EXERCISE - NUMERICS

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

Plug into first eqn:

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

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

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

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

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

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

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

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

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

$$\partial_z [\alpha b^3 - \ldots] = \underbrace{3\alpha b^2 \partial_z b}_{\text{non-linear term.}} - \partial_z (\ldots)$$

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 these are not small we get non-linear terms. Hence, both equations can be called non-linear.~~

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

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

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

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

is discrete time step.

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

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

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

This is called forward Euler method.

Now, ~~consider~~ we derive central difference method.

We have

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

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

add these two together to get

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

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

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

$$b'^{n+1}_j = b'^n_j \cancel{+} - \Delta t \left(3\alpha D_0^2 \, \partial_z b' \right) + \underbrace{\ldots}_{\text{other terms}}$$

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

$$\partial_z b' \approx \frac{(b'^n_j - b'^n_{j-1})}{\Delta x}. \quad (***)$$

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

$$b'^n_{j-1} = b'^n_j - \Delta z \, \partial_z b'^n_j + O((\Delta z)^2)$$

$$\Leftrightarrow \quad \Delta z \, \partial_z b'^n_j = b'^n_j - b'^n_{j-1} + O((\Delta z)^2)$$

Hence, we get

$$\partial_z b'^n_j \approx \frac{b'^n_j - b'^n_{j-1}}{\Delta z}$$

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

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

becomes

$$\frac{b'^{n+1}_j - b'^n_j}{\Delta t} + 3\alpha D_0^2 \frac{b'^n_j - b'^n_{j-1}}{\Delta z} - \beta D_0^3 \frac{b'^n_{j+1} - 2b'^n_j + b'^n_{j-1}}{(\Delta z)^2} = 0$$

Rearranging for b'^{n+1}_j we get

$$b'^{n+1}_j = b'^n_j - \frac{\Delta t}{\Delta z} 3\alpha D_0^2 \left(b'^n_j - b'^n_{j-1}\right) + \frac{\Delta t}{(\Delta z)^2} \beta D_0^2 \Big(\overbrace{\qquad}^{b'^n_{j+1} - 2b'^n_j + b'^n_{j-1}}\Big)$$ two

It remains to approximate equ ~~(6)~~ (5):

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

becomes

$$\frac{b^{n+1}_j - b^n_j}{\Delta t} + 3\alpha \left(b^n_j\right)^2 \frac{\left(b^n_j - b^n_{j-1}\right)}{\Delta z} - 3\beta \left(b^n_j\right)^2 \left(\frac{b^n_j - b^n_{j-1}}{\Delta z}\right)^2 - \beta \left(b^n_j\right)^3 \Big(\underbrace{\qquad}_{\frac{b^n_{j+1} - 2b^n_j + b^n_{j-1}}{(\Delta z)^2}}\Big) = 0$$

Don't differentiate diffusion term as said: done next I see.

Now, linearize by setting $b^n_j = D_0 + b'^n_j$ and similarly for b^{n+1}_j, b^n_{j-1}, b^n_{j+1}. We get

$$\frac{b^{n+1}_j - b^n_j}{\Delta t} = \frac{D_0 + b'^{n+1}_j - D_0 - b'^n_j}{\Delta t} = \frac{b'^{n+1}_j - b'^n_j}{\Delta t}$$

$$3\alpha \left(b_j^n\right)^2 \frac{b_j^n - b_{j-1}^n}{\Delta z} = 3\alpha \left(D_0 + b'^n_j\right)^2 \frac{\cancel{D_0} + b'^n_j - \cancel{D_0} - b'^n_{j-1}}{\Delta z}$$

linearise to get:

$$3\alpha D_0^2 b'^n_j \frac{b'^n_j - b'^n_{j-1}}{\Delta z}$$

Note that term

$$-3\beta \left(b_j^n\right)^2 \left(\frac{b_j^n - b_{j-1}^n}{\Delta z}\right)^2 = -3\beta \left(D_0 + b'^n_j\right)^2 \left(\frac{b'^n_j - b'^n_{j-1}}{\Delta z}\right)^2$$

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

Lastly

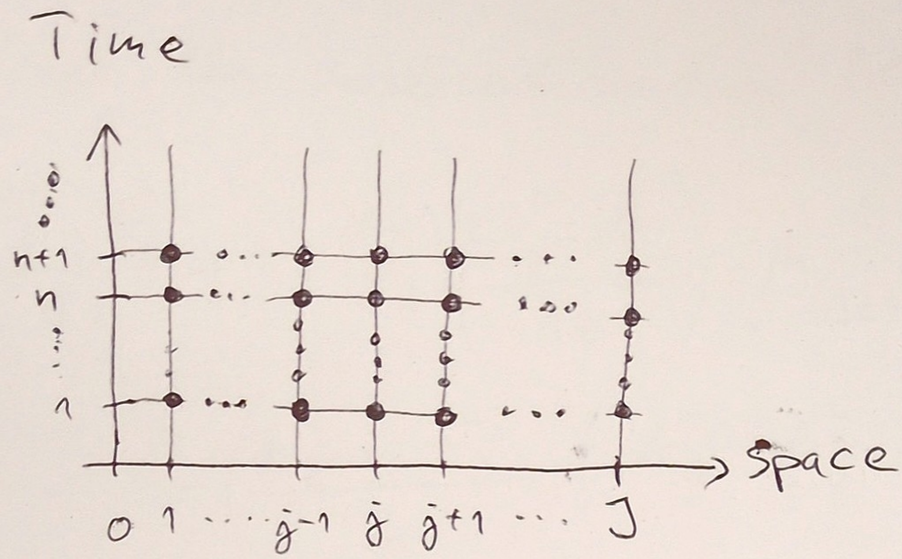
$$\beta \left(b_j^n\right)^3 \left(\frac{b_{j+1}^n - 2b_j^n + b_{j-1}^n}{\Delta z}\right) = \beta \left(D_0 + b'^n_j\right)^3 \left(\frac{\cancel{D_0} + b'^n_{j+1} - 2\cancel{D_0} - 2b'^n_j + \cancel{D_0} + b'^n_{j-1}}{(\Delta z)^2}\right)$$

This becomes

$$\beta \left(D_0\right)^3 \left(\frac{b'^n_{j+1} - 2b'^n_j + b'^n_{j-1}}{(\Delta z)^2}\right)$$

after linearisation.

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



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

$$\partial_z[p\, \partial_z b] \approx \frac{1}{(\Delta z)^2}\left(p^n_{j+\frac{1}{2}}(b^n_{j+1} - b^n_j) - p^n_{j-\frac{1}{2}}(b^n_j - b^n_{j-1})\right)$$

from Morton & Mayers (2005).

Hence, the discretisation becomes

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

Rewrite the equation

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

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

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

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

Linearise the above scheme, i.e. set

$$b_j^n = D_0 + b'^n_j, \cancel{\text{then}}$$

then

$$r_j^n = \left(b_j^n\right)^3 = \left(D_0 + b'^n_j\right)^3 = D_0^3 + 3D_0^2 b'^n_j + \dots$$

higher order terms

However, note that

$$\frac{b_j^n - b_{j-1}^n}{\Delta z} = \frac{\cancel{D_0} + b'^n_j - \cancel{D_0} - b'^n_{j-1}}{\Delta z}$$

these kind of terms are always linear, hence

$\cancel{r_j^n z}$ $\qquad r_j^n = D_0^3$

is the only surviving term, and the scheme becomes:

$$b'^{n+1}_j = -3\alpha (D_0)^2 \left(b'^n_j - b'^n_{j-1}\right)\frac{\Delta t}{\Delta z} + \beta \frac{\Delta t}{(\Delta z)^2}\left(\frac{D_0^3}{2}\left(b'^n_{j+1} - b^n_j\right) - \frac{D_0^3}{2}\left(b'^n_j - b'^n_{j-1}\right)\right) + \cancel{D_0}\, b'^n_j$$

$(S2)$

c) Let

$$b_j^n = \lambda^n e^{ik(j\Delta z)}$$

Then (♡) becomes

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

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

$$+ \lambda^n e^{ikj\Delta z}.$$

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

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

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

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

Now, note that $\lambda = \lambda_R + i\lambda_{II}$ and $\lambda^2 = \lambda_R^2 + \lambda_{II}^2$. Hence

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

CASE: $\alpha = 0$

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

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 $\sin^2(\cdot)$ is non-negative!

CASE $b=0$

$$\lambda^2 = 9\alpha^2 D_0^4 \left(\frac{\Delta t}{\Delta z}\right)^2 \sin^2(k\Delta z) + \left(1 - 6\sin^2\left(\frac{k\Delta z}{2}\right)\frac{\Delta t}{\Delta z} D_0^2 \alpha\right)^2$$

$$= 9\alpha^2 D_0^4 \left(\frac{\Delta t}{\Delta z}\right)^2 \sin^2(k\Delta t) + 1 - 12\sin^2\left(\frac{k\Delta z}{2}\right)\frac{\Delta t}{\Delta t} D_0^2 \alpha$$

$$+ 36\left(\frac{\Delta t}{\Delta z}\right)^2 D_0^4 \alpha^2 \sin^4\left(\frac{k\Delta z}{2}\right) \le 1$$

iff

$$9\alpha^2 D_0^4 \left(\frac{\Delta t}{\Delta z}\right)^2 \sin^2(k\Delta z) - 12\sin^2\left(\frac{k\Delta z}{2}\right)\frac{\Delta t}{\Delta z} D_0^2 \alpha$$

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

iff

$$\cancelto{3}{9}\alpha^{\cancel{2}} D_0^{\cancelto{2}{4}} \left(\frac{\Delta t}{\Delta z}\right)^{\cancelto{1}{2}} \left(\sin^2(k\Delta z) + 4\sin^4\left(\frac{k\Delta z}{2}\right)\right) - \cancelto{1}{\frac{\Delta t}{\Delta z}} \cancelto{1}{D_0^2\alpha}\, \cancelto{4}{12} \sin^2\left(\frac{k\Delta z}{2}\right) \le 0$$

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

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

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

Some factor off since should be dz/(3 alpha D0^2). -0.5

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

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

~~Case $\beta = 0$:~~

$$|\lambda| \leq \left|1 - 6\alpha \frac{D_0^2 \Delta t}{\Delta z}\right| \leq 1$$

iff

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

iff

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

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

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d) Recall the discretization of (6):

$$b'^{n+1}_j = b'^n_j - \frac{\Delta t}{\Delta z} 3\alpha D_0^2 \left(b'^n_j - b'^n_{j-1}\right) + \frac{\Delta t}{(\Delta z)^2} \beta D_0^2 \left(b'^n_{j+1} - 2b'^n_j + b'^n_{j-1}\right)$$

Require that $b'^n_j \geq 0$ under maximum principle ~~require~~ we need to establish condition under which $b'^{n+1}_j \geq 0$.

Rearrange terms to get

$$b'^{n+1}_j = b'^n_{j-1}\left(\frac{\Delta t}{\Delta z} 3\alpha D_0^2 + \frac{\Delta t}{(\Delta z)^2}\beta D_0^2\right) + b'^n_j\left(1 - \frac{\Delta t}{\Delta z} 3\alpha D_0^2 - 2\frac{\Delta t}{(\Delta z)^2}\beta D_0^2\right)$$

$$+ b'^n_{j+1}\left(\frac{\Delta t}{(\Delta z)^2}\beta D_0^2\right)$$

$$\geq b'^n_j\left(1 - \frac{\Delta t}{\Delta z} 3\alpha D_0^2 - 2\frac{\Delta t}{(\Delta z)^2}\beta D_0^2\right) \geq 0$$