

# 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 Cranck-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

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

The implementation of this system of equation uses SciPy's sparse matrix library. After creating sparse realizations of  $A$ , SciPy's `splu` is used to generate the LU decomposition LU of  $A$ . This is an object with methods such as `.solve()`, which utilizes the LU decomposition. The wrapper `simulate` then loops over  $N_t - 1$  steps, using `solve(V) = lambda V: LU.solve(V)`, where  $V$  is as given above.

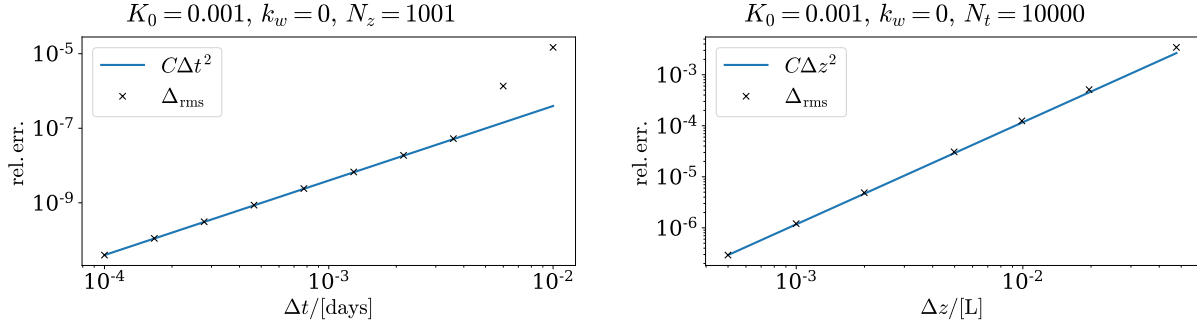


Figure 1: Error, measured as the root mean square deviation from a reference value, after 1 day simulation of an gaussian initial concentration.

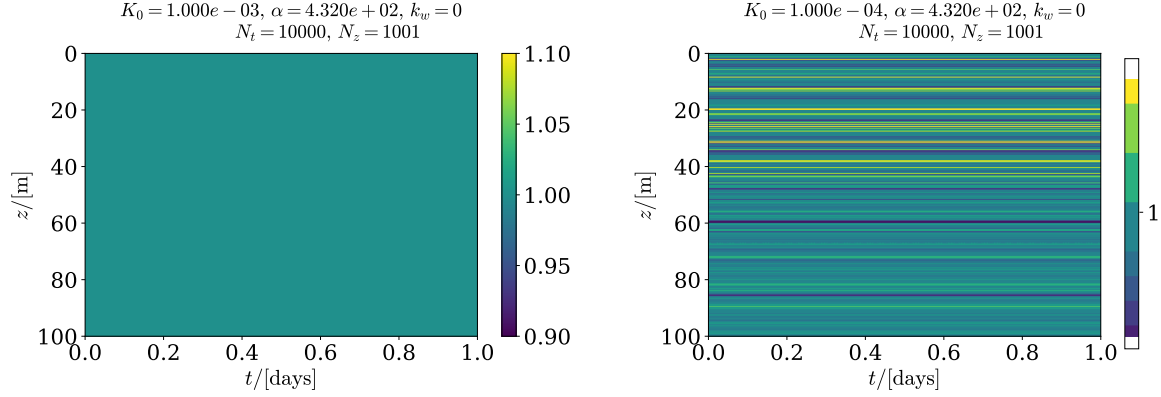


Figure 2: The time evolution of an constant concentration. The system on the left has a constant  $K(z)$ , while system of the right has an oscillatory  $K$ . The largest deviation of the system is of order  $10^{-16}$  and  $10^{-15}$ , respectively.

## 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  $\text{CO}_2$  should remain constant, regardless of  $K(z)$ , as long as it is positive. This test is shown in Figure 2, with a both a constant  $K(z)$ , and a smooth step function between two values of  $K$ . For both, the constant initial concentration is close to unchanged, save for numerical errors.

The systems should also, given  $k_w = 0$ , conserve mass. To test this, a initial distribution of two gaussian functions were evolved in time, with a non-constant diffusivity. The result is shown in Figure 3, where the mass is conserved to a good approximation.

A sharply peaked gaussian package should have a variance that increases linearly with time, then approach a steady state. This is shown in Figure 4.

Figure 5 shows the depletion of  $\text{CO}_2$  from the ocean, given a zero partial pressure in the atmosphere. For a small Biot number, this should follow a exponential decay, as this test shows.

Lastly, Figure 6 shows how the ocean reaches a equilibrium with the atmosphere, given a non-zero, positive mass-transfer coefficient  $k_w$  and either constant or non-constant diffusivity.

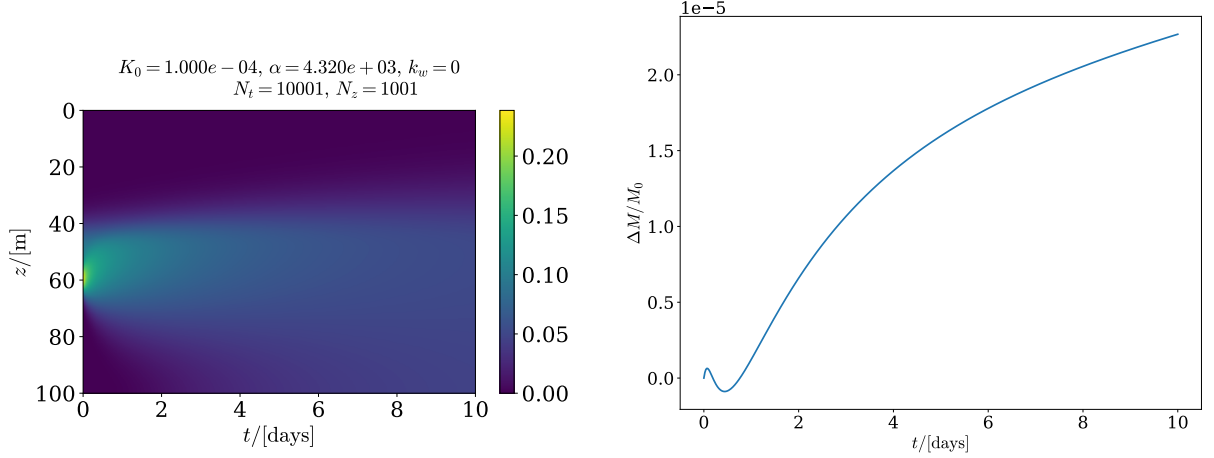


Figure 3: The evolution of a gaussian distribution of CO<sub>2</sub> is shown on the left. On the right, the relative change in mass as a function of time is plotted.

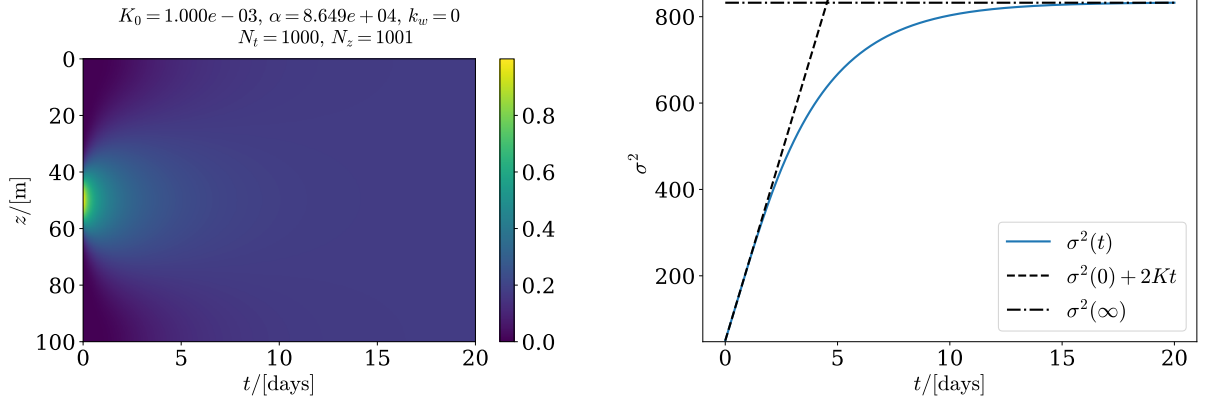


Figure 4

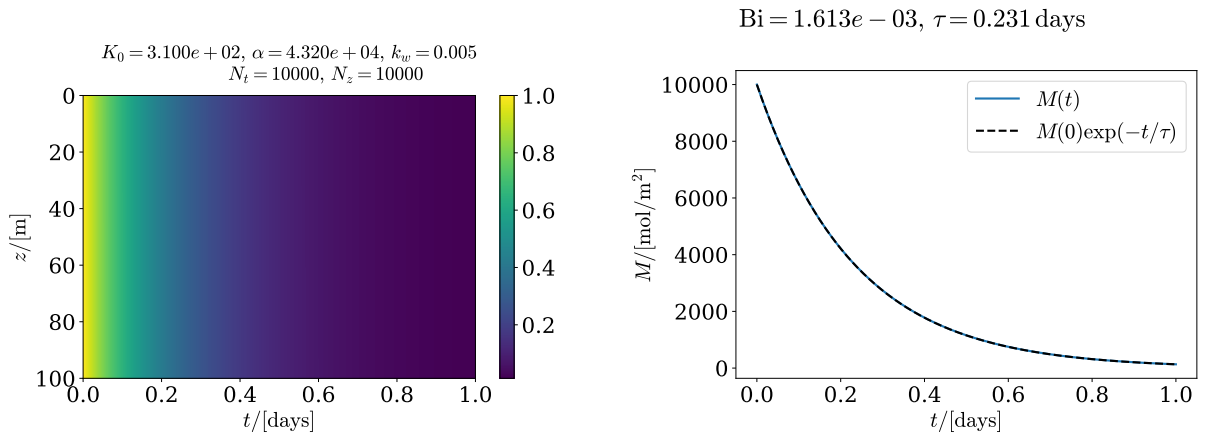


Figure 5: The slow removal of CO<sub>2</sub> from the ocean, when the atmosphere contains a partial pressure of 0.

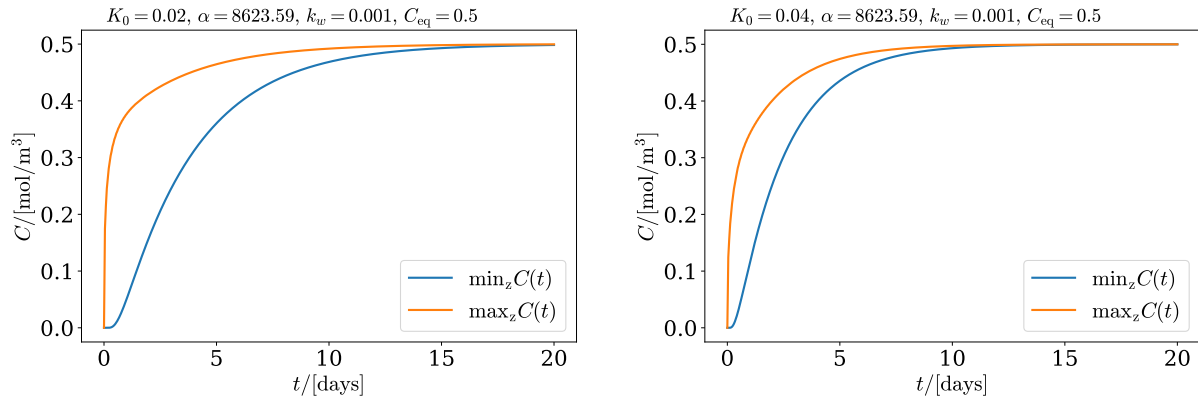


Figure 6: Equilibration of the ocean with a atmosphere with  $C_{\text{eq}} = 0.5$ . The figure on the left is a system with constant diffusivity, the left side has a oscillating but always positive diffusivity.

## References

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