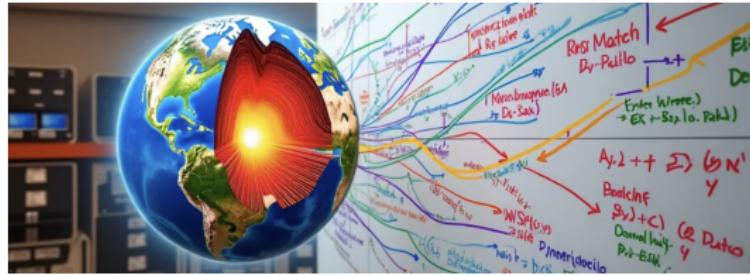


Principles of Numerical Modelling in Geosciences

Lecture 3: From ODEs to PDEs – Conservation and Spatial Variation

Mattia de' Michieli Vitturi

PhD Course in Earth Sciences



Outline

1 Introduction to PDEs

- From ODEs to PDEs

2 Physics of fluids and conservation laws

- The continuum hypothesis
- Conservation laws
- Eulerian and Lagrangian description

3 Governing equations

- Mass equation
- Heat equation

4 Boundary Conditions

5 Numerical discretization

- Finite differences

6 Python implementation

Lesson Goals

In this lesson, we begin transitioning from ordinary differential equations (ODEs) to partial differential equations (PDEs). Our goals are:

- Understand how PDEs generalize ODEs by incorporating spatial variation.
- Learn the physical and mathematical foundation of conservation laws.
- See how time and space interact in natural processes.
- Explore practical examples from geosciences: lava flows, soil infiltration, ash dispersion.
- Introduce the basic tools for solving PDEs numerically.

From ODE to PDE: What's the Key Difference?

An Ordinary Differential Equation (ODE) describes how a quantity u changes with respect to a single independent variable.

- Typically, this is time t : $u(t)$. Example:

Radioactive decay $\frac{dN(t)}{dt} = -\lambda N$. The amount $N(t)$ changes only with time.

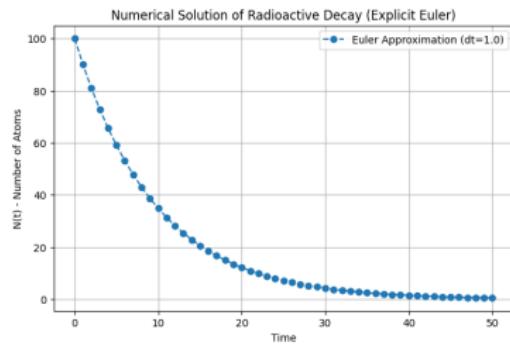
- Or, less commonly in our context so far, a single spatial dimension x . Example:

Steady-state temperature profile

through a rock layer of thickness L with fixed temperatures T_1 at $x = 0$ and T_2 at $x = L$.

$$\kappa \frac{d^2 T(x)}{dx^2} = 0$$

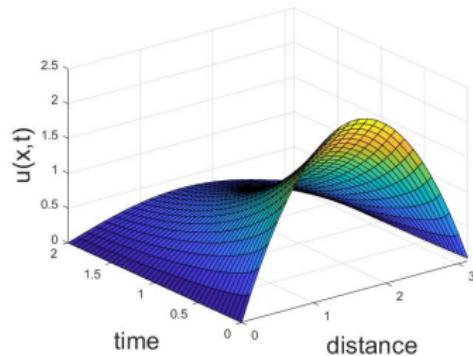
The solution gives the value of the variable of interest at different points (or times).



From ODEs to PDEs: What is the Key Difference?

A **Partial Differential Equation (PDE)** describes how a quantity u changes with respect to **multiple independent variables**.

- Commonly, these are time t AND one or more spatial dimensions (e.g., x , or x, y , or x, y, z): $u(x, t)$, $u(x, y, t)$.
- Example: $\frac{\partial u(t,x)}{\partial t} + \frac{\partial u(t,x)}{\partial x} = 0$.
- The solution varies in both space and time.



Many Earth science processes are spatially distributed (temperature in ground, water in soil, volcanic ash in atmosphere), requiring PDEs to capture these spatial interactions and their evolution over time.

A Familiar ODE: Newton's Cooling Law

We recall the model for the cooling of a body, introduced in Lecture 1:

$$\frac{dT(t)}{dt} = -k(T(t) - T_{\text{env}})$$

where:

- $T(t)$ is the temperature of the body at time t .
- T_{env} is the constant ambient (environment) temperature.
- k is the cooling coefficient (related to heat transfer properties and surface area).

This is a first-order linear ODE. Assuming an initial temperature $T(0) = T_0$, the **analytical solution** is:

$$T(t) = T_{\text{env}} + (T_0 - T_{\text{env}})e^{-kt}$$

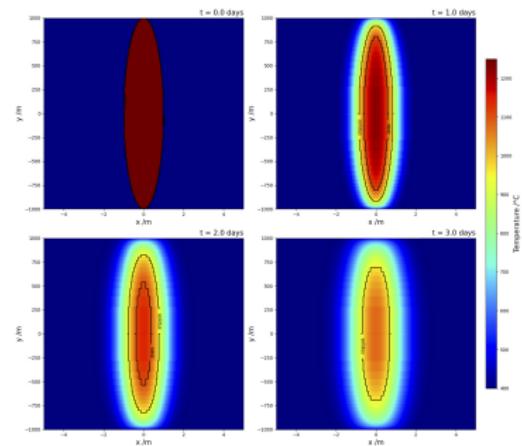
It is a lumped model: we assume the temperature is uniform. Suitable for small or well-mixed objects.

When Space Matters: Heat Flow in Geosciences

In many geological scenarios, temperature is not uniform but varies significantly within a body or region. This spatial variation directly affects how temperature changes over time.

Consider these examples:

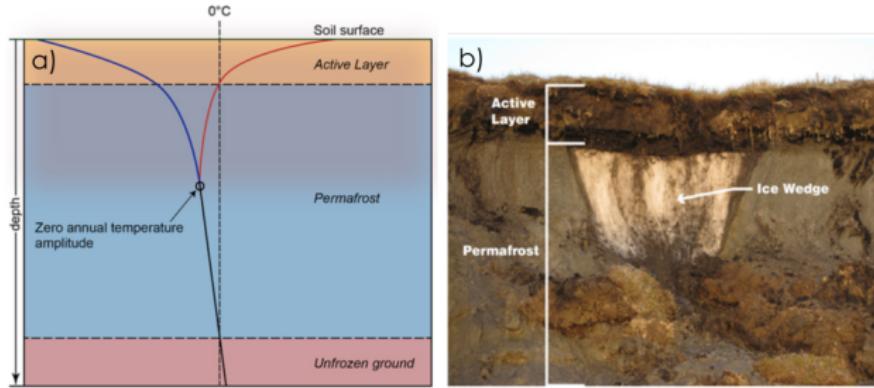
- **Lava Flow Cooling:** The surface exposed to air cools much faster than the insulated interior. Heat flows from the hot core to the cooler surface.
- **Magmatic Dike Intrusion:** A hot dike intrudes cooler host rock. The dike cools while heating the surrounding rock, creating temperature gradients in both.



From Loncart and Huppert 2022 EPSL.

When Space Matters: Heat Flow in Geosciences

- **Geothermal Systems:** Heat from depth is conducted upwards through the Earth's crust, establishing a geothermal gradient.
- **Permafrost Thawing/Freezing:** Temperature changes at the surface propagate downwards, affecting the freeze-thaw boundary.



In all these cases, temperature T is a function of both position (e.g., x or depth z) and time t , i.e., $T(x, t)$.

When Space Matters: The Heat (Diffusion) Equation

If we denote with $T(x, t)$ the temperature T , the main equation governing the processes described in the previous slides is the **Heat Equation**:

$$\underbrace{\frac{\partial T}{\partial t}}_{\text{Rate of change of } T \text{ at a point}} = \underbrace{\kappa}_{\text{Thermal Diffusivity}} \cdot \underbrace{\frac{\partial^2 T}{\partial x^2}}_{\text{Curvature of } T \text{ profile (Laplacian)}}$$

Key Components Explained:

- $\frac{\partial T}{\partial t}$: How fast temperature changes at a location.
- κ (kappa, m^2/s): **Thermal Diffusivity**. Measures how quickly heat spreads.
- $\frac{\partial^2 T}{\partial x^2}$: The **second spatial derivative**. It drives heat flow from hotter to colder regions to smooth out temperature differences.

This is a **parabolic PDE**, characteristic of diffusion processes that evolve towards equilibrium by smoothing initial variations.

Other Geoscience Examples of PDEs

Many other fundamental processes in Earth Sciences are described by PDEs. Here are a few more examples:

- Unsaturated Soil Water Flow (Richards' Equation - 1D vertical):

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z} \left[D(\theta) \frac{\partial \theta}{\partial z} \right] - \frac{\partial K(\theta)}{\partial z}$$

Models the change in volumetric water content θ in unsaturated soil. This is highly nonlinear as hydraulic conductivity $K(\theta)$ and diffusivity $D(\theta)$ depend strongly on θ .

- $\frac{\partial \theta}{\partial t}$: Rate of change of water content.
- $\frac{\partial}{\partial z} [D(\theta) \frac{\partial \theta}{\partial z}]$: Diffusive flux.
- $\frac{\partial K(\theta)}{\partial z}$: Advection flux due to gravity (and pressure gradients if K includes them).

Other Geoscience Examples of PDEs

- Advection-Diffusion Equation (e.g., for Ash/Pollutant Dispersion):

$$\frac{\partial c}{\partial t} + \vec{u} \cdot \nabla c = \nabla \cdot (D \nabla c) + S$$

Describes how the concentration c of a substance (e.g., volcanic ash, pollutant) changes due to transport by a fluid flow (advection by wind \vec{u}) and spreading due to mixing (diffusion D). S represents sources (e.g., erupting volcano) or sinks (e.g., deposition).

- $\frac{\partial c}{\partial t}$: Rate of change of concentration.
- $\vec{u} \cdot \nabla c$: Advective transport (movement with the mean flow).
- $\nabla \cdot (D \nabla c)$: Diffusive/dispersive transport (spreading).
- This equation combines *hyperbolic* (advective) and *parabolic* (diffusive) characteristics.

All these equations involve both time and spatial derivatives, capturing the dynamic interplay of processes in space and time.

Outline

1 Introduction to PDEs

- From ODEs to PDEs

2 Physics of fluids and conservation laws

- The continuum hypothesis
- Conservation laws
- Eulerian and Lagrangian description

3 Governing equations

- Mass equation
- Heat equation

4 Boundary Conditions

5 Numerical discretization

- Finite differences

6 Python implementation

Describing Physical Conservation with PDEs

Most of these equations can be derived from **conservation laws**. These laws state that certain quantities are conserved within a system unless acted upon by external influences.

- Conservation of Mass
- Conservation of Momentum (Newton's Second Law)
- Conservation of Energy (First Law of Thermodynamics)

To model systems governed by these physical laws, we translate them into mathematical language. This translation often results in **Partial Differential Equations (PDEs)**.

PDEs provide the framework to describe how these conserved quantities and their fluxes vary in both space and time. Therefore, to simulate such physical processes, we often need to solve these PDEs, frequently using numerical methods.

Physics of fluids

Introduction

In many text books of fluid dynamics the word **fluid** refers to *one of the states of matter, either liquid or gaseous, in contrast to the solid state.* This definition is much too restrictive. In fact, **the definition of a fluid rests in its tendency to deform irrecoverably.** Basically any material that appears as elastic or non-deformable, with a crystalline structure (i.e., belonging to the solid state) or with a disordered structure (e.g., a glass, which from a thermodynamic point of view belongs to the liquid state) can be deformed when subjected to stresses for a long enough time.

The characteristic time constant of the geological processes related to mantle convection, typically 10 Myrs ($3 \times 10^{14} \text{ s}$), is so long that the mantle, although stronger than steel and able to transmit seismic shear waves, can be treated as a fluid.

Physics of fluids

The continuum hypothesis

- Most materials can therefore behave like elastic solids on very short time scales and like fluids at long times.
- The physics of fluid behavior is based on the general continuum hypothesis and this hypothesis requires that quantities like density, temperature, or velocity are defined everywhere.
- The continuum hypothesis is basically an approximation, because at a small scale fluids are composed of molecules that collide with one another and solid objects, and this approximation results in approximate solutions. Consequently, assumption of the continuum hypothesis can lead to results which are not of desired accuracy. However, under the right circumstances, the continuum hypothesis produces extremely accurate results.

Modeling philosophy

From the physical principles to the equation

In order to simulate fluid flow, heat transfer, and other related physical phenomena, it is necessary to describe the physics associated with these processes in mathematical terms.

- Choose a physical principle:
 - conservation of mass
 - conservation of momentum
 - conservation of energy
- Apply it to a suitable flow model
 - Eulerian/Lagrangian approach
 - for a finite/infinitesimal CV
- Extract integral equations or partial differential equations (PDEs) which embody the physical principle.

Conservation laws

The physical principles

The equations of fluid-dynamics represent the mathematical transposition of some **conservation** laws of physics.

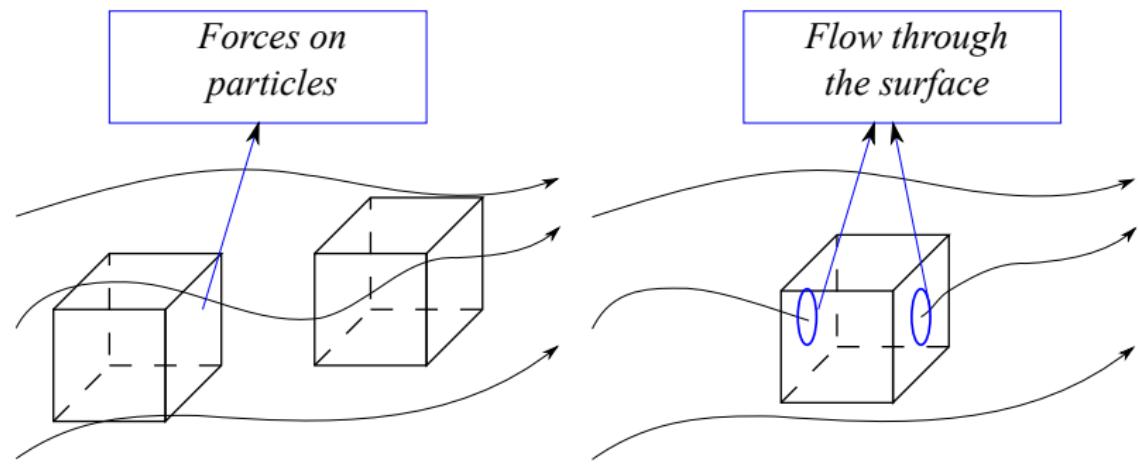
In particular, we will use these three physical principles:

- **Conservation of mass:** *the mass of a closed system (in the sense of a completely isolated system) will remain constant over time.* Or alternatively: *the rate of change of mass inside a fixed control volume V equals the net flux through the surface of the control volume.*
- **Conservation of momentum** (second Newton's law): *if no external force acts on a closed system of objects, the momentum of the closed system remains constant.*
- **Conservation of energy:** *the total amount of energy in a closed system remains constant over time.*

Lagrangian and Eulerian view

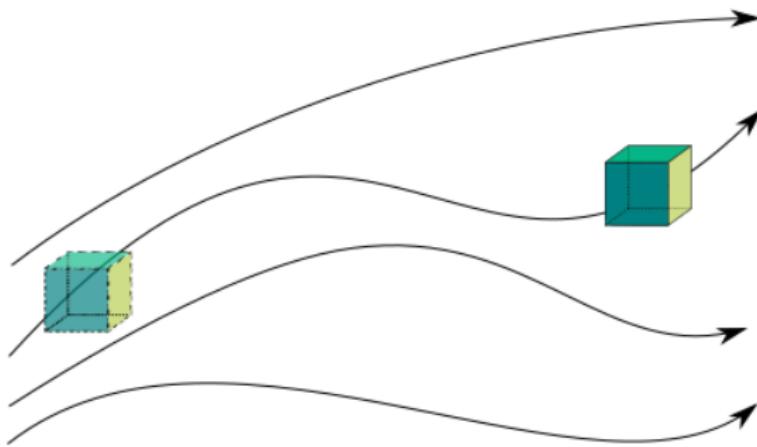
It is possible to describe the motion of fluids with two different approaches:

- in the **Lagrangian** description we track individual fluid particles as they move through the flow field
- in the **Eulerian** description we are interested in the flow characteristics in a fixed control volume



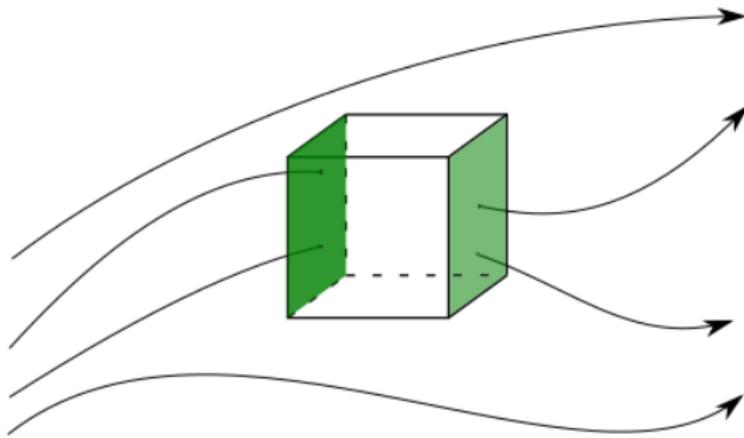
Lagrangian approach

The **Lagrangian approach** is a way of looking at fluid motion where the observer follows an individual fluid parcel as it moves through space and time, therefore in the Lagrangian description the individual fluid particles are tracked as they move and deform (it is possible that both the shape and size change) through the flow field, as in Figure.



Eulerian approach

The **Eulerian approach** is a way of looking at the fluid motion by focusing on a fixed location in space. The characteristics of the flow are evaluated with respect to an imaginary and fixed *control volume*.



Lagrangian and Eulerian view

An example of an Eulerian frame of reference is a web-cam that does not move.

An example of Lagrangian description is a weather balloon measuring the temperature while it is advected by the wind.

Questions:

- In the Eulerian description, what is the best choice for the unknown of the problem?

Position

Velocity

Lagrangian and Eulerian view

An example of an Eulerian frame of reference is a web-cam that does not move.

An example of Lagrangian description is a weather balloon measuring the temperature while it is advected by the wind.

Questions:

- In the Eulerian description, what is the best choice for the unknown of the problem?
- In the Lagrangian description, what is the best choice for the unknown of the problem?

Position

Velocity

Eulerian and Lagrangian description

Time derivative

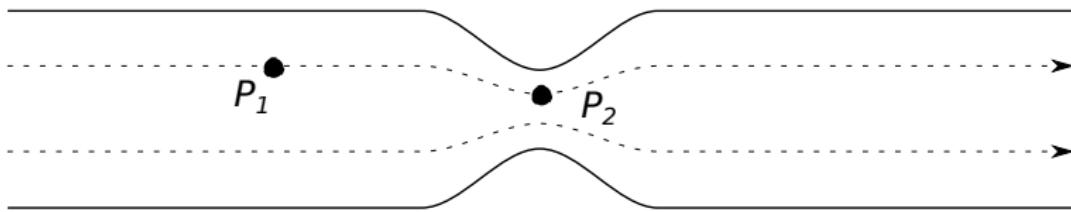
- In the *Eulerian* formalism, the spatial coordinates $\mathbf{x} = (x, y, z)$ are the independent variables and they refer to a fixed reference system. Each physical quantity q related to the flow, be it a scalar (such as density, pressure, and temperature) or a vector quantity (like velocity), is defined in each point \mathbf{x} and for every time t and it constitutes a scalar field or vector field respectively, hence $q = q(\mathbf{x}, t)$, $\forall t, \forall \mathbf{x}$.
- In the *Lagrangian* framework, the focus is on a single fluid parcel which is followed during the flow. The position of a fluid parcel initially located in $\mathbf{r}_0 = (x_0, y_0, z_0)$ is a function of time expressed as

$$\mathbf{x}_{\mathbf{r}_0}(t) = (x_{\mathbf{r}_0}(t), y_{\mathbf{r}_0}(t), z_{\mathbf{r}_0}(t)).$$

Eulerian and Lagrangian description

Time derivative

Let consider the water in a river where the cross-section changes width. If the solution is steady, what can we tell about the velocity changes with time?



In the Eulerian view the steadiness of the flow means that in every point the quantities (velocity) describing the flow are constant in time. In the Lagrangian view, the flow accelerates when we track the fluid particles passing through a narrower section. Thus, two different time derivatives arise in the Eulerian and Lagrangian approaches.

Eulerian and Lagrangian description

Time derivative

We have seen that in the Lagrangian point of view we “follow” the motion of the fluid particle. Thus, when we consider a quantity seen by the particle along its motion, there are two reasons that can produce changes in the considered quantity:

- variations related to changes in the fluid with time ($\frac{\partial}{\partial t}$);
- variations due to the fact that the particles moves to a new position where the conditions can be different ($\mathbf{u} \cdot \nabla$).

The sum of these two variation rates for a quantity ϕ is called **substantial derivative** (also called the Lagrangian derivative, convective derivative, material derivative, total derivative or particle derivative) and we use the notation $\frac{D\phi}{Dt}$ for it:

$$\frac{D\phi}{Dt} = \frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi$$

Eulerian view

Remarks

- The Eulerian description is better suited to fluid dynamics problems, whereas the Lagrangian description is more appropriate for problems related to solid particles and objects (particle tracking, traces, etc.).
- In the Eulerian description of the flow field, the flow quantities are depicted as a function of position (x, y, z) and time t . Specifically, the flow is described by a function

$$\mathbf{u}(\mathbf{x}, t)$$

giving the flow velocity at position (x, y, z) at time t .

- In the following we will use the Eulerian description to derive the conservation equations from physical principles expressing the conservation laws.

Conservation laws

Governing equations

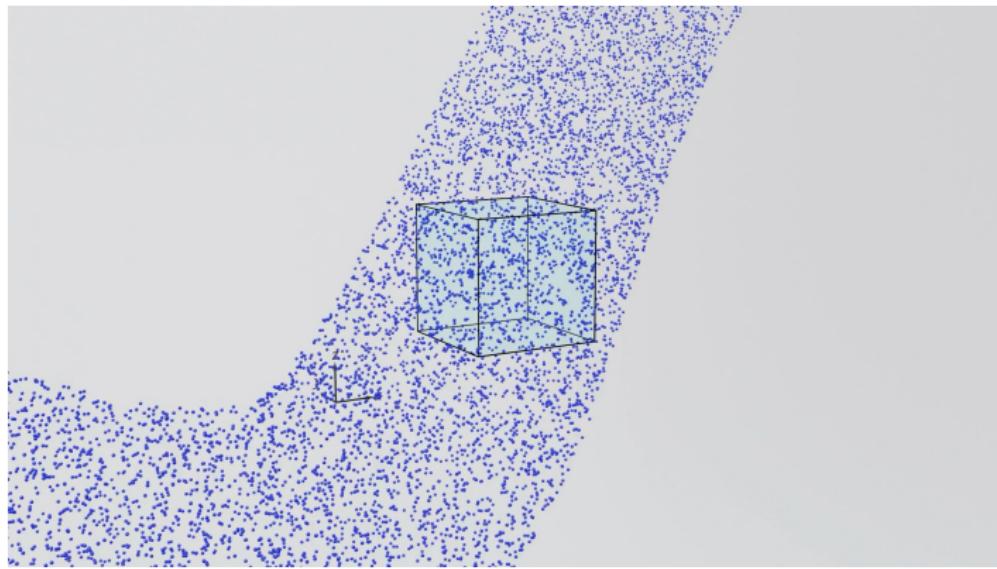
Typical governing equations describing the conservation of **momentum, energy, or chemical species** are written in terms of specific quantities - i.e., quantities **associated with the mass** (or with the volumetric density ρ).

For example, the momentum equation expresses the principle of conservation of linear momentum in terms of the momentum per unit mass, i.e., velocity.

The equation for conservation of chemical species expresses the conservation of the mass of the species in terms of its mass fraction.

Conservation laws

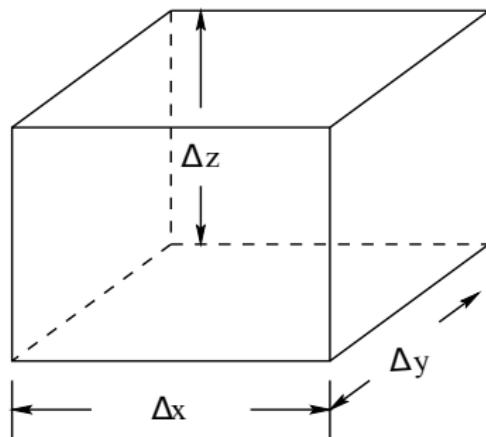
Governing equations



Conservation laws

Governing equations

Let us consider a **specific quantity** ϕ , which may be momentum per unit mass (velocity), or the energy per unit mass (specific energy), or any other such quantity. Consider a control volume V of size $\Delta x \times \Delta y \times \Delta z$. We want to express the variation of ϕ in the control volume over time. Let us assume that ϕ is governed by a conservation principle that states:



Accumulation of ϕ in the control volume over time Δt =
 Net influx of ϕ into the control volume V through the surface S +
 Net generation of ϕ inside control volume V .

Conservation laws

Governing equations

Accumulation of ϕ in the control volume over time Δt =
Net influx of ϕ into the control volume V through the surface S +
Net generation of ϕ inside control volume V .

- If ϕ is expressed on a per unit mass basis, the accumulation in the control volume over time Δt is given by:

$$(\rho\phi\Delta V)_{t+\Delta t} - (\rho\phi\Delta V)_t$$

where ρ is the density of the fluid, ΔV is the volume of the control volume ($\Delta x \times \Delta y \times \Delta z$) and t is the time.

Conservation laws

Governing equations

Accumulation of ϕ in the control volume over time Δt =
Net influx of ϕ into the control volume V through the surface S +
Net generation of ϕ inside control volume V .

- The net generation of ϕ inside the control volume over time Δt is given by

$$S\Delta V\Delta t$$

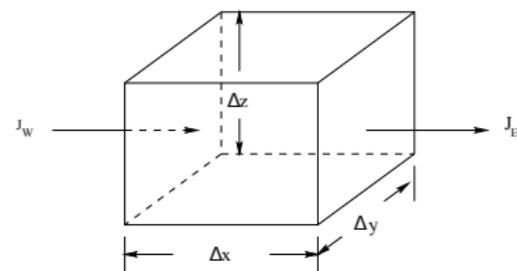
where S is the generation of ϕ per unit volume and per unit time. S is also sometimes called the source term.

Conservation laws

Governing equations

Accumulation of ϕ in the control volume over time $\Delta t =$
Net influx of ϕ into the control volume V through the surface S +
Net generation of ϕ inside control volume V .

Let us consider the remaining term,
the net influx of ϕ into the control
volume. Let J_W represent the flux of ϕ
through face W at x , and J_E the flux
through face E at $x + \Delta x$.



Similar fluxes exist on the y and z faces respectively. The net influx of ϕ into the control volume over time Δt is

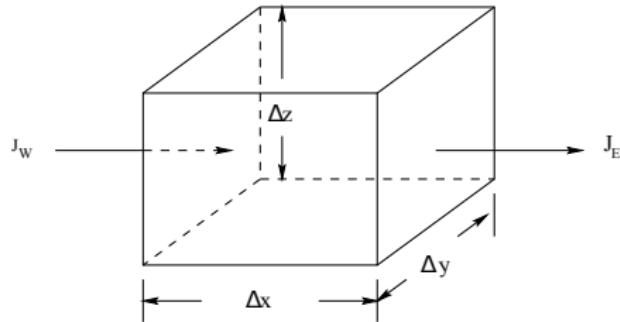
$$(J_W - J_E) \Delta y \Delta z \Delta t + (J_N - J_S) \Delta x \Delta z \Delta t + (J_T - J_B) \Delta x \Delta y \Delta t.$$

Conservation laws

Diffusion and convection

Accumulation of ϕ in the control volume over time $\Delta t =$
Net influx of ϕ into the control volume V through the surface S +
Net generation of ϕ inside control volume V .

We have not yet said what physical mechanism causes the **influx of ϕ** . For physical phenomena of interest to us, ϕ is transported by two primary mechanisms: **diffusion** due to molecular collisions, and **convection** due to the motion of fluid.

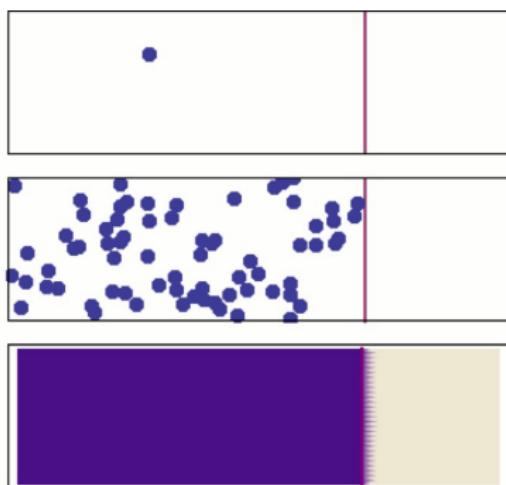


Diffusive flux

Fick's law

Fick's first law relates the diffusive flux to the concentration under the assumption of steady state. It postulates that the flux goes from regions of high concentration to regions of low concentration, with a magnitude that is proportional to the concentration gradient (spatial derivative). In many cases, the diffusion flux may be written as

$$J_{\text{diffusion},x} = -\Gamma \frac{\partial \phi}{\partial x}$$



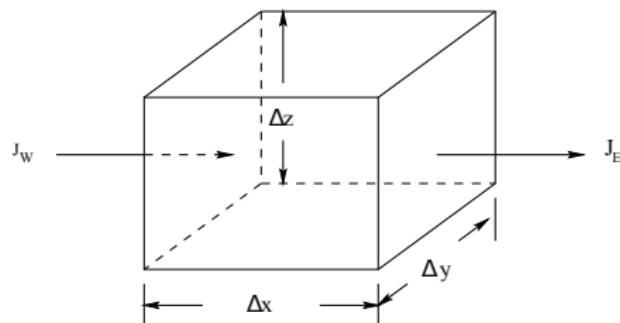
Influx

Convective flux

The convective flux of ϕ in the x -direction may be written as

$$J_{convection,x} = \rho u \phi$$

where u is component in the x -direction of the velocity.



Although the term "convection" is often reserved for flows driven by internal buoyancy anomalies of thermal origin, here we more generally use "convection" for any motion of a fluid driven by internal or external forcing. Convection can be kinematically forced by boundary conditions or induced by density variations. The term **advection** sometimes serves as a synonym for this meaning of convection.

Conservation laws

Convection and diffusion

Thus, summing the two contributions of the influx in the x -direction, the net convective and diffusive flux may be written as

$$J_W = \left(\rho u \phi - \Gamma \frac{\partial \phi}{\partial x} \right)_W, \quad J_E = \left(\rho u \phi - \Gamma \frac{\partial \phi}{\partial x} \right)_E$$

Similar expressions may be written for the y and z directions respectively:

$$J_S = \left(\rho v \phi - \Gamma \frac{\partial \phi}{\partial y} \right)_S, \quad J_N = \left(\rho v \phi - \Gamma \frac{\partial \phi}{\partial y} \right)_N,$$

$$J_B = \left(\rho w \phi - \Gamma \frac{\partial \phi}{\partial z} \right)_B, \quad J_T = \left(\rho w \phi - \Gamma \frac{\partial \phi}{\partial z} \right)_T.$$

Conservation laws

Governing equations

We can now express the conservation principles stated by:

Accumulation of ϕ in the control volume over time $\Delta t =$
Net influx of ϕ into the control volume V through the surface $S +$
Net generation of ϕ inside control volume V .

in a mathematical form as:

$$\begin{aligned} & (\rho\phi\Delta V)_{t+\Delta t} - (\rho\phi\Delta V)_t = \\ & (J_W - J_E)\Delta y\Delta z\Delta t + (J_N - J_S)\Delta x\Delta z\Delta t + (J_T - J_B)\Delta x\Delta y\Delta t + \\ & S\Delta V\Delta t. \end{aligned}$$

Conservation laws

Governing equations

Rearranging the terms and dividing both the sides by Δt and ΔV , the generic conservation equation may be written as

$$\frac{(\rho\phi)_{t+\Delta t} - (\rho\phi)_t}{\Delta t} = \frac{(J_W - J_E)}{\Delta x} + \frac{(J_N - J_S)}{\Delta y} + \frac{(J_T - J_B)}{\Delta z} + S$$

Taking the limit $\Delta x, \Delta y, \Delta z, \Delta t \rightarrow 0$, we get the differential form of the conservation equation:

$$\frac{\partial(\rho\phi)}{\partial t} = \frac{\partial J_x}{\partial x} + \frac{\partial J_y}{\partial y} + \frac{\partial J_z}{\partial z} + S$$

where (J_x, J_y, J_z) are the components of the flux (convective and diffusive).

Transport equation

Differential form

Let us write now the differential form of the transport equation we have derived expanding the flux term:

$$\frac{\partial}{\partial t} (\rho\phi) + \frac{\partial}{\partial x} (\rho u\phi) + \frac{\partial}{\partial y} (\rho v\phi) + \frac{\partial}{\partial z} (\rho w\phi) =$$

$$\frac{\partial}{\partial x} \left(\Gamma \frac{\partial \phi}{\partial x} \right) + \frac{\partial}{\partial y} \left(\Gamma \frac{\partial \phi}{\partial y} \right) + \frac{\partial}{\partial z} \left(\Gamma \frac{\partial \phi}{\partial z} \right) + S$$

or, in vector notation:

$$\frac{\partial}{\partial t} (\rho\phi) + \nabla \cdot \rho \mathbf{u}\phi = \nabla \cdot (\Gamma \nabla \phi) + S.$$

Transport equation

Differential form

The equation we have derived is called the **differential form** of the transport equation:

$$\frac{\partial}{\partial t} (\rho\phi) + \nabla \cdot \rho\mathbf{u}\phi = \nabla \cdot (\Gamma\nabla\phi) + S.$$

The transport equation written in this form clearly highlights the various transport processes:

- the *rate of change* term $\frac{\partial}{\partial t} (\rho\phi)$
- the *convective* term $\nabla \cdot \rho\mathbf{u}\phi$
- the *diffusive* term $\nabla \cdot (\Gamma\nabla\phi)$
- the *source* term S .

Outline

1 Introduction to PDEs

- From ODEs to PDEs

2 Physics of fluids and conservation laws

- The continuum hypothesis
- Conservation laws
- Eulerian and Lagrangian description

3 Governing equations

- Mass equation
- Heat equation

4 Boundary Conditions

5 Numerical discretization

- Finite differences

6 Python implementation

Governing equations

The mass equation

The governing laws for fluid flow, heat and mass transfer, as well as other transport processes, may be represented by the equation we have derived:

$$\frac{\partial}{\partial t} (\rho\phi) + \nabla \cdot \rho\mathbf{u}\phi = \nabla \cdot (\Gamma\nabla\phi) + S.$$

Let us now consider some specific cases.

First of all, if we take $\phi = 1$, and we neglect diffusive and source terms, we obtain the following conservation equation:

$$\frac{\partial\rho}{\partial t} + \nabla \cdot \rho\mathbf{u} = 0.$$

This equation is the Eulerian formulation of the differential form of the conservation equation of mass (also called continuity equation).

Continuity equation

Lagrangian form

We use the definition of the substantial derivative to rewrite the differential form of the continuity equation we have derived with the Eulerian approach:

$$\frac{\partial}{\partial t} \rho + \nabla \cdot (\rho \mathbf{u}) = 0$$

Expanding the divergence term we have:

$$\frac{\partial}{\partial t} \rho + \mathbf{u} \cdot \nabla \rho + \rho \nabla \cdot \mathbf{u} = 0$$

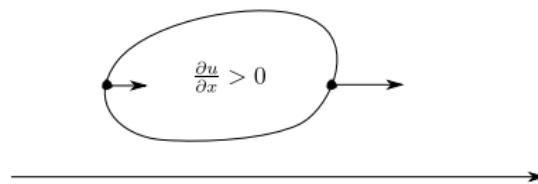
The first two terms are the substantial derivative of the density, thus we can write the following Lagrangian form for the continuity equation:

$$\frac{D}{Dt} \rho = -\rho \nabla \cdot \mathbf{u}$$

Continuity equation

Divergence

It is possible to give a physical interpretation to this form of the continuity equation: $\frac{D}{Dt}\rho = -\rho \nabla \cdot \mathbf{u}$.



The equation states that a fluid particle increases its density when the motion of the fluid converges, and decreases its density when the motion is diverging. In other words, the density of a fluid particle changes along the motion when the motion compresses, or expands, the particle. This compression (expansion) is expressed mathematically by the divergence $\nabla \cdot \mathbf{u}$.

Continuity equation

Lagrangian framework



From the General Transport Equation to the Heat Equation

We start now from the general scalar transport equation:

$$\frac{\partial(\rho\phi)}{\partial t} + \nabla \cdot (\rho \vec{u}\phi) = \nabla \cdot (\Gamma \nabla \phi) + S$$

and we consider a simplified case:

- No convection: $\vec{u} = 0$
- No sources or sinks: $S = 0$
- Constant properties: $\rho = 1, \Gamma = \kappa$

Then the equation reduces to:

$$\frac{\partial \phi}{\partial t} = \kappa \nabla^2 \phi$$

When $\phi = T$, this is called the **heat (diffusion) equation**.

In the next slides we will see how to solve numerically this equation.

Outline

1 Introduction to PDEs

- From ODEs to PDEs

2 Physics of fluids and conservation laws

- The continuum hypothesis
- Conservation laws
- Eulerian and Lagrangian description

3 Governing equations

- Mass equation
- Heat equation

4 Boundary Conditions

5 Numerical discretization

- Finite differences

6 Python implementation

Why Do We Need Boundary Conditions?

- In partial differential equations (PDEs), like the heat equation from the previous slide, we describe how a quantity (for example the temperature T) changes with both time and space.
- To obtain a unique solution, we need to specify values or behavior at the boundaries of the domain.
- These are called **boundary conditions**.
- Boundary conditions represent the interaction of the system with its surroundings.
- *Example:* when modeling the temperature of a lava flow, the surrounding air or ground affects how heat is lost through the surface.

What Is a Boundary Condition?

- A **boundary condition** tells us what happens at the edge of the physical domain.
- It can fix the value (temperature, concentration), fix the flux (heat, mass), or combine both.
- Without boundary conditions, the PDE has an infinite number of possible solutions.
- They are essential to close the problem mathematically and physically.

If we model the cooling of a vertical magma dike and assume symmetry along its central axis, we can simulate only half of the dike. At the symmetry plane, we use a boundary condition to impose zero heat flux (zero temperature gradient). At the outer edge, which is in contact with cold surrounding rock, we apply a boundary condition to fix the temperature.

Types of Boundary Conditions

- **Dirichlet condition:** impose the value of the variable.

$$T(0, t) = T_{\text{left}}, \quad T(L, t) = T_{\text{right}}$$

- **Neumann condition:** impose the derivative (flux).

$$\left. \frac{\partial T}{\partial x} \right|_{x=0} = 0$$

- **Robin (mixed) condition:** combine value and flux.

$$-k \frac{\partial T}{\partial x} = h(T - T_{\infty})$$

Geoscience Examples of Boundary Conditions

- Lava cooling:
 - Dirichlet: fixed temperature at the surface (e.g., contact with cold air)
 - Neumann: zero heat flux at symmetry plane or insulated bottom
 - Robin: convective cooling at the lava-air interface
- Soil moisture:
 - Neumann: rainfall as imposed surface flux
 - Dirichlet: saturation or known water content at depth
- Ash dispersion:
 - Dirichlet: concentration zero at the top of the domain
 - Neumann: no flux at domain boundaries

Summary: Boundary Conditions

Boundary conditions are essential to solve a PDE. They represent how the system interacts with its physical environment. *Choosing realistic boundary conditions is part of accurate modelling.*

Outline

1 Introduction to PDEs

- From ODEs to PDEs

2 Physics of fluids and conservation laws

- The continuum hypothesis
- Conservation laws
- Eulerian and Lagrangian description

3 Governing equations

- Mass equation
- Heat equation

4 Boundary Conditions

5 Numerical discretization

- Finite differences

6 Python implementation

From Time Derivatives to Spatial Derivatives

In the previous lectures, and when solving Ordinary Differential Equations (ODEs) like $\frac{dT}{dt} = f(T, t)$, we focused on approximating the time derivative.

Recall: Approximating $\frac{dT}{dt}$ for ODEs

- We used schemes like Forward Euler:

$$\frac{T^{n+1} - T^n}{\Delta t} \approx f(T^n, t^n)$$

This approximates $\frac{dT}{dt}$ using temperature values at two different *time points* (t^n and t^{n+1}) separated by Δt .

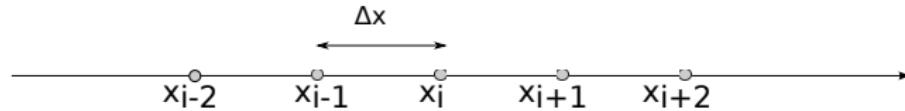
- The core idea was to replace the continuous derivative with a ratio of finite differences in time.
- The scheme above is explicit, because f is computed at time n .

From Time Derivatives to Spatial Derivatives

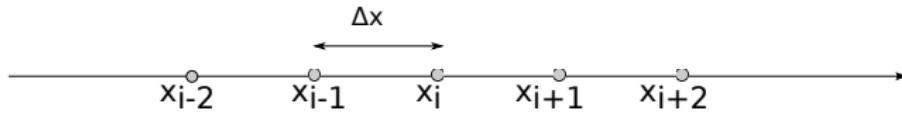
Now, for **Partial Differential Equations (PDEs)**, such as the Heat Equation $\left(\frac{\partial T}{\partial t} = \kappa \frac{\partial^2 T}{\partial x^2}\right)$, we have partial derivatives with respect to **both time AND space**.

- We still need to approximate the time derivative $\frac{\partial T}{\partial t}$ (and we can often use similar ideas, like Forward Euler, for this part).
- Crucially, we now also need to approximate **spatial derivatives** like $\frac{\partial T}{\partial x}$ (first derivative) or $\frac{\partial^2 T}{\partial x^2}$ (second derivative).

The approach will be analogous: we will replace continuous spatial derivatives with ratios of finite differences using function values at discrete *spatial grid points* (x_i, x_{i+1}, x_{i-1} , etc.) separated by Δx .



Second Derivative Approximation: Central Difference



- Consider values of a function $T(x)$ at discrete points: $T_i = T(x_i)$.
- The second derivative at point x_i is approximated as:

$$\left. \frac{\partial^2 T}{\partial x^2} \right|_{x_i} \approx \frac{T_{i+1} - 2T_i + T_{i-1}}{\Delta x^2}$$

- This is called the **central difference** approximation.
- It has **second-order accuracy** (error $\mathcal{O}(\Delta x^2)$).

Deriving the Central Difference for $\frac{\partial^2 T}{\partial x^2}$ (1/2)

To approximate the second spatial derivative, $\frac{\partial^2 T}{\partial x^2}$, we use Taylor series expansions. Consider the function $T(x)$.

Let $T_i = T(x_i)$, $T_{i+1} = T(x_i + \Delta x)$, and $T_{i-1} = T(x_i - \Delta x)$. The Taylor expansions around x_i for T_{i+1} and T_{i-1} are:

1. For T_{i+1} (expanding forward from x_i by Δx):

$$T_{i+1} = T_i + \Delta x \frac{\partial T}{\partial x} \Big|_i + \frac{\Delta x^2}{2!} \frac{\partial^2 T}{\partial x^2} \Big|_i + \frac{\Delta x^3}{3!} \frac{\partial^3 T}{\partial x^3} \Big|_i + \mathcal{O}(\Delta x^4)$$

2. For T_{i-1} (expanding backward from x_i by Δx):

$$T_{i-1} = T_i - \Delta x \frac{\partial T}{\partial x} \Big|_i + \frac{\Delta x^2}{2!} \frac{\partial^2 T}{\partial x^2} \Big|_i - \frac{\Delta x^3}{3!} \frac{\partial^3 T}{\partial x^3} \Big|_i + \mathcal{O}(\Delta x^4)$$

(Here, $|_i$ denotes evaluation at x_i .)

Deriving the Central Difference for $\frac{\partial^2 T}{\partial x^2}$ (2/2)

Recall the Taylor expansions:

$$(Eq.1) : \quad T_{i+1} = T_i + \Delta x \frac{\partial T}{\partial x} \Big|_i + \frac{\Delta x^2}{2} \frac{\partial^2 T}{\partial x^2} \Big|_i + \frac{\Delta x^3}{6} \frac{\partial^3 T}{\partial x^3} \Big|_i + \dots$$

$$(Eq.2) : \quad T_{i-1} = T_i - \Delta x \frac{\partial T}{\partial x} \Big|_i + \frac{\Delta x^2}{2} \frac{\partial^2 T}{\partial x^2} \Big|_i - \frac{\Delta x^3}{6} \frac{\partial^3 T}{\partial x^3} \Big|_i + \dots$$

Now, add Equation 1 and Equation 2:

$$\begin{aligned} T_{i+1} + T_{i-1} &= (T_i + T_i) + (\Delta x - \Delta x) \frac{\partial T}{\partial x} \Big|_i \\ &\quad + \left(\frac{\Delta x^2}{2} + \frac{\Delta x^2}{2} \right) \frac{\partial^2 T}{\partial x^2} \Big|_i \\ &\quad + \left(\frac{\Delta x^3}{6} - \frac{\Delta x^3}{6} \right) \frac{\partial^3 T}{\partial x^3} \Big|_i + O(\Delta x^4) \end{aligned}$$

Deriving the Central Difference for $\frac{\partial^2 T}{\partial x^2}$ (2/2)

This simplifies to:

$$T_{i+1} + T_{i-1} = 2T_i + \Delta x^2 \frac{\partial^2 T}{\partial x^2} \Big|_i + \mathcal{O}(\Delta x^4)$$

Rearranging for $\frac{\partial^2 T}{\partial x^2} \Big|_i$ and neglecting terms of $\mathcal{O}(\Delta x^4)$ and higher (which become part of the truncation error):

$$\frac{\partial^2 T}{\partial x^2} \Big|_i \approx \frac{T_{i+1} - 2T_i + T_{i-1}}{\Delta x^2}$$

This approximation has a truncation error of $\mathcal{O}(\Delta x^2)$.

Discretizing Both Space and Time for PDEs

So far, we have focused on approximating spatial derivatives like $\frac{\partial^2 T}{\partial x^2}$ at a generic point x_i . However, our temperature T in the Heat Equation $\left(\frac{\partial T}{\partial t} = \kappa \frac{\partial^2 T}{\partial x^2} \right)$ is a function of **both space x and time t** , i.e., $T(x, t)$.

To solve this PDE numerically, we need to discretize **both** independent variables:

- **Spatial Discretization:** We divide our spatial domain (e.g., a 1D rod of length L) into a finite number of grid points x_i , where $i = 0, 1, 2, \dots, N_x$. The spacing between points is Δx .
- **Temporal Discretization:** We advance the solution in discrete time steps t^n , where $n = 0, 1, 2, \dots$. The duration of each time step is Δt .

Introducing the Notation T_i^n : We will denote the approximate numerical solution for temperature as:

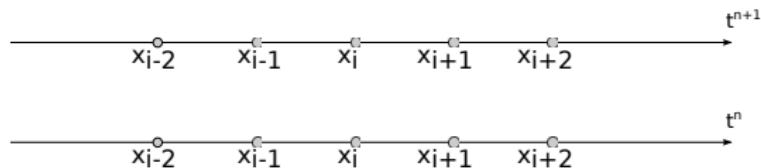
$$T_i^n \approx T(x_i, t^n)$$

Discretizing Both Space and Time for PDEs

This means:

- T_i^n is the temperature at spatial grid point x_i and at the time step t^n .
- T_i^{n+1} is the temperature at spatial grid point x_i and at the time step t^{n+1} .

Our goal is to find a formula to calculate T_i^{n+1} (temperature at all points i at the next time step $n + 1$) using values from time step n , i.e. the values T_0^n, \dots, T_{-1}^n .



Above we used a Pythonic indexing, with 0 for the first index and -1 for the last one.

Applying This to the Heat Equation

- The heat (diffusion) equation in 1D:

$$\frac{\partial T}{\partial t} = \kappa \frac{\partial^2 T}{\partial x^2}$$

- Time derivative: use forward Euler (as in Lesson 1)
- Space derivative: use central difference (just introduced)

$$\frac{T_i^{n+1} - T_i^n}{\Delta t} = \kappa \frac{T_{i+1}^n - 2T_i^n + T_{i-1}^n}{\Delta x^2}$$

- Gives a full update formula for each node:

$$T_i^{n+1} = T_i^n + \kappa \frac{\Delta t}{\Delta x^2} (T_{i+1}^n - 2T_i^n + T_{i-1}^n)$$

or

$$T_i^{n+1} = T_i^n + \alpha (T_{i+1}^n - 2T_i^n + T_{i-1}^n), \quad \alpha = \kappa \frac{\Delta t}{\Delta x^2}$$

What Does This Mean Physically?

$$T_i^{n+1} = T_i^n + \alpha(T_{i+1}^n - 2T_i^n + T_{i-1}^n), \quad \alpha = \kappa \frac{\Delta t}{\Delta x^2}$$

- The temperature at a point updates based on its neighbors.
- Heat Flow from Neighbors:
 - The term $\alpha(T_{i-1}^n - T_i^n)$ represents (proportional to) the heat flowing toward point i from point $i - 1$. If $T_{i-1}^n > T_i^n$, this term is positive, contributing to heating T_i .
 - The term $\alpha(T_{i+1}^n - T_i^n)$ represents (proportional to) the heat flowing toward point i from point $i + 1$. If $T_{i+1}^n > T_i^n$, this term is positive, also heating T_i .
 - Combining these (as done in the $T_{i+1}^n - 2T_i^n + T_{i-1}^n$ form) effectively calculates the net heat gain/loss for point i due to its neighbors.
- The scheme explicitly models how temperature differences between adjacent points drive heat transfer, causing temperatures to **diffuse and smooth out** over time.

Outline

1 Introduction to PDEs

- From ODEs to PDEs

2 Physics of fluids and conservation laws

- The continuum hypothesis
- Conservation laws
- Eulerian and Lagrangian description

3 Governing equations

- Mass equation
- Heat equation

4 Boundary Conditions

5 Numerical discretization

- Finite differences

6 Python implementation

Numerical Exercise: 1D Heat Diffusion in Python

We will simulate the 1D Heat Equation $\frac{\partial T}{\partial t} = \kappa \frac{\partial^2 T}{\partial x^2}$ in Python using finite differences.

We will use:

- Forward Euler in time
- Central difference in space

We simulate temperature diffusion along a rod or a vertical lava flow profile.

Problem Domain and Discretization:

- Length of domain: $L = 1.0$ m
- Number of spatial grid points: $N_x = 51$ (giving $\Delta x = L/(N_x - 1)$)
- Thermal diffusivity: e.g., $\kappa = 1 \times 10^{-6}$ m²/s

Numerical Exercise Setup: 1D Heat Diffusion

Scenario 1: Dirichlet-Dirichlet Boundary Conditions

- Initial Condition ($t = 0$): A hot pulse in the center.

$$T(x, 0) = \begin{cases} 100^\circ C & \text{if } 0.4L \leq x \leq 0.6L \\ 20^\circ C & \text{elsewhere} \end{cases}$$

- Boundary Conditions (for $t > 0$): Fixed temperatures at both ends.
 - At $x = 0$: $T(0, t) = 20^\circ C$
 - At $x = L$: $T(L, t) = 20^\circ C$
- Simulation End Time (t_{final}): We will choose a t_{final} (e.g., 100,000 s) sufficient to observe significant diffusion. The time step Δt will be chosen to satisfy stability ($\alpha \leq 0.5$).

Later in the notebook, we will explore a second scenario with a Neumann boundary condition.

Numerical Scheme: Update Formula

Before looking at the notebook, let's have a look at the explicit numerical scheme we will use, and let's try to understand if the scheme is conditionally or unconditionally stable.

At each interior point i :

$$T_i^{n+1} = T_i^n + \kappa \frac{\Delta t}{\Delta x^2} (T_{i+1}^n - 2T_i^n + T_{i-1}^n)$$

- This updates the temperature using the heat from neighbors.
- Works well if the time step satisfies a stability condition:

$$\Delta t \leq \frac{\Delta x^2}{2\kappa}$$

Stability of the Numerical Scheme for Heat Equation

We have the update formula for the 1D heat equation (FTCS scheme):

$$T_i^{n+1} = T_i^n + \alpha (T_{i+1}^n - 2T_i^n + T_{i-1}^n)$$

where $\alpha = \kappa \frac{\Delta t}{\Delta x^2}$ is a crucial dimensionless parameter, often called the **Courant number for diffusion** or numerical diffusivity.

A Key Question: Will this scheme always produce a physically reasonable and stable solution for any choice of Δt and Δx ? The answer is **NO**.

Explicit schemes like this often have *stability conditions*.

The FTCS Stability Condition

For the Explicit Forward-Time Central-Space (FTCS) scheme for the 1D heat equation, the solution remains stable and physically meaningful only if:

$$\alpha = \kappa \frac{\Delta t}{\Delta x^2} \leq \frac{1}{2}$$

This can be rewritten as a condition on the time step Δt :

$$\Delta t \leq \frac{\Delta x^2}{2\kappa}$$

What does this mean intuitively (without formal proof)?

- **Information Propagation:** The scheme calculates T_i^{n+1} based on its neighbors at time t^n . The condition ensures that "information" (heat) does not try to diffuse "too far" in a single time step relative to the grid spacing.

The FTCS Stability Condition

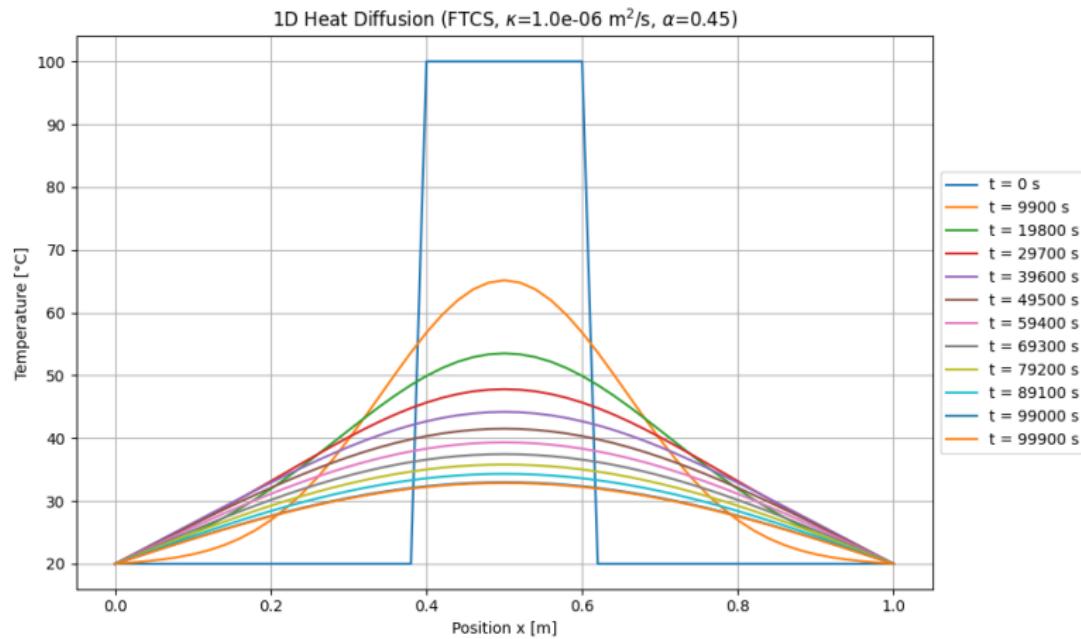
- **Preventing Oscillations:** If Δt is too large (i.e., $\alpha > 1/2$), the term T_i^n in the update formula can become negative if its neighbors are very different. This can lead to unphysical oscillations that grow and destroy the solution.
 - Consider rewriting the update as:
$$T_i^{n+1} = \alpha T_{i+1}^n + (1 - 2\alpha) T_i^n + \alpha T_{i-1}^n.$$
 - If $(1 - 2\alpha) < 0$ (i.e., $\alpha > 1/2$), T_i^{n+1} can become "anti-correlated" with T_i^n , leading to oscillations. For stability, we want all coefficients of T^n terms to be non-negative.
- **Practical Implication:** For finer spatial grids (smaller Δx), you must use a much smaller time step (Δt decreases with Δx^2). This can make explicit schemes computationally expensive for high-resolution simulations.

We will test this in the Python exercise!

Dirichlet Boundary condition

Stable solution

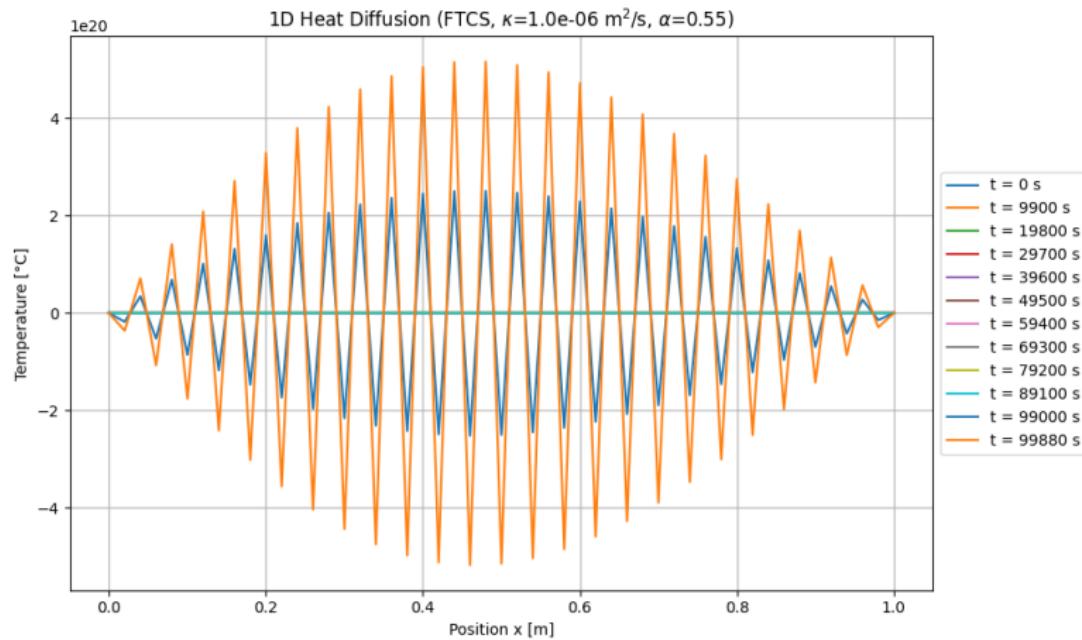
$$\alpha = 0.45$$



Dirichlet Boundary condition

Unstable solution

$$\alpha = 0.55$$



Numerical Exercise: Scenario 2 - Neumann BC

Now, let's modify the setup in the Jupyter Notebook to explore a different boundary condition.

Scenario 2: Neumann (Zero-Flux) at Left, Dirichlet at Right

- Spatial Domain and κ : Same as Scenario 1.
- Initial Condition ($t = 0$): Hot pulse near the left boundary.

$$T(x, 0) = \begin{cases} 100^\circ C & \text{if } 0 \leq x \leq 0.2L \\ 20^\circ C & \text{elsewhere} \end{cases}$$

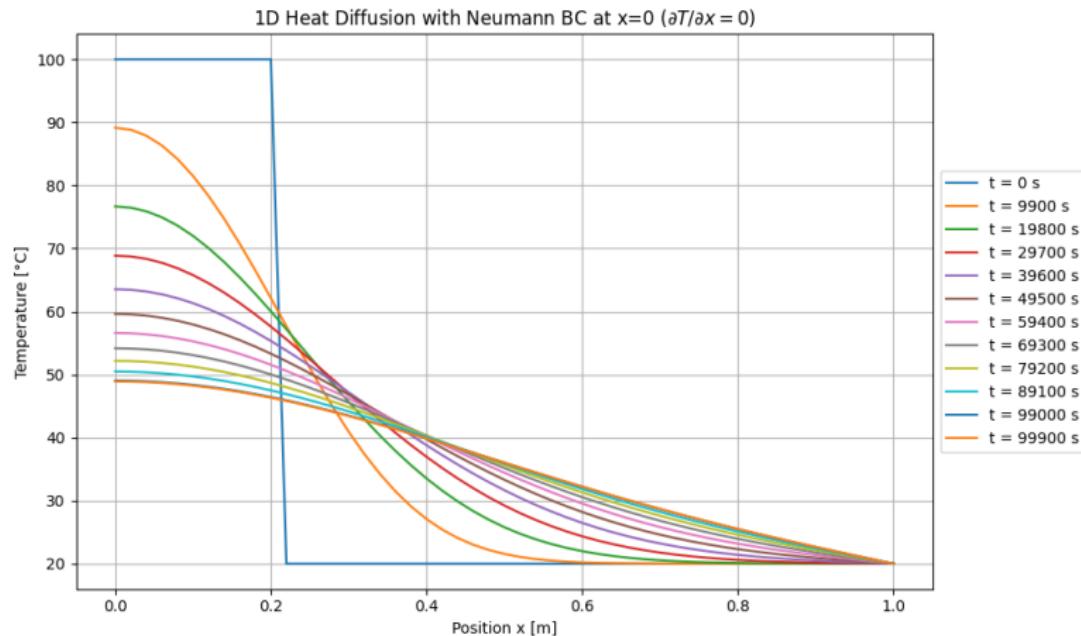
- Boundary Conditions (for $t > 0$):
 - At $x = 0$: Zero-flux (Neumann condition): $\left. \frac{\partial T}{\partial x} \right|_{x=0} = 0$
 - At $x = L$: Fixed temperature (Dirichlet): $T(L, t) = 20^\circ C$
- Simulation End Time (t_{final}) and Δt : Similar to Scenario 1, ensuring stability.

This setup models an insulated left boundary or a plane of symmetry at $x = 0$.

Neumann/Dirichlet Boundary condition

Stable solution

$$\alpha = 0.45$$



Numerical Exploration in Jupyter Notebook: Key Takeaways (1/3)

In the accompanying Jupyter Notebook, we implemented the 1D Heat Equation:

$$\frac{\partial T}{\partial t} = \kappa \frac{\partial^2 T}{\partial x^2}$$

using an explicit Forward-Time Central-Space (FTCS) numerical scheme:

$$T_i^{n+1} = T_i^n + \alpha(T_{i+1}^n - 2T_i^n + T_{i-1}^n), \quad \text{with } \alpha = \kappa \frac{\Delta t}{\Delta x^2}$$

Experiments with Dirichlet Boundary Conditions (T fixed at ends):

- Varying Thermal Diffusivity (κ):
 - Higher $\kappa \Rightarrow$ faster diffusion, quicker smoothing of the initial pulse.
 - Lower $\kappa \Rightarrow$ slower diffusion.
- Varying Spatial Discretization (Δx via N_x):
 - Smaller Δx (more points) \Rightarrow potentially smoother solution, but requires much smaller Δt for stability (since $\Delta t \propto \Delta x^2$).

Numerical Exploration in Jupyter Notebook: Key Takeaways (2/3)

- **Testing Stability Condition ($\alpha \leq 0.5$):**
 - If $\alpha > 0.5$, the numerical solution becomes unstable, showing unphysical oscillations that grow exponentially. This highlights the conditional stability of the explicit FTCS scheme.
- **Initial and Boundary Temperature Values:** Changing these directly alters the problem being solved and the resulting temperature evolution (e.g., diffusion towards a non-uniform steady state if boundary temperatures differ).

Implementing Neumann Boundary Conditions (Zero-Flux): We modified the problem to have a zero-flux (insulation/symmetry) condition at one boundary ($x = 0$):

$$\left. \frac{\partial T}{\partial x} \right|_{x=0} = 0$$

Numerical Exploration in Jupyter Notebook: Key Takeaways (3/3)

This was implemented numerically using a "ghost point" concept, leading to an update for the boundary node T_0^{n+1} :

$$T_0^{n+1} = T_0^n + 2\alpha(T_1^n - T_0^n)$$

- **Effect Observed:** The temperature profile near the $x = 0$ boundary became flat (zero gradient), as expected for an insulated or symmetry boundary. Heat did not escape through this boundary, causing the temperature near it to behave differently than with a fixed (Dirichlet) temperature.
- This demonstrated how different physical boundary conditions translate into different numerical implementations at the boundary nodes.