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):
  \[ \kappa \cdot \left( T_{xx} + T_{yy} + T_{zz} \right) = \kappa \cdot \left( \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2} \right) = \frac{\partial T}{\partial t} = T, \]
  or shortly $\kappa \cdot \Delta T = T$, with the Laplace operator $\Delta$

- 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
  \[ \frac{\partial}{\partial t} \int_D \rho \, c \, T \, dV = \int_D q \, dV + \int \kappa \nabla T : \vec{n} \, dS \]
  - density $\rho$, specific heat $c$, external term $q$, heat conductivity $k$, outer normal vector $\vec{n}$, volume/surface element $dV/dS$
Modelling Heat Conduction 2

- derivation of the heat equation (continued):
  - transform the above equation according to Gauß' theorem:
    \[ \int_D \left( \rho c T_t - q - k \Delta T \right) dV = 0 \]
  - 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:
    \[ \frac{\partial T}{\partial n}(x, y, z) = \varphi (x, y, z) \]
  - 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 cannot be proven.

Types of PDE

- The heat equation is a linear PDE of second order:
  \[ \sum_{i,j=1}^{d} a_{ij}(x) \cdot u_{i,j}(x) + \sum_{i=1}^{d} a_i(x) \cdot u_i(x) + a(x) \cdot u(x) = f(x) \]

- three types are distinguished:
  - elliptic PDE: the matrix A of the \( a_{ij} \) 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 v v v.

- examples:
  - elliptic: Laplace equation \( \Delta u = 0 \)
  - parabolic: heat equation \( \Delta u = u_t \)
  - hyperbolic: wave equation \( \Delta u = u_{tt} \)