Continuous Models 2: PDE

- so far: only time as independent variable
- ODE-based population models sometimes too coarse:
  - population in the USA during California gold rush in the 1850s
  - predictions of the UN concerning world population (industrialized countries versus third world)
- therefore: suppose p(x,t) or p(x,y,t) instead of p(t)
  - California gold rush: 1D sufficient (east-west)
  - world population: perhaps 1D (north-south), perhaps 2D
- taking space into account makes models
  - more accurate (spatial effects are no longer neglected)
  - more complicated (analytical solution becomes harder, numerical solution means a lot of additional work)
- standard example: heat conduction

Modelling with PDE

- taking space into account is typical for many problems or phenomena from physics or continuum mechanics:
  - fluid mechanics: where will we get a tornado?
  - structural mechanics: where will be the crack?
  - process engineering: where is it how hot in the reactor?
  - electromagnetism: where is which electron density?
  - geology: where will the earthquake happen?
- more independent variables entail *partial* derivatives
- we distinguish:
  - *stationary* problems: no time-dependence
  - *unsteady* problems: time-dependence (perhaps, but not necessarily, with a stationary limit for increasing time)

Heat Conduction

- central problem of thermodynamics
- let heat affect an object's boundary – propagation?
  - a wire, heated at one end
  - a metal plate, heated at one side
  - water cooling the reactor in a nuclear power plant
  - a room in winter: where to place the heating
  - a room in summer: effect of direct sunshine
  - boiling water in a pot on a ceramic hob
- central function of interest: temperature T

$$T(x;t) \text{ or } T(x,y;t) \text{ or } T(x,y,z;t)$$

- The values of T will depend on the material and its heat conductivity.

Modelling Heat Conduction 1

- part 1 of the model: the PDE, indicating the relations of changes of T with respect to time and space (3D):

$$\kappa \cdot (T_{xx} + T_{yy} + T_{zz}) = \kappa \cdot \left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2} \right) = \frac{\partial T}{\partial t} = T_t$$

or shortly $\kappa \cdot \Delta T = T_t$ with the Laplace operator Δ

- short derivation (excursion to physics):
  - starting point is the basic principle of energy conservation
  - changes of heat in some part D of our domain are due to flux in/out D's surface and to external sources and drains in D

$$\frac{\partial}{\partial t} \int_D \rho\, cT \mathrm{d}V = \int_D q \,\mathrm{d}V + \int_{\partial D} k \nabla T \cdot \vec{\mathrm{n}}\, \mathrm{d}S$$

  - density ρ, specific heat c, external term q, heat conductivity k, outer normal vector, n volume/surface element dV/dS

Modelling Heat Conduction 2

- derivation of the heat equation (continued):
  - transform the above equation according to Gauß' theorem:

$$\int_D (\rho\, c T_t - q - k\,\Delta T)\,\mathrm{d}V = 0$$

  - This holds for an arbitrary part D of our domain. Hence, the integrand must vanish:

$$T_t = \kappa\,\Delta T + \frac{q}{\rho\, c}, \quad \kappa = \frac{k}{\rho\, c}$$

  - $\kappa > 0$ is called the *thermal diffusion coefficient* (since the Laplace operator stands for a (heat) diffusion process)
  - For vanishing external influence q=0, we get (and, thus, have derived) the famous **heat equation**:

$$T_t = \kappa\,\Delta T$$

Modelling Heat Conduction 3

- part 2 of the model: the PDE needs boundary or initial-boundary conditions to provide a unique solution:
  - **Dirichlet** boundary conditions: fix T on (part of) the boundary

$$T(x,y,z) = \varphi(x,y,z)$$

  - **Neumann** boundary conditions: fix T's normal derivative on (part of) the boundary:

$$\frac{\partial T}{\partial \mathrm{n}}(x,y,z) = \varphi(x,y,z)$$

  - pure Dirichlet and mixtures are allowed, pure Neumann b.c. do not lead to a unique solution (with T solves T+constant the PDE, too)
  - in case of time-dependence: initial conditions for t=0
- in case of no time-dependence: Laplace equation

Modelling Heat Conduction 4

- meaning of boundary conditions:
  - Dirichlet: the temperature T is prescribed itself along (part of) the boundary (some defined heating or cooling)
  - Neumann: the temperature flux through (part of) the boundary is prescribed (if vanishing: complete isolation, no orthogonal transport of heat into or out of the domain
- analytical solutions:
  - In simple (1D) configurations, solutions can be given explicitly via *separation of variables (Fourier's method).* We will discuss these in the exercises.
  - The heat equation is a simple case of a PDE, where general statements concerning existence and uniqueness of solutions are possible. Often, such theorems can not be proven.

Types of PDE

- The heat equation is a *linear PDE of second order:*

$$\sum_{i,j=1}^{d} a_{i,j}(\vec{x}) \cdot u_{x_i,x_j}(\vec{x}) + \sum_{i=1}^{d} a_i(\vec{x}) \cdot u_{x_i}(\vec{x}) + a(\vec{x}) \cdot u(\vec{x}) = f(\vec{x})$$

- three types are distinguished:
  - elliptic PDE: the matrix A of the $a_{i,j}$ is pos. or neg. definite
  - parabolic PDE: one eigenvalue of A is zero, the others have the same sign, and the rank of A together with the vector of the a_i is full (d)
  - hyperbolic PDE: A has 1 pos. and d-1 neg. eigenvalues or vv.
- examples:
  - elliptic: Laplace equation $\Delta u = 0$
  - parabolic: heat equation $\Delta u = u_t$
  - hyperbolic: wave equation $\Delta u = u_{tt}$