out.

Assuming u is sufficiently smooth and applying the Divergence theorem

$$\int_\Omega \frac{\partial u}{\partial t}\,d\vec{x} = - \int_\Omega \vec{\nabla}\cdot\vec{J}\,d\vec{x} + \int_\Omega f(\vec{x},t,u)\,d\vec{x}$$

If the integrands are continuous then since the <u>domain is arbitrary</u> the integrands on each side must match:

$$(1) \quad \boxed{\frac{\partial u}{\partial t} = -\vec{\nabla} \cdot \vec{J} + f(\vec{x}, t, u)}$$

Differential form of conservation law.

Functional forms for $\vec{J}$ and f are assumptions based off "constitutive laws".

A constituitive law is a measured or assumed mathematical relationship between physical quantities.

For instance, the ideal gas law

$$PV = nRT$$

may be viewed as a "constituitive law".

Generally for models there may be many different kinds of fluxes and sources so that (1) becomes

$$u_t = -\sum_{i=1}^{N} \vec{\nabla} \cdot \vec{J}_i + \sum_{j=1}^{M} f_j(\vec{x}, t, u)$$
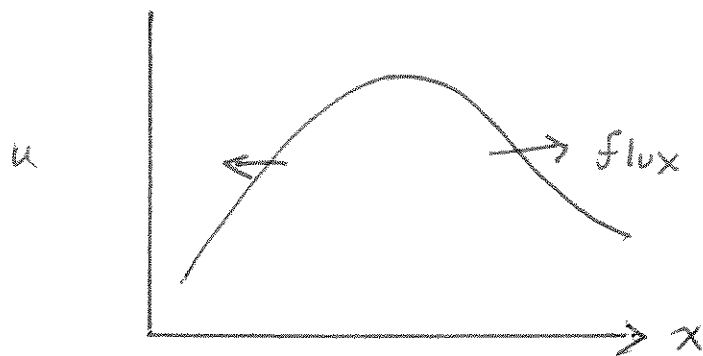
EXAMPLE   Diffusion

Let u = concentration of a substance

(1) $\vec{J} = -D\vec{\nabla}u$ Fick's Law

is an assumed law for the flux. Here
D is the <u>diffusivity</u> of the substance
in the medium.

        $\vec{\nabla}u$ = direction u ↑ most rapidly

Thus flux in (1) indicates substance
moves in direction u decreasing
most rapidly

In some media D depends on $\vec{x}$.

Large molecules typically have a small D.

Spatial dependence of D on $\vec{x}$ may be
due to the medium is not homogeneous
(perhaps stratified in some manner)

If one assumes $\vec{J} = -D(\vec{x})\vec{\nabla}u$ in the conservation equation we arrive at

$$(2) \qquad \frac{\partial u}{\partial t} = \vec{\nabla} \cdot (D(\vec{x})\vec{\nabla}u)$$

and when $D > 0$ is constant, eqn (2) becomes the <u>diffusion eqn</u>

$$(3) \qquad u_t = D\vec{\nabla}^2 u \qquad\qquad \vec{x} \in \Omega,\ t > 0$$

with sources present

$$(4) \qquad u_t = D\vec{\nabla}^2 u \quad + f(\vec{x}, t, u)$$

is a <u>reaction-diffusion equation</u>

<u>Remarks on units:</u>

Let M, L, T be mass, time and length.

$$[u] = ML^{-3}$$

$$[u_{xx}] = ML^{-5}$$

Thus since $[u_t] = [D][\vec{\nabla}^2 u]$ we have

$$[D] = L^2 T^{-1}$$

$$[\vec{J}] = ML^{-2}T^{-1}$$

EXAMPLE   Heat Eqn (Thermal Transport)

$$\vec{T}(\vec{x}, t) = \text{temperature} \qquad [T] = °$$

$$u(\vec{x}, t) = \text{energy density} \qquad [u] = J/m^3$$

$$\rho = \text{medium density} \qquad [\rho] = kg/m^3$$

$$C = \text{specific heat} \qquad [C] = J/(m-°)$$

$$K = \text{thermal conductivity} \qquad [K] = J/(m\,sec\,°)$$
of medium

Most generally $\underline{K}$, C and ρ could depend on $\vec{x}$. For example the medium insular properties could vary.

Empirical (Constitutive) laws

$$u(\vec{x}, t) \equiv C\rho\, T(\vec{x}, t)$$

$$\vec{J}(x, t) = -\underline{K} \vec{\nabla} T$$

in which case

$$C\rho\, T_t = \nabla \cdot (\underline{K} \vec{\nabla} T) + f$$

If $C, \rho, \underline{K}$ are constant

$$\frac{\partial T}{\partial t} = D \nabla^2 T + F(\vec{x}, t, T) \quad, \quad \vec{x} \in \Omega$$

is a PDE whose solution yields the spatiotemporal variations of temperature

$$D = \frac{K}{C\rho} \qquad\qquad F = \frac{f}{C\rho}$$

EXAMPLE   Advection/Diffusion

$$\vec{J}_{Diff} = -D(x)\vec{\nabla}u \qquad\qquad Diffusion$$

$$\vec{J}_{Adv} = +u\,\vec{v}(\vec{x}) \qquad\qquad Advection$$

where $D =$ diffusivity and $\vec{v}(\vec{x})$ is the velocity of the fluid that u is in.

Conservation of u implies

$$u_t = \vec{\nabla}\cdot(D(x)\vec{\nabla}u) - \vec{\nabla}\cdot(\vec{v}u) + f$$

Is a reaction-diffusion-advection eqn.

If D, are constant

$$u_t = D\nabla^2 u - \vec{v}\cdot\vec{\nabla}u + f$$

which in one dimensional spatial domain becomes

$$u_t = Du_{xx} - vu_x + f$$

Remark   For diffusion the "$-$" sign is needed for u to move toward lower concentrations

For advection the "$+$" sign implies u moves along with the fluid flow
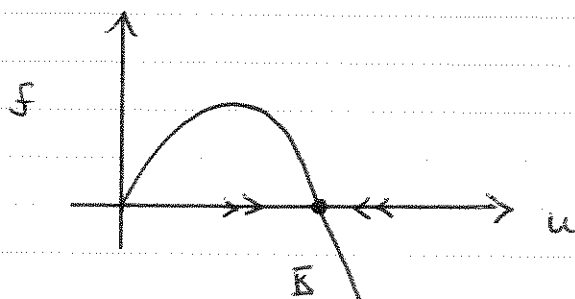
EXAMPLE   Population Models

$$u(\vec{x}, t) = \text{population density at } \vec{x} \in \Omega.$$

Notion of density works better for bacteria or cells. Could be trees, etc.

Logistic source term

$$f(u) = ru\left(1 - \frac{u}{K}\right)$$

where K = carrying capacity of environment.

Fact $f(u) < 0$ for $u > K$ meant to reflect death due to overcrowding (competition)

Other source terms

Suppose a substance $c(\vec{x}, t)$ is the primary food source.

$$f = f(u, c)$$

may have the generic property $f_c > 0$ to reflect (bacterial) birth rate is higher if c is larger. Perhaps

$$f(u, c) = \eta \frac{uc}{c + K} \qquad \eta, K \in \mathbb{R}$$

Constitutive laws for organism movement

$$\vec{J} = -D\,\vec{\nabla} u \qquad\qquad \text{Diffusive (random)}$$

$$\vec{J} = +u\,\vec{v} \qquad\qquad \text{Advection}$$

$$\vec{J} = +\alpha u\,\vec{\nabla} c \qquad\qquad \text{Chemotaxis}$$

$$\vec{J} = +\alpha u\,\vec{\nabla} T \qquad\qquad \text{Thermotaxis}$$

where $\vec{v}$ = fluid velocity, c = food concentration, T = temperature

Some bacteria are chemotactic. They tend to move toward food.

Slime mold and nematodes are thermotactic

MODEL ONE

$$\frac{\partial u}{\partial t} = D_1 \nabla^2 u + f_1(u, c)$$

$$\frac{\partial c}{\partial t} = D_2 \nabla^2 c + f_2(u, c)$$

Both organism and food diffuse through homogeneous medium.

$$f_1 > 0 \qquad \frac{\partial f_1}{\partial c} > 0$$

and f_2 reflects a loss of c that u eats.

MODEL TWO (Logistic)

$$\vec{J} = -D\vec{\nabla}u \qquad\qquad D \in \mathbb{R}^+ \text{ const.}$$

$$f = ru(1 - \frac{u}{K})$$

yields in one spatial domain

$$u_t = Du_{xx} + ru(1 - \frac{u}{K})$$

MODEL THREE (very slow fluid flow)

$$\vec{J}_1 = -D_1\vec{\nabla}u \qquad\qquad D \in \mathbb{R}^+ \text{ const.}$$

$$\vec{J}_2 = +\alpha u\vec{\nabla}c \qquad\qquad \alpha \in \mathbb{R}^+ \text{ const}$$

and certain source terms f_k. Conservation law implies

$$(1) \qquad \frac{\partial u}{\partial t} = -\vec{\nabla}\cdot\vec{J}_1 - \vec{\nabla}\cdot\vec{J}_2 + f_1$$

If c merely diffuses we obtain coupled equations for u, c

$$(2) \qquad \frac{\partial u}{\partial t} = \underbrace{D_1\vec{\nabla}^2 u}_{\text{diff}} - \underbrace{\alpha\vec{\nabla}\cdot(u\vec{\nabla}c)}_{\text{chemotaxis}} + f_1$$

$$(3) \qquad \frac{\partial c}{\partial t} = D_2\vec{\nabla}^2 c \qquad\qquad\qquad + f_2$$

For $\Omega \subset \mathbb{R}$ eqn (2) would be

$$u_t = D_1 u_{xx} - \alpha(uc_x)_x + f_1$$

EXAMPLE   Electro Diffusion

Charged particles diffuse through
a medium having electric field
$\vec{E}(\vec{x})$.

$$u(\vec{x}, t) = \text{charge density}$$

Ohmic flux law

$$\vec{J} = z\sigma\vec{E} \qquad\qquad z = \text{valence}$$

and σ is conductivity (generally a
matrix for anisotropic non homogeneous
media)

If the electric field is given by

$$\vec{E} = -\vec{\nabla}\phi$$

where ϕ is the electric potential
one obtains

$$\frac{\partial u}{\partial t} = \underbrace{D\nabla^2 u}_{\text{diff}} + \underbrace{z\sigma\nabla^2\phi}_{\text{electric}}$$

The eqn for ϕ is obtained using Maxwell's
eqn. Steady state version is

$$0 = D\nabla^2 u + z\sigma\nabla^2\phi$$

$$-\beta u = \nabla^2\phi \qquad\qquad (\vec{\nabla}\cdot\vec{E} = 4\pi\rho)$$

for an appropriate constant β