GEF4510 PROBLEM SET 02

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Vertical Diffusive Mixing

a) To delevop a numerical scheme we seek to find finite difference approximations (FDA's) for the two terms in the diffusion equation

$$\frac{\partial \psi}{\partial t} = \kappa \frac{\partial^2 \psi}{\partial z^2} \tag{1}$$

We start by using the definition of Taylor series, for $\psi(z \pm \Delta z, t)$ and $\psi(z, t \pm \Delta t)$ around the point (z, t), to write the following equations

$$\psi|^t_{z+\Delta z} = \sum_{k=0}^{\infty} \frac{1}{k!} \frac{\partial^k \psi}{\partial z^k}\Big|^t_z \Delta z^k = \psi|^t_z + \frac{\partial \psi}{\partial z}\Big|^t_z \Delta z + \frac{1}{2}\frac{\partial^2 \psi}{\partial z^2}\Big|^t_z \Delta z^2 + \mathcal{O}(\Delta z^3) \tag{2}$$

$$\psi|^t_{z-\Delta z} = \sum_{k=0}^{\infty} \frac{1}{k!} \frac{\partial^k \psi}{\partial z^k}\Big|^t_z (-\Delta z)^k = \psi|^t_z - \frac{\partial \psi}{\partial z}\Big|^t_z \Delta z + \frac{1}{2}\frac{\partial^2 \psi}{\partial z^2}\Big|^t_z \Delta z^2 - \mathcal{O}(\Delta z^3) \tag{3}$$

$$\psi|^{t+\Delta t}_z = \sum_{k=0}^{\infty} \frac{1}{k!} \frac{\partial^k \psi}{\partial t^k}\Big|^t_z \Delta t^k = \psi|^t_z + \frac{\partial \psi}{\partial t}\Big|^t_z \Delta t + \frac{1}{2}\frac{\partial^2 \psi}{\partial t^2}\Big|^t_z \Delta t^2 + \mathcal{O}(\Delta t^3) \tag{4}$$

$$\psi|^{t-\Delta t}_z = \sum_{k=0}^{\infty} \frac{1}{k!} \frac{\partial^k \psi}{\partial t^k}\Big|^t_z (-\Delta t)^k = \psi|^t_z - \frac{\partial \psi}{\partial t}\Big|^t_z \Delta t + \frac{1}{2}\frac{\partial^2 \psi}{\partial t^2}\Big|^t_z \Delta t^2 - \mathcal{O}(\Delta t^3) \tag{5}$$

To find a forward-in-time (FT) FDA for the LHS of (1) we contract the two last terms on the RHS of (4) into $\mathcal{O}(\Delta t^2)$ and solve (4) for $\partial\psi/\partial t|^t_z$ to get

$$\frac{\partial \psi}{\partial t}\Big|^t_z = \frac{\psi|^{t+\Delta t}_z - \psi|^t_z}{\Delta t} + \mathcal{O}(\Delta t) \qquad \Rightarrow \qquad \left[\frac{\partial \psi}{\partial t}\right]^n_j = \frac{\psi^{n+1}_j - \psi^n_j}{\Delta t} \tag{6}$$

where we have switched to numerical notation where space point j and time point n corresponds to $z_j = (j-1)\Delta z$, $j = 1, 2, ..., J$ and $t_n = n\Delta t$, $n = 0, 1, ..., N-1$, respectively (J and N being the total number of space- and time points). We have also dropped the $\mathcal{O}(\Delta t)$ term, meaning we have truncated the Taylor series and we have obtained a first order accurate FDA. To get an FDA for the RHS of (1) we add (2) and (3) and solve for $\partial^2\psi/\partial z^2$:

$$\psi|^t_{z+\Delta z} + \psi|^t_{z-\Delta z} = 2\psi|^t_z + \frac{\partial^2 \psi}{\partial z^2}\Big|^t_z \Delta z^2 + \mathcal{O}(\Delta z^4)$$

where we got the $\mathcal{O}(\Delta z^4)$ term because the third-order term cancelled when adding the two equations together. If we then rearrange, divide through by Δz^2 and apply the numerical notation, we get

$$\left[\frac{\partial^2 \psi}{\partial z^2}\right]_j^n = \frac{\psi_{j+1}^n - 2\psi_j^n + \psi_{j-1}^n}{\Delta z^2} \tag{7}$$

as an FDA for the second-order space derivative. We see that this is a centered-in-space FDA and that it has second order accuracy (dividing by Δz^2 gives error term $\mathcal{O}(\Delta z^2)$ which is truncated). Using the to found FDA'a we can delevope the numerical FTCS scheme for the diffusion eqution. Inserting (6) and (7) into (1) gives

$$\frac{\psi_j^{n+1} - \psi_j^n}{\Delta t} = \kappa \frac{\psi_{j+1}^n - 2\psi_j^n + \psi_{j-1}^n}{\Delta z^2}$$

and furthermore through defining $K = \kappa \Delta t / \Delta z^2$ and rearranging we get

$$\psi_j^{n+1} = \psi_j^n + K\left(\psi_{j+1}^n - 2\psi_j^n + \psi_{j-1}^n\right) \tag{8}$$

as an explicit forward-in-time and centered-in-space numerical scheme for (1). To show the stability condition we apply Von Neumann stability analysis. We define a discrete Fourier component

$$\psi_j^n = \Psi_n e^{i\alpha z_j} = \Psi_n e^{i\alpha(j-1)\Delta z}$$

and substitute it in to our discrete diffusion approximation to get

$$\Psi_{n+1} e^{i\alpha(j-1)\Delta z} = \Psi_n e^{i\alpha(j-1)\Delta z} + K\left(e^{i\alpha\Delta z} + e^{-i\alpha\Delta z} - 2\right)\Psi_n e^{i\alpha(j-1)\Delta z}$$

$$\Rightarrow \qquad \frac{\Psi_{n+1}}{\Psi_n} = G = 1 + K\left(e^{i\alpha\Delta z} + e^{-i\alpha\Delta z} - 2\right) = 1 - 2K[1 - \cos(\alpha\Delta z)]$$

where the definition of the growth factor $G = \Psi_{n+1}/\Psi_n$ has been used. In the analysis we require $|G| \leq 1 \quad \Rightarrow \quad -1 \leq G \leq 1$ for the cheme to be stable and for the amplitude Ψ_n not to grow without limits. Hence we are interesed in the maximum value (+ or -) our G can have. The expression inside the brackets (at the far right in the above equation) will always be between 0 and 2 and therefore $G < 1$ always ($K > 0$). So the right inequality is taken care of. Now we look at the left and insert $1 - \cos(\alpha\Delta z) = 2$ (min. G):

$$-1 \leq 1 - 4K \qquad \Rightarrow \qquad K = \frac{\kappa\Delta t}{\Delta z^2} \leq \frac{1}{2} \qquad \Rightarrow \qquad \Delta t \leq \frac{\Delta z^2}{2\kappa}$$

So according to the Von Neumann stability analysis the FTCS scheme for the diffusion equation (1) is stable under the condition $K \leq 1/2$.

b) We are here to delevop a CTCS scheme for (1) and therefore need an centered-in-time FDA for $\partial\psi/\partial t$. We find this by subtracting (5) from (4):

$$\psi_j^{n+1} - \psi_j^{n-1} = 2\frac{\partial\psi}{\partial t}|_j^n \Delta t + \mathcal{O}(\Delta t^3) \quad \Rightarrow \quad \left[\frac{\partial\psi}{\partial t}\right]_j^n = \frac{\psi_j^{n+1} - \psi_j^{n-1}}{2\Delta t} \tag{9}$$

where the $\mathcal{O}(\Delta t^2)$ cancels upon subtraction. And when diving through by Δt we see that this is a second order accurate FDA. Again by substituting our FDA's (7) and (9) into (1) and rearranging the resulting equation we get

$$\psi_j^{n+1} = \psi_j^{n-1} + 2K\left(\psi_{j+1}^n - 2\psi_j^n + \psi_{j-1}^n\right) \tag{10}$$

which is our centered-in-time and centered-in-space (CTCS) scheme. This is second order accurate in both space and time. To analyse the stability we do as in **a)**. Substituting the discrete Foruier component into (10) gives

$$\begin{aligned}
&\Psi_{n+1}e^{i\alpha(j-1)\Delta z} = \Psi_{n-1}e^{i\alpha(j-1)\Delta z} + 2K\left(e^{i\alpha\Delta z} + e^{-i\alpha\Delta z} - 2\right)\Psi_n e^{i\alpha(j-1)\Delta z} \\
\Rightarrow \quad &\frac{\Psi_{n+1}}{\Psi_n} = \frac{\Psi_{n-1}}{\Psi_n} + 2K\left(e^{i\alpha\Delta z} + e^{-i\alpha\Delta z} - 2\right) \\
\Rightarrow \quad &G = G^{-1} - 4K[1 - \cos(\alpha\Delta z)] \\
\Rightarrow \quad &G^2 + 4K[1 - \cos(\alpha\Delta z)] - 1 = 0 \\
\Rightarrow \quad &G = -2K[1 - \cos(\alpha\Delta z)] \pm \sqrt{4K^2[1 - \cos(\alpha\Delta z)]^2 + 1}
\end{aligned}$$

After solving the quadratic equation for G we got two solutions G^+, G^- and both must satisfy $|G| \leq 1$ for the scheme to be stable. First we investigate G^-; we see that this expression is entirely negativ (both terms being negative) and taking the absolute value corresponds to replacing both $(-)$ with $(+)$ and the we must require this to be less or equal to 1. In the process we will substitute $[1 - \cos(\alpha\Delta z)] = 2$ to view the extreme case:

$$\begin{aligned}
&2K[1 - \cos(\alpha\Delta z)] + \sqrt{4K^2[1 - \cos(\alpha\Delta z)]^2 + 1} \leq 1 \\
&\Rightarrow \qquad 4K + \sqrt{16K^2 + 1} \leq 1
\end{aligned}$$

Since $K > 0$ we see that $|G^-| > 0$ and conclude that the CTCS scheme is unconditionally unstable; there is no possible condition on K that could make $G^- \leq 1$.

c) Based on the introduction to the problem set we have $H = 270$m, $D = 30$m and $J_{max} = 27$. This defines $\Delta z = H, D/(J_{max} - 1)$ (where $(J_{max} - 1)$ is the number of space-steps) which gives a value of $\Delta z = 10.38$m and $\Delta z = 1.15$m for the atmosphere and ocean respectively. So since we have a given number of grid points in space and the hegiht of the atmospeheric boundary layer is larger than the depth of the oceanic boundary layer, we get a larger Δz for the atmosphere. When we combine this togehter with the numbers given in this exercise (**c)**) and the definition $\Delta t = K\Delta z^2/\kappa$ we get get a time step $\Delta t = 1.62$s and $\Delta t = 199.70$s for the atmosphere and ocean respectively. These choices of Δt satisfy the stability condition from **a)** since they are based on $K = 0.45 < 1/2$. As indicated by the exercise the time steps for the two spheres are very different; it is much larger in the ocean (123 times larger actually). From the definition of Δt written above we see that this comes from the differences in the diffusion coefficients κ_A and κ_O. This difference is a reflection of how heat diffuses at a much faster rate in the atmosphere than in the ocean. Therefore, to resolve the more rapid changes in the atmosphere we need a shorter time step. This can be experienced on an everyday basis as well in terms of how much faster things happen in the atmosphere than in the ocean. Mixing/turbulence is generally a lot faster in the atmosphere. When it comes to the consequences of this difference we note that if we have a specified number of time steps, say 1200, our simulation in the ocean will reach a time of 66 hours in to the future, but for the same amount of time steps we are only able to simulate 0.5 hours in the atmosphere. So this seem to indicate that running the diffusion simulation in the atmsophere requires a lot more computations and data storage for a given time to simulate into the future.

d) The numerical FTCS scheme (8) in **a)** with the given inital- and boundary conditions (from the exercise) is implemented in the source file `atmosphere_application.f90`. Next follows a derivation of the analytical solution and then a comparison of the result. For the analytical case we assume a component solution $\psi_m(z,t) = Z_m(z)T_m(t)$ (of the total solution ψ) attempt a separation of variables. Insertion into (1) gives

$$Z\frac{dT}{dt} = \kappa T\frac{d^2Z}{dz^2} \qquad \Rightarrow \qquad \frac{1}{T}\frac{dT}{dt} = \frac{\kappa}{Z}\frac{d^2Z}{dz^2}$$

Here we have that a function of only t (left side) is equal to a function of only z (right side). For this to hold for all z, t we must have that both of

these sides are equal to a (the same) constant, say $-k^2$. This gives us the following ordinary linear differential equations

$$\frac{dT}{dt} = -k^2 T \qquad \Rightarrow \qquad T(t) = T_0 e^{-k^2 t}$$

$$\frac{d^2 Z}{dz^2} = -\frac{k^2}{\kappa} Z \qquad \Rightarrow \qquad Z(z) = A \sin\left(\frac{kz}{\sqrt{\kappa}}\right) + B \cos\left(\frac{kz}{\sqrt{\kappa}}\right)$$

where these equations are solved respectively by integration factor (for T_m) and characteristic quadratic equation (for Z_m). Here T_0, A, B are integration constants. Next we apply the boundary conditions on ψ_m. We conclude that $\psi(0,t) = \psi(H,t) = 0 \quad \Rightarrow \quad Z_m(0) = Z_m(H) = 0$ for the BC to hold for all t. Imposing the BC's gives

$$Z(0) = 0 \qquad \Rightarrow \qquad B = 0$$

$$Z(H) = 0 \qquad \Rightarrow \qquad A \sin\left(\frac{kH}{\sqrt{\kappa}}\right) = 0 \qquad \Rightarrow \qquad k = \frac{n\pi\sqrt{\kappa}}{H}$$

Where for the last BC we have assumed $A \neq 0$ since this would just give us the trivial zero-solution. So we get a condtition on k for the solution to satisfy the BC's. Insertion of this k in T_m and Z_m gives the component solution

$$\psi_m = A'_m e^{-(m^2\pi^2\kappa/H^2)t} \sin\left(\frac{m\pi}{H} z\right)$$

where A'_m is the merged constant of T_0 and A. Now the full solution ψ is the sum of ψ_m over all m's. We write this simultanously as imposing the initial condition on ψ:

$$\psi(z,0) = \psi_0 \sin\left(\frac{\pi z}{H}\right) = \sum_{m=1}^{\infty} \psi_m(z,0) = \sum_{m=1}^{\infty} A'_m \sin\left(\frac{m\pi}{H} z\right)$$

We see that the initial condition corresponds to the first term in the Fourier series on the right-hand-side so only the term $m = 1$ is represented and furthermore we see that $A'_1 = \psi_0$. So we arrive at the full analytical solution including inital- and boundary conditions written as

$$\psi(z,t) = \psi_0 e^{-(\pi^2\kappa/H^2)t} \sin\left(\frac{\pi z}{H} z\right) \tag{11}$$

So we see that the analytical solution consist of a time decating part and sinusoidal part in space. This seems reasonable with our general impression of diffusion processes.

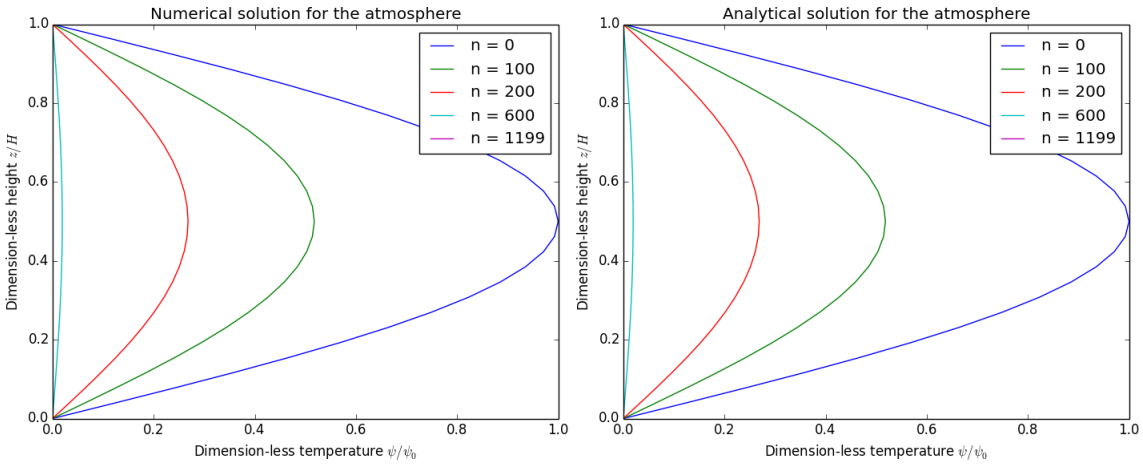

Figure 1: Plots of both the numerical ($K = 0.45$) and analytical solution to (1) for time steps $n = 0, 100, 200, 600, 1200$.

In Figure 1, we see plots of the numerical and analytical solution. To begin with we note that both solutions smooth out in time and the diffusion process looks to act as to lessen the differences, which is consistent with our physical understanding of diffusion. After enough time, the temperature in the column tends toward a uniform 0 degree (because of the voundary conditions). The numerical and analytical solution seem similar and it looks like the numerical schem worked well in computing the solution. The conditionally stable FTCS scheme (8) is definetly a decent way of handling the diffusion problem in this case. However, we could see (if zoomed in and closely inspected) that at the later time steps, the numerical solution had somewhat smaller ψ-values than the analytical. This could potentially come from numerical dissipation and might be improved if we would choose a K closer to $K = 1/2$.

Then we run the simulation with $K = 0.55$. Here it is only plotted for $n = 0, 115$ as the solution became massively unstable and blew up for larger n-values generating unplottable values for ψ. When using this K-value, we see a saw tooth pattern emerge as times passes (illustrated in Figure 2). We didn't see this for the stable case of $K = 0.45$ so here we get a confirmation that the scheme (8) with $K > 1/2$ is in fact unstable. When we found the stablity condition for (8) we saw that the first case where $K > 1/2$ corresponded with $1 - \cos(\alpha\Delta z) = 2$ or $\cos(\alpha\Delta z) = -1$ which is $\alpha\Delta z = m\pi \quad \Rightarrow \quad \lambda = 2\pi/\alpha = 2\Delta z/m \quad m = 1, 3, 5, ...$ where λ is the wavelength

corresponding to the wavenumber α. So the first part of the solution to break the stability condition is components of the solution with wavelengths $\lambda = 2\Delta z/m$. So this is what we would experience as the saw tooth pattern.

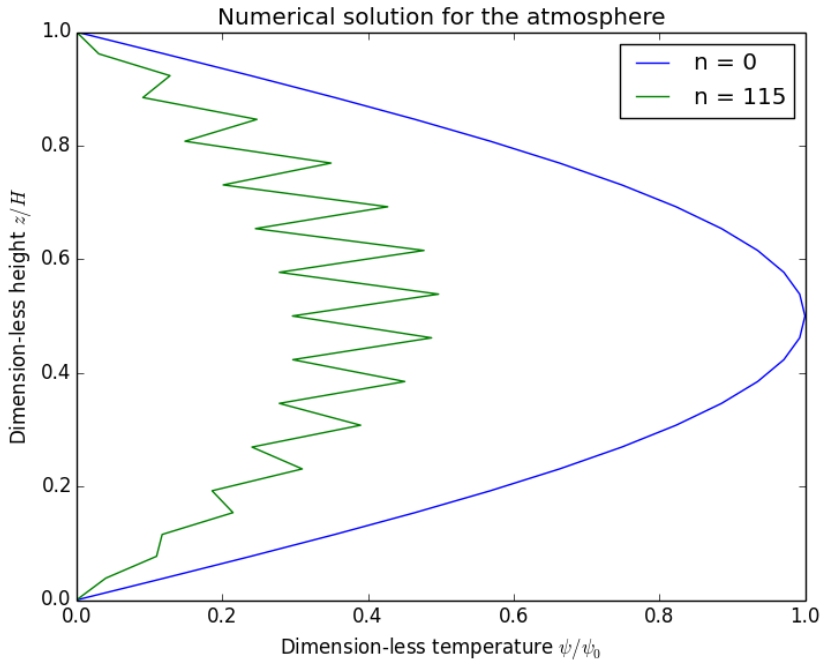

Figure 2: Plot of numerical solution with $K = 0.55$ for time steps $n = 0, 115$.

e) The numerical implementation of (8) and the ascossiated initial- and boundary conditions specified by this exercise can be found in the souce file `ocean_application.f90`. Here the surface boundary condition is defined through the hyperbolic tangent function as suggested in the exercise text. Before looking at the result we derive the steady-state analytical solution. By definition, steady-state is when we don't have any variation in time. This corresponds to ∞ and is when the system has reached equilibrium. The left-hand-side of the diffusion equation vanishes. So the temperature ψ is function of only z and this simplifies our surface boundary condition which becomes $\psi(0) = \psi_0$ (in this state the surface has reached its maximum temperature) and furthermore the initial condition becomes irrelevant. The

bottom boundary condition remains the same and integrating twice gives

$$\frac{d^2\psi}{dz^2} = 0 \qquad \Rightarrow \qquad \psi(z) = Az + B$$

where $A, B \in \mathbb{R}$ are integration constants. Then imposing the surface BC $\psi(0) = \psi_0$ implies $B = \psi_0$. Finally the bottom BC then gives $A = B/D = \psi_0/D$ which gives us the steady-state solution

$$\psi(z) = \frac{\psi_0}{D} z + \psi_0 = \psi_0 \left(\frac{z}{D} + 1 \right) \tag{12}$$

So we see that the steady-state solution gives a linear temperature from 0 at the bottom to ψ_0 at the top. Part of a verification process on our numerical solution could then be to check our result and see if it approached the analytically found steady-state solution. And from Figure 3, we see that this in fact seems to be the case. We see that the surface BC really impacts

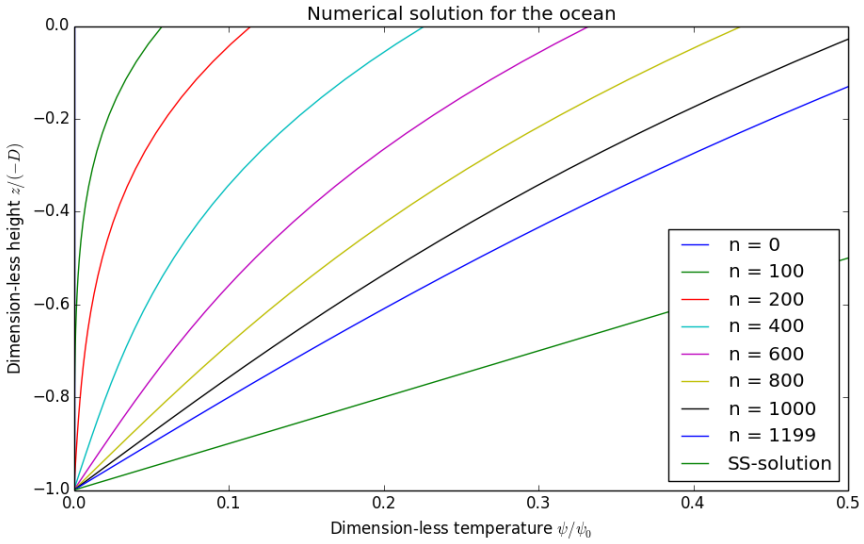

Figure 3: Plot of numerical solution with $K = 0.45$ for a water column in the ocean. Solution is stable.

the temperature evolution in the water column where it's heated at the top and then it diffuses down the column to even out the temperature differences. The numerical solution doesn't quite reach the full steady-state, but that is because our simulation time is too short. To fix this we could for example simulate for a longer time or tweak the γ and t_c parameters.