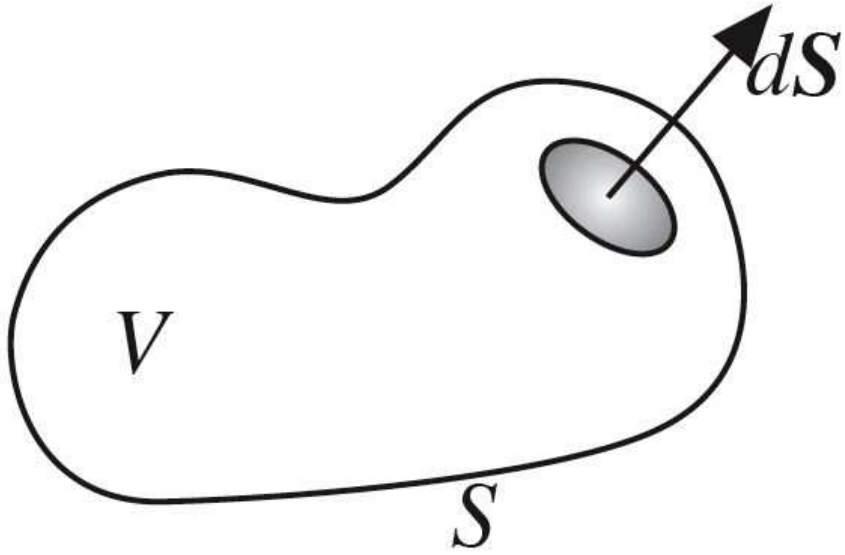
Modeling Advection

Nearly all of the modeling of physical phenomena is based on the simple statement that certain important physical properties must be conserved.

1. Conservation of anything

Consider an arbitrary inertial frame in space of volume V enclosed by a surface S, i.e.



Here, dS is the vector normal to a small patch on the surface S. This vector points outwards by convention.

If we now consider how any quantity Φ (in units of stuff per unit volume) can change within this volume, the only way to change the amount of Φ with time is to flux it through the boundary or create it within the volume. If we let $\boldsymbol{F}$ be the flux of Φ in the absence of fluid transport (e.g. heat conduction), $\Phi \cdot \boldsymbol{v}$ be the transport flux (stuff per unit area per unit time) and H be a source or sink of Φ then the statement of conservation of Φ for the volume V becomes

$$\frac{d}{dt}\int_V \Phi \, dV = -\int_S \boldsymbol{F} \cdot dS - \int_S \Phi \boldsymbol{v} \cdot dS + \int_V H \, dV \qquad (1)$$

The negative signs in front of the surface integrals are present because a positive outward flux corresponds to a negative rate of change of the integral on the left side of eq. (1).

This equation is always true, independent of the size of the blob and even if the fields are not continuous; however, because of the integrals, any information on the spatial structure of the fields on a scale smaller than the “blob” size is lost (sorry to the mineralogists/petrologists !).

Given the existence of a suitable continuum length scale, we can now rewrite eq. (1) as a local partial differential equation.
Because the property of interest is differentiable, we can replace the surface integrals in eq. (1) using Gauss’ theorem

$$-\int_S \boldsymbol{F}\cdot d\boldsymbol{S} - \int_S \Phi\boldsymbol{v}\cdot d\boldsymbol{S} = -\int_V \nabla\cdot(\boldsymbol{F}+\Phi\boldsymbol{v})\,dV \qquad (2)$$

Moreover, because the surface S and volume V are fixed in an inertial frame, the time derivative of the summed properties is equal to the sum of the local time derivatives or

$$\frac{d}{dt}\int_V \Phi\,dV = \int_V \frac{\partial\Phi}{\partial t}\,dV \qquad (3)$$

Substituting eqs. (2) and (3) into (1) yields

$$\int_V \left[\frac{\partial \Phi}{\partial t} + \nabla \cdot (\boldsymbol{F} + \Phi \boldsymbol{v}) - H \right] dV = 0 \tag{4}$$

Because V is of arbitrary shape and size, eq. (4) can only be satisfied if the term in square brackets is zero everywhere,

therefore

$$\boxed{\frac{\partial \Phi}{\partial t} + \nabla \cdot (\boldsymbol{F} + \Phi \boldsymbol{v}) = H} \tag{5}$$

This is the general form which all conservation laws take in continuum mechanics.

2. Conservation of mass and energy

Given eq. (5) for the conservation of anything, it is now straightforward to consider conservation of the 3 most important quantities, mass, energy and momentum (force balance).

Conservation of mass

To derive conservation of mass, we just substitute $\Phi = \rho$ (density is the amount of mass per unit volume), $\boldsymbol{F} = 0$ (mass flux can only change due to transport) and $H = 0$ (mass cannot be created or destroyed) into eq. (5) to get

$$\boxed{\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \boldsymbol{v}) = 0} \tag{6}$$

This equation is often referred to as the *continuity equation*.

Conservation of energy (heat)

For a single phase material, the amount of heat per unit volume is $\Phi = \rho c_p T$, where c_p is the specific heat (energy per unit mass per degree Kelvin) at constant pressure and T is the temperature.
The heat flux has two components due to conduction and transport. In the absence of transport the heat flux is $\boldsymbol{F} = -k\nabla T$ where k is the *thermal conductivity*. Note that heat flows opposite to ∇T, i.e., heat flows from hot to cold. The transport flux is $\rho c_p T \cdot \boldsymbol{v}$.
Finally, unlike mass, heat can be created in a region due to terms like radioactive decay or viscous dissipation and shear heating. We will just lump all the source terms into H.
Thus the simplest conservation of heat equation reads

$$\frac{\partial \rho c_p T}{\partial t} + \nabla \cdot (\rho c_p T \boldsymbol{v}) = \nabla \cdot k \nabla T + H \tag{7}$$

For constant c_p and k, this equation can also be rewritten using eq. (6) as

$$\boxed{\frac{\partial T}{\partial t} + \boldsymbol{v} \cdot \nabla T = \kappa \nabla^2 T + H} \tag{8}$$

where $\kappa = k/\rho c_p$ is the *thermal diffusivity* with units $m^2 s^{-1}$.

Note: terms that look like

$$\frac{D}{Dt} = \frac{\partial}{\partial t} + \boldsymbol{v} \cdot \nabla \tag{9}$$

are known as the *material derivative* and can be shown to be the change in time of a materials property as observed in a moving frame of reference (material moves with velocity $\boldsymbol{v}$).

Example: Heat flow and the Peclet number

In the absence of any heat sources, and assuming constant material properties, the simples 1D equation for heat flow is

$$\frac{\partial T}{\partial t} + W\frac{\partial T}{\partial z} = \kappa\frac{\partial^2 T}{\partial z^2} \tag{10}$$

This equation includes two processes, advection of heat at velocity W, and diffusion of heat with thermal diffusivity κ.
As an example problem, this equation could be used to solve for the temperature distribution directly beneath an upwelling mantle plume or mantle ridge (see Figure 1).

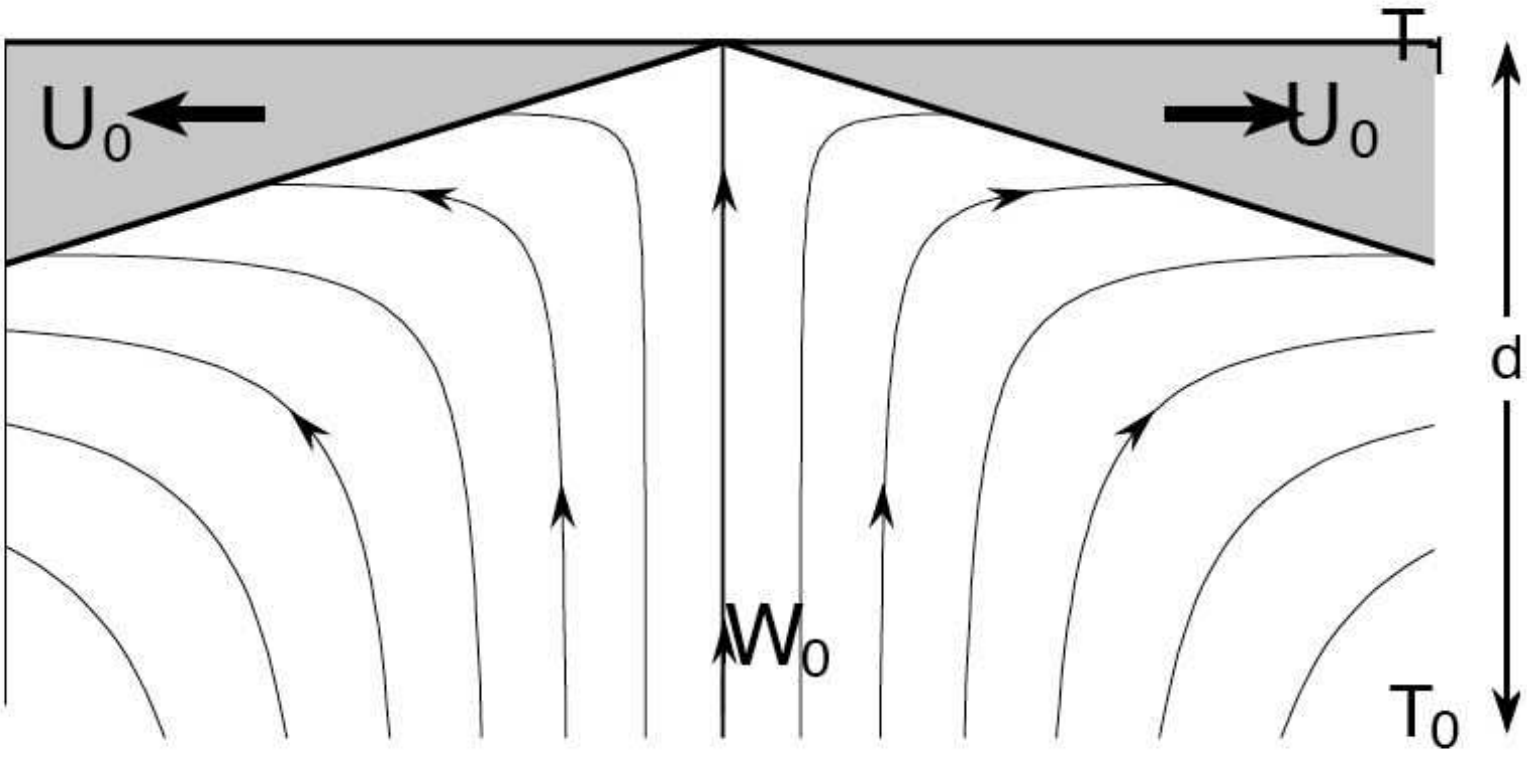


Figure 1: Corner flow beneath an ocean ridge. Layer depth is d, upwelling rate at axis is W_0

While it may appear that that are at least two free parameters (W and κ as well as some temperatures), there is in fact only *one* parameter and it is independent on temperature.

To show this, we begin by replacing the dimensional variables with dimensionless ones. The cholice of scaling values is a bit of an art. Examination of Fig. 1.1 shows that for the case of an upwelling through a thermal layer of depth d, which has constant temperatures T_0 at $z = 0$ and T_1 at $z = d$ and has a characteristic velocity W_0, the sensible scaling is

$$\begin{aligned} z &= d \cdot z' \\ t &= d/W_0 \cdot t' \\ \partial/\partial z &= 1/d \cdot \partial/\partial z' \\ W &= W_0 \cdot W' \\ T &= T_0 + (T_1 - T_0) \cdot T' \end{aligned} \tag{11}$$

where the primes denotes dimensionless variables.

Brute force substitution of eq. (11) into eq. (10) gives

$$\frac{\Delta T W_0}{d}\left[\frac{\partial T'}{\partial t'} + W'\frac{\partial T'}{\partial z'}\right] = \frac{\kappa \Delta T}{d^2}\frac{\partial^2 T'}{\partial {z'}^2} \tag{12}$$

where $\Delta T = T_1 - T_0$.

Multiplying both sides by $d/(\Delta T W_0)$ and dropping the primes yields
(we assume a constant advection velocity in 1D with $\vec{\boldsymbol{v}} = W_0 \vec{n}_z$, i.e. $W' = 1$)

$$\frac{\partial T}{\partial t} + \frac{\partial T}{\partial z} = \frac{1}{Pe} \cdot \frac{\partial^2 T}{\partial z^2} \tag{13}$$

where

$$Pe = \frac{W_0 d}{\kappa} \tag{14}$$

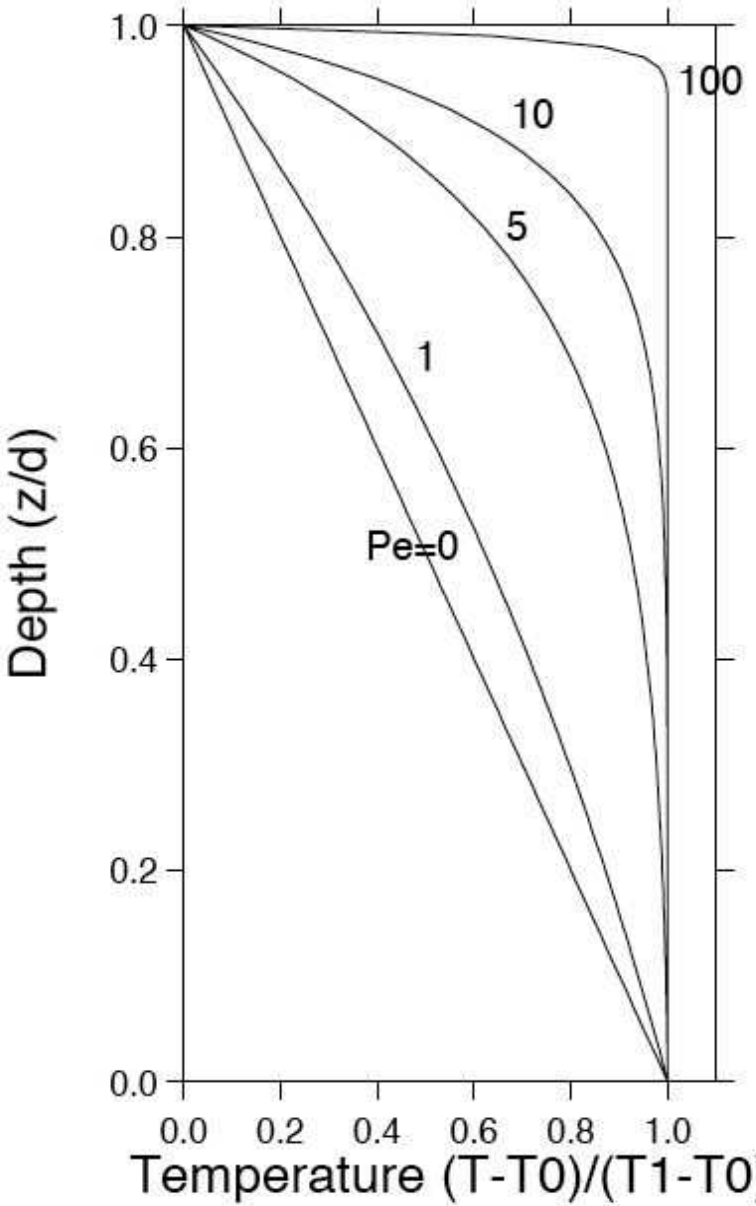
is the *Peclet number* which controls the relative strength of advection to diffusion.

If Pe is large, advection dominates and the last term is negligible[1].
If Pe is small, diffusion dominates.

[1] except in narrow boundary layers

However, there is only one parameter that controls all solutions. Figure 2 shows shows the analytic steady state solution to eq. (13) with dimensionless boundary conditions $T(0) = 1$, $T(1) = 0$ and a range of the Peclet number Pe.

Figure 2 (next slide):
Analytic solution to the simplest steady-state advection-diffusion problem. The solution is $T(z) = (e^{Pe \cdot z} - e^{Pe})/(1 - e^{Pe})$. This problem is a good estimate for the thermal structure direct on the axis. Note that the Peclet number controls the width of the thermal boundary layers which are of order $1/Pe$.


1.0
0.8
0.6
0.4
0.2
0.0
Depth (z/d)
100
10
5
1
Pe=0
0.0 0.2 0.4 0.6 0.8 1.0
Temperature (T-T0)/(T1-T0)

b

Another, more physical way to derive the Peclet number is to consider the time it takes each process to affect the entire layer. The time it takes to advect across the layer at speed W_0 is

$$t_{adv} = d/W_0$$

while the time it takes for heat to diffuse a distance d is

$$t_{diff} = d^2/\kappa$$

.

Thus the Peclet number simply is the ratio of the diffusion time to the advection time scale, i.e. $Pe = t_{diff}/t_{adv}$.

This is a characteristic property of almost all dimensionless numbers that are important for mantle dynamics. They are mostly simple ratios of time scales generated by independent processes and reflecting the relative importance of their corresponding driving forces (mechanisms).

	Earth Mantle	Gulf Stream	Your Bathtub
W_0	10^{-9} m/s (3 cm/yr)	1 m/s	0.01 m/s
d	3000 km	100 km	1 m
ν	10^{18} m^2/s	10^{-6} m^2/s	10^{-6} m^2/s
κ	10^{-6} m^2/s	$1.4 \cdot 10^{-7}$ m^2/s	$1.4 \cdot 10^{-7}$ m^2/s
t_{adv} $(= d/W_0)$			
t_{diff} $(= d^2/\kappa)$			
Pe $(= W_0 d/\kappa)$			
Pr $(= \nu/\kappa)$			

Table 1: Some scales for three fluid problems

(to be completed !)

Numerical Implementation

In the absence of thermal diffusion (κ = 0) and internal heating (H=0), the equation for energy conservation, eq. (8), reads

$$\frac{\partial T}{\partial t} + \boldsymbol{v} \cdot \nabla T = \kappa \nabla^2 T + H = 0 \quad , \tag{15}$$

that is, in 1-D we have

$$\frac{\partial T}{\partial t} + v_z \frac{\partial T}{\partial z} = 0 \quad . \tag{16}$$

We will now evaluate some options on how to solve this equation with a finite difference scheme on a fixed grid.

Even though the equation appears simple, it is quite tricky to solve it accurately, more so than for the diffusion problem. This is particularly the case if there are large gradients in the quantity that is to be advected.

If not done carefully, one can easily end up with strong numerical artifacts such as wiggles (oscillatory artifacts) and numerical diffusion (artificial smoothing of the solution).

FTCS method

In 1-D, the simplest way to discretize eq. (21) is by employing a central difference scheme in space, and go forward in time (another example of a forward-time, central space, FTCS, scheme):

$$\frac{T_i^{n+1} - T_i^n}{\Delta t} = -v_{z,i} \cdot \frac{T_{i+1}^n - T_{i-1}^n}{2\Delta z} \quad , \tag{17}$$

where $v_{z,i}$ is the v_z velocity at location i.

As a exercise, we will consider an exponential pulse of temperature getting advected along the z axis with constant velocity v_z (see matlab script `advection_ftcs_template.m`).

Please download this file from the course homepage, fill in the questions marks as necessary and try to answer the related questions.

- complete the FTCS method, run the file and see what happens
- change e.g. the sign of the velocity v_z
- change the time step and grid spacing and compute the so-called non-dimensional Courant number $\alpha = |v_z|\Delta t/\Delta z$
- When do unstable results occur?
  Can you find a Δt small enough to avoid blow-up?

It turns out, that the FTCS method does not work at all !

In fact, it is a nice example of a scheme that looks logical on paper, but looks can be deceiving. The FTCS method is unconditionally unstable, blows up for any Δt, as can be shown by von Neumann stability analysis.

The instability is related to the fact that this scheme produces negative diffusion, which is numerically unstable.

Lax method

The Lax approach consists of replacing the T_i^n at the left-hand-side of eq. (22) with $(T_{i+1}^n + T_{i-1}^n)/2$.

The resulting equation is

$$\frac{T_i^{n+1} - (T_{i+1}^n + T_{i-1}^n)/2}{\Delta t} = -v_{z,i} \cdot \frac{T_{i+1}^n - T_{i-1}^n}{2\Delta z} \quad . \tag{18}$$

- Program the Lax method by modifying the script of the last exercise
- Try different v_z and Δt settings and compute the Courant number
- Is the numerical scheme stable for all Courant numbers α?
- What is the physical meaning of α?
  What happens for α = 1 and why?

As you can see, the Lax method does not blow up, but does have a lot of numerical diffusion for $\alpha \neq 1$ (which is hard to attain for realistic problems, as v_z will vary in space and time).

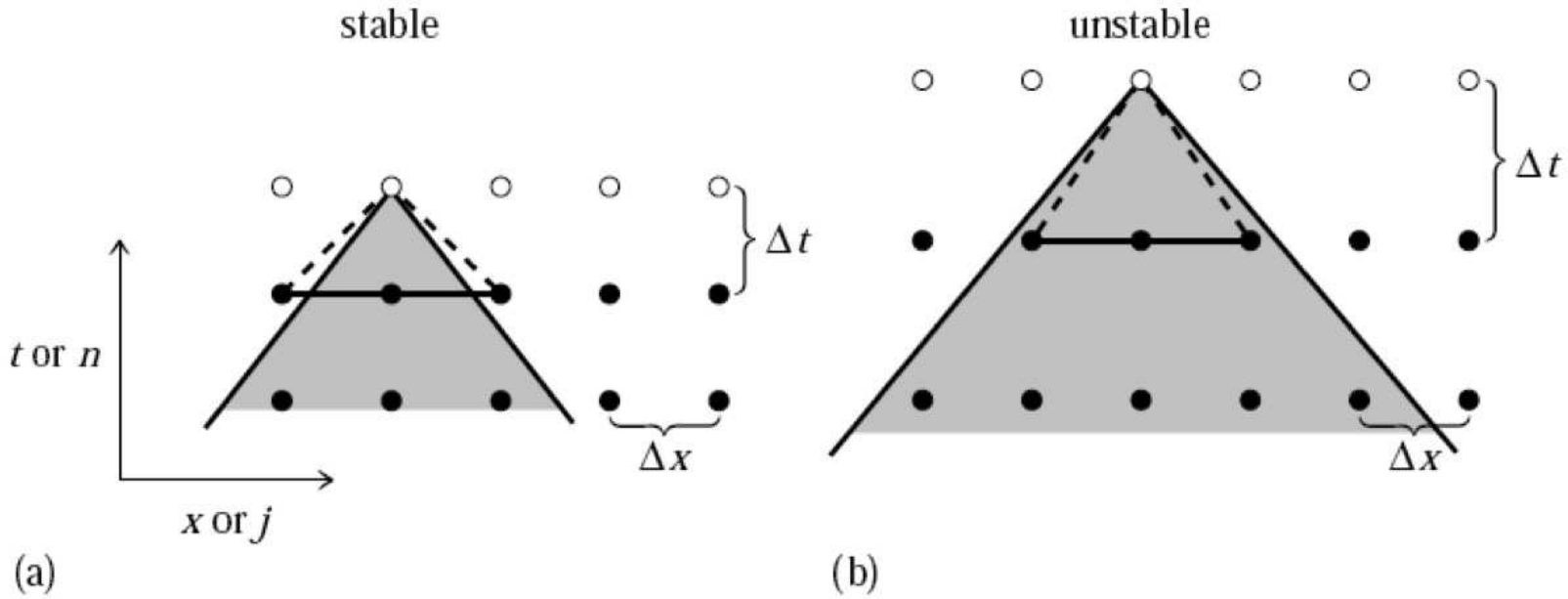
In fact, the Lax criterion stabilized the discretized advection equation by adding some artificial diffusion. So, it is an improvement of the situation – but it's far from being perfect (!) since you may now loose details of the solution purely due to numerical diffusion.

As for the case of the implicit versus explicit solution of the diffusion equation, you see that there are trade-offs between stability and accuracy.

The stability requirement

$$\alpha = \frac{|v_z|\Delta t}{\Delta z} \leq 1 \tag{19}$$

is called the *Courant criterion* (see Figure).



Courant condition for stability of a differencing scheme: The solution of a hyperbolic problem at a point depends on information within some domain of depencency to the past, shown here shaded. The differencing scheme has its own domain of dependency determined by the choice of points on one time slice (shown as connected solid dots) whose values are used in determining a new point (shown connected by dashed lines). A differencing scheme is called Courant stable if the differencing domain of dependency is larger than that of the PDE's, as in (a).

Streamline upwind scheme

A popular scheme is the so-called (streamline) upwind approach. Here, the spatial finite difference scheme depends on the sign of the velocity:

The resulting equation is

$$\begin{aligned} \frac{T_i^{n+1} - T_i^n}{\Delta t} &= -v_{z,i} \cdot (T_i^n - T_{i-1}^n)/\Delta z \qquad \text{if} \quad v_{z,i} > 0 \\ &= -v_{z,i} \cdot (T_{i+1}^n - T_i^n)/\Delta z \qquad \text{if} \quad v_{z,i} < 0 \end{aligned} \tag{20}$$

Note that we have replaced central with forward or backward derivatives, depending on the flow direction.

The idea is that the flux into the local cell at z_i will only depend on the gradient of temperature in the direction “upstream”, i.e. where the inflowing velocity is coming from.

The upwind scheme also suffers from numerical diffusion, and it is only first order accurate in space.

For some applications, particularly if there's also diffusion, it might just be good enough because the simple trick of doing FD forward or backward is closer to the underlying physics of transport than, say, FTCS. There are some mantle convection codes that use streamline upwind schemes.

So far, we employed explicit discretizations. You're probably wondering whether implicit discretizations will save us again this time. Bad news: they are not well-suited for this type of problem. Implicit schemes behave like parabolic partial differential equations (e.g. the diffusion equation) in that a perturbation at node (i,n) will affect the solution at all nodes at time level n+1.

With an advection type equation, disturbances travel at a finite speed (the speed of the material displacement) and will not affect all nodes at time level n+1. So we have to come up with something else.