Exercise 3, TFY4235 Computational physics

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Introduction

This is an implementation of [1].

Theory

The diffusion equation, with the addition of a source at $z = 0$, can be written as

$$\Delta t \frac{\partial}{\partial t} C(z,t) = \Delta t \left(K(z) \frac{\partial^2}{\partial z^2} + \frac{\mathrm{d}K(z)}{\mathrm{d}z} \frac{\partial}{\partial z} \right) C(z,t) = \mathcal{D} C(z,t).$$

This differential operator can be discretized as

$$\mathcal{D}_{nm} = K_{nk} D^2_{km} + D^a_{nk} K_{k\ell} D^b_{\ell m}$$

where $K_{nm} = K(z_n)\delta_{nm}$, D, D^2 are finite difference matices. In the bulk, with $\alpha = \frac{\Delta t}{2\Delta z^2}$

$$D_{nn} = 0, D_{nn\pm1} = \pm\sqrt{\alpha}, \quad D^2_{nn} = -4\alpha, D_{nn\pm1} = 2\alpha$$

The no-flux boundary condition at the bottom means that $C_{NN+1} = C_{NN-1}$, so

$$D^b_{NN-1} = 0, D^2_{NN-1} = 4\alpha.$$

At the surface, $C_{-1} = C_1 + (2\Delta z k_w / K_0)(C_0 - C_{eq})$, so

$$D^2_{00} = -4\alpha + 2\alpha \frac{2\Delta z k_2}{K_0}, \; D^2_{01} = 2\alpha, \quad D^b_{01} = \sqrt{\alpha} \frac{2\Delta z k_2}{K_0}$$

The Chranck-Nichelson scheme then yields

$$C_{n,i+1} = C_{n,i} + \frac{1}{2}\Delta t (\mathcal{D}_{nm,i} C_{m,i} + s_{ni}) + \frac{1}{2}\Delta t \mathcal{D}_{nm,i+1} C_{m,i+1},$$

so

$$\left(\delta_{nm} - \frac{1}{2}\Delta t \mathcal{D}_{nm,i} \right) C_{m,i+1} = \left(\delta_{nm} + \frac{1}{2}\Delta t \mathcal{D}_{nm,i+1} \right) C_{m,i}$$

References

[1] Exercise 3, 2021, tfy4235 computational physics.