

EXERCISE - NUMERICS

a) $\partial_t b + \partial_z [\mu_2 b] = 0, \mu = \alpha b^2 - \beta b^2 \partial_z b, z \in [0, H]$

Plug into first eqn:

$$\partial_t b + \partial_z [\alpha b^3 - \beta \partial_z b b^3] = 0 \quad (5)$$

Linearize by using $b = D_0 + b'$ & assume b' is small & D_0 is constant. We get

$$\partial_t b' + \partial_z [\underbrace{\alpha (D_0 + b')^3 - \beta (D_0 + b')^3 \partial_z b'}_{\dots} = 0]$$

$$\dots + \partial_z [(D_0 + b')^3 (\alpha - \beta \partial_z b')] = 0$$

$$\dots + 3(D_0 + b')^2 \partial_z b' (\alpha - \beta \partial_z b') + (D_0 + b') (-\beta \partial_z^2 b') = 0$$

Assuming b' is small only D_0 terms survive in polynomial expansion, so:

$$\partial_t b' + 3D_0^2 \partial_z b' (\alpha - \beta \partial_z b') + D_0^3 \beta \partial_z^2 b' = 0$$

$$\partial_t b' + 3D_0^2 \cancel{\partial_z b'} - 3D_0^2 \beta (\partial_z b')^2 - D_0^3 \beta \partial_{zz} b' = 0$$

↑
small in
comparison to]

Hence, we get

$$\partial_t b' + 3\alpha D_0^2 \partial_z b' - \beta D_0^3 \partial_{zz} b' = 0 \quad (6)$$

Note that $(\partial_t + \partial_z) b = 0$ describes wave transport of quantity b , while i.e. convection. Meanwhile, $(\partial_t - \partial_{zz}) b = 0$ describes diffusion, or spreading effect.

Using these operators together we get convection-diffusion equation.

Equation (5) is non-linear as after differentiating w.r.t. z we get

$$\partial_z [\alpha b^3 - \dots] = \underbrace{3\alpha b^2 \partial_z b - \partial_z (\dots)}$$

non-linear term.

Although, all terms contain constant coefficients in eqn. (6), this is the result of linearising the equation (5), i.e. neglecting non-linear terms as being too small. ~~If there are not small we get non-linear terms.~~ Hence, ~~the equations can be called non-linear.~~

$$(b) \partial_t b + \partial_z [ab^3 - b^5 \partial_z b] = 0$$

$$\partial_t b + 3ab^2 \partial_z b - 5b^3 (\partial_z b)^2 - b^5 \partial_{zz} b = 0$$

Let $n \in \mathbb{N}$ & $j \in \{0, \dots, J\}$, then

$$b_j^n = b(j \Delta z, n \Delta t), \text{ where } \Delta z = \frac{1}{J} \text{ & } \Delta t$$

is discrete time step.

$$b_j^{n+1} = b_j^n + \Delta t \partial_t b_j^n + O((\Delta t)^2)$$

$$\frac{b_j^{n+1} - b_j^n}{\Delta t} = \partial_t b_j^n + O((\Delta t)^2)$$

$$\therefore \partial_t b_j^n \approx \frac{b_j^{n+1} - b_j^n}{\Delta t} \quad (*)$$

This is called forward Euler method.

Now, consider central difference method.
we derive

We have

$$b_j^{n+1} = b_j^n + \Delta z \partial_z b_j^n + \frac{(\Delta z)^2}{2} \partial_{zz} b_j^n + O((\Delta z)^3)$$

$$b_j^{n-1} = b_j^n + \Delta z \partial_z b_j^n + \frac{(\Delta z)^2}{2} \partial_{zz} b_j^n - O((\Delta z)^3)$$

Add these two together to get

$$b_j^{n+1} + b_j^{n-1} = 2b_j^n + (\Delta z)^2 \partial_{zz} b_j^n + O((\Delta z)^4)$$

$$\therefore \partial_{zz} b_j^n \approx \frac{b_j^{n+1} - 2b_j^n + b_j^{n-1}}{(\Delta z)^2} \quad (**) \quad (3)$$

If we discretize convective part of eqn (6) we get

$$b_j^{(n+1)} = b_j^{(n)} - \Delta t \left(3x D_0^2 \partial_z b \right) + \dots$$

in
other
terms

Note that $3x D_0^2 > 0$, so to construct upwind scheme we need to use

$$\partial_z b \approx \frac{(b_j^{(n)} - b_{j-1}^{(n)})}{\Delta x}. \quad (**)$$

We obtain it similarly as ~~temporal~~ temporal approximation. We have

$$b_{j-1}^{(n)} = b_j^{(n)} - \Delta z \partial_z b_j^{(n)} + O((\Delta z)^2)$$

$$\Leftrightarrow \Delta z \partial_z b_j^{(n)} = b_j^{(n)} - b_{j-1}^{(n)} + O((\Delta z)^2)$$

Hence, we get

$$\partial_z b_j^{(n)} \approx \frac{b_j^{(n)} - b_{j-1}^{(n)}}{\Delta z}$$

Using (*), (**), (***) we can easily discretize eqn (6):

$$\partial_t b' + 3\alpha D_0^2 \partial_2 b' - \beta D_0^3 \partial_{22} b' = 0$$

becomes

$$\frac{b_j^{n+1} - b_j^n}{\Delta t} + 3\alpha D_0^2 \frac{b_j^n - b_{j-1}^n}{\Delta z} - \beta D_0^3 \frac{b_{j+1}^n - 2b_j^n + b_{j-1}^n}{(\Delta z)^2} = 0$$

Rearranging for b_j^{n+1} we get

$$b_j^{n+1} = b_j^n - \frac{\Delta t}{\Delta z} 3\alpha D_0^2 (b_j^n - b_{j-1}^n) + \frac{\Delta t}{(\Delta z)^2} \beta D_0^3 (b_{j+1}^n - 2b_j^n + b_{j-1}^n)$$

It remains to approximate eqn (5):

$$\partial_t b + 3\alpha b^2 \partial_2 b - 3\beta b^2 (\partial_2 b)^2 - \beta b^3 \partial_{22} b = 0$$

becomes

$$\frac{b_j^{n+1} - b_j^n}{\Delta t} + 3\alpha \left(\frac{b_j^n}{\Delta z} \right)^2 \left(\frac{b_j^n - b_{j-1}^n}{\Delta z} \right) - 3\beta \left(\frac{b_j^n}{\Delta z} \right)^2 \left(\frac{b_j^n - b_{j-1}^n}{\Delta z} \right)^2 - \beta \left(\frac{b_j^n}{\Delta z} \right)^3 \left(\frac{b_{j+1}^n - 2b_j^n + b_{j-1}^n}{(\Delta z)^2} \right) = 0$$

Now, linearize by setting $b_j^n = D_0 + b_j'$ and similarly for $b_j^{n+1}, b_{j-1}^n, b_{j+1}^n$. We get

$$\frac{b_j^{n+1} - b_j^n}{\Delta t} = \frac{D_0 + b_j^{n+1} - D_0 - b_j^n}{\Delta t} = \frac{b_j^{n+1} - b_j^n}{\Delta t}$$

(5.)

$$3\alpha \left(\frac{b_j^u}{\Delta z}\right)^2 \frac{b_j^u - b_{j-1}^u}{\Delta z} = 3\alpha \left(D_0 + \frac{b_j^u}{\Delta z}\right)^2 \frac{D_0 + b_j^u - D_0 - b_{j-1}^u}{\Delta z}$$

linearise to get:

$$3\alpha D_0^2 \frac{b_j^u}{\Delta z} \frac{b_j^u - b_{j-1}^u}{\Delta z}$$

Note that term

$$-3\beta \left(\frac{b_j^u}{\Delta z}\right)^2 \left(\frac{b_j^u - b_{j-1}^u}{\Delta z}\right)^2 = -3\beta \left(D_0 + \frac{b_j^u}{\Delta z}\right)^2 \left(\frac{b_j^u - b_{j-1}^u}{\Delta z}\right)^2$$

is non-linear because of power 2, so it must be ignored.

Lastly

$$\beta \left(\frac{b_j^u}{\Delta z}\right)^3 \left(\frac{b_{j+1}^u - 2b_j^u + b_{j-1}^u}{\Delta z}\right) = \beta \left(D_0 + \frac{b_j^u}{\Delta z}\right)^3 \left(\frac{D_0 + b_{j+1}^u - 2D_0 - 2b_j^u}{(\Delta z)^2}\right)$$

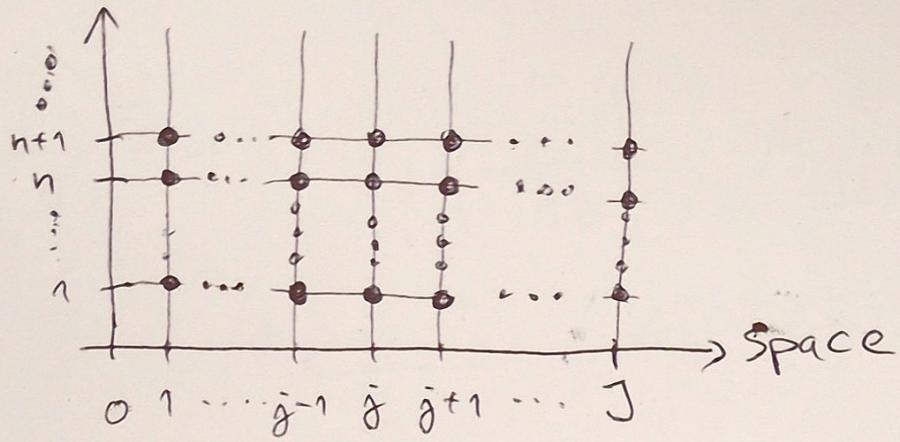
This becomes

$$\beta \left(\frac{b_j^u}{\Delta z}\right)^3 \left(\frac{b_{j+1}^u - 2b_j^u + b_{j-1}^u}{(\Delta z)^2}\right)$$

after linearisation.

Hence, discretising and then linearising eqn. (5) is the same as linearising and then discretising eqn. (5).

Time



For boundary condition require:

$$b_0^n = b_B \quad \& \quad b_J^n = b_T$$

also require initial condition:

$$b_j^0 = b_i(\Delta z_j)$$

Recall that non-linear eqn is

$$\partial_t b + \partial_z [\alpha b^3 - \beta b^3 \partial_z b] = 0$$

$$\Leftrightarrow \partial_t b + 3\alpha b^2 \partial_z b - \beta \partial_z [b^3 \partial_z b] = 0$$

Now, set $p(z, t) = b^3$, then the non-linear diffusion term can be approximated using

$$\partial_z [p \partial_z b] \approx \frac{1}{(\Delta z)^2} \left(p_{j+\frac{1}{2}}^n (\partial_{j+1}^n - \partial_j^n) - p_{j-\frac{1}{2}}^n (\partial_j^n - \partial_{j-1}^n) \right)$$

from Morton & Mayers (2005).

Hence, the discretisation becomes

$$\frac{b_j^{n+1} - b_j^n}{\Delta t} + 3\alpha \left(b_j^n \right)^2 \left(\frac{b_j^n - b_{j-1}^n}{\Delta z} \right) - \beta \frac{1}{(\Delta z)^2} \left(\left(\frac{r_{j+1}^n + r_j^n}{2} \right) \left(b_{j+1}^n - b_j^n \right) \right. \\ \left. - \left(\frac{r_{j-1}^n + r_j^n}{2} \right) \left(b_j^n - b_{j-1}^n \right) \right) = 0$$

Rewrite the equation

$$b_j^{n+1} = -3\alpha \left(b_j^n \right)^2 \frac{\left(b_j^n - b_{j-1}^n \right) \Delta t}{(\Delta z)} + \beta \frac{\Delta t}{(\Delta z)^2} \left(\left(\frac{r_{j+1}^n + r_j^n}{2} \right) \left(b_{j+1}^n - b_j^n \right) \right. \\ \left. - \left(\frac{r_{j-1}^n + r_j^n}{2} \right) \left(b_j^n - b_{j-1}^n \right) \right) + b_j^n$$

The advantage of using this discretisation is that we maintain "additional term" after the discretisation. This term

$$\partial_z [b^3 \partial_z b] = \underline{3b^2 (\partial_z b)^2} + b^3 \partial_z \partial_z b$$

would disappear after linearisation, but by not expanding & discretising we somehow include it!

Linearise the above scheme, i.e. set

$$b_j^n = D_0 + b_j^{n-1} \Delta t, \text{ then}$$

then

$$p_j^n = (b_j^n)^3 = (D_0 + b_j^{n-1} \Delta t)^3 = D_0^3 + 3D_0^2 b_j^{n-1} \Delta t + \dots$$

higher
order terms

However, note that

$$\frac{b_j^n - b_{j-1}^n}{\Delta z} = \frac{D_0 + b_j^{n-1} \Delta t - D_0 - b_{j-1}^{n-1} \Delta t}{\Delta z}$$

These kind of terms are always linear, hence

$$p_j^n = D_0^3$$

is the only surviving term and the scheme becomes:

$$b_j^{n+1} = -5\alpha(D_0) \left(b_j^n - b_{j-1}^n \right) \frac{\Delta t}{\Delta z} + \beta \frac{\Delta t}{(\Delta z)^2} \left(\frac{D_0^3}{2} \left(b_{j+1}^n - b_j^n \right) - \frac{D_0^3}{2} \left(b_j^n - b_{j-1}^n \right) \right) + D_0 b_j^n \quad (S2)$$

(a)

c) Let

$$b_j^n = \lambda^n e^{ikj\Delta z}$$

Then (9) becomes

$$\lambda^{n+1} e^{ikj\Delta z} = -3\kappa D_0^2 \left(e^{ik(j+1)\Delta z} - e^{ik(j-1)\Delta z} \right) \frac{\Delta t}{\Delta z} \lambda^n$$

$$+ \lambda^n \beta \frac{\Delta t}{(\Delta z)^2} \left(\frac{D_0^3}{2} \right) \left(e^{ik(j+1)\Delta z} - e^{ikj\Delta z} - e^{ik(j-1)\Delta z} + e^{ik(j-2)\Delta z} \right)$$
$$+ \lambda^n e^{ikj\Delta z}.$$

Now, divide by $\lambda^n e^{ikj\Delta z}$ to get

$$\lambda = -3\kappa D_0^2 \frac{\Delta t}{\Delta z} \left(1 - e^{-ik\Delta z} \right) + \beta \frac{\Delta t}{(\Delta z)^2} D_0^3 \left(\cos(k\Delta z) - 1 \right) + 1$$

$$= -3\kappa D_0^2 \frac{\Delta t}{\Delta z} \left(1 - \cos(k\Delta z) + i \sin(k\Delta z) \right) + \dots$$

$$= -3\kappa D_0^2 \frac{\Delta t}{\Delta z} \sin(k\Delta z) + \underbrace{\left(1 - \left(1 - \cos(k\Delta z) \right) \frac{\Delta t}{\Delta z} D_0^2 \left(3\kappa + \frac{\beta D_0}{\Delta z} \right) \right)}_{2 \sin^2 \left(\frac{k\Delta z}{2} \right)}$$

Now, note that $\lambda = \lambda_R + i\lambda_I$ and $\lambda^2 = \lambda_R^2 + \lambda_I^2$. Hence

$$\lambda^2 = 9\kappa^2 D_0^4 \left(\frac{\Delta t}{\Delta z} \right)^2 \sin^2(k\Delta z) + \left(1 - 2 \sin^2 \left(\frac{k\Delta z}{2} \right) \frac{\Delta t}{\Delta z} D_0^2 \left(3\kappa + \frac{\beta D_0}{\Delta z} \right) \right)^2$$

CASE: $\kappa = 0$

$$\lambda^2 = 1 - 2 \sin^2 \left(\frac{k\Delta z}{2} \right) \frac{\Delta t}{\Delta z} \left(\frac{\beta D_0}{\Delta z} \right) \leq 1$$

iff

$$\sin^2 \left(\frac{k\Delta z}{2} \right) \frac{\Delta t}{(\Delta z)^2} \beta D_0 \geq 0$$

which always holds as $\sin^2(0)$ is non-negative!

CASE $b=0$

$$\gamma^2 = q \alpha^2 D_0^4 \left(\frac{\Delta t}{\Delta z} \right)^2 \sin^2(k \Delta z) + \left(1 - 6 \sin^2(k \frac{\Delta z}{2}) \right) \frac{\Delta t}{\Delta z} D_0^2 \alpha^2$$
$$= q \alpha^2 D_0^4 \left(\frac{\Delta t}{\Delta z} \right)^2 \sin^2(k \Delta z) + 7 - 12 \sin^2(k \frac{\Delta z}{2}) \frac{\Delta t}{\Delta z} D_0^2 \alpha^2$$
$$+ 36 \left(\frac{\Delta t}{\Delta z} \right)^2 D_0^4 \alpha^2 \sin^4 \left(\frac{k \Delta z}{2} \right) \leq 1$$

iff

$$q \alpha^2 D_0^4 \left(\frac{\Delta t}{\Delta z} \right)^2 \sin^2(k \Delta z) - 12 \sin^2 \left(\frac{k \Delta z}{2} \right) \frac{\Delta t}{\Delta z} D_0^2 \alpha^2$$
$$+ 36 \left(\frac{\Delta t}{\Delta z} \right)^2 \sin^4 \left(\frac{k \Delta z}{2} \right) \leq 0$$
$$D_0^4 \alpha^2$$

iff

~~$$q \alpha^2 D_0^4 \left(\frac{\Delta t}{\Delta z} \right)^2 \left(\sin^2(k \Delta z) + 4 \sin^4 \left(\frac{k \Delta z}{2} \right) \right) - \frac{\Delta t}{\Delta z} D_0^2 \alpha^2 \sin^2 \left(\frac{k \Delta z}{2} \right) \leq 0$$~~

$$3 \alpha D_0^2 \frac{\Delta t}{\Delta z} \left(\sin^2(k \Delta z) + 4 \sin^4 \left(\frac{k \Delta z}{2} \right) \right) \leq 4 \sin^2 \left(\frac{k \Delta z}{2} \right)$$

$$\Delta t \leq \frac{4 \sin^2 \left(\frac{k \Delta z}{2} \right) \Delta z}{3 \alpha D_0^2 \left(\sin^2(k \Delta z) + 4 \sin^4 \left(\frac{k \Delta z}{2} \right) \right)}$$

$$\leq \frac{4 \Delta z}{3 \alpha D_0^2 (1 + 4)} = \frac{4 \Delta z}{15 \alpha D_0^2}$$

* If $\lambda^2 \leq 1$, then $|\gamma| \leq 1$.

Hence, use $\Delta t \leq \frac{4 \Delta z}{15 \alpha D_0^2}$

Case $\gamma/b = 0$:

$$|\lambda| \leq b - 6 \times \frac{D_0^2 \Delta t}{\Delta z} P \leq 1$$

iff

$$-2 \leq -6 \times \frac{D_0^2 \Delta t}{\Delta z} \leq 0$$

iff

$$\frac{\Delta t}{\Delta z} \leq \frac{1}{3 \times D_0^2}$$

Hence, choose $\Delta t \leq \frac{\Delta z}{3 \times D_0^2}$ to ensure stability.

d) Recall the discretization of (6):

$$b_j^{(n+1)} = b_j^{(n)} - \frac{\Delta t}{\Delta z} 3 \times D_0^2 (b_j^{(n)} - b_{j-1}^{(n)}) + \frac{\Delta t}{(\Delta z)^2} 5 D_0^2 ()$$

Require that $b_j^{(n)} \geq 0$ under maximum principle ~~require we~~

need to establish condition under which $b_j^{(n+1)} \geq 0$.

Rearrange terms to get

$$b_j^{(n+1)} = b_{j-1}^{(n)} \left(\frac{\Delta t}{\Delta z} 5 \times D_0^2 + \frac{\Delta t}{(\Delta z)^2} \beta D_0^2 \right) + b_j^{(n)} \left(1 - \frac{\Delta t}{\Delta z} 3 \times D_0^2 - 2 \frac{\Delta t}{(\Delta z)^2} \beta D_0^2 \right)$$

$$+ b_{j+1}^{(n)} \left(\frac{\Delta t}{(\Delta z)^2} \beta D_0^2 \right)$$

$$\geq b_j^{(n)} \left(1 - \frac{\Delta t}{\Delta z} 3 \times D_0^2 - 2 \frac{\Delta t}{(\Delta z)^2} \beta D_0^2 \right) \geq 0$$

$$b_{j+1}^{(n)} - 2b_j^{(n)} + b_{j-1}^{(n)}$$