PS.1 Engineering Simulation

Fundamentally, engineers seek "*solutions* to *problems*"

conservation principles (mass, momentum, energy,...)

physics closure models (conduction, turbulence,...)

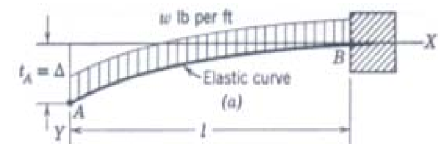
$\Rightarrow$ vector differential calculus

Conservation principles, *Lagrangian* viewpoint

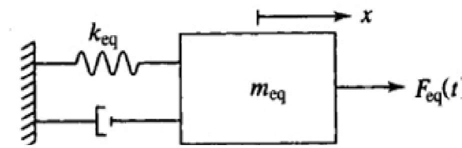
mass:	$\mathrm{d}M = 0, \quad M = \Sigma\, m_i$
linear momentum:	$\mathrm{d}\mathbf{P} = \Sigma\,\mathbf{F}, \quad \mathbf{P} = M\,\mathbf{V}$
energy:	$\mathrm{d}E = \mathrm{d}Q - \mathrm{d}W$
thermodynamic process:	$\mathrm{d}S \geq 0$

PS.2 Continuum Mechanics Viewpoint

Lagrangian form illustrative applications



strength of materials: $d^2y/dx^2 = M/EI$

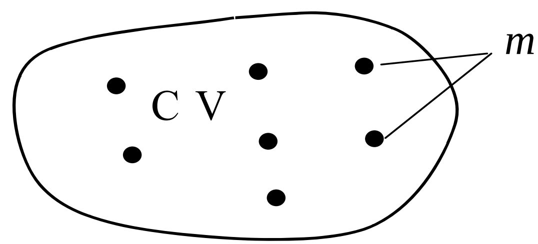


mechanical vibrations: $m\ddot{x} + c\dot{x} + kx = F(t)$

rigid body dynamics: $\mathbf{a}_{XYZ} = \mathbf{a}_{xyz} + \ddot{\mathbf{R}} + 2\boldsymbol{\omega} \times \mathbf{V}_{xyz} + \boldsymbol{\omega} \times \boldsymbol{\rho} + \boldsymbol{\omega} \times \boldsymbol{\omega} \times \boldsymbol{\rho}$

Continuum mechanics concept

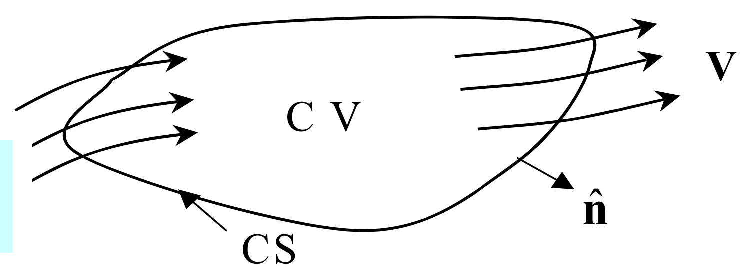
$$\rho(\mathbf{x},t) = \lim_{CV \to 0} \frac{1}{CV} \sum_i m_i$$



Control volume (CV) with enclosing surface (CS)

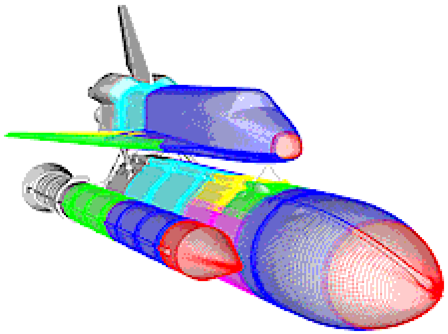
Reynolds transport theorem

$$d(\ ) \Rightarrow D(\ ) \equiv \frac{\partial}{\partial t}\int_{CV} (\ )\, d\tau + \oint_{CS} (\ )\, \mathbf{V} \cdot \hat{\mathbf{n}}\, d\sigma$$



PS.3 Continuum Mechanics Principles

Continuum descriptions with $\rho(\mathbf{x}, t)$:



- structures
- fluids
- heat transfer
- electromagnetics
- mass transport
- mechanical vibrations

Conservation principles, *Eulerian* viewpoint:

$$\mathrm{D}M = \frac{\partial}{\partial t}\int_{CV} \rho \, d\tau + \oint_{CS} \rho \mathbf{V} \cdot \hat{\mathbf{n}} \, d\sigma = 0$$

$$\mathrm{D}\mathbf{P} \Rightarrow \frac{\partial}{\partial t}\int_{CV} \rho \mathbf{V} \, d\tau + \oint_{CS} \mathbf{V} \rho \mathbf{V} \cdot \hat{\mathbf{n}} \, d\sigma = \int_{CV} \rho \mathbf{B} \, d\tau + \int_{CS} \mathbf{T} \, d\sigma$$

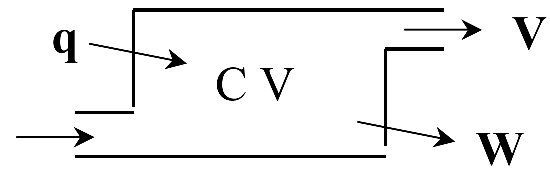
$$\mathrm{D}E \Rightarrow \frac{\partial}{\partial t}\int_{CV} \rho e \, d\tau + \oint_{CS} (e + p/\rho) \rho \mathbf{V} \cdot \hat{\mathbf{n}} \, d\sigma = \int_{CV} s \, d\tau + \oint_{CS} (W - \mathbf{q} \cdot \hat{\mathbf{n}}) \, d\sigma$$

PS.4 Continuum Mechanics Forms

Control volume conservation forms rarely used

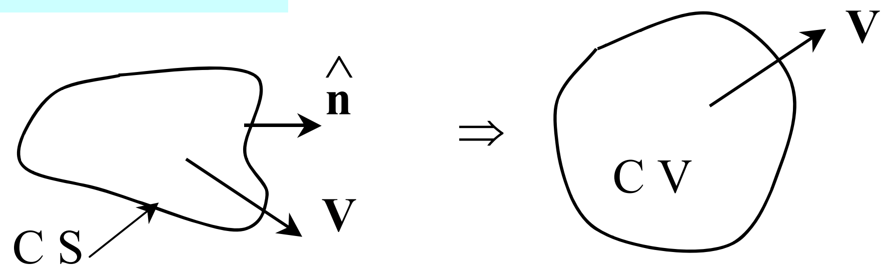
"network" simulations

"coarsest mesh" possible



For stationary CV, *Divergence Theorem*

$$\oint_{CS} \rho \mathbf{V} \cdot \hat{\mathbf{n}} d\sigma = \int_{CV} \nabla \cdot \rho \mathbf{V} d\tau$$

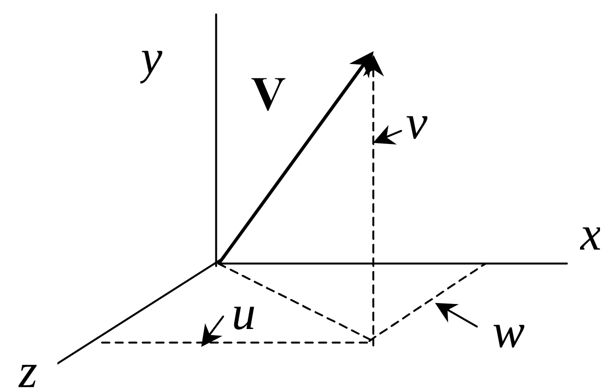


gradient **vector** derivative

$$\nabla = \hat{\mathbf{i}} \frac{\partial}{\partial x} + \hat{\mathbf{j}} \frac{\partial}{\partial y} + \hat{\mathbf{k}} \frac{\partial}{\partial z}$$

divergence operation

$$\nabla \cdot \rho \mathbf{V} = \frac{\partial \rho u}{\partial x} + \frac{\partial \rho v}{\partial y} + \frac{\partial \rho w}{\partial z}$$

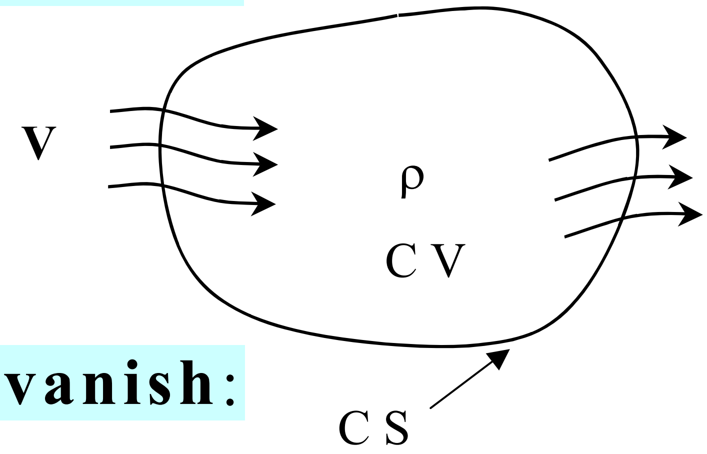


vectors!! calculus!!

PS.5 Continuum Mechanics PDEs

Reynolds transport + Divergence theorem

$$\mathrm{D}M = \int_{CV} \left(\frac{\partial \rho}{\partial t} + \nabla \cdot \rho \, \mathbf{V} \right) d\tau = 0$$



For arbitrary CV, integrand must vanish:

$$\mathrm{D}M : \frac{\partial \rho}{\partial t} + \nabla \cdot \rho \mathbf{V} = 0$$

$$\mathrm{D}\mathbf{P} : \frac{\partial \rho \mathbf{V}}{\partial t} + \nabla \cdot \rho \mathbf{V}\mathbf{V} = \rho \mathbf{g} + \nabla \mathbf{T}$$

$$\mathrm{D}E : \frac{\partial \rho e}{\partial t} + \nabla \cdot (\rho e + p)\mathbf{V} = s - \nabla \cdot \mathbf{q}$$

for traction vector **T**, gravity body force **g**, heat flux **q**

PS.6 Physics Closure Models

Continuum PDEs universally valid!

solids, fluids, EM, vibrations $\Rightarrow$ *how*?!

Distinction for discipline $\rightarrow$ *physics closure models*

example, Fourier *conduction law*: $\mathbf{q} \equiv -k\nabla T$

k = thermal conductivity $\Rightarrow k(\mathbf{x}, T)$
- sign for heat flow direction

Unsteady heat conduction: for $\mathbf{V} = \mathbf{0}$, $e = c_V T$

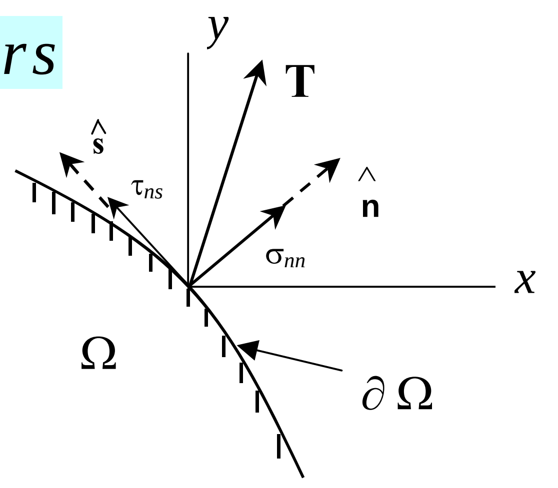
$$\mathrm{DE}: \quad \frac{\partial T}{\partial t} = \kappa\nabla^2 T + s$$

$\kappa = k/\rho c_p \Rightarrow$ material *thermal diffusivity*

$$\nabla^2 \equiv \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} = \text{Laplace PDE operator}$$

PS.7 Physics Closure for DP, Structures

Structural mechanics: DP involves *tensors*



stress: $\mathbf{T}_{\mathbf{cs}} \Rightarrow \tau_{ij}\hat{\mathbf{n}}_j$

Statics: $\partial/\partial t = 0 = \mathbf{V}$

$$\mathrm{DP}: \frac{\partial\sigma_x}{\partial x}+\frac{\partial\tau_{xy}}{\partial y}+\rho g_x=0,\ \frac{\partial\tau_{xy}}{\partial x}+\frac{\partial\sigma_y}{\partial y}+\rho g_y=0$$

closure model: *linear* Hooke's law, $n = 2$

$$\begin{Bmatrix}\sigma_x\\ \sigma_y\\ \tau_{xy}\end{Bmatrix}=\frac{E}{1-\upsilon^2}\begin{bmatrix}1 & \upsilon & 0\\ \upsilon & 1 & 0\\ 0 & 0 & (1-\upsilon)/2\end{bmatrix}\begin{Bmatrix}\varepsilon_x\\ \varepsilon_y\\ \gamma_{xy}\end{Bmatrix}$$

kinematics (strain-displacement): $\varepsilon_x=\frac{\partial u}{\partial x},\quad \gamma_{xy}=\frac{\partial u}{\partial y}+\frac{\partial v}{\partial x}$

$$\mathrm{DP}: \left.\begin{aligned}\nabla^2 u-\frac{1}{1-2\upsilon}\frac{\partial}{\partial x}\left(\frac{\partial u}{\partial x}+\frac{\partial v}{\partial y}\right)+\frac{\rho g_x}{G}=0\\ \nabla^2 v-\frac{1}{1-2\upsilon}\frac{\partial}{\partial y}\left(\frac{\partial u}{\partial x}+\frac{\partial v}{\partial y}\right)+\frac{\rho g_y}{G}=0\end{aligned}\right\}\ \text{laplacian PDE system}$$

PS.8 Structural Mechanics D*E* Principle

Structural analyses employ an *energy principle*

$$\text{D}E: \qquad \Pi \equiv \int_{\Omega} \mathrm{d}e = \frac{1}{2}\int_{\Omega} \mathrm{d}vol \int_0^{\varepsilon} \tau_{ij}\,\mathrm{d}\varepsilon_{ij} - \int_{\partial\Omega} u_j T_j \,\mathrm{d}surf$$

Principle of Virtual Work: inserting Hooke's law

$$\text{D}E: \qquad \Pi = \int_{\Omega}\left(\frac{1}{2}\{\varepsilon\}^T[\mathbf{E}]\{\varepsilon\} - \{\mathbf{u}\}^T\{\mathbf{B}\}\right)\mathrm{d}vol - \int_{\partial\Omega}\{\mathbf{u}\}^T\{\mathbf{T}_s\}\mathrm{d}surf$$

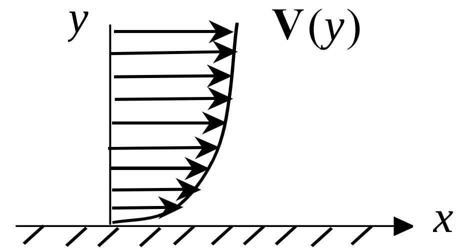
Extremum of D*E* ⇒ DP, e.g.,

$$\text{DP}: \quad \mathcal{L}(\mathbf{u}) = -\nabla^2\mathbf{u} - g(\upsilon)\,\nabla(\nabla\bullet\mathbf{u}) - \mathbf{b} = \mathbf{0}$$

PS.9 Physics Closure for Fluids

Fluid mechanics: strain ⇒ *strain-rate*, hence velocity $\mathbf{V} \Rightarrow u_i$

viscosity closure model: Stoke's law



$$\tau_{ij} = \upsilon\left[\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right] - \frac{2}{3}\lambda\nabla\cdot\mathbf{V}\,\delta_{ij}$$

Navier-Stokes PDE system: incompressible, 2D, steady

D*M*: $\nabla\cdot\mathbf{V} = 0$

D**P**:

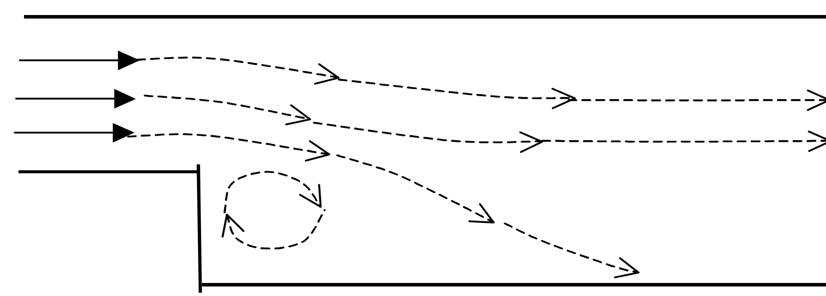
$$\upsilon\nabla^2 u - \frac{1}{\rho_o}\frac{\partial p}{\partial x} - \frac{\partial uu}{\partial x} - \frac{\partial uv}{\partial y} = 0$$

$$\upsilon\nabla^2 v - \frac{1}{\rho_o}\frac{\partial p}{\partial x} - \frac{\partial uv}{\partial x} - \frac{\partial vv}{\partial y} = 0$$

⇒ laplacian PDE system

non-linear(!)

constrained



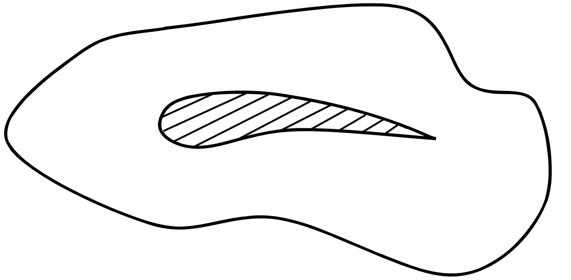
PS.10 Continuum Laplacian PDE Systems

Fluid mechanics: irrotational $(\nabla \times \mathbf{V} = 0)$

\+ incompressible $(\nabla \cdot \mathbf{V} = 0)$

D *M*: $\nabla^2 \Phi = 0\,, \quad \mathbf{V} = -\nabla \Phi$

potential theory



Wave propagation: Maxwell's equations, plane wave

D*M*: $\nabla^2 \phi - \omega^2 \phi = 0$

$\Rightarrow$ perfect medium, ϕ = volts, ω = frequency

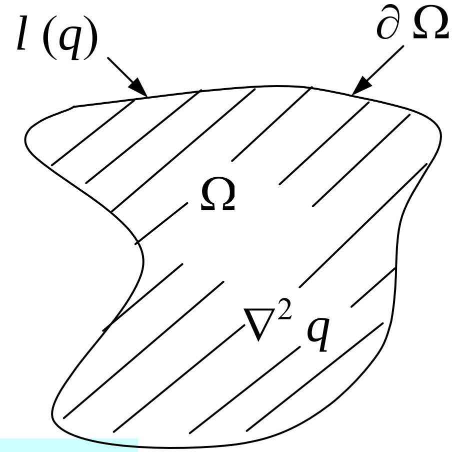
Mass transport: conservation of species (*implicitly* non-linear)

D*M*: $\nabla^2 \phi + s(\phi) = 0$

Creeping flow: saturated aquifer (*explicitly* non-linear)

D*M*: $\nabla \cdot \phi \nabla \phi = 0$

PS.11 Engineering Problem Statements



Summary: problem statements are PDEs!

Laplace operator (∇^2) is highest derivative
$\Rightarrow$ physics closure model

with sources, non-linearities, unsteady terms

Generic *elliptic* boundary value (EBV) problem

$$\mathrm{L}(q) \;=\; -\nabla^2 q - s\,(q) = 0, \quad on \quad \Omega$$

boundary conditions required on total $\partial\Omega$

$$l\,(q) \;=\; \nabla q \cdot \widehat{\mathbf{n}} + g(q) = 0 \quad on \quad \partial\Omega$$

q	= constant	(Dirichlet)
$\nabla q \cdot \widehat{\mathbf{n}}$	= fixed	(Neumann)
$\nabla q \cdot \widehat{\mathbf{n}}$	$= -g(q)$	(Robin)

PS.12 Computational Simulation

Engineering design problems: PDEs + physics + BCs

unknown called *state variable* ≡ $q\ (\mathbf{x},\ t)$

solution is distribution of q on $(\mathbf{x},\ t > t_0)$

analytically *intractible*!

Computer simulation ⇒ seek an *approximate* solution

$$q(\mathbf{x},t) \approx q^N(\mathbf{x},t)$$

finite difference - historical, archaic

finite element analysis

$$q^N(\mathbf{x},t) \equiv q^h(\mathbf{x},t) = \cup_e q_e(\mathbf{x},t)$$

optimal
encompassing
real world problems