

Code skeleton

1. Inputs to be read in from a "dat" file:

MM, tend, dtout, factor, D, a, b

2. Set grid

$$Dx = 1.0 / MM, M = (b - a) * MM$$

CALL MESH(M, a, b, Dx, x)

returns x array

3. Set timestep (for stability of explicit scheme, ... more later)

$$Dt_{EXPL} = Dx * Dx / (2 * D)$$

$$Dt = factor * Dt_{EXPL}$$

$$N_{max} = \text{int}(tend / Dt) + 1$$

CALL INIT(...); CALL OUTPUT(...)

profile at t=0

4. Initialize

$$nsteps = 0$$

$$\text{time} = 0.0$$

$$\text{tout} = \text{MAX}(dtout, Dt)$$

5. Execute timestepping

for nsteps = 1 : Nmax

CALL FLUX(

returns F array

CALL PDE(

returns U array

$$\text{time} = (\text{time} + Dt) \Rightarrow nsteps * Dt$$

if (time >= tout)

CALL OUTPUT(M, x, U, time, nsteps)

$$\text{tout} = \text{tout} + dtout$$

endif

endfor

6. Finish

print: 'DONE, at time = ', time, ' after nsteps = ', nsteps

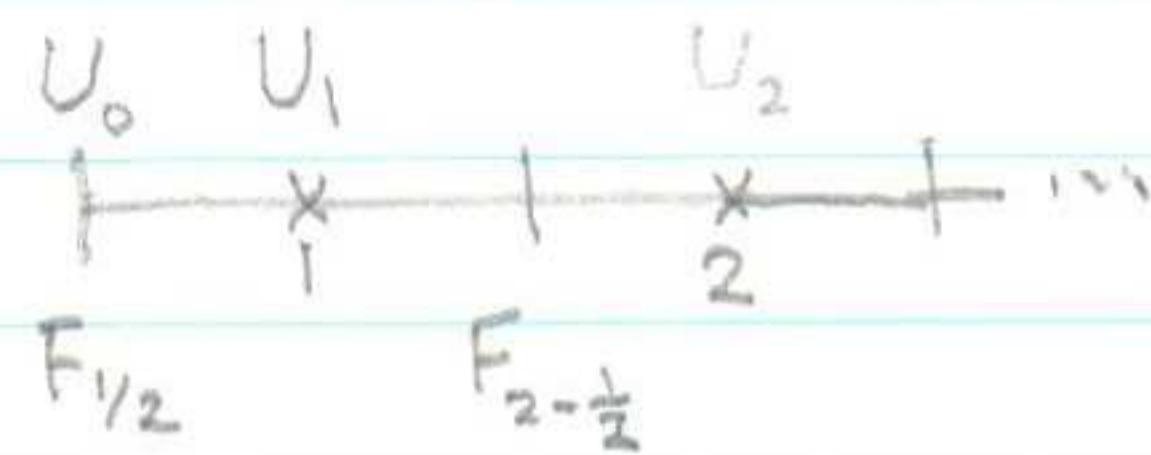
END

Boundary Conditions in FV scheme for diffusion

A PDE problem consists of: PDE eg. $u_t = Du_{xx}$, $x \in \Omega$, $t_0 < t < t_{\text{end}}$
 for $u(x, t)$
 IC $u(x, 0) = u_{\text{init}}(x)$, $x \in \Omega$
 BCs some BC at each pt of $\partial\Omega$ for all time

Standard BCs at $x=a$ or $x=b$ coded in FLUX routine

I. Dirichlet (or 1st kind): impose value at $x=a$: $u(a, t) = u_a(t)$ given



$$\text{so } U_0^n \approx u(a, t_n) = u_a(t_n) \text{ known bry value}$$

$$\Rightarrow F_{1/2}^n = -D \frac{U_1^n - U_0^n}{\Delta x / 2}$$

II. Neumann (or 2nd kind): impose flux at $x=a$: $F(a, t) = F_a(t)$ given

$$\text{so } F_{1/2}^n = F_a(t_n) \text{ known bry flux}$$

$$\text{then bry value } U_0^n \text{ can be found from } F_{1/2} = -D \frac{U_1 - U_0}{\Delta x / 2} = F_a(t_n)$$

solve for U_0

$$\Rightarrow U_0^n = U_1^n + \frac{\Delta x}{2D} F_{1/2}^n \quad \text{for outputting}$$

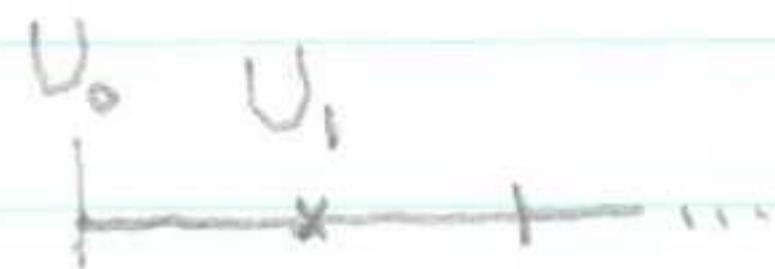
In particular, impermeable/insulated bry: $F(a, t) = F_a(t) \equiv 0$

$$\Rightarrow U_0^n = U_1^n$$

BCs ...

III. Convective BC (or Robin or 3rd kind):

most realistic BC physically



$$F(a, t) = h [u_{\text{amb}}(t) - u(a, t)]$$

h = film coeff,
heat transfer coeff,

$u_{\text{amb}}(t)$ = ambient u , given

$F_{1/2}$

$$F_{1/2}^n = h [u_{\text{amb}}(t_n) - U_o^n] \stackrel{\text{want}}{=} -D \frac{U_i^n - U_o^n}{\Delta x / 2}$$

solve for U_o :

$$U_o = \frac{U_i + \frac{h \Delta x}{2D} u_{\text{amb}}}{1 + \frac{h \Delta x}{2D}}$$

for Output

$$\Rightarrow F_{1/2}^n = -D \frac{U_i - u_{\text{amb}}}{\frac{D}{h} + \frac{\Delta x}{2}}$$

so u_{amb} plays role of U_o
but with $\frac{D}{h} + \frac{\Delta x}{2}$ instead of $\frac{\Delta x}{2}$

Note: $h \rightarrow \infty \Rightarrow u(a, t) = u_{\text{amb}}$ (for χ to be finite).
Dirichlet BC!

$h = 0 \Rightarrow F = 0$, insulated by
homogeneous Neumann BC

IV. Periodic BC ... later

V. Radiation BC

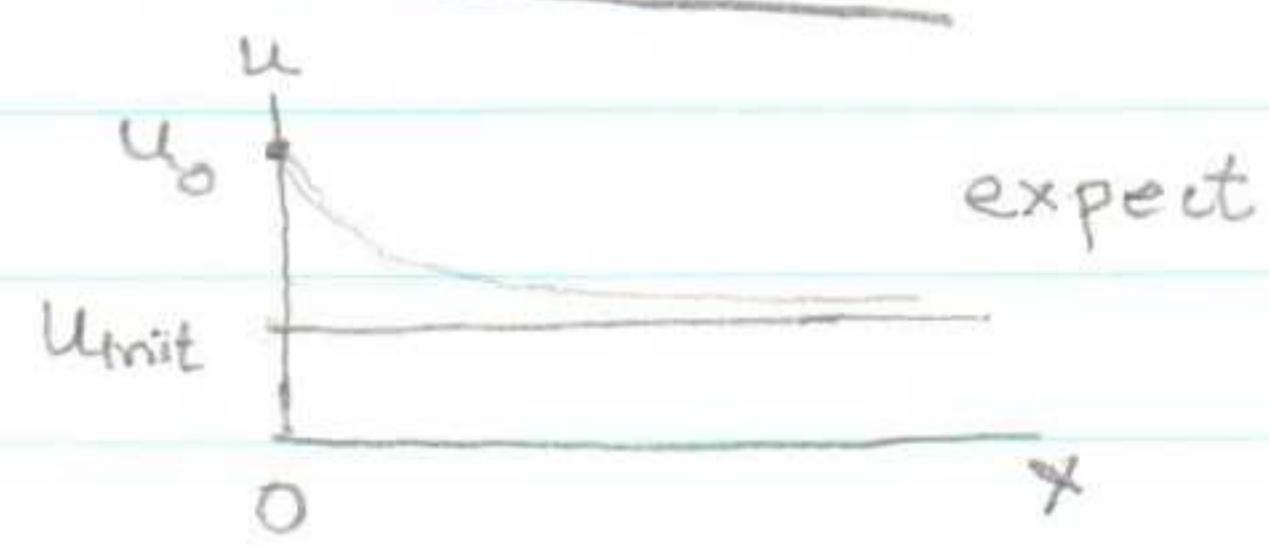
Explicitly solvable diffusion problem for debugging 1D diffusion

The diffusion problem in semi-infinite rod, with constant data u_{init}, u_0

PDE $u_t = D u_{xx}, 0 < x < \infty, t > 0$

IC $u(x, 0) = u_{\text{init}}, 0 \leq x < \infty$

BC $u(0, t) = u_0, \lim_{x \rightarrow \infty} u(x, t) = u_{\text{init}}$

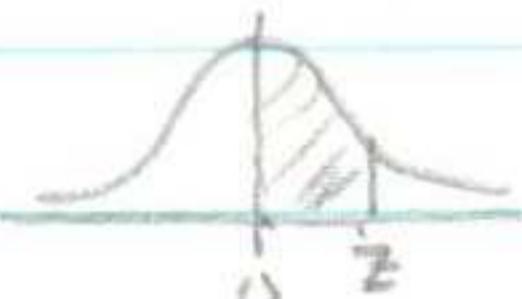


admits exact (similarity) solution: (HW1)

$$u(x, t) = u_0 + (u_{\text{init}} - u_0) \operatorname{erf}\left(\frac{x}{2\sqrt{Dt}}\right), 0 \leq x < \infty, t \geq 0$$

error function: $\operatorname{erf}(z) = \frac{2}{\sqrt{\pi}} \int_0^z e^{-s^2} ds$

$\operatorname{erf}(0) = 0, \operatorname{erf}(\infty) = 1$



To test/debug diffusion code over a finite interval $[a, b]$: set $a = 0$

impose exact solution at boundaries: Dirichlet BCs

$$U_0^n = u_0, U_{M+1}^n = u_b(t_n) = u_0 + (u_{\text{init}} - u_0) \operatorname{erf}\left(\frac{b}{2\sqrt{Dt_n}}\right)$$

time-dependent bry value

For simplicity, take $u_{\text{init}} = 0, u_0 = 1$

$$\Rightarrow u(x, t) = 1 - \operatorname{erf}\left(\frac{x}{2\sqrt{Dt}}\right) \equiv \operatorname{erfc}\left(\frac{x}{2\sqrt{Dt}}\right)$$

complementary error function