Exercise 3, TFY4235 Computational physics

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Introduction

This is an implementation of [1].

Theory

The diffusion equation, can be written as

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

Discretizing the spatial part, and applying boundary conditions, gives

$$\Delta t \frac{\partial}{\partial t} C_n(t) = \mathcal{D}_{nm} C_n(t) + S_n(t),$$

where

$$\mathcal{D} = \begin{pmatrix} 4\alpha K_0 + 2\Gamma & -4\alpha K_0 & 0 & \dots & 0 \\ \alpha K_1'/2 - 2\alpha K_1 & 4\alpha K_1 & -\alpha K_1'/2 - 2\alpha K_1 & & \\ 0 & \ddots & \ddots & \ddots & 0 \\ 0 & \dots & \alpha K_{N-1}'/2 - 2\alpha K_{N-1} & 4\alpha K_{N-1} & -\alpha K_{N-1}'/2 - 2\alpha K_{N-1} \\ 0 & \dots & 0 & 4\alpha K_N & 4\alpha K_N \end{pmatrix}, \quad S(t) = \begin{pmatrix} 2\Gamma C_{\mathrm{eq}}(t) \\ 0 \\ \vdots \\ 0 \end{pmatrix}$$

The Chranck-Nichelson scheme then yields

$$C_n^{i+1} = C_n^i + \frac{1}{2}(\mathcal{D}_{nm} C_m^i + S_n^i) + \frac{1}{2}(\mathcal{D}_{nm} C_m^{i+1} + S_n^{i+1}),$$

so

$$\left(\delta_{nm} - \frac{1}{2}\mathcal{D}_{nm} \right) C_m^{i+1} = \left(\delta_{nm} + \frac{1}{2}\mathcal{D}_{nm} \right) C_m^i + \frac{1}{2}(S_n^i + S_n^{i+1})$$

References

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