Mathematical models of physical processes

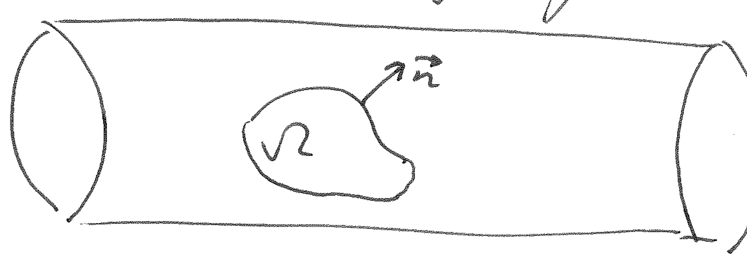
Physical processes $\rightarrow$ physical laws $\rightarrow$ mathematical assumptions

$\rightarrow$ mathematical model (PDE)

Gas dynamics $\rightarrow$ flow of gas in a large container

Denote $\rho(x,t)$ density of gas, $v(x,t)$ velocity $\Big\}$ at time t and location x.

Let Ω denote an arbitrary region in the container



Mass of ~~g~~ substance (gas) in Ω at time t

$$m(t) = \int_\Omega \rho(x,t)\,dx$$

Rate of change of mass in Ω

= rate of mass flow over the boundary $\partial\Omega$ + $\boxed{\text{rate of mass put in / taken out of } \Omega}$

assume is zero.

flux of mass per unit time per unit surface area $F(x,t) = \rho(x,t)\, v(x,t)$ → vector

$$\boxed{m'(t) = -\int_{\partial\Omega} F\cdot\vec{n}\, ds} = -\int_{\Omega} \operatorname{div} F\, dx .$$

$$\boxed{\frac{d}{dt}\int_{\Omega} \rho\, dx = -\int_{\Omega} \operatorname{div} F\, dx}$$

integral form of the conservation of mass

$$\boxed{\rho_t + \operatorname{div}(\rho v) = 0}$$ continuity equation

differential form of the conservation of mass

if $v(x,t) \equiv v(t)$ (i.e. v is constant in space (homogeneous flow))

then $\operatorname{div}(\rho v) = (\nabla\rho)\cdot v$

and we have $\boxed{\rho_t + v\cdot\nabla\rho = 0}$ transport equation

in 1-D: $\rho_t + v\rho_x = 0$

with solution $\underline{\rho(x,t) = \phi(x - vt)}$

Heat equation : model the time evolution of the temperature distribution of an object.

Temperature $\leftrightarrow$ heat $\leftrightarrow$ energy

Use conservation of thermal energy

Let Ω an arbitrary region (bounded, open, connected set)

Let $e(x,t)$ = thermal energy density

Thermal energy in Ω	Rate of change
$\int_\Omega e(x,t)\,dx$	$\frac{d}{dt}\int_\Omega e\,dx = -\int_{\partial\Omega} \phi\cdot n + \int_\Omega f\,dx$

where $\phi(x,t)$ = flux of energy vector per unit area per unit time

$f(x,t)$ = thermal energy source / sink per unit time per unit volume

Conservation of thermal energy

$$\left.\begin{array}{c} \int_\Omega \left[e_t + \operatorname{div}\phi - f\right]dx = 0 \\ \Omega \text{ arbitrary region} \end{array}\right\}$$

$$\Rightarrow \boxed{e_t + \operatorname{div}\phi = f}$$ differential form of the conservation law

$$\boxed{e(x,t) = \rho(x)\, c(x)\, u(x,t)}$$

$\rho(x)$ = material density

$c(x)$ = specific heat

$u(x,t)$ = object temperature

Fourier's law $\boxed{\phi(x,t) = -K \cdot \nabla u}$

where $K > 0$ is the <u>thermal conductivity</u> coefficient

Then $\boxed{\rho c u_t = \operatorname{div}(K \nabla u) + f}$

if ρ, c, K are constants

$$u_t = k \Delta u + Q, \qquad \boxed{k = \frac{K}{\rho c} = \text{thermal diffusivity}}$$

Equilibrium

$Q=0$: $\boxed{\Delta u = 0}$ Laplace's equation

$\boxed{-\Delta u = Q}$ Poisson's equation

<u>Diffusion - dispersion processes</u>

Model time-space evolution of the concentration (density) of pollutant in the atmosphere.

$\rho(x,t)$

Mass conservation: $\boxed{\rho_t + \operatorname{div} \phi = 0}$.

$\phi(x,t)$ = concentration flux vector

<u>Fick's law of diffusion</u> $\boxed{\phi = -D\nabla\rho + \rho v}$

where $v = (v_1, v_2, v_3)$ is the wind field vector and it is assumed to be known

$D > 0$ is the diffusion coefficient

PDE model
if D = constant $\boxed{\rho_t = D\Delta\rho - \operatorname{div}(\rho v)}$ diffusion-dispersion

if v is constant

$$\boxed{\rho_t + v\cdot\nabla\rho - D\Delta\rho = 0}$$ advection-diffusion equation.

initial conditions $\quad u(x,0) = u_0(x)$

Boundary conditions (heat equation)

→ prescribed values (Dirichlet, first kind)

$$u(x,t) = g(x,t), \quad x \in \Gamma, \quad t > 0.$$

→ prescribed flux (Neumann, second kind)

$$\phi \cdot n = f(x,t) \quad : \quad -K\nabla u \cdot n = f$$

in particular, insulated boundary $\frac{\partial u}{\partial n} = 0$

→ Robin (Third kind)

$$\phi \cdot n = h(u - \tilde{u})$$

$$-K\nabla u \cdot n = h(u - \tilde{u})$$

(Newton's law of cooling)

Exercise: Let $\Omega \subset \mathbb{R}^n$ open, bounded domain

Show that

$$\begin{cases} u_t = \operatorname{div}(K\nabla u) + Q & \text{in } \Omega \\ u|_{\Gamma_1} = f \\ -K\nabla u \cdot n|_{\Gamma_2} = g \\ u(x,0) = u_0(x) \end{cases}$$

has at most one solution.

Nonlinear PDEs

Gas dynamics (revised)

Continuity equation $\boxed{\rho_t + \operatorname{div}(\rho v) = 0}$

if the velocity vector v is not known we need to model its evolution.

→ use Newton's second law $f = ma$

→ conservation of momentum : mv

For an arbitrary region Ω, the total momentum in Ω is

$$\int_\Omega \rho(x,t)\, v(x,t)\, dx \quad \to \text{vector}$$

Then, conservation law :

$$\boxed{\frac{d}{dt}\int_\Omega \rho(x,t)\, v(x,t)\, dx = F - \underbrace{\int_{\partial\Omega} (\rho v)\, v\cdot n\, ds}_{\text{momentum flux (rate of flow) over the boundary}}}$$

vector equality $v = (v_1, v_2, v_3)$

forces

Forces that act on Ω : $F = F_1 + F_2$

F_1 = body forces → act on particles in Ω

F_2 = surface forces → act on the boundary $\partial\Omega$

Assume that the only body forces are due to gravity

$$F_1 = -\int_\Omega \rho \vec{g}\, dx \quad , \text{ where } \vec{g} = (0, 0, g)$$

positive direction for x_3 is upward

Surface forces per unit area are given by the pressure $p(x,t)$ acting normal to $\partial\Omega$

$\vec{P} = p\vec{n}$ where p is scalar (magnitude) and $\vec{n}$ is the direction (normal unit outward vector)

$$F_2 = -\int_{\partial\Omega} p\vec{n}\, ds = -\int_\Omega \nabla p\, dx$$

→ movement takes place from high pressure to low pressure.

"−" sign: if $p > 0$ then outside pressure is lower so loss of momentum.

Conservation of momentum law:

$$\boxed{\frac{d}{dt}\int_\Omega \rho v\, dx = -\int_{\partial\Omega} (\rho v)\, v\cdot n\, ds - \int_\Omega \rho \vec{g}\, dx - \int_\Omega \nabla p\, dx}$$

Componentwise,

$$\int_\Omega (\rho v_i)_t \, dx = -\int_{\partial\Omega} \rho v_i \, v\cdot n \, ds - \int_\Omega \rho g_i - \int_\Omega p_{x_i}$$

$$\int_\Omega (\rho v_i)_t = -\int_\Omega \operatorname{div}(\rho v_i v)\, dx - \int_\Omega \rho g_i \, dx - \int_\Omega p_{x_i}$$

$$\boxed{(\rho v_i)_t + \operatorname{div}(\rho v_i v) + p_{x_i} = -\rho g_i , \quad i=1,2,3}$$

Continuity equation: $\rho_t + \operatorname{div}(\rho v) = 0$.

$$\Rightarrow \quad \rho v_{i,t} + \rho v\cdot\nabla v_i + p_{x_i} = -\rho g_i$$

Vector equation: (3 equations for conservation of momentum)

$$\boxed{\rho\left[v_t + (v\cdot\nabla) v\right] + \nabla p = -\rho \vec{g}}$$

We have 4 equations $\to$ 1 continuity, $\to$ 3 momentum

and 5 unknowns: $\rho, p, v = (v_1, v_2, v_3)$.

We need additional information about the gas itself.

Equation of state for the gas

$$\frac{p}{p_0} = \left(\frac{\rho}{\rho_0}\right)^{\lambda}, \quad \lambda > 0 \text{ constant}$$

Euler equations An additional equation is provided using conservation of energy

$$E = \underbrace{\rho e}_{\substack{\text{internal}\\ \text{energy}}} + \underbrace{\tfrac{1}{2}\rho(v_1^2 + v_2^2 + v_3^2)}_{\text{Kinetic energy}}$$

e = specific internal energy per unit mass, gas specific, assumed to be known as a function of pressure and density

$$e = e(p, \rho)$$

Conservation of energy: $\boxed{E_t + \operatorname{div}[(E+p)v] = 0}$

→ total energy advects with the flow leading to a flux term Ev

→ in addition, the momentum flux measured by p leads to a flux in Kinetic energy $\rightarrow pv$

if the conservation laws are applied to an incompressible fluid, then $\underline{\rho = \text{constant}}$

Continuity equation $\rho_t + \operatorname{div}(\rho v) = 0$

implies $\boxed{\operatorname{div} v = 0}$

Assume the fluid is viscous (adhesive, sticky)

then

$$\boxed{\begin{aligned} &\operatorname{div} v = 0 \\ &\rho\left[v_t + (v \cdot \nabla) v\right] + \nabla p = \mu \Delta v \end{aligned}}$$

Navier-Stokes equations

<u>Advection-diffusion-reaction systems</u>

→ model chemically reactive pollutants

$A + B \longrightarrow C$

$$\frac{\partial c_i}{\partial t} + \operatorname{div}(v c_i) - D \Delta c_i = f_i(c)$$

where $c = (c_1, \dots, c_s)$ vector of concentrations.

Minimal surface problem

Find $u : \Omega \subset \mathbb{R}^2 \to \mathbb{R}$

$u|_{\partial\Omega} = f$ of minimal surface area.

$$S(u) = \int_\Omega \sqrt{1+|\nabla u|^2} = \int_\Omega \sqrt{1+u_x^2+u_y^2}\, dx\,dy$$

$$\left\{ \begin{array}{l} \min S(u) \\ u|_{\partial\Omega} = f \end{array} \right.$$

$\to$ minimizing function may be expressed as the solution to a B.V.P.

Let $v : \Omega \to \mathbb{R}$, $v|_{\partial\Omega} = 0$, arbitrary.

Then $u + \varepsilon v$ is admissible function

if u is the minimizer then $\varepsilon = 0$ is min point to

$$g(\varepsilon) = S(u+\varepsilon v)$$

$$g'(\varepsilon) = \int_\Omega \frac{(u_x+\varepsilon v_x)v_x + (u_y+\varepsilon v_y)v_y}{\sqrt{1+|\nabla(u+\varepsilon v)|^2}}\, dx\,dy.$$

$$g'(0) = \int_\Omega \frac{u_x v_x + u_y v_y}{\sqrt{1+|\nabla u|^2}}\, dx\,dy = \int_\Omega \frac{\nabla u \cdot \nabla v}{\sqrt{1+|\nabla u|^2}}$$

Remark : $\int_\Omega \operatorname{div}(F(u)v) = \int_\Omega F(u)\cdot\nabla v + v \operatorname{div} F(u)$.

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$$\int_{\partial\Omega} v F(u)\cdot n = 0 \quad \text{iff} \quad v\big|_{\partial\Omega} = 0.$$

Then, $\quad g'(0) = \int_\Omega \frac{\nabla u\cdot\nabla v}{\sqrt{1+|\nabla u|^2}} = -\int_\Omega v \operatorname{div}\left(\frac{\nabla u}{\sqrt{1+|\nabla u|^2}}\right) dx$

Then, the minimizing function must satisfy

$$\boxed{\operatorname{div}\left(\frac{\nabla u}{\sqrt{1+|\nabla u|^2}}\right) = 0}$$

minimal surface equation

$$\boxed{u\big|_{\partial\Omega} = f}$$