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

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

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

$$\mathcal{D} = \begin{pmatrix} -4\alpha K_0 - 2\Gamma & 4\alpha K_0 & 0 & \dots & 0 \\ -\frac{\alpha}{2} K_1' + 2\alpha K_1 & -4\alpha K_1 & \frac{\alpha}{2} K_1' + 2\alpha K_1 & \dots & 0 \\ 0 & \ddots & \ddots & \ddots & 0 \\ 0 & \dots & -\frac{\alpha}{2} K_{N-1}' + 2\alpha K_{N-1} & -4\alpha K_{N-1} & \frac{\alpha}{2} K_{N-1}' + 2\alpha K_{N-1} \\ 0 & \dots & 0 & 4\alpha K_N & -4\alpha K_N \end{pmatrix},$$

$$S(t) = \begin{pmatrix} 2\Gamma C_{\mathrm{eq}}(t) & 0 & \dots & 0 \end{pmatrix}^T \quad \Gamma = 2 \frac{\alpha k_w \Delta z}{K_0} \left(K_0 - \frac{1}{2}(-\frac{3}{2} K_0 + 2K_1 - \frac{1}{2} K_2) \right), \quad \alpha = \frac{\Delta t}{2 \Delta z^2},$$

$$K_n' = K_{n+1} - K_{n-1}$$

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 the equation to be solved to get the next timestep is

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

...

Tests

Make sure the implementation gives good answers, it is compared to known solutions. The method used in this implementation has quadratic convergence, both in time and space. A convergence test was implemented for a simple test case, to check this. Figure 1 shows the result of this.

A constant concentration of CO_2 should remain constant, regardless of $K(z)$, as long as it is positive. This test is shown in Figure 2, both for constant and varying diffusivity $K(z)$.

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

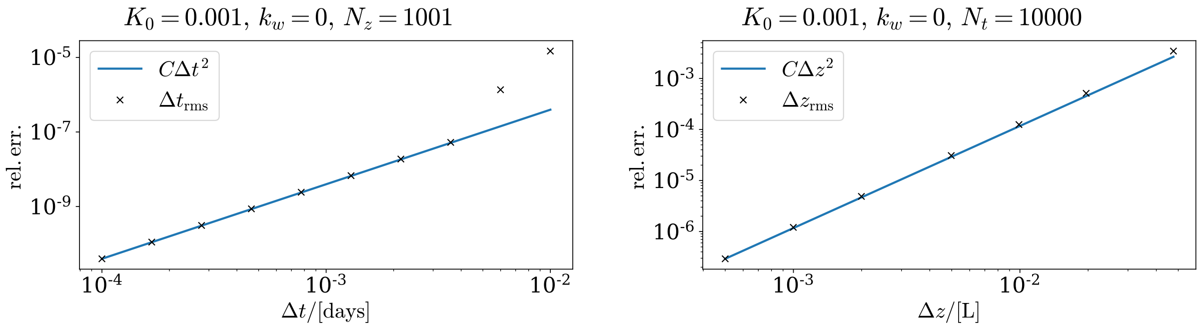

Figure 1: Error, measured as the root mean square deviation from a reference value, after 1 day simulation of an gaussian initial concentration.

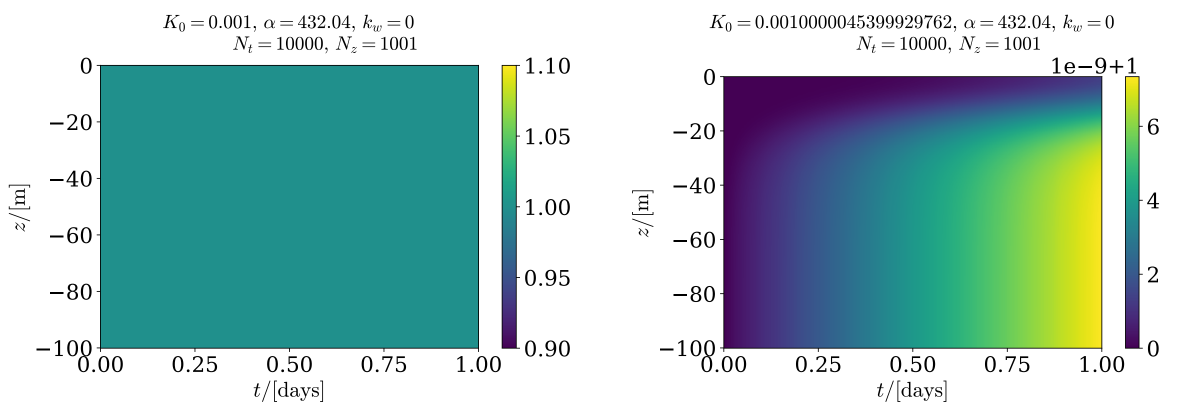

Figure 2: The time evolution of an constant concentration. The system on the left has a constant $K(z)$, while system of the right has an oscillatory K. The largest deviation of the system is of order 10^{-16} and 10^{-12}, respectively.

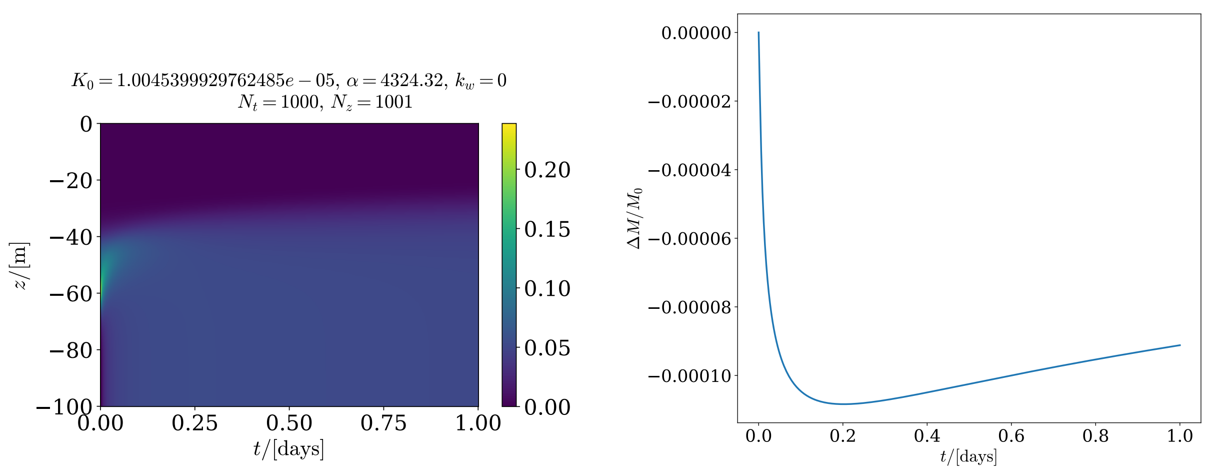

Figure 3: The evolution of a gaussian distribution of CO_2 is shown on the left. On the right, the relative change in mass as a function of time is plotted.

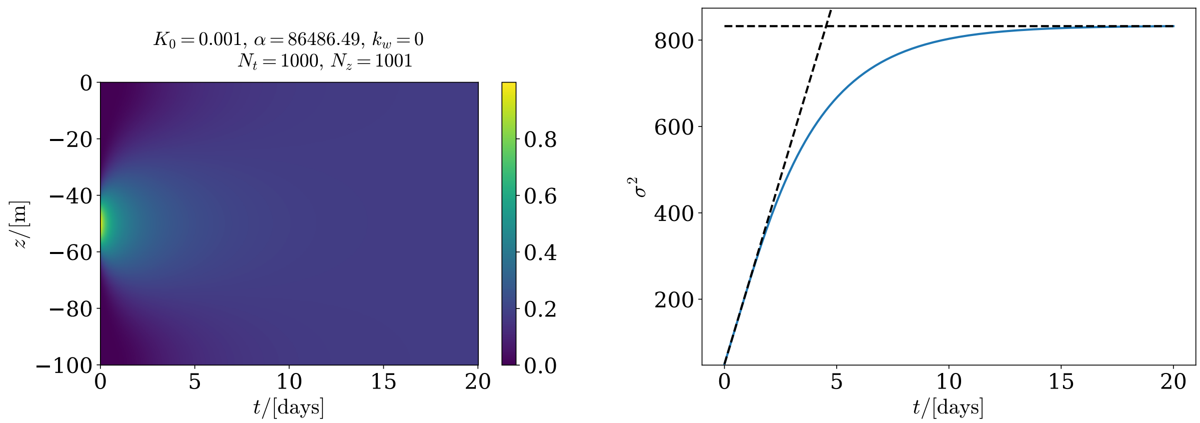

Figure 4

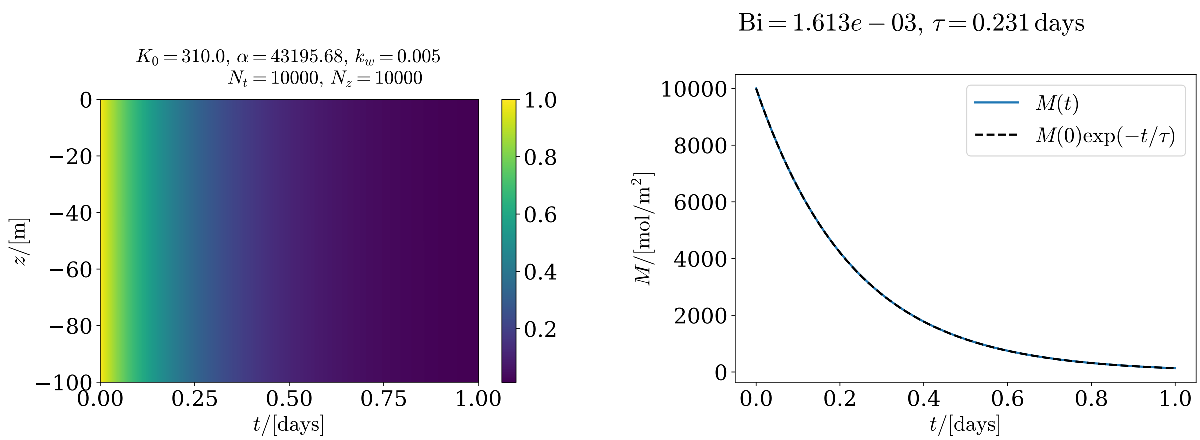

Figure 5: The slow removal of CO_2 from the ocean, when the atmosphere contains a partial pressure of 0.

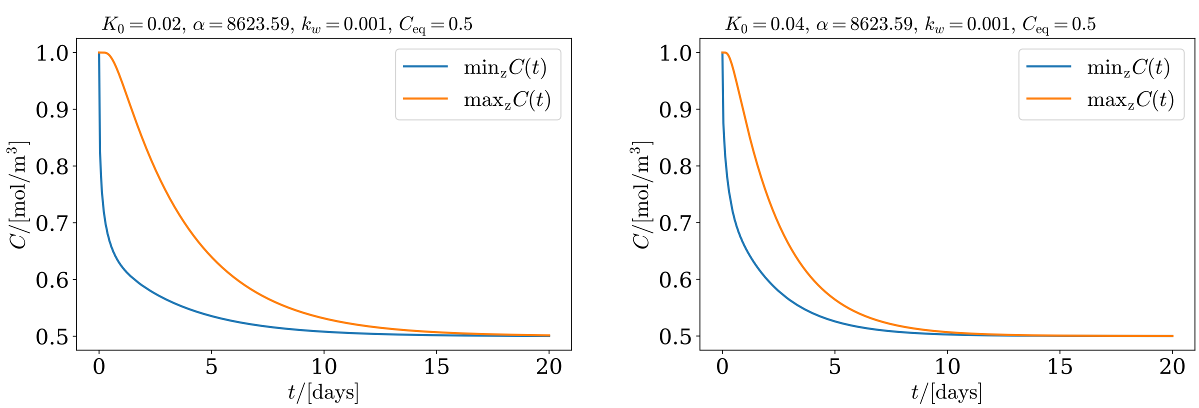

Figure 6: The slow removal of CO_2 from the ocean, when the atmosphere contains a partial pressure of 0.

References

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