Partial Differential Equations

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The Seven Golden Rules of Numerical Modeling

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Golden Rule 3. Numerical modelling consists of solving partial differential equations (PDEs).
There are only a few equations to learn. They are generally not complicated, but it is essential to learn and understand them gradually and properly.

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Functions of More Than One Coordinate

Almost all processes relevant in geosciences are described by variables varying in time and space. The spatial component is a scalar in case of a one-dimensional description and a vector in case of a two- or three-dimensional description.

Examples:

- $T(\vec{x}, t)$ as the temperature
- $\rho(\vec{x}, t)$ as the density in a gas
- $p(\vec{x}, t)$ as the fluid pressure in a reservoir
- $\vec{v}(\vec{x}, t)$ as the flow velocity in a fluid
- $P(\vec{x}, t)$ and $Q(\vec{x}, t)$ as the population densities of prey and predators

Spatial Interactions

Spatial interactions often refer to the spatial variation in the variables.

- Heat conduction is driven by spatial differences in temperature; in direction of ______ temperature.
- Fluid flow is driven by spatial differences in pressure; acceleration in direction of ______ pressure.
- Prey may preferably move in direction of
  ______ prey population and
  ______ predator population.
- Predators may preferably move in direction of
  ______ prey population and
  ______ predator population.

Partial Derivatives

- If a function u depends on more than one coordinate, e. g., $u(x_1, x_2, x_3, t)$ $(= u(\vec{x}, t))$, the derivative with respect to one of the coordinates (while the others are constant) is called partial derivative.
- Partial derivatives are written with the symbol ∂, e. g.,

$$\frac{\partial}{\partial x_1} u(\vec{x}, t), \ \frac{\partial}{\partial x_2} u(\vec{x}, t), \ \frac{\partial}{\partial x_3} u(\vec{x}, t), \text{ and } \frac{\partial}{\partial t} u(\vec{x}, t).$$

Examples of Partial Derivatives

1D harmonic wave

$$u(x,t) = A\sin(\omega t - kx) \quad \text{with} \quad \begin{aligned} A &= \text{amplitude} \\ \omega &= \text{angular frequency} \\ k &= \text{wave number} \end{aligned}$$

$$\frac{\partial}{\partial x}u(x,t) = $$

$$\frac{\partial}{\partial t}u(x,t) = $$

Examples of Partial Derivatives

Density of an ideal gas

$$\rho(p, T) = \frac{M}{R}\frac{p}{T} \quad \text{with} \quad \begin{aligned} M &= \text{molar mass} \\ R &= \text{gas constant} \end{aligned}$$

$$\frac{\partial}{\partial p}\rho(p, T) = $$

$$\frac{\partial}{\partial T}\rho(p, T) = $$

The Gradient

The partial derivatives with respect to the spatial coordinates are often subsumed in a vector

$$\text{grad}(u(\vec{x},t)) = \nabla u(\vec{x},t) = \begin{pmatrix} \frac{\partial}{\partial x_1} u(\vec{x},t) \\ \frac{\partial}{\partial x_2} u(\vec{x},t) \\ \frac{\partial}{\partial x_3} u(\vec{x},t) \end{pmatrix}$$

Examples:

$$H(x_1, x_2) = x_1^2 - x_2^2, \quad \nabla H(x_1, x_2) = \begin{pmatrix} \\ \end{pmatrix}$$

$$H(x_1, x_2) = x_1\, x_2, \quad \nabla H(x_1, x_2) = \begin{pmatrix} \\ \end{pmatrix}$$

Properties of the Gradient

- $\nabla u(\vec{x})$ is ______ to the lines (in 2D) or the surfaces (in 3D) where $u(\vec{x})$ is constant.
- $\nabla u(\vec{x})$ points in direction of ______ in $u(\vec{x})$.
- The length of $\nabla u(\vec{x})$ is the slope of $u(\vec{x})$ in direction of ______.

What Is a Partial Differential Equation?

Ordinary differential equation (ODE): equation for an unknown function only one variable involving derivatives

Partial differential equation (PDE): equation for an unknown function depending on more than one coordinate involving partial derivatives

Several definitions are the same for ODEs and PDEs:

- Order
- Systems of differential equations
- Initial conditions
- Fixed points

Geologists in Numerical Modeling

. . . popular 'myths' among geologists, who often declare (or think) something like:

Numerical modelling is very complicated; it is too difficult for people with a traditional geological background and should be performed by mathematicians.

I used to think like that before I started. I always remember my feeling when I heard for the first time the expression, 'Navier–Stokes equation'. 'Ok, forget it! This is hopeless,' I thought at that time, and that was wrong.

Examples of Partial Differential Equations

The Navier-Stokes Equations of a Viscous Fluid

$$\rho\left(\frac{\partial}{\partial t}\vec{v} + v_1\frac{\partial}{\partial x_1}\vec{v} + v_2\frac{\partial}{\partial x_2}\vec{v} + v_3\frac{\partial}{\partial x_3}\vec{v}\right)$$
$$= \rho\,\vec{g} - \nabla p + \eta\left(\frac{\partial^2}{\partial x_1^2}\vec{v} + \frac{\partial^2}{\partial x_2^2}\vec{v} + \frac{\partial^2}{\partial x_3^2}\vec{v}\right)$$

where

$$\begin{aligned} \vec{v}(\vec{x}, t) &= \text{velocity} \\ p(\vec{x}, t) &= \text{pressure} \end{aligned}$$

The 1D Advection Equation

$$\frac{\partial}{\partial t}u(x,t) \;=\; -\,v\,\frac{\partial}{\partial x}u(x,t)$$

General solution with the initial condition

$$u(x,0) \;=\; u_0(x)$$

where $u_0(x)$ is a given function:

$$u(x,t) \;=\; u_0(x-vt)$$

Treatment of the Time Coordinate

The procedure is basically the same as for the time in ordinary differential equations:

- If second-order derivatives occur, the first-order derivatives must be introduced as separate variables.
- Approximate solutions are computed step by step (in steps of length δt), starting from the initial time t_0.
- The time derivative is approximated by

$$\frac{\partial}{\partial t} u(\vec{x}, t) \approx \frac{u(\vec{x}, t + \delta t) - u(\vec{x}, t)}{\delta t}.$$

- All schemes (explicit and fully implicit Euler, mixed, e. g., Crank-Nicholson) can be used.

The Finite-Difference Method in One Dimension

One-dimensional case: only one spatial coordinate x (and time)

First step:

- Discrete points $x_1, x_2, \ldots, x_n$ are defined on the considered part of the x-axis (from the left-hand boundary to the right-hand boundary).
- These points are called nodes and are the points where an approximate solution will be computed.
- The nodes may be equidistant (having all the same distance δx), but spacing may also be non-uniform.

The Finite-Difference Method in One Dimension

Second step: The partial derivatives $\frac{\partial}{\partial x} u(x,t)$ are approximated by difference quotients.

Right-handed difference quotient:

$$\frac{\partial}{\partial x} u(x,t) \approx \frac{u(x+\delta x, t) - u(x,t)}{\delta x}$$

Left-handed difference quotient:

$$\frac{\partial}{\partial x} u(x,t) \approx \frac{u(x,t) - u(x-\delta x, t)}{\delta x}$$

The Finite-Difference Method in One Dimension

Central (symmetric) difference quotients:

$$
\begin{aligned}
\frac{\partial}{\partial x} u(x,t) &\approx \frac{u(x+\delta x,t) - u(x-\delta x,t)}{2\delta x} \\
\frac{\partial}{\partial x} u(x,t) &\approx \frac{u(x+\frac{\delta x}{2},t) - u(x-\frac{\delta x}{2},t)}{\delta x} \\
\frac{\partial}{\partial x} u(x+\tfrac{\delta x}{2},t) &\approx \frac{u(x+\delta x,t) - u(x,t)}{\delta x} \\
\frac{\partial}{\partial x} u(x-\tfrac{\delta x}{2},t) &\approx \frac{u(x,t) - u(x-\delta x,t)}{\delta x}
\end{aligned}
$$

Only the first version can be applied directly, the others are only useful for combining them to second-order derivatives.

The Finite-Difference Method in One Dimension

- The accuracy of all these difference quotients decreases with increasing δx.
- As long as there is no preferred direction, right-hand and left-hand difference quotients are equivalent.
- Central difference quotients provide a higher accuracy than the one sided versions.

Balance Equations

General Concept

Rate of change of the amount contained in a given volume

=

Amount per time entering at the boundaries

-

Amount per time leaving at the boundaries

+

Amount per time produced within the volume

-

Amount per time consumed within the volume

Density and Flux Density

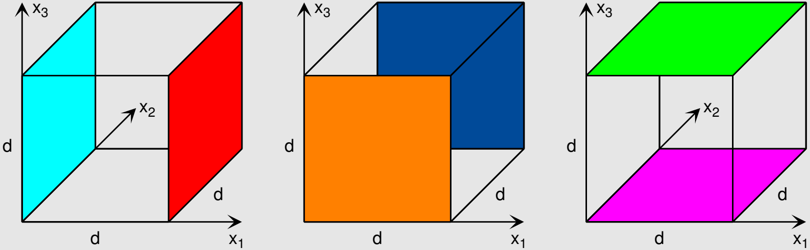
Density $u(\vec{x}, t)$ = amount per volume

Flux density $\vec{q}(\vec{x}, t)$ = amount passing a surface per time and surface area

$\vec{q}$ is a vector, so that the amount per time passing a (small) surface of size A with a unit normal vector $\vec{n}$ is $\vec{q} \cdot \vec{n} A$.

The Equation of Continuity

Balance of the amount contained in a cube:



$$\frac{\partial u}{\partial t} d^3 \quad = \quad q_1 d^2 - q_1 d^2 + q_2 d^2 - q_2 d^2 + q_3 d^2 - q_3 d^2 + Q\, d^3$$

where Q = rate of production (amount per time and volume)

Balance Equations

The Equation of Continuity

$$\frac{\partial}{\partial t} u(\vec{x}, t) = -\operatorname{div}(\vec{q}(\vec{x}, t)) + Q(\vec{x}, t)$$

where

$$\begin{aligned}\operatorname{div}(\vec{q}(\vec{x}, t)) &= \frac{\partial}{\partial x_1} q_1(\vec{x}, t) + \frac{\partial}{\partial x_2} q_2(\vec{x}, t) + \frac{\partial}{\partial x_3} q_3(\vec{x}, t) \\ &= \text{divergence of the flux density } \vec{q}\end{aligned}$$

Fundamental Transport Mechanisms

Advection

Assume that the considered amount moves at a given velocity $\vec{v}(\vec{x}, t)$:

$$\vec{q}(\vec{x}, t) \;=\; u(\vec{x}, t)\,\vec{v}(\vec{x}, t)$$

$$\Downarrow$$

$$\frac{\partial}{\partial t} u(\vec{x}, t) \;=\; -\operatorname{div}\left(u(\vec{x}, t)\,\vec{v}(\vec{x}, t)\right) + Q(\vec{x}, t)$$

In 1D:

$$\frac{\partial}{\partial t} u(x, t) \;=\; -\frac{\partial}{\partial x}\left(u(x, t)\, v(x, t)\right) + Q(x, t)$$

The equation of advection is of first order in both time and space (hyperbolic differential equation).

Advection

Simplest version of the equation of advection:
$\vec{v}(\vec{x}, t) = \text{const.}, \; Q(\vec{x}, t) = 0$:

$$\frac{\partial}{\partial t} u(\vec{x}, t) \; = \; -\vec{v} \cdot \nabla u(\vec{x}, t)$$

In 1D:

$$\frac{\partial}{\partial t} u(x, t) \; = \; -v \frac{\partial}{\partial x} u(x, t)$$

Diffusion

- Flux follows the direction of steepest descent of the density $u(\vec{x}, t)$.
- Flux density is proportional to the decrease of density per length.

$$\Downarrow$$

$$\vec{q}(\vec{x}, t) = -D\,\nabla u(\vec{x}, t) = -D \begin{pmatrix} \frac{\partial}{\partial x_1} u(\vec{x}, t) \\ \frac{\partial}{\partial x_2} u(\vec{x}, t) \\ \frac{\partial}{\partial x_3} u(\vec{x}, t) \end{pmatrix}$$

where

D = diffusivity (coefficient of diffusion) $[\quad]$

Diffusion

Insert the flux density into the equation of continuity:

$$\begin{aligned} \frac{\partial}{\partial t} u(\vec{x}, t) &= -\operatorname{div}\left(\vec{q}(\vec{x}, t)\right) + Q(\vec{x}, t) \\ &= \operatorname{div}\left(D \nabla u(\vec{x}, t)\right) + Q(\vec{x}, t) \end{aligned}$$

In 1D:

$$\frac{\partial}{\partial t} u(x, t) = \frac{\partial}{\partial x}\left(D \frac{\partial}{\partial x} u(x, t)\right) + Q(x, t)$$

The diffusion equation is of first order in time and of second order in space (parabolic differential equation).

Fundamental Transport Mechanisms

Diffusion

Simplest version: $D = \text{const.}$, $Q(\vec{x}, t) = 0$:

$$\begin{aligned}
\frac{\partial}{\partial t} u(\vec{x}, t) &= D \operatorname{div}\left(\nabla u(\vec{x}, t)\right) \\
&= D \left(\frac{\partial^2}{\partial x_1^2} u(\vec{x}, t) + \frac{\partial^2}{\partial x_2^2} u(\vec{x}, t) + \frac{\partial^2}{\partial x_3^2} u(\vec{x}, t) \right) \\
&= D \, \Delta u(\vec{x}, t)
\end{aligned}$$

where $\Delta = \frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} + \frac{\partial^2}{\partial x_3^2}$ is the Laplace operator.

In 1D:

$$\frac{\partial}{\partial t} u(x, t) = D \frac{\partial^2}{\partial x^2} u(x, t)$$

Initial Conditions and Boundary Conditions

- Time is distinct from the spatial coordinates as it is directed.
- For a unique solution, partial differential equations require

  Initial conditions: The solution for all points $\vec{x}$ of the domain at a time t_0 must be given.

  Boundary conditions: The solution (or, e. g., its derivatives) must be given at (least at a part of) the boundary of the domain for all times $t > t_0$.