

Advection - Diffusion Overview

Recall that conservation of a quantity u (per unit volume) is expressed by the conservation law:

$$u_t + \nabla \cdot \vec{F} = 0, \quad \vec{F} = \text{flux of } u$$

In general, the flux F consists of the advective flux

$$\vec{F}^{\text{adv}} = u \vec{v} \quad \text{due to a velocity field } \vec{v}$$

plus any non-advective fluxes that may be present; their form depends on the phenomena being modeled, specified by a constitutive law, of which we mentioned several very important examples (Fick's law, Fourier law, D'Arcy, ...)

The most important non-advective phenomenon is diffusion of mass in which case Fick's Law: $F^{\text{diff}} = -D \nabla u$, where u = concentration of diffusing species,

or of heat (thermal energy) in which case Fourier's Law: $F^{\text{cond}} = -k \nabla T$, T = temperature.

In fact, the most important non-advective phenomena are described by "gradient flows", i.e. flux is proportional to the gradient of some field, so in fact they behave pretty much "diffusively".

Science is very partial to this sort of description, and prefers gradient flows because of their satisfactory properties (physically and mathematically), and sometimes new quantities have been "invented" in order to express fluxes as gradients! Such (often invented) quantities are called potentials! e.g. voltage was "invented" to express the electric field (strength) as $\vec{E} = -\nabla V$, whence current flux $\vec{J} = \sigma \vec{E} = -\sigma \nabla V$.

All this is to point out that the case of diffusion is rather generic, a good representative of many important non-advective phenomena, and that's an additional reason we studied it (in addition to its intrinsic importance).

Note that all gradient type theories lead to 2nd order Parabolic PDEs, so for a well-posed problem we need Initial and boundary conditions on all exterior boundaries.

The hallmarks of such equations are:

- Smoothing: rough initial data are smoothed out (instantaneously! \rightarrow loss of information)
- infinite speed of propagation of signals
- time-irreversible: ^{only} forward in time problems are well-posed
but backward in time are not (the initial data cannot be determined from future data)

Contrast with hyperbolic behavior:

- no smoothing (no loss of information)
- finite speed of propagation
- time-reversible; both forward and backward well-posed

It follows that phenomena not complying with this picture cannot be modelled by diffusion-type (gradient) laws!

Indeed, time-reversible, non-smoothing phenomena are modelled by hyperbolic PDEs, the prototype of which is such phenomena is advection, (which we shall study next. (wave propagation)).

The third, and last, broad category is steady-state phenomena, which result from either of the above under time-independence. They are modelled by elliptic PDEs, the model equation being

$$\text{the Laplace eqn. } \nabla^2 u = 0 \quad \text{or} \quad \nabla \cdot (\nabla u) = 0$$

$$\text{or Poisson eqn. } \nabla^2 u = f$$

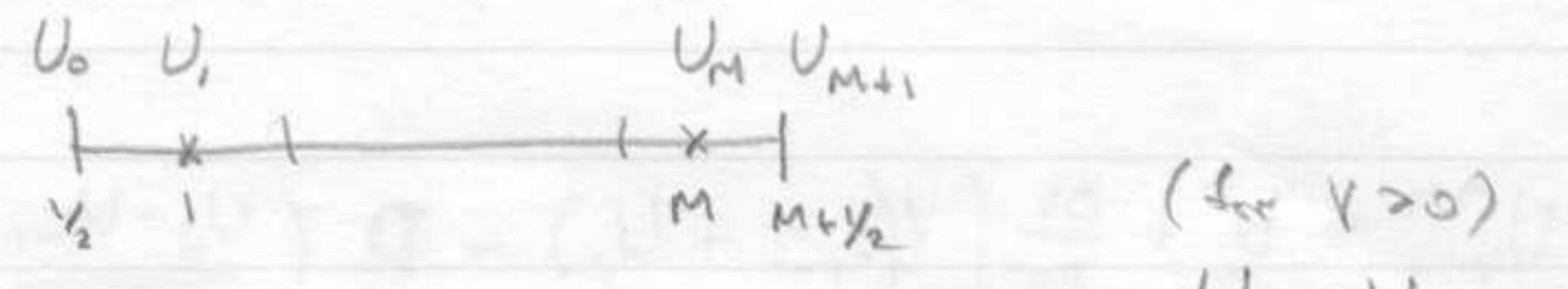
Advection + Diffusion : Boundary Conditions

Total Flux is $F = F^{\text{adv}} + F^{\text{diff}}$
 $= Vu - Du_x$

so boundary fluxes are
(for $V > 0$)

$$F_{\frac{V}{2}} = Vu_0 - D \frac{U_1 - U_0}{\Delta x/2}$$

for $V < 0$: $= Vu_1 - D$ _____



$$F_{\frac{V}{2}} = Vu_0 - D \frac{U_1 - U_0}{\Delta x/2} \quad \text{and} \quad F_{\frac{V}{2}} = Vu_M - D \frac{U_{M+1} - U_M}{\Delta x/2}$$

for $V < 0$: $= Vu_{M+1} - D$ _____

1. Dirichlet: $U_0 = \text{given}$

$F_{\frac{V}{2}}$ from the above formula

If $D=0$: OK if $V > 0$, no BC if $V < 0$

$U_{M+1} = \text{given}$

$F_{\frac{V}{2}}$ from above formula

If $D=0$: $F_{\frac{V}{2}} = Vu_{M+1} - D \frac{U_{M+1} - U_M}{\Delta x/2}$ if $V < 0$
 - no BC if $V > 0$

2. Neumann: $F_{\frac{V}{2}} = q_a = \text{given}$

$F_{\frac{V}{2}} = q_b = \text{given}$

Solve for U_0 :

$$U_0 = \frac{q_a \frac{\Delta x}{2} + DU_1}{V \frac{\Delta x}{2} + D}$$

If $D=0$: $V > 0$ then $U_0 = \frac{q_a}{V}$
 $V < 0$ no BC

Solve for U_{M+1} :

$$U_{M+1} = \frac{[V \frac{\Delta x}{2} + D] U_M - q_b \frac{\Delta x}{2}}{D} \quad \text{if } V > 0$$

$$U_{M+1} = \frac{-q_b \frac{\Delta x}{2} + D U_M}{-V \frac{\Delta x}{2} + D} \quad \text{if } V < 0$$

If $D=0$: $V > 0$: no BC

$$V < 0$$
: OK, $U_{M+1} = \frac{q_b}{V}$

3. Convective BC: $F_{\frac{V}{2}} = h [U_\infty - U_0]$

$$VU_0 - D \frac{U_1 - U_0}{\Delta x/2} = h [U_\infty - U_0]$$

$$\Rightarrow U_0 = \frac{\frac{2D}{\Delta x} U_1 + h U_\infty}{V + \frac{2D}{\Delta x} + h}$$

$$\Rightarrow F_{\frac{V}{2}} = \frac{VU_\infty - D \frac{U_1 - U_\infty}{\Delta x/2}}{1 + \frac{V}{h} + \frac{D}{h \Delta x/2}}$$

$$F_{\frac{V}{2}} = -h [U_\infty - U_{M+1}]$$

$$VU_M - D \frac{U_{M+1} - U_M}{\Delta x/2} = h U_{M+1} - h U_\infty$$

$$\Rightarrow U_{M+1} = \frac{(V + \frac{2D}{\Delta x}) U_M + h U_\infty}{\frac{2D}{\Delta x} + h}$$

$$\Rightarrow F_{\frac{V}{2}} = \frac{VU_M + \frac{2D}{\Delta x} (U_M - U_\infty)}{1 + \frac{2D}{h \Delta x}}$$

as $h \rightarrow \infty$ we get $F_{\frac{V}{2}}$ for Dirichlet with U_∞ as U_0

as $h \rightarrow \infty$, $F_{\frac{V}{2}} = VU_M - D \frac{U_\infty - U_M}{\Delta x/2} = \text{Dirichlet}$
 with U_∞ as U_{M+1}

Advection = Diffusion : CFL condition $U_t + (Vu)_x = (Du_x)_x + S$

Explicit upwind scheme

$$U_i^{n+1} = U_i^n + \frac{\Delta t}{\Delta x} [F_{i-\frac{1}{2}} - F_{i+\frac{1}{2}}] , \quad F_{i-\frac{1}{2}} = \begin{cases} VU_{i-1} - D \frac{U_i - U_{i-1}}{\Delta x}, & V > 0 \\ VU_i - D \frac{U_{i+1} - U_i}{\Delta x}, & V < 0 \end{cases}$$

$$\begin{aligned} V > 0 \Rightarrow U_i^{n+1} &= U_i^n + \frac{\Delta t}{\Delta x} [V(U_{i-1} + U_i) - D \left(\frac{U_i - U_{i-1}}{\Delta x} - \frac{U_{i+1} - U_i}{\Delta x} \right)] \\ &= \left[1 - \frac{V\Delta t}{\Delta x} - \frac{2D\Delta t}{\Delta x^2} \right] U_i^n + \frac{V\Delta t}{\Delta x} U_{i-1} + \frac{D\Delta t}{\Delta x^2} (U_{i-1} + U_{i+1}) \end{aligned}$$

Positive Coeff Rule: $\underbrace{\frac{|V|\Delta t}{\Delta x}}_{\text{Courant Number}} + 2 \frac{D\Delta t}{\Delta x^2} \leq 1 \quad \text{CFL condition}$

$$\Rightarrow \Delta t \leq \frac{1}{\frac{|V|}{\Delta x} + 2 \frac{D}{\Delta x^2}} = \frac{\Delta x^2}{V\Delta x + 2D} = \Delta t_{\text{exp}}$$

$$= \frac{\Delta x^2/D}{Pe + 2}, \quad Pe = \frac{V\Delta x}{D} = \text{cell Pelet Number}$$

$= \frac{\text{advection effect}}{\text{diffusion effect}}$

small $|Pe|$ means diffusion dominated

large $|Pe| \rightarrow$ advection

Dimensionless form: $U_t + Vu_x = Du_{xx}$
 $\bar{x} = \frac{x}{\hat{x}}, \quad \tau = \frac{t}{\hat{t}}, \quad w(\bar{x}, \tau) = \frac{u(x, t) - u_{\text{ref}}}{\hat{u}}$

$$\Rightarrow \frac{\hat{u}_t}{\hat{x}} = \frac{\hat{u}}{\hat{x}} \cdot \hat{w}_\tau, \quad u_x = \frac{\hat{u}}{\hat{x}} w_\tau, \quad u_{xx} = \frac{\hat{u}}{\hat{x}^2} w_{\tau\tau}$$

$$\Rightarrow \frac{\hat{u}_t}{\hat{x}} w_\tau + V \frac{\hat{u}}{\hat{x}} \hat{w}_\tau = D \frac{\hat{u}}{\hat{x}^2} w_{\tau\tau}$$

Choose $D \frac{\hat{x}}{\hat{x}^2} = 1 \Rightarrow \frac{\hat{x}}{\hat{x}} = \frac{V\hat{t}}{D} = Pe$

$$\Rightarrow w_\tau + Pe w_{\tau\tau} = w_{\tau\tau}$$

$$\hat{x}^2 = D\hat{t} \text{ is the diffusive scaling}$$

in unit time ($\hat{t}=1$) $\hat{x} = \sqrt{D}$ units of space are affected
to cover unit space ($\hat{x}=1$) $\hat{t} = \frac{1}{D}$ units of time it takes

Large $|Pe| \Rightarrow$ advection dominated

Small $|Pe| \Rightarrow$ diffusion dominated

When $D > 0$, PDE is parabolic, needs some BC at each pt of the bry.

Consistency - Stability - Convergence

Discretization replaces the PDE $[u] = 0$ by a Finite-Difference Equation FDE $[U_i^n] = 0$
 $U_i^n \approx u(x_i, t_n)$

Consistency error (local truncation error) is the amount by which the exact sol. of the PDE fails to satisfy the FDE:

$$te_i^n := FDE[u(x_i, t_n)]$$

$\equiv FDE[u] - PDE[u]$ so = difference between

FDE and PDE applied to u

If $te_i^n = O(\Delta x^p)$ then scheme is of p-th order in space.

A discretization is consistent if the consistency error $\rightarrow 0$ as $\Delta x, \Delta t \rightarrow 0$,

so that the FDE does approximate the PDE (and not some other PDE)

Discretization error is the difference between exact and numerical solution

$$de_i^n := U_i^n - u(x_i, t_n)$$

A method is convergent if $de_i^n \rightarrow 0$ as $\Delta x, \Delta t \rightarrow 0$,

so that the discrete sol. does tend to the exact sol.

(at ∞ precision).

Note that U_i^n denotes the exact sol. of the FDE. The actual numerical solution \tilde{U}_i^n may be contaminated by roundoff errors:

$$re_i^n := \tilde{U}_i^n - U_i^n$$

These are due to the finite-precision arithmetic and may be introduced at any point in the computation.

Each roundoff error is negligibly small, but the concern is that they may propagate and pile up. The best we can hope for is the scheme does not amplify errors so that they grow faster than the exact discrete sol. Then the scheme is called stable.

Unstable schemes are entirely useless! These concepts are related via the famous

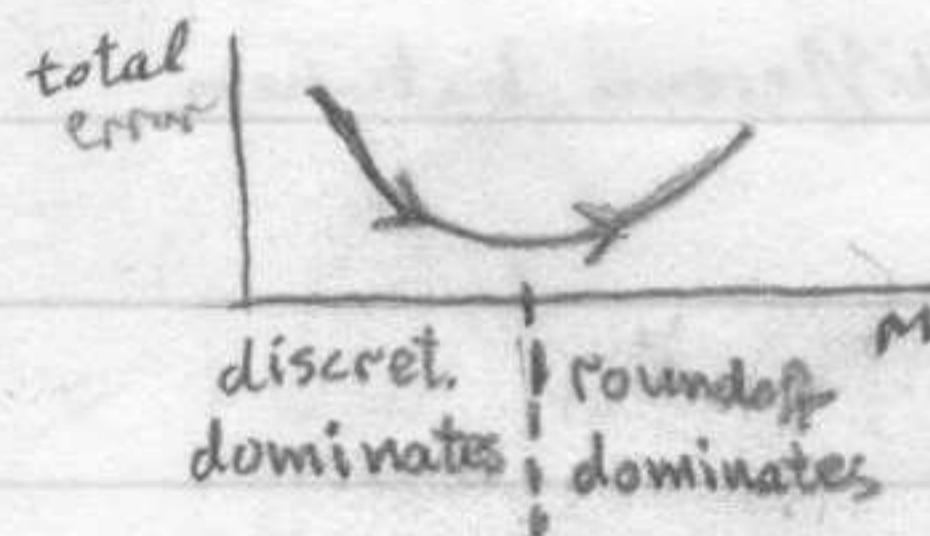
Lax Equivalence Theorem: A consistent scheme for a well-posed problem is convergent iff it is stable.

$$\text{The actual overall error} = \tilde{U}_i^n - u(x_i, t_n) = \tilde{U}_i^n - U_i^n + U_i^n - u(x_i, t_n)$$

(at time t_n)

$$= \text{roundoff} + \text{discretization error}$$

In a convergent scheme, we can reduce de_i^n by using smaller $\Delta x, \Delta t$,
but then more computations must be performed, increasing the roundoff!



For each problem and num. method, there is an "optimal" mesh, which however can only be guessed at by refining the mesh to see if the error decreases

(assuming we can estimate error, rare event! only on an exactly solvable (debugging) problem,

Since optimal mesh cannot be determined a priori

typically we compute with some seemingly reasonable mesh, then with a finer mesh

(say $\frac{\Delta x}{2}$) to see if computed solution (or some meaningful measure, e.g. total mass) changes appreciably. If it does, then refine again till no appreciable change, obtaining "grid converged" solution, or error goes up: over-refined!

Estimating order of convergence p : scheme of order p : error = $O(\Delta x^p) \approx C \cdot \Delta x^p$

$$\text{Compute with } \Delta x \text{ and with } \frac{\Delta x}{f}: \frac{\text{err}(\Delta x)}{\text{err}(\frac{\Delta x}{f})} \approx \frac{C \cdot \Delta x^p}{C \cdot (\frac{\Delta x}{f})^p} = f^p$$

$$\Rightarrow p \approx \frac{\ln(\text{err}(\Delta x)) - \ln(\text{err}(\frac{\Delta x}{f}))}{\ln f}$$