Advection - Diffusion

Conservation law: for $u(x,t)$: $u_t + F_x = S$ in $a<x<b$
$t_0 < t < t_{end}$

Constitutive law for flux: $F = F_{adv} + F_{diff}$

$= vu - Du_x$, v = given vel. D = diffusivity

so PDE for $u(x,t)$: $\boxed{u_t + (vu - Du_x)_x = S}$
advection-diffusion-reaction ~~equ.~~ equ.

(As long as $D \neq 0$) this is a parabolic equ, so
needs IC: $u(x,0) = u_{init}(x)$ = given
and BCs: some BC at each boundary pt. for all time.

standard BCs: at $x=a$, $t_0 < t < t_{end}$

I. Dirichlet BC: $u(a,t) = u_a(t)$ given

II. Neumann BC: $F(a,t) = F_a(t)$ given

so $vu - Du_x \big|_{x=a} = F_a(t)$

In particular, insulated (impermeable) bry: $F(a,t) \equiv 0$

III. Convective BC: $F(a,t) = h \cdot [u_{amb}(t) - u(a,t)]$, h = film coeff. heat transfer coeff.

IV. Periodic BCs: $u(a,t) = u(b,t)$ and $F(a,t) = F(b,t)$

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(p.2)

<u>Undimensionalization</u>: make all variables dimensionless

Simplest case: $v \equiv V = \text{const.}$, $D = \text{const.}$

$$u_t + V u_x = D u_{xx}$$

Choose a length scale L, a u-scale $\hat{u}$, a reference u_{ref}

[redacted], a time-scale τ

Set: $\xi = \frac{x}{L}$, $w(\xi, \tau) = \frac{u(x,t) - u_{ref}}{\hat{u}} \Rightarrow u(x,t) = \hat{u} \cdot w(\xi,\tau) + u_{ref}$

$\tau = \frac{D}{L^2} t$: diffusion time-scale : <u>Fourier Number</u>.

$$\Rightarrow u_t = \hat{u} \cdot w_\tau \cdot \tau_t = \hat{u} \cdot w_\tau \cdot \frac{D}{L^2}$$

$$u_x = \hat{u} \cdot w_\xi \cdot \xi_x = \hat{u} \cdot w_\xi \cdot \frac{1}{L}$$

$$u_{xx} = \hat{u} \cdot w_{\xi\xi} \cdot \frac{1}{L^2}$$

$$\overset{\text{PDE}}{\Longrightarrow} \cancel{\hat{u}} \cdot w_\tau \cdot \frac{D}{L^2} + \frac{V}{L} \cdot \cancel{\hat{u}} \cdot w_\xi = \frac{D}{L^2} \cdot \cancel{\hat{u}} \cdot w_{\xi\xi}$$

$\Rightarrow \; w_\tau + \frac{VL}{D} w_\xi = w_{\xi\xi}$ only one coeff. $\boxed{Pe = \frac{VL}{D} : \text{Peclet Number}}$

strength of $\frac{\text{advection}}{\text{diffusion}}$

Dimensionless advection-diffusion equ:

$$w_\tau + Pe \cdot w_\xi = w_{\xi\xi} \quad \text{for} \quad 0 \lneq Pe \lneq \infty$$

$Pe = 0 \Leftrightarrow V = 0$: pure diffusion : $w_\tau = w_{\xi\xi}$

$Pe = \infty \Leftrightarrow D = 0$: pure advection : $w_\tau + w_\xi = 0$

choose $\tau = \frac{V}{L} t$: advection time-scale

$$\Rightarrow w_\tau + w_\xi = \frac{1}{Pe} w_{\xi\xi}$$

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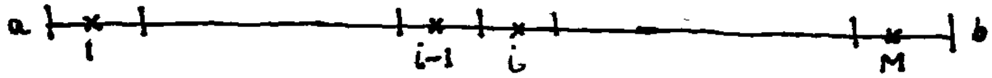
Finite Volume discretization of $u_t + (vu - Du_x)_x = S$

It is a conservation law $u_t + F_x = S$, $a<x<b$, $t_0<t<t_{end}$
with flux $F = vu - Du_x = F_{adv} + F_{diff}$

We know how to discretize each piece.
Mesh of M control volumes: $x(0:M+1)$, $\Delta x = \frac{b-a}{M}$



Integrating $u_t + F_x = S$ over each $CV_i = [x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}]$
and each timestep $[t_n, t_{n+1}]$ and setting

$$U_i^n = \frac{1}{\Delta x}\int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} u(x,t_n)\,dx = \text{mean } u \text{ over } CV_i \text{ at time } t_n$$
$$\approx u(x_i, t_n)$$

$$\overline{F}_{i-\frac{1}{2}}^{n+\theta} = \frac{1}{\Delta t}\int_{t_n}^{t_{n+1}} F(x_{i-\frac{1}{2}}, t)\,dt = \text{mean } F \text{ over } [t_n, t_{n+1}] \text{ at face } x_{i-\frac{1}{2}}$$

$$S_i^{n+\theta} = \frac{1}{\Delta t}\int_{t_n}^{t_{n+1}} \frac{1}{\Delta x}\int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} S(x,t)\,dx\,dt = \text{mean source}$$

we get, as before

$$U_i^{n+1} = U_i^n + \frac{\Delta t}{\Delta x}\left[\overline{F}_{i-\frac{1}{2}}^{n+\theta} - \overline{F}_{i+\frac{1}{2}}^{n+\theta}\right] + \Delta t\, S_i^{n+\theta}$$

$$i = 1:M, \quad n = 0:N, \quad 0 \le \theta \le 1$$

$$F_{i-\frac{1}{2}} = (vu)_{i-\frac{1}{2}} + (-Du_x)_{i-\frac{1}{2}}, \quad i = 2:M, \quad F_{\frac{1}{2}}, F_{M+\frac{1}{2}} \text{ from BCs}$$

$$\approx \underset{\text{adv. flux}}{\text{upwind}} \quad - D\,\frac{U_i - U_{i-1}}{\Delta x}$$

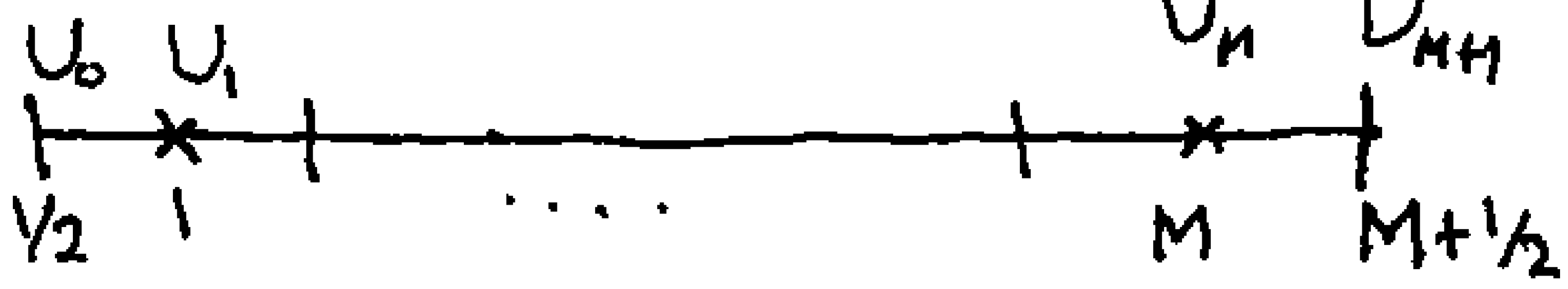
$$= \begin{cases} v_{i-\frac{1}{2}} U_{i-1} & \text{if } v_{i-\frac{1}{2}} > 0 \\ v_{i-\frac{1}{2}} U_i & \text{if } v_{i-\frac{1}{2}} < 0 \end{cases} \quad - D\,\frac{U_i - U_{i-1}}{\Delta x}$$

Advection - Diffusion: Boundary Conditions

Total Flux: $F = F^{adv} + F^{diff}$

$= Vu - Du_x$

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



$$F_{1/2} = VU_0 - D\frac{U_1 - U_0}{\Delta x/2} \quad (V>0) \qquad F_{M+1/2} = VU_M - D\frac{U_{M+1} - U_M}{\Delta x/2}$$

for $V<0$: $= VU_1 - D$ —— $\quad (V<0) \qquad = V \cdot U_{M+1} - D$ ——

I. Dirichlet BC: U_0 = given

$F_{1/2}$ from above formula

If $D=0$: $F_{1/2} = VU_0$ if $V>0$ (incoming) but NO BC if $V<0$ (outgoing)

U_{M+1} given

$F_{M+1/2}$ from above formula

If $D=0$: NO BC if $V>0$ (outgoing)

$F_{M+1/2} = V\,U_{M+1}$ if $V<0$ (incoming)

II. Neuman BC: $F_{1/2} = q_a$ given

solve for U_0:

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

For $D=0$: $U_0 = \frac{q_a}{V}$ if $V>0$

$F_{M+1/2} = q_b$ given

solve for U_{M+1}:

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

$$= \frac{DU_M - q_b\frac{\Delta x}{2}}{D + V\frac{\Delta x}{2}} \quad \text{if } V<0$$

For $D=0$: No BC if $V>0$

$U_{M+1} = \frac{q_b}{V}$

III. Convective BC: $F_{1/2} = h\cdot[U_\infty - U_0]$

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

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

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

as $h\to\infty$ we get $F_{1/2}$ for Dirichlet with U_∞ as U_0

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

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

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

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

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

as Dirichlet with U_∞ as U_{M+1}

CFL condition

So, say for $V > 0$:

$$U_j^{n+1} = U_j^n + \frac{\Delta t}{\Delta x}\left[V U_{j-1}^n \overset{-V U_j^n}{} - D_{j-1/2}\frac{U_j - U_{j-1}}{\Delta x} + D_{j+1/2}\frac{U_{j+1} - U_j}{\Delta x}\right]$$

and for $D \equiv$ const:

$$U_j^{n+1} = U_j^n\left[1 - V\frac{\Delta t}{\Delta x} - 2\frac{D\Delta t}{\Delta x^2}\right] + V\frac{\Delta t}{\Delta x}U_{j-1}^n + D\frac{\Delta t}{\Delta x^2}\left(U_{j-1}^n + U_{j+1}^n\right)$$

Stability via the "positive coefficient rule":

$$1 - V\frac{\Delta t}{\Delta x} - 2D\frac{\Delta t}{\Delta x^2} > 0$$

so $\boxed{0 < V\frac{\Delta t}{\Delta x} + 2D\frac{\Delta t}{\Delta x^2} \leq 1 \quad \text{is the CFL condition}}$

This restricts the time step to; $\quad \Delta t \leq \dfrac{\Delta x^2}{|V|\Delta x + 2D} = \dfrac{1}{\frac{|V|}{\Delta x} + \frac{2D}{\Delta x^2}}$

Pure advection case ($D \equiv 0$): Courant number $|V|\frac{\Delta t}{\Delta x} \leq 1$, CFL: $\Delta t \leq \frac{\Delta x}{V_{max}}$

Pure diffusion case ($V \equiv 0$): Courant number $D\frac{\Delta t}{\Delta x^2} \leq \frac{1}{2}$, CFL: $\Delta t \leq \frac{\Delta x^2}{2D_{max}}$

Advection-diffusion: Courant number $|V|\frac{\Delta t}{\Delta x} + 2\frac{D\Delta t}{\Delta x^2} \leq 1 \implies \Delta t \leq \frac{\Delta x^2}{|V|\Delta x + 2D}$

Note: taking $\Delta t = \min(\Delta t_{ad}, \Delta t \ldots)$