Boundary Conditions

for advection-diffusion eqs.

A. Donev, Spring 2021

Consider now solving adv-diff

$$u_t + (a\,u)_x = (d\,u_x)_x$$

on $[0, L]$ with BCs.

One of the first challenges we need to deal with is that the allowed BCs are different if $d > 0$ vs. $d = 0$

This means that in general we expect boundary layers for advection-dominated problems

To make this explicit, consider

$$u_t + a u_x = d\, u_{xx}, \quad a > 0$$
$$0 < x < L = 1$$

$u(0,t) = 1$ (inflow boundary)

$d > 0$

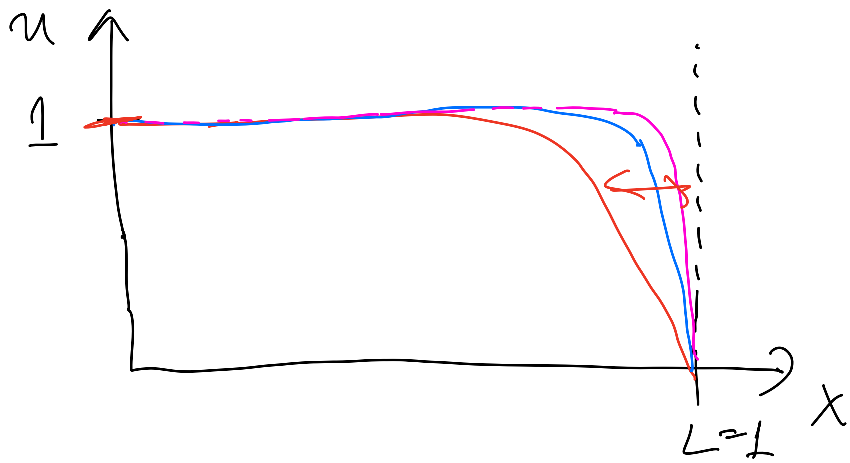
and either $\begin{cases} u(1,t) = 0 & \text{(Dirichlet)} \\ u_x(1,t) = 0 & \text{(Flux or Neumann)} \end{cases}$

on the outflow boundary

For Dirichlet BC, the steady state solution

$$u_t = 0 = -a u_x + d u_{xx}$$

is
$$u(x,t) = \frac{e^{a/d} - e^{ax/d}}{e^{a/d} - 1}$$



Boundary layer of width

$$\ell_b \sim d/a \to 0 \text{ as } d \to 0$$

If the problem is advection-dominated, i.e.,

Peclet number $P_e = \dfrac{aL}{d} \gg 1$,

then $\dfrac{\ell_b}{L} \approx \dfrac{d}{aL} \ll 1$

so the boundary layer is very thin.

This means that even a fine grid is unlikely to resolve the solution near the boundary.

Does this matter?

Depends!

For flow over the wing of an airplane, we can compute the lift without worrying about the boundary layer. But the (viscous) drag is dominated by the boundary layer.

At an outflow boundary, we mostly care that "stuff" leaves the domain without reflection, so we don't want a boundary layer.

In fact, often a boundary is an open boundary (artificial), meaning there is not an actual physical boundary there and so the BC is fake anyway.

At such "boundaries" we better choose a Neumann BC $u_x = 0$, since this makes the steady solution be

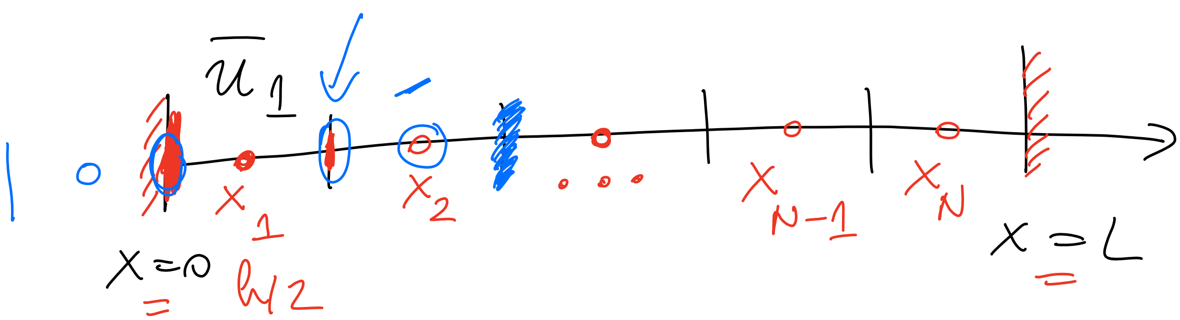
$$u(x, t \to \infty) = 1$$

with no boundary layer.

It is important to know what kind of boundary one has physically before solving PDE!

Let's first consider <u>advection</u> (– dominated) problems

$$\begin{cases} u_t + (au)_x = 0 \,, & x \in (0,L) \\ u(0,t) = \gamma_0(t) & \text{(Inflow)} \\ \underline{\text{No}} \text{ BC at outflow!} & \end{cases}$$



$$x_j = (j - 1/2)\,h \,, \quad h = \frac{L}{N}$$

Remember that for FV schemes the <u>faces</u> of the grid overlap the boundaries:

$x_{1/2} = 0$ $\qquad$ $x_{N+1/2} = L$

The inflow boundary flux is trivial. We need the flux

$$F_{1/2}(t) = a_{1/2}\, u(x_{1/2}, t)$$

$$= a_{1/2}\, g_0(t)$$

For example, to second order

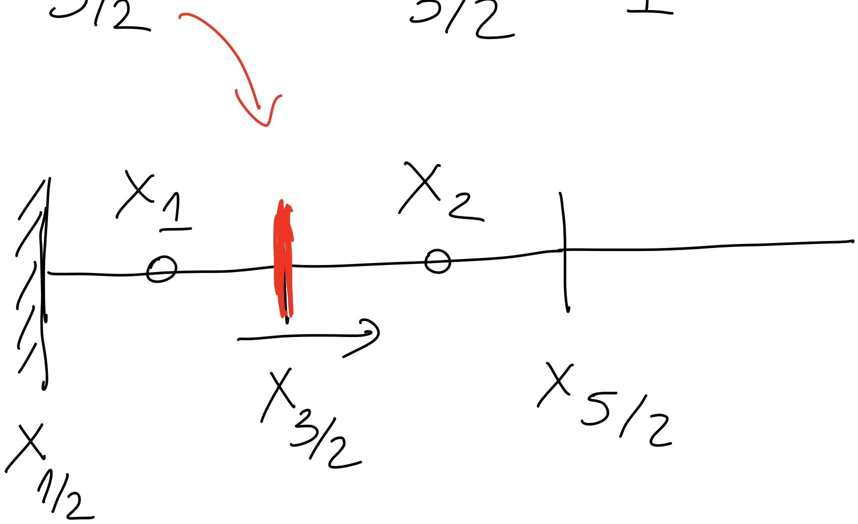
$$F^{n+1/2}_{1/2} \approx a_{1/2}\, g_0\left(t^n + \frac{2}{2}\right)$$

Don't forget the half step!

But what about $F^{n+1/2}_{3/2}$?

For first order upwinding, there would be no issue

$$F^{n}_{3/2} = a_{3/2}\, u^{n}_{1}$$



We may worry that this will only lead to first-order schemes, but in fact, as we show later,
it is OK to use first-order schemes right on the boundary & still get 2^{nd} order, sometimes!
Harder issue is stability & hard to analyze & prove

Another option is to use a centered flux on this face,

$$F^n_{3/2} = a_{3/2}\left(\frac{u_1+u_2}{2}\right)$$

but we may worry about stability.

Yet a third option is "ghost cells", as we discuss shortly.

In practice: We try things out & see stability/accuracy/robustness

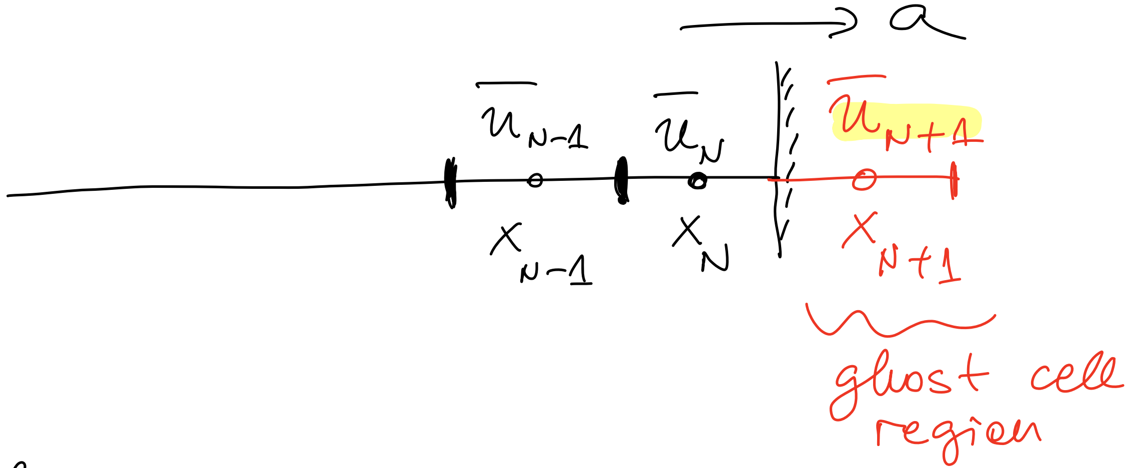
The harder part is the outflow boundary, where there is no BC

Options:

a) In the last one or two cells, switch to a fully one-sided method such as upwind or beam-warming

b) Use "ghost cells" and continue to use the same formulas as in the interior. This is good also for computational performance (no branching in code), is simple, and often works well.

Let's illustrate this approach for the outflow boundary for $a = \text{const}$.



The idea is to set the values in the ghost cell using extrapolation from the interior using the BC if there is one. For example:

a) Piecewise constant extrapolation:

$$u_{N+1} = u_N$$

b) Linear extrapolation:

$$u_{N+1} = 2u_N - u_{N-1}$$

Let's see what these do if we use Lax-Wendroff <u>NOT</u> in flux form:

$$\bar{u}_N^{n+1} = \bar{u}_N^n - \nu h \underbrace{\left(\frac{\bar{u}_{N-1} - \bar{u}_{N+1}}{2h} \right)}_{\text{centered advection}}$$

$$+ \frac{(\nu h)^2}{2} \left(\frac{\bar{u}_{N-1} - 2\bar{u}_N + \bar{u}_{N+1}}{h^2} \right)$$

Piecewise constant

$$\bar{u}_N^{n+1} = \bar{u}_N^n - \nu h \left(\frac{\bar{u}_{N-1} - \bar{u}_N}{2h} \right)$$

$$+ \frac{(\nu h)^2}{2} \left(\frac{\bar{u}_{N-1} - 2\bar{u}_N + \bar{u}_N}{h^2} \right)$$

$$\bar{u}_N^{n+1} = \bar{u}_N^{n} - \frac{\nu(1-\nu)}{2} h \left(\frac{\bar{u}_{N-1} - \bar{u}_N}{h} \right)$$

which is not consistent with the PDE and so is a bad idea.

If we used linear extrapolation

$$\bar{u}_{N+1} = 2\bar{u}_N - \bar{u}_{N-1} \implies$$

$$\bar{u}_N^{n+1} = \bar{u}_N^{n} - \nu h \left(\frac{\bar{u}_{N-1} - \bar{u}_N}{h} \right)$$

which means we are using upwind in the outflow cell, so this makes sense.

Is it second order?

(return to this later)

Now, imagine we wrote LW or Fromm or Beam Warming in flux form. The problem would be on the outflow face

slope estimate

$$F_{N+1/2} = a\left(\bar{u}_N + \frac{h}{2} S_N (1-\nu)\right)$$

But what is S_N ?

For LW, we used downwind slopes,

linear extra

$$S_N = \frac{\bar{u}_{N+1} - \bar{u}_N}{h}, \quad a > 0$$

So if we use constant extrapolation for the ghost cell $(\bar{u}_{N+1} = \bar{u}_N)$ then $S_N = 0$

$\Rightarrow$ upwind flux $F_{N+1/2} = a\bar{u}_N$

which is consistent with the ODE though looks only first order (to be checked!). So now constant extrapolation is OK.

If we used <u>linear extrapolation</u> then

$$S_N = \frac{u_N - u_{N-1}}{h}$$

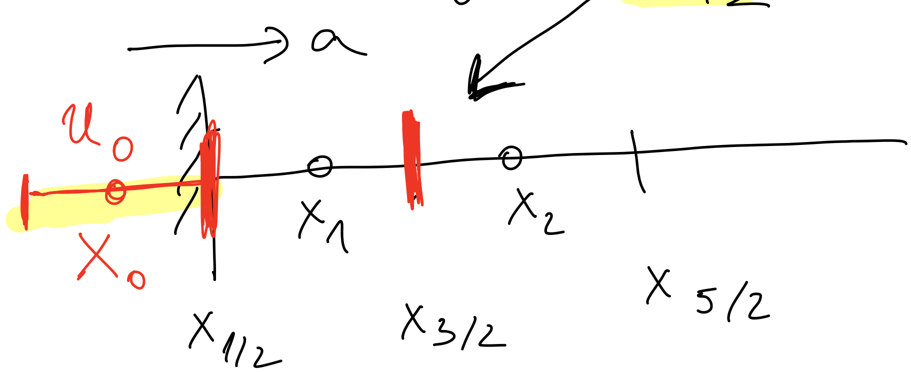
which is the same as the Beam Warming scheme for the last <u>face</u> (<u>NOT</u> the same as switching to BW in last <u>cell</u>)

We see that depending on what the code does ghost cells do different things!

$$\boxed{\text{Ghost cells are NOT real cells!}}$$

They are just a (computational) tool to implement one-sided stencils (finite differences) at the boundaries.

Let's go back to the inflow boundary & computing $F_{3/2}$



ghost cell

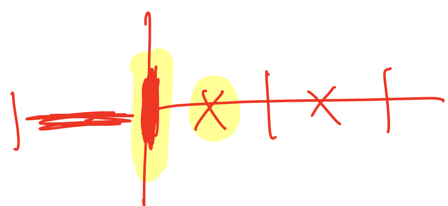
$$F_{3/2} = a\left(\bar{u}_1 + \frac{h}{2} s_1 (1-\nu)\right)$$

If we use downwind slopes as in LW, there is no issue,

$$s_1 = \frac{\bar{u}_2 - \bar{u}_1}{h}$$

But what if we are doing Fromm's method

$$s_1 = \frac{\bar{u}_2 - \bar{u}_0}{2h}$$

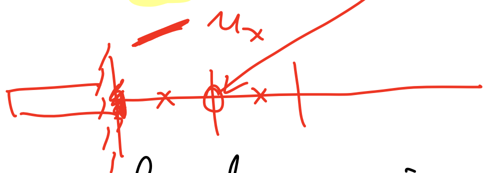


Linear extrapolation

$$\bar{u}_0^n = \underbrace{2\gamma_0(t)}_{\text{uses BC!}} - \bar{u}_1$$

$$\Rightarrow s_1 = \frac{(\bar{u}_2 + \bar{u}_1) - 2\gamma_0(t)}{2h}$$

$$S_1 = \frac{\frac{\bar{u}_2 + \bar{u}_1}{2} - \gamma_0(t)}{h}$$



which is a consistent slope estimate, so looks like a good choice. But this also makes sense:

$$S_1 = \frac{u_1 - \gamma_0(t)}{h/2}$$

To get this using ghost cells we would have needed

$$u_0 = u_2 - 4u_1 + 4\gamma_0$$

which is weird & is not quadratic extrapolation, which would be

$$u_0 = \frac{8\gamma_0}{3} - 2u_1 + u_2/3$$

Which choice is "good"?

Demo in class

Getting clear second-order convergence up to the boundary is <u>difficult</u> when both advection & diffusion compete.

More important is to avoid spurious reflections from artificial boundaries, since these polute the solution in the domain we care about.

In 2D/3D, corners are even harder & sometimes singular & not even well-posed in the PDE itself.

BCs for diffusion

It is useful here to consider first elliptic PDE

$$\mathcal{L} u = f$$

elliptic operator WITH BCs

with BCs. General rule:

Discretize elliptic operator with BCs to (say) 2nd order to get linear system:

$$LU + F^{(BC)} = F \quad \text{(elliptic)}$$

From inhomogeneous BCs

$$\Rightarrow \quad U_t = LU + F^{(BC)} \quad \text{(parabolic) MOL}$$

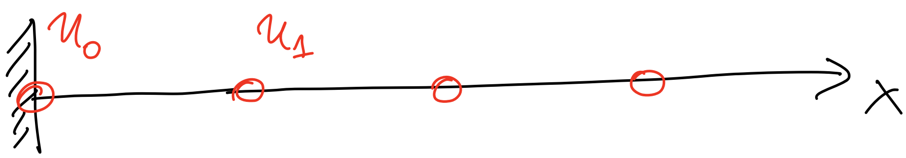
and you will get 2nd order for the parabolic eq. as well

Let us consider both FD & FV schemes, i.e., grids where the boundary is either a grid point or a face

[Both appear in FV in 2D sometimes, say incompressible Navier-Stokes on staggered grid]

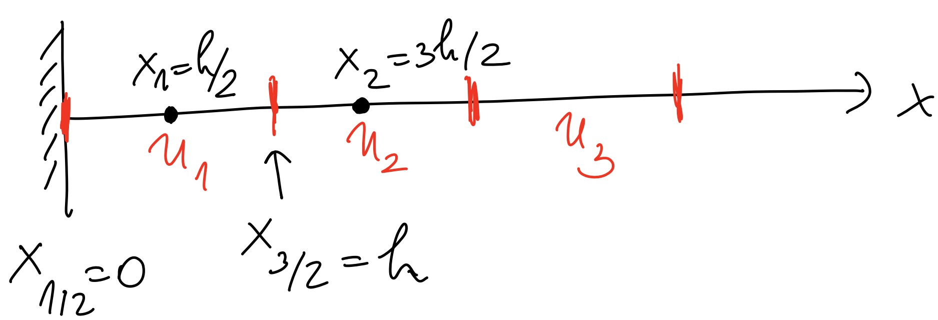
$$u_{xx} = f \quad , \quad x \in (0, L)$$

FD



$x_0 = 0$, $x_1 = h$, $x_2 = 2h$

FV



For FD, Dirichlet BC is easy, just set "ghost" cell:

$$u_0 = u(0)$$

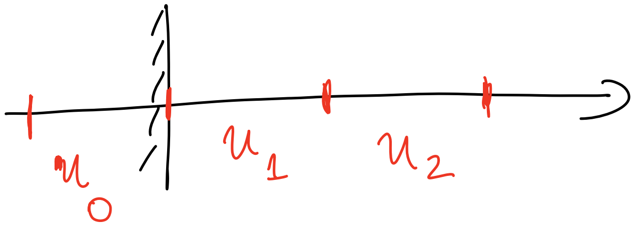
$$\Rightarrow \left(u_{xx}\right)_{x=h} \approx \frac{u_2 - 2u_1 + \overset{u(0)}{\overset{\shortparallel}{u_0}}}{h^2}$$

$$\Rightarrow \begin{cases} (Lu)_1 = \dfrac{u_2 - 2u_1}{h^2} \\ F_1^{(BC)} = \dfrac{u(0)}{h^2} \end{cases}$$

(FD - Dirichlet)

For FV, homogeneous Neumann is easy since it really means no flux through boundary.

For inhomogeneous BCs, set



$$\frac{u_1 - u_0}{h} \simeq u_x(x=0)$$

$$\Rightarrow \quad u_0 = u_1 - h\, u_x(x=0)$$

$$(u_{xx})_{x=h/2} \simeq \frac{u_2 - 2u_1 + u_0}{h^2}$$

$$= \frac{u_2 - u_1}{h^2} - \frac{u_x(x=0)}{h} \Rightarrow$$

$$\begin{cases} (Lu)_1 = \dfrac{u_2 - u_1}{h^2} \\ F_1^{BC} = -\dfrac{u_x(x=0)}{h} \end{cases}$$

(FV-Neumann)

Is this second order?
the easiest way to check is to check if exact for quadratic functions. That is,

take

$$u(x) = ax^2 + bx + c$$

$$u_1 = u(h/2)$$

$$u_2 = u(3h/2)$$

& confirm that

$$\frac{u_2 - u_1}{h^2} - \frac{u_x(x=0)}{h} = u_{xx}(0) = 2a$$

which shows 2nd order

For FD, however, Neumann BC is less obvious.

One option (Section 2.12 in FD book of Le Veque):

$$\frac{u_1 - u_0}{h} = u_x(x=0)$$

and use this equation instead of the PDE & the first point (u_0). This makes it harder to do parabolic for which we need PDE at $x=0$.

Instead, let's put a ghost point u_{-1} & use BC to fill it in:

E.g.

$$\frac{u_1 - u_{-1}}{2h} = u_x(x=0) \Rightarrow$$

$$u_{-1} = u_1 - 2h\,u_x(0)$$

$$(u_{xx})_{x=0} \simeq \frac{1}{h^2}\left(u_{-1} - 2u_0 + u_1\right)$$

$$= \frac{2}{h^2}\left(u_1 - u_0 - h\,u_x(0)\right) \Rightarrow$$

$$\begin{cases} (Lu)_0 = \dfrac{2}{h^2}(u_1 - u_0) \\ F_0^{BC} = -\dfrac{2}{h}u_x(0) \end{cases}$$

FD Neumann

This makes sense for the elliptic PDE since

$$(Lu)_0 + F_0^{BC} \to (\mathcal{L}u)(x=0)$$

$$\frac{2}{h^2}\left(u_1 - u_0 - h\,u_x(0)\right) = f(0)$$

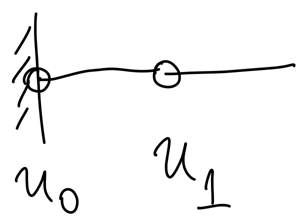
$$\Rightarrow \quad \frac{u_1 - u_0}{h} = u_x(0) + \frac{h}{2} f(0)$$

$$\frac{u(h) - u(0)}{h} = u_x(0) + \frac{h}{2} u_{xx}(0)$$

PDE

which is a one-sided Taylor series, one order more accurate than the previous attempt $\frac{u_1 - u_0}{h} = f(0)$

Yet another approach is to use a 2nd order one-sided difference instead of ghost cells:



$$u(x \text{ near } 0) = ax^2 + bx + c$$

$$u_x(0) = b$$

$$u(0) = u_0 = c$$

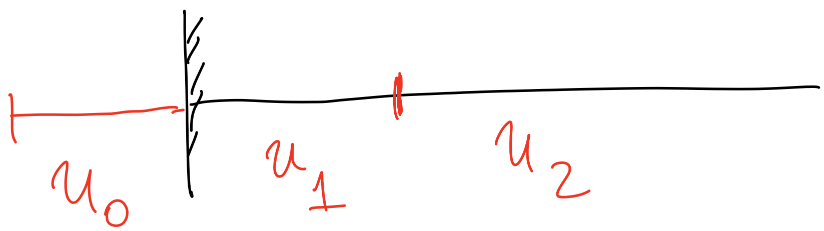
$$u(1) = ah^2 + bh + c = u_1$$

$$u_{xx}(0) = 2a = \frac{2}{h^2}(u_1 - u_0) - \frac{2}{h} u_x(0)$$

same as what we got before

Since this is exact for quadratic functions, expect 2nd order

For FV, Dirichlet is less obvious. Let's try using a ghost cell



BC

$$\frac{u_0 + u_1}{2} \approx u(x=0)$$

$$\Rightarrow \quad u_0 = 2u(0) - u_1$$

(linear extrapolation)

$$(u_{xx})(x = h/2) = \frac{1}{2}\left(u_0 - 2u_1 + u_2\right)$$

$$= \frac{1}{h^2}\left(-3u_1 + u_2 + 2u(0)\right)$$

$$\Rightarrow \begin{cases} (Lu)_1 = \frac{1}{h^2}\left(u_2 - 3u_1\right) \\ f_1^{BC} = \frac{2u(0)}{h^2} \end{cases}$$ FV Dirichlet #1

The matrix L looks like

$$L = \frac{1}{h^2}\begin{bmatrix} -3 & 1 & & & \\ 1 & -2 & 1 & & \\ & 1 & -2 & 1 & \\ & & 1 & \ddots & \\ & & & & \end{bmatrix}$$

which is symmetric negative definite, just like the Laplacian operator with Dirichlet BCs.
So this is a good discretization in terms of robustness & physical fidelity? Is it 2^{nd} order accurate?

If we plug in a quadratic function like before, we would get

$$\frac{1}{h^2}\left(-3u_1+u_2+2u(0)\right) =$$

$$\frac{3a}{2} \neq 2a = u_{xx}(h/2)$$

so this is not consistent with PDE at boundary.

Yet numerically this is 2^nd order for diffusion equation.

But, if we also have advection, the error introduced into the domain is advected into the domain & we loose 2^nd order (demo code)

Can we get 2^{nd} order accuracy at boundary?

We want

$$u_{xx}(x = h/2) = \alpha\, u(h/2) + \beta(3h/2) + \gamma\, u(0)$$

to be exact for <u>all</u> quadratic functions

$$u(x) = ax^2 + bx + c \quad \Rightarrow$$

(simple 3x3 linear solve)

$$\alpha = -\frac{4}{h^2} \qquad \beta = \frac{4}{3h^2} \qquad \delta = \frac{8}{3h^2}$$

$$\begin{cases} (Lu)_1 = \dfrac{4}{3h^2}(3u_1 - u_0) \\ F_1^{BC} = \dfrac{8\,u(0)}{3h^2} \end{cases}$$

FV Dirichlet #2

Note that the matrix L is no longer symmetric! Eigenvalues may not all be real ... so we could be sacrificing stability for accuracy.

An easier & more flexible way to derive the same BC & put it in codes (including non-constant diffusion!) is to use quadratic extrapolation to ghost cell

$$u_0 \simeq u(-h/2) = -2u_1 + \frac{u_2}{3} + \frac{8u(0)}{3}$$

$$\Rightarrow \frac{u_0 - 2u_1 + u_2}{h^2} = \frac{4}{3h^2}\left(3u_1 - u_0\right) + \frac{8u(0)}{3h^2}$$

as before

With non-constant diffusion:

$$F_{1/2} = -d_{1/2}\left(\frac{u_1 - u_0}{h}\right)$$

$$F_{3/2} = -d_{3/2}\left(\frac{u_2 - u_1}{h}\right)$$

$$\left((d u_x)_x\right)(x = h/2) = -\frac{F_{3/2} - F_{1/2}}{h}$$

$$= -\frac{\left(3 d_{1/2} + d_{3/2}\right)}{h^2} u_1$$

$$+ \left(\frac{\frac{1}{3} d_{1/2} + d_{3/2}}{h^2}\right) u_2$$

Matrix L

$$+ \frac{8 d_{1/2}\, u(0)}{3h^2}$$

We will not have time to discuss theory in any detail here, and the general theory is called GKSO theory (Gustafsson, Kreiss, Oliger, Osher) and is complicated.

An important point to realize is that the error follows the same (discretized) PDE as the solution, (This follows from linearity) with the local truncation error as a source term on the r.h.s.

E.g. error at an inflow boundary will be <u>advected</u> <u>into</u> the domain (and is important)

For elliptic PDEs:

Let $\hat{u}$ be numerical solution

& u be discretized true solution

Error $E = \hat{u} - u$

$$L\hat{u} = f \quad \text{(Discrete system)}$$

Local Truncation error (LTE):

$$\tau = Lu - f$$

$$L(u - \hat{u}) = LE = \tau$$

If we make a larger error at a boundary, how it affects the interior depends on solution of $LE = \tau$ which approximates

$\simeq \mathcal{L}e = \tau$ (elliptic PDE + source on boundary)

For $\mathcal{L} = \partial_{xx}$ + periodic

$$\bar{\tau} = \frac{h^2}{12} u_{xxxx} + O(h^4)$$

(Taylor series)

$$\mathcal{L} e = \bar{\tau} \Rightarrow$$

$$e_{xx} \approx \frac{h^2}{12} u_{xxxx} \Rightarrow$$

$$e \simeq \frac{h^2}{12} u_{xx} = \frac{h^2}{12} f$$

which is an excellent error estimate in the absence of boundaries.

Now imagine we have BCs, say Neumann on right & Dirichlet on left, and we modify L accordingly.

E.g. imagine

$$\tau = \begin{bmatrix} c_L\, O(h^p) \\ O(h^2) \\ c_R\, O(h^q) \end{bmatrix} \quad \begin{matrix} \leftarrow \text{Left e.g. } p=0 \text{ (inconsistent)} \\ \\ \leftarrow \text{Right e.g. } q=1 \text{ (first order)} \end{matrix}$$

$$L = \frac{1}{h^2} \begin{bmatrix} -1 & 1 & & & \\ 1 & -2 & \ddots & & \\ & 1 & \ddots & \ddots & \\ & & \ddots & \ddots & 1 \\ & & & 1 & -3 \end{bmatrix} \quad \left(\begin{matrix}\text{Discrete} \\ \text{Laplacian} \\ + \text{BCs}\end{matrix}\right)$$

Solve $LE = \tau$ & you will see that

$$E = O(h^2) \quad \underline{\text{everywhere}}$$

This is because $L^{-1} = h^2 O(1)$ has an h^2 in front which helps us! Specifically

$$L^{-1}\begin{bmatrix}1\\0\\0\\0\end{bmatrix} = -\frac{h^2}{2}\begin{bmatrix}1\\1\\1\\1\\\vdots\end{bmatrix}$$

$$L^{-1}\begin{bmatrix}0\\0\\\vdots\\1\end{bmatrix} = h^2\begin{bmatrix}1\\2\\3\\\vdots\\N\end{bmatrix} - \frac{h^2}{2}$$

$\leftarrow$ <u>error grows</u>

So

$$E = h^2\left[C_L\, O(h^p) + N \cdot C_R \cdot O(h^q)\right]$$

$$E = C_L\, O(h^{p+2}) + L\, C_R\, O(h^{q+1})$$

This means we can get a 2^{nd} order scheme <u>even</u> if $p=0$ & $q=\underline{1}$!

To see this from the PDE perspective $\mathcal{L} e = \tau$, note that e satisfies:

$$\begin{cases} e_{xx} = \dfrac{h^2}{12} u_{xxxx} & \text{(interior)} \\ e(x=0) = \alpha\, O(h^p) \\ e_x(x=L) = \beta\, O(h^q) \end{cases}$$

$$\Rightarrow \quad e(x) = \frac{h^2}{12} f(x) + \underbrace{\alpha}_{\text{constant}} + \underbrace{\beta x}_{\text{grows}}$$

which tells us that error introduced at Dirichlet BC will propagate <u>unchanged</u> through interior, but error at Neumann boundary will grow in interior

For time-dependent PDEs, consider MOL for simplicity

$$u'(t) = \underbrace{L}_{\text{assume constant}} u(t) + g(t)$$

LTE $\hat{u}'(t) = L\hat{u} + g + \tau$

$$e'(t) = \hat{u}' - u' = Le + \tau$$

$$e' = Le + \tau$$

$$\left.\mathcal{E}_t = \mathcal{L}\mathcal{E} + \tau\ \right]$$ error approx. satisfies same PDE + source

$$e' = L(e + L^{-1}\tau)$$

$$= L(e + \xi(t))$$

If scheme is stable, then perturbation/error ξ won't grow too fast

So if $\xi = O(h^p)$ then $e = O(h^p)$ for finite time. This means that we need to control / bound / estimate ξ!

$$L\xi = \tau$$

which is the steady-state equation $\mathcal{L}\xi = \tau$, i.e., elliptic PDE for parabolic eqs.
This shows that if we discretize elliptic PDE + BCs to second order, we will get second order for the parabolic one if time integrator is stable & sufficiently accurate.
For advection-diffusion, error at inflow boundaries gets advected into the domain