

# Exercise 3, TFY4235 Computational physics

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## Introduction

This is an implementation of [1].

## Theory and implementation

The diffusion equation, can be written as

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

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

$$\mathcal{D} = \begin{pmatrix} -4\alpha K_0 - 2\Gamma & 4\alpha K_0 & 0 & \dots & 0 \\ -\frac{\alpha}{2} K'_1 + 2\alpha K_1 & -4\alpha K_1 & \frac{\alpha}{2} K'_1 + 2\alpha K_1 & \dots & 0 \\ 0 & \ddots & \ddots & \ddots & 0 \\ 0 & \dots & -\frac{\alpha}{2} K'_{N-1} + 2\alpha K_{N-1} & -4\alpha K_{N-1} & \frac{\alpha}{2} K'_{N-1} + 2\alpha K_{N-1} \\ 0 & \dots & 0 & 4\alpha K_N & -4\alpha K_N \end{pmatrix},$$
$$S(t) = (2\Gamma C_{\text{eq}}(t) \quad 0 \quad \dots \quad 0)^T \quad \Gamma = 2 \frac{\alpha k_w \Delta z}{K_0} \left( K_0 - \frac{1}{2} \left( -\frac{3}{2} K_0 + 2K_1 - \frac{1}{2} K_2 \right) \right), \quad \alpha = \frac{\Delta t}{2\Delta z^2},$$

$$K'_n = K_{n+1} - K_{n-1}$$

The Crank-Nicholson 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 the equation to be solved to get the next timestep is

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

...

## Tests

Make sure the implementation gives good answers, it is compared to known solutions. First, a constant concentration of CO<sub>2</sub> should remain constant, regardless of  $K(z)$ , as long as it is positive. This test is shown in Figure ??.

The systems should also, given  $k_w = 0$ , conserve mass.

## References

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

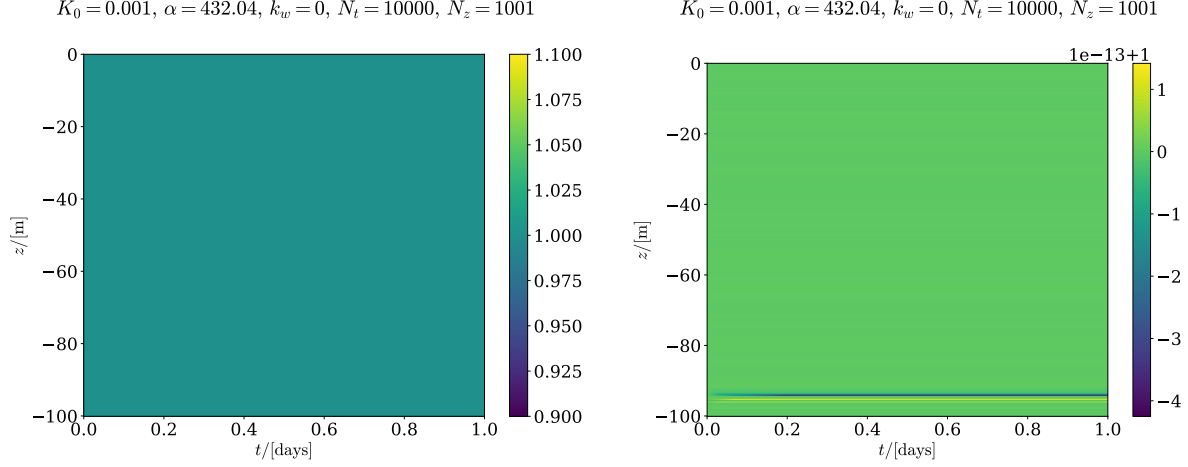


Figure 1: The time evolution of an constant concentration. The system on the left has a constant  $K(z)$ , while system of the right has an oscillatory  $K$ . The largest deviation of the system is of order  $10^{-16}$  and  $10^{-12}$ , respectively.

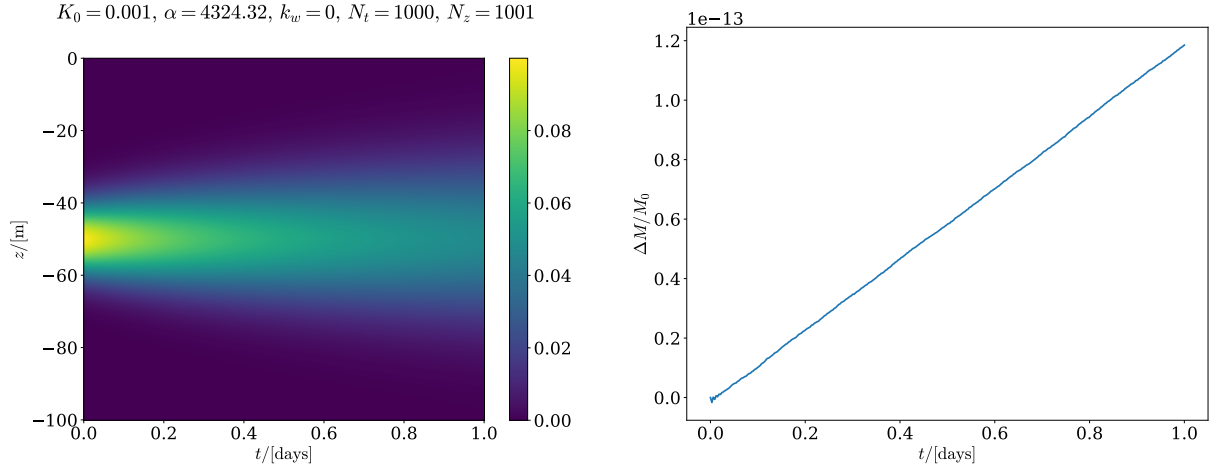


Figure 2: The evolution of a gaussian distribution of  $\text{CO}_2$  is shown on the left. On the right, the relative change in mass as a function of time is plotted.

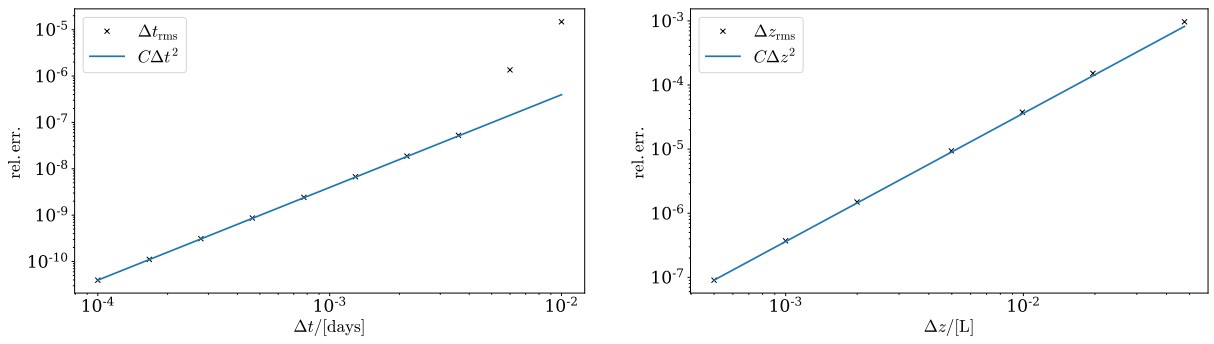


Figure 3