Partial Differential Equations

Stefan Hergarten

Institut für Geo- und Umweltnaturwissenschaften
Albert-Ludwigs-Universität Freiburg

Functions of More Than One Variable

- 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
  $p(\vec{x}, t)$ as the fluid pressure in a reservoir
  $\rho(\vec{x}, t)$ as the density in a gas
  $\vec{v}(\vec{x}, t)$ as the flow velocity in a fluid

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

  Examples:

  Heat conduction is driven by spatial differences in temperature.
  Fluid flow is driven by spatial differences in pressure.

Partial Derivatives

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

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

- Partial derivatives are computed by assuming that the other variables are constant.

Examples of Partial Derivatives

- Density of an ideal gas

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

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

- One-dimensional harmonic wave

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

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

The Gradient

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

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

Examples:

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

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

Fundamentals

Properties of the Gradient

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

What Is a Partial Differential Equation?

A partial differential equation (PDE) is an equation for an unknown function depending on more than variable involving partial derivatives.

A differential equation for a function of only one variable is called ordinary differential equation (ODE).

Examples of Partial Differential Equations

The One-Dimensional Advection Equation

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

The Equation of Continuity (mass conservation) in a Fluid

$$\begin{aligned}
\frac{\partial}{\partial t}\rho(\vec{x},t) \quad &= \quad -\mathrm{div}\left(\rho(\vec{x},t)\,\vec{v}(\vec{x},t)\right) \\
&= \quad -\frac{\partial}{\partial x_1}\left(\rho(\vec{x},t)\,v_1(\vec{x},t)\right) - \frac{\partial}{\partial x_2}\left(\rho(\vec{x},t)\,v_2(\vec{x},t)\right) \\
&\qquad -\frac{\partial}{\partial x_3}\left(\rho(\vec{x},t)\,v_3(\vec{x},t)\right)
\end{aligned}$$

The Heat Conduction Equation

Simplest version (1D with constant parameters):

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

General version (3D):

$$\begin{aligned}
\rho c \frac{\partial}{\partial t} T(\vec{x},t) &= \operatorname{div}\left(\lambda \nabla T(\vec{x},t)\right) \\
&= \frac{\partial}{\partial x_1}\left(\lambda \frac{\partial}{\partial x_1} T(\vec{x},t)\right) + \frac{\partial}{\partial x_2}\left(\lambda \frac{\partial}{\partial x_2} T(\vec{x},t)\right) \\
&\quad + \frac{\partial}{\partial x_3}\left(\lambda \frac{\partial}{\partial x_3} T(\vec{x},t)\right)
\end{aligned}$$

Examples of Partial Differential Equations

The Navier-Stokes Equations of a Viscous Fluid (without gravity)

$$\rho\left(\frac{\partial}{\partial t}\vec{v}(\vec{x},t)+\left(\vec{v}(\vec{x},t)\cdot\nabla\right)\vec{v}(\vec{x},t)\right) = -\nabla p(\vec{x},t)+\eta\Delta\vec{v}(\vec{x},t)$$

with

$$\begin{aligned}\left(\vec{v}(\vec{x},t)\cdot\nabla\right)\vec{v}(\vec{x},t) &= v_1(\vec{x},t)\frac{\partial}{\partial x_1}\vec{v}(\vec{x},t)+v_2(\vec{x},t)\frac{\partial}{\partial x_2}\vec{v}(\vec{x},t)\\ &\quad +v_3(\vec{x},t)\frac{\partial}{\partial x_3}\vec{v}(\vec{x},t)\\ \Delta\vec{v}(\vec{x},t) &= \frac{\partial^2}{\partial x_1^2}\vec{v}(\vec{x},t)+\frac{\partial^2}{\partial x_2^2}\vec{v}(\vec{x},t)+\frac{\partial^2}{\partial x_3^2}\vec{v}(\vec{x},t)\end{aligned}$$

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

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

Treatment of the Time Coordinate

- All schemes (explicit and fully implicit Euler, mixed, e. g., Crank-Nicholson) can be used.
- If the explicit Euler scheme is used, the solution $u(\vec{x}, t + \delta t)$ can be directly obtained from $u(\vec{x}, t)$ by computing partial derivatives of $u(\vec{x}, t)$ with respect to the spatial coordinates $\vec{x}$.
- For all implicit schemes, a partial differential equation with respect to the spatial coordinates $\vec{x}$ remains to be solved in each timestep.

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, ..., 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) or not.

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 quotient:

$$\frac{\partial}{\partial x}u(x,t) \approx \frac{u(x+\delta x,t)-u(x-\delta x,t)}{2\delta x}$$

or

$$\frac{\partial}{\partial x}u(x,t) \approx \frac{u(x+\frac{\delta x}{2},t)-u(x-\frac{\delta x}{2},t)}{\delta x}$$

or

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

or

$$\frac{\partial}{\partial x}u(x-\tfrac{\delta x}{2},t) \approx \frac{u(x,t)-u(x-\delta x,t)}{\delta x}$$

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 (mass, energy, ...)

General Concept

Consider the amount of anything that is worth keeping track of (mass, energy, ...) in a volume

rate of change of the amount stored within the 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 removed within the volume

Balance Equations (mass, energy, ...)

Density and Flux Density

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

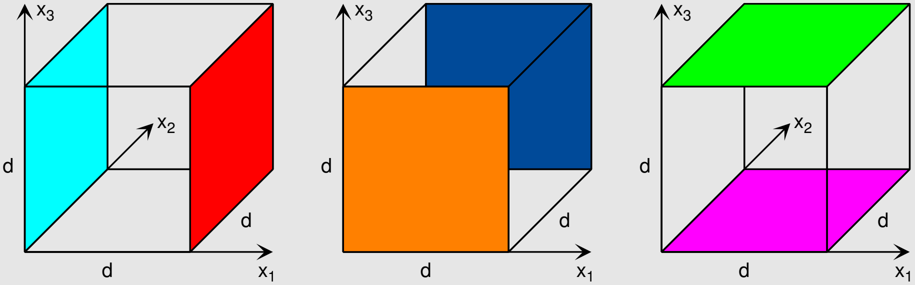
Flux density $\vec{q}(\vec{x}, t) =$ amount passing a surface per time and surface area

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

Balance Equations (mass, energy, . . .)

The Equation of Continuity

Balance of a 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 is the rate of production (amount per time and volume)

Balance Equations (mass, energy, ...)

The General Balance Equation

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

where

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

The Equation of 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:

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

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

The Equation of Advection

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

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

In 1D:

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

Balance Equations (mass, energy, ...)

The Diffusion Equation

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

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

with

$$D \;=\; \text{diffusivity (coefficient of diffusion) } [\tfrac{\mathrm{m}^2}{\mathrm{s}}]$$

The Diffusion Equation

Insert flux density into the balance equation:

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

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).

The Diffusion Equation

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

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

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:

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

Initial Conditions and Boundary Conditions

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

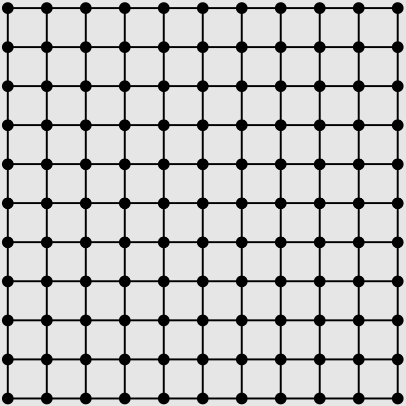
  Initial conditions: The solution for all points $\vec{x}$ of the domain at a time t_0 must be given.

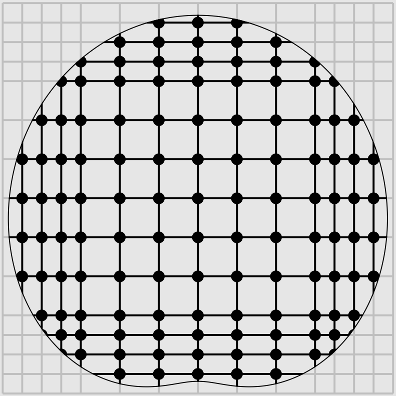
  Boundary conditions: The solution (or, e. g., its derivatives) must be given at (least at a part of) the boundary of the domain for all times $t > t_0$.

The Finite-Difference Method in Two Dimensions

Two-dimensional case: Spatial coordinates x_1 and x_2.

First step: The domain is covered by a lattice where the lines are parallel to the coordinate axes.





The Finite-Difference Method in Two Dimensions

Second step: The partial derivatives $\frac{\partial}{\partial x_1} u(x,t)$ and $\frac{\partial}{\partial x_2} u(x,t)$ are approximated by difference quotients.

Right-handed difference quotients:

$$\begin{aligned} \frac{\partial}{\partial x_1} u(x_1, x_2, t) &\approx \frac{u(x_1 + \delta x, x_2, t) - u(x_1, x_2, t)}{\delta x} \\ \frac{\partial}{\partial x_2} u(x_1, x_2, t) &\approx \frac{u(x_1, x_2 + \delta x, t) - u(x_1, x_2, t)}{\delta x} \end{aligned}$$

Left-handed difference quotients:

$$\begin{aligned} \frac{\partial}{\partial x_1} u(x_1, x_2, t) &\approx \frac{u(x_1, x_2, t) - u(x_1 - \delta x, x_2, t)}{\delta x} \\ \frac{\partial}{\partial x_2} u(x_1, x_2, t) &\approx \frac{u(x_1, x_2, t) - u(x_1, x_2 - \delta x, t)}{\delta x} \end{aligned}$$

The Finite-Difference Method in Two Dimensions

Central difference quotients:

$$
\begin{aligned}
\frac{\partial}{\partial x_1} u(x_1, x_2, t) &\approx \frac{u(x_1 + \delta x, x_2, t) - u(x_1 - \delta x, x_2, t)}{2\delta x} \\
\frac{\partial}{\partial x_1} u(x_1, x_2, t) &\approx \frac{u(x_1 + \frac{\delta x}{2}, x_2, t) - u(x_1 - \frac{\delta x}{2}, x_2, t)}{\delta x} \\
\frac{\partial}{\partial x_2} u(x_1, x_2, t) &\approx \frac{u(x_1, x_2 + \delta x, t) - u(x_1, x_2 - \delta x, t)}{2\delta x} \\
\frac{\partial}{\partial x_2} u(x_1, x_2, t) &\approx \frac{u(x_1, x_2 + \frac{\delta x}{2}, t) - u(x_1, x_2 - \frac{\delta x}{2}, t)}{\delta x}
\end{aligned}
$$

and all other variants discussed in the one-dimensional case

The Energy Balance

$$\frac{\partial}{\partial t}\epsilon(\vec{x}, t) \;=\; -\,\mathrm{div}\vec{q}(\vec{x}, t) + Q(\vec{x}, t)$$

where

$$\begin{aligned}
\epsilon(\vec{x}, t) &= \text{energy density } [\tfrac{\mathrm{J}}{\mathrm{m}^3}] \\
\vec{q}(\vec{x}, t) &= \text{heat flux density } [\tfrac{\mathrm{W}}{\mathrm{m}^2}] \\
Q(\vec{x}, t) &= \text{rate of production of thermal energy per volume } [\tfrac{\mathrm{W}}{\mathrm{m}^3}]
\end{aligned}$$

The Specific Heat Capacity

The specific heat capacity

$$c = \frac{1}{\rho}\frac{\partial \epsilon}{\partial T}$$

describes the change in thermal energy with temperature.

⬇

$$\frac{\partial}{\partial t}\epsilon(\vec{x}, t) = \rho c \frac{\partial}{\partial t} T(\vec{x}, t) = -\operatorname{div}\vec{q}(\vec{x}, t) + Q(\vec{x}, t)$$

Water: $c = 4180 \, \frac{\mathrm{J}}{\mathrm{kg\,K}}$

Rocks: $c = 800\text{–}1000 \, \frac{\mathrm{J}}{\mathrm{kg\,K}}$

The Three Mechanisms of Heat Transport

Heat conduction: Driven by spatial differences in temperature.

Advective transport: Heat is carried by a moving (flowing) medium.

$$\vec{q}(\vec{x},t) \;=\; \epsilon(\vec{x},t)\,\vec{v} \;=\; \rho c\, T(\vec{x},t)\,\vec{v}$$

Radiation: Does not require a medium, but is only significant at very high temperatures.

Fourier's Law of Heat Conduction (1822)

1. Heat flux follows the direction of steepest descent of the temperature field $T(\vec{x}, t)$.
2. The heat flux density is proportional to the decrease of temperature per length.

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

with

$$\lambda \;=\; \text{thermal conductivity } [\tfrac{\mathrm{W}}{\mathrm{m\,K}}]$$

Typical Values of λ

Material	λ $[\frac{W}{m\,K}]$
diamond	2300
iron	80
quartz	1.4
sand	0.6
expanded polystyrene	0.033
water	0.6
air	0.026

Rocks	λ $[\frac{W}{m\,K}]$
granite	2.8
basalt	2
dolomite	2.5
limestone	2.5
sandstone	2.5
shale	2
widely used value	2.5

The Full Heat Equation (conduction, advection, production)

Energy balance + Fourier's law + advective heat flux

$$\Downarrow$$

$$\rho c \, \frac{\partial}{\partial t} T(\vec{x}, t) \;=\; \mathrm{div}\left(\lambda \nabla T(\vec{x}, t) - \rho c T(\vec{x}, t)\vec{v}\right) + Q$$

The Thermal Diffusivity

If ρ, c, and λ are constant (mass balance implies $\operatorname{div}\vec{v} = 0$ then), the heat equation can be simplified to

$$\begin{aligned}\frac{\partial}{\partial t} T(\vec{x}, t) &= \kappa \Delta T(\vec{x}, t) - \vec{v} \cdot \nabla T(\vec{x}, t) + \frac{Q}{\rho c} \\ &= \kappa \left(\frac{\partial^2}{\partial x_1^2} T(\vec{x}, t) + \frac{\partial^2}{\partial x_2^2} T(\vec{x}, t) + \frac{\partial^2}{\partial x_3^2} T(\vec{x}, t) \right) \\ &\qquad - \vec{v} \cdot \nabla T(\vec{x}, t) + \frac{Q}{\rho c}\end{aligned}$$

with the thermal diffusivity

$$\kappa = \frac{\lambda}{\rho c}$$

Water: $\kappa = 1.4 \times 10^{-7} \, \frac{\mathrm{m}^2}{\mathrm{s}}$

Rocks: $\kappa \approx 10^{-6} \, \frac{\mathrm{m}^2}{\mathrm{s}} \approx 30 \, \frac{\mathrm{m}^2}{\mathrm{a}}$

Boundary Conditions

Boundary conditions for a second-order (concerning space) differential equation concern the values or their derivatives (or a combination of both).

Dirichlet boundary conditions define the temperatures at the boundaries:

$$T(\vec{x}, t) = T_b$$

Interpretation: System is coupled to a big reservoir held a a given temperature.

Boundary Conditions

(Von) Neumann boundary conditions define the conductive heat flux density across the boundaries:

$$-\lambda \nabla T(\vec{x}, t) \cdot \vec{n} \;=\; q_b$$

where $\vec{n}$ is the outer unit normal vector on the surface.

In 1D:

$$\pm\lambda \frac{\partial}{\partial x} T(x, t) \;=\; q_b$$

Homogeneous (von) Neumann boundary condition: $q_b = 0$

$$\Downarrow$$

$$\nabla T(\vec{x}, t) \cdot \vec{n} \;=\; 0 \quad (2D/3D), \qquad \frac{\partial}{\partial x} T(x, t) \;=\; 0 \quad (1D)$$

Boundary Conditions

Mixed boundary conditions define a combination of temperature and temperature gradient normal to the surface.

Examples:

- Total (conductive + advective) heat lux density across the boundary is given:

$$(-\lambda \nabla T(\vec{x}, t) + \rho c T(\vec{x}, t)\vec{v}) \cdot \vec{n} \;=\; q_b$$

- Radiating surface (without advection):

$$-\lambda \nabla T(\vec{x}, t) \cdot \vec{n} \;=\; \sigma T(\vec{x}, t)^4$$