1a) $\partial_t b + \partial_z(\alpha b^3 - \beta b^3 \partial_z b) = 0$

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

$\qquad (1) \qquad\qquad (2)$

Linearize : $b = D_0 + b'$

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

b' terms sufficiently small $b' \times b' \sim 0$

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

$\qquad (1) \qquad\qquad (2)$

The equations are refered to as the convection - diffusion equations as the (1) terms represent a convective flux, and the (2) terms represent a diffusive flux.

$$\text{b)}\quad \overbrace{\frac{b_j^{n+1} - b_j^n}{\Delta t}}^{\partial_t b} + \overbrace{3\alpha (b_j^n)^2 \left(\frac{b_j^n - b_j^n{}_{-1}}{\Delta z}\right)}^{\partial_z b \text{ (upwind)}} \qquad (5)$$

$$\underbrace{-\beta\,(q_{j+1/2}^n - q_{j-1/2}^n)\cdot\frac{1}{\Delta z^2}}_{\partial_{zz} b \text{ (2nd order CD)}} = 0$$

where $q = b^3 \partial_{zz} b$

$$\Rightarrow \quad q_{j+1/2}^n = (b_{j+1/2}^n)^3 (b_{j+1}^n - b_j^n)$$

$$q_{j-1/2}^n = (b_{j-1/2}^n)^3 (b_j^n - b_{j-1}^n)$$

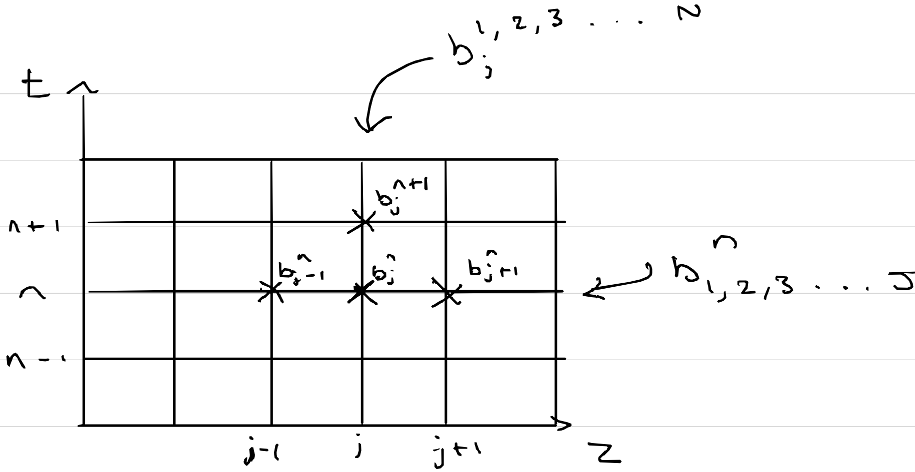
$$b_{j+1/2}^n = \frac{1}{2}(b_{j+1}^n + b_j^n)$$

$$b_{j-1/2}^n = \frac{1}{2}(b_j^n + b_{j-1}^n)$$

Complete discretization

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

$$\frac{b_j^{n+1} - b_j^n}{\Delta t} + 3\alpha D_0^2 \left(\frac{b_j^n - b_{j-1}^n}{\Delta z}\right) - \beta D_0^3 \left(\frac{b_{j+1}^n - 2 b_j^n + b_{j-1}^n}{(\Delta z)^2}\right) = 0 \qquad (6)$$



Linearizing (5) : $b = D_0 + b' \rightarrow b_j^n = D_0 + b'^n_j$

Time Derivative unchanged $\Rightarrow \dfrac{b_j^{n+1} - b_j^n}{\Delta t}$

Convective term

$$3\frac{d}{\Delta z}(b_j^n)^2(b_j^n - b_{j-1}^n)$$

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

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

$2D_0 b'^n_j \cdot b'^n_j$ or $\cdot b'^n_{j-1} \sim 0$ leaving:

$3\frac{d}{\Delta z} D_0^2 (b'^n_j - b^n_{j-1}) \Rightarrow$ same as the discretization of (6).

Diffusive term

Considering term in term $-\frac{\beta}{\Delta z}(q^n_{j+1/2} - q^n_{j-1/2})$

$$q^n_{j+1/2} = \frac{1}{\Delta z}(b^n_{j+1/2})^3 (b^n_{j+1} - b^n_j)$$

$$(b^n_{j+1/2})^3 \Rightarrow (D_0 + b'^n_{j+1/2})^3$$

$$= D_0^3 + \underbrace{3D_0^2 b'^n_{j+1/2}}_{\sim 0 \text{ when multiplied by } (b'^n_{j+1} - b'^n_j)} + 3D_0 \underbrace{(b'^n_{j+1/2})^2}_{\sim 0} + \underbrace{(b'^n_{j+1/2})^3}_{\sim 0}$$

$$\Rightarrow q^n_{j+1/2} = \frac{1}{\Delta z} D_0^3 (b'_{j+1} - b'^n_j (+D_0 - D_0))$$

$$\Rightarrow q^n_{j-1/2} = \frac{1}{\Delta z} D_0^3 (b'^n_j - b^n_{j-1} (+D_0 - D_0))$$

Diffusive term $\Rightarrow -\frac{\beta}{(\Delta z)^2} D_0^3 (b^n_{j+1} - 2b^n_j + b^n_{j-1})$

$\Rightarrow$ The linearization of the discretization of (5) yields the same as the discretization of the linearized (6).

The adjoint method is conservative, retaining the original form of the PDE, hence is more stable, meaning it's advantageous to use.

The boundary conditions are implemented such that

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

→ for $n > 0$

$$b_0^n = b_B \quad \text{and} \quad b_J^n = b_T$$

where $z_J = H \Rightarrow \Delta z = H/J$

1c) Fourier analysis: $\alpha = 0$, $\beta \neq 0$

⇒ equation becomes

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

which can also be written as:

$$b_j^{n+1} = b_j^n + \nu \left(b_{j+1}^n - 2b_j^n + b_{j-1}^n \right)$$

where $\nu = \beta D_0^3 \frac{\Delta t}{(\Delta z)^2}$

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

$$\Rightarrow \lambda = 1 + \nu \left(-2 + e^{ik\Delta z} + e^{-ik\Delta z} \right)$$

$$\Rightarrow \lambda = 1 + \nu \left(-4 \sin^2\left(\frac{k \Delta z}{2} \right) \right)$$

Scheme stable where $|\lambda|^n \leq 1$

$\nu > 0 \Rightarrow \lambda > -1 \,/\, \lambda \leq 1$

$$1 + \nu\left(-4\sin^2\left(\frac{k\Delta z}{2}\right)\right) > -1$$

$$\nu\left(-4\sin^2\left(\frac{k\Delta z}{2}\right)\right) > -2$$

$$\Rightarrow \quad \nu < \frac{2}{4\sin^2\left(\frac{k\Delta z}{2}\right)}, \quad \nu < \frac{1}{2\sin^2\left(\frac{k\Delta z}{2}\right)}$$

worst possible case : $\sin^2(k) = 1$

$$\Rightarrow \quad \Delta t < \frac{(\Delta z)^2}{2\beta D_0^3}$$

where $\alpha \neq 0$, $\beta = 0$

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

$$\mu = \frac{\Delta t}{\Delta z}\left(-3\alpha D_0^2\right)$$

$$\Rightarrow \quad b_j^{n+1} = b_j^n + \mu\left(b_j^n - b_{j-1}^n\right)$$

$$\lambda - 1 = \mu\left(1 - e^{-ik\Delta z}\right)$$

$$= \mu\left(1 - \left(\cos k\Delta z - i\sin k\Delta z\right)\right)$$

$$\lambda_R = 1 - \mu\left(1 - \cos k\Delta z\right)$$

$$\lambda_I = \mu \sin k\Delta z$$

$$|\lambda|^2 = |\lambda_R|^2 + |\lambda_I|^2$$

$$|\lambda_R|^2 = \left[(1-\mu) + \mu\cos k\Delta z\right]^2 + \left[\mu \sin k\Delta z\right]^2$$

$$= (1-\mu)^2 + \mu^2 + 2\mu(1-\mu)\cos k\Delta z$$

$$= 1 - 2\mu(1-\mu)(1 - \cos k\Delta z)$$

$$= 1 - 4\mu(1-\mu)\sin^2\left(\frac{k\Delta z}{2}\right)$$

$|\lambda|^n < 1$

$\lambda < 1$ / $\lambda > -1$

$$1 - 4(1-\mu)\sin^2\left(\frac{K\Delta z}{2}\right) > -1$$

$$4(1-\mu)\sin^2\left(\frac{K\Delta z}{2}\right) > -2$$

worst possible case: $\sin^2(K) = 1$

$$\Rightarrow \quad 4(1-\mu) < 2$$

$$1-\mu < \frac{1}{2}$$

$$\mu > \frac{1}{2}$$

$$\frac{\Delta t}{\Delta z^2}\left(-3\alpha D_0^2\right) > \frac{1}{2}$$

$$\Rightarrow \quad \Delta t < \frac{(\Delta z)^2}{6\alpha D_0^2}$$

$$\Rightarrow \quad \Delta t < \min\left(\frac{\Delta z}{2\beta D_0^3}, \frac{(\Delta z)^2}{6\alpha D_0^3}\right)$$

1d) Considering update scheme for b_j^{n+1}

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

which can also be written as

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

To satisfy the maximum principle, the coefficients of discrete b values must be > 0. For b_{j+1}^n and b_{j-1}^n, the values are all real and positive. Provides the condition for b_j^n:

$$1 - \left(\frac{\Delta t}{\Delta z} 3\alpha D_0^2 + \frac{\Delta t}{(\Delta z)^2} 2\beta D_0^3\right) > 0$$

$$\Delta t < \frac{(\Delta z)^2}{3\alpha D_0^2 \Delta z + 2\beta D_0^3}$$

1e) To derive variable ~~time~~ step, consider update scheme such that

$$b_j^{n+1} = b_j^n - \Delta t\left[\frac{B_{con}}{\Delta z} - \frac{B_{dif}}{(\Delta z)^2}\right]$$

where $B_{dif} = \beta\left[(b_{j+1/2}^n)^3(b_{j+1}^n - b_j^n) - (b_{j-1/2}^n)^3(b_j^n - b_{j-1}^n)\right]$

and $B_{con} = 3\alpha(b_j^n)^2(b_j^n - b_{j-1}^n)$

Given condition $b_j^{n+1} > 0$

$$b_j^n - \Delta t\left[\frac{B_{con}}{\Delta z} - \frac{B_{dif}}{(\Delta z)^2}\right] > 0$$

$$\Rightarrow \quad \Delta t < \frac{b_j^n(\Delta z^2)}{B_{con}\cdot\Delta z - B_{dif}}$$

1f) Consider the convection approximation

using a central approximation

$\Rightarrow \quad \partial_z b_j^n \approx \dfrac{b_{j+1}^n - b_{j-1}^n}{2\Delta z}$

Similar to previously

$b_j^{n+1} = b_j^n - \Delta t \left(\dfrac{B_{2con}}{\Delta z} - \dfrac{B_{dif}}{(\Delta z)^2} \right)$

where $B_{2con} = 3\alpha (b_j^n)^2 (b_{j+1}^n - b_{j-1}^n) \cdot \dfrac{1}{2\Delta z}$

$\Rightarrow \Delta t < \dfrac{b_j^n (\Delta z)^2}{B_{2con}\Delta z - B_{dif}}$

2a) $\partial_t b + \partial_z (\alpha b^3 - \beta b^3 \partial_z b) = 0$ (5)

Steady state $\Rightarrow \partial_t b = 0$

$\partial_z (\alpha b^3 - \beta b^3 \partial_z b) = 0$

integrating $\rightarrow$ $\alpha b^3 - \beta b^3 \partial_z b = Q$ (integration constant

$\Rightarrow \beta b^3 \dfrac{\partial b}{\partial z} = \alpha b^3 - Q$

$\dfrac{db}{dz} = \dfrac{\alpha}{\beta} - \dfrac{Q}{\beta} b^{-3}$

$\Rightarrow b_{j+1} = b_j + \Delta z \left(\dfrac{\alpha}{\beta} - \dfrac{Q}{\beta} b_j^{-3} \right)$

2c) Through variation of spatial step (Δz) the solution $b(z,t)$ can be compared with the solution to the high resolution solution to the steady state solution. The rate of change of error with respect to the change in the spatial step can be used as the order of spatial accuracy $\Rightarrow$ here it is 1^{st} order accurate. (plots for L^2, L^∞ in code)

2d) For travelling wave $b(z,t) = b(s)$

where $s = z - z_{r0} - ct$

$$\partial_t b = \frac{\partial b}{\partial s} \partial_t s = -cb'(s), \; \partial_z b = b'(s)$$

$\rightarrow$ substituting into PDE.

$$-cb' + \alpha b^3 - \beta b^3 b' = Q \quad \text{(constant of integration)}$$

$$\beta b^3 b' = \alpha b^3 - cb - Q \quad [1^{st} \text{ order PDE for } b(s)]$$

$\Rightarrow$ any $b(s)$ satisfying equation provides travelling wave solution.

Where $Q = 0$

$$\times b^{-3} \curvearrowright \quad \beta b^3 b' = \alpha b^3 - cb$$

$$\beta b' = \alpha - cb^{-2}$$

seperating variables : $\dfrac{db}{\alpha - cb^{-2}} = \dfrac{1}{\beta} ds$

$$\Rightarrow \int \frac{b^2}{\alpha b^2 - c} \, db = \frac{1}{\beta} s + k_1$$

$$\left(\frac{b^2}{\alpha b^2 - c} = \frac{\alpha b^2 - c + c}{\alpha(\alpha b^2 - c)} = \frac{1}{\alpha} + \frac{c}{\alpha} \frac{1}{\alpha b^2 - c} \right)$$

$$\int \left(\frac{1}{\alpha} + \frac{c}{\alpha} \cdot \frac{1}{\alpha b^2 - c} \right) db = \frac{1}{\beta} s + k_1$$

$$\frac{b}{\alpha} - \frac{1}{\alpha} \sqrt{\frac{c}{\alpha}} \operatorname{atanh}\left(\sqrt{\frac{\alpha}{c}} b\right) + k_2 = \frac{1}{\beta} s + k_1$$

$$\Rightarrow s = \frac{\beta}{\alpha} \left(b - \sqrt{\frac{c}{\alpha}} \operatorname{atanh}\left(\sqrt{\frac{\alpha}{c}} b\right)\right) + k_3$$

$(= k_2 - k_1)$

Constant absorbed by z_0 $\Rightarrow$ (12) provides an exact solution to the PDE.

2e) Applying crank-nicholson scheme to problem

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

$$+ \beta \frac{\Delta t}{16 (\Delta z)^2} \left[(b_{j+1/2}^n)^3 (b_{j+1}^n - b_j^n) - (b_{j-1/2}^n)^3 (b_j^n - b_{j-1}^n) \right.$$

can be written as

$$b_j^{n+1} = b_j^n - C_1\left[(b_j^n)^3 - (b_{j-1}^n)^3 + (b_j^{n+1})^3 - (b_{j-1}^{n+1})^3\right]$$
$$+ C_2\left[(b_{j+1}^n + b_{j-1}^n)^3 (b_{j+1}^n - b_j^n) - (b_j^n + b_{j-1}^n)^3 (b_j^n - b_{j-1}^n)\right]$$
$$+ C_2\left[(b_{j+1}^{n+1} - b_{j-1}^{n+1})^3 (b_{j+1}^{n+1} - b_j^{n+1}) - (b_j^{n+1} + b_{j-1}^{n+1})^3 (b_j^{n+1} - b_{j-1}^{n+1})\right]$$

where $C_1 = \alpha \frac{\Delta t}{2\Delta z}$ and $C_2 = \beta \frac{\Delta t}{16(\Delta z)^2}$

$$J_{ij} = \frac{\partial R_{ij}}{\partial b_{ij}} = \frac{R_{ij,pert} - R_{ij}}{\varepsilon}$$

Solve for $J\delta b = -R$

$$\Rightarrow b^{n+1} = b^n + \delta b$$

- Crank-nicholson takes longer to compute given more calculations at each step of the calculation.
- Slightly more accurate solution achieved.