**Part I: Discrete Models**

### Motivation: Heat Transfer

- **objective:** compute the temperature distribution of some object
- under certain prerequisites:
  - temperature at object boundaries given
  - heat sources
  - material parameters
- observation from physical experiments:
  
  \[ q \approx k \cdot \delta T \]

  heat flux proportional to temperature differences

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### A Wiremesh Model

- consider rectangular plate as fine mesh of wires
- compute temperature \( x_{i,j} \) at nodes of the mesh

```
  x_{i,j}
  x_{i+1,j}
  ...
  x_{i,j+1}
```

- model assumption:
  - temperatures in equilibrium at every mesh node
  - equilibrium: steady state (of temperature), energy balance (inflow = outflow) in each node of the mesh
  - incoming temperature fluxes at point \( i,j \) via the four wires:
    - from the left: \( k \cdot \left( x_{i-1,j} - x_{i,j} \right) \)
    - from the right: \( k \cdot \left( x_{i+1,j} - x_{i,j} \right) \)
    - from below: \( k \cdot \left( x_{i,j-1} - x_{i,j} \right) \)
    - from above: \( k \cdot \left( x_{i,j+1} - x_{i,j} \right) \)
  - equation for steady state: sum over all fluxes = zero:
    
    \[ x_{i,j} = \frac{1}{4} \left( x_{i-1,j} + x_{i+1,j} + x_{i,j-1} + x_{i,j+1} \right) \]

  for all temperatures \( x_{i,j} \).

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### A Wiremesh Model (2)

- temperature known at (part of) the boundary; for example
  \[ x_{0,j} = T_j \]

  models a heated/cooled wall with constant temperature \( T_j \) at the left boundary.
- temperature flux known at (part of) the boundary; for example
  \[ x_{i,0} = x_{i,1} \Leftrightarrow x_{i,1} - x_{i,0} = 0 \]

  models an isolated wall at the lower boundary.
- heat sources: temperature given at a certain position \( i,j \):
  \[ x_{i,j} = T_s \]

  task: solve Linear System of Equations

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### A Wiremesh Model (3)

- object: a rectangular metal plate (again)
- model as a collection of small connected rectangular cells

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### A Finite Volume Model

- examine the heat flux across the cell edges
A Finite Volume Model (2)

- model assumption: temperatures in equilibrium in every grid cell
- heat flux across a given edge is proportional to
  - temperature difference \((T_i - T_j)\) between the adjacent cells
  - length \(h\) of the edge
- e.g.: heat flux across the left edge:
  \[
  q_{ij}^{\text{left}} = k_y (T_i - T_{i-1,j}) h_y
  \]
- note: heat flux out of the cell (and \(k_y > 0\))
- heat flux across all edges determines change of heat energy:
  \[
  \frac{d}{dt} \sum_i h_i \frac{\partial T_i}{\partial t} = - \sum_{\text{edges}} k_y \frac{\partial q_y}{\partial T} \frac{\partial T}{\partial t} + \sum_{\text{sources}} F_i
  \]

Towards a Time Dependent Model

- idea: set up an ODE for each cell
- simplification: no external heat sources or sinks, i.e. \(f_i = 0\)
- change of temperature per time is proportional to heat flux \(q_{ij}(t)\) into the cell (no longer 0):
  \[
  \frac{dT_i}{dt} = -c \cdot q_{ij}(t)
  \]
  \[
  \frac{c}{2} \left(-2T_i + T_{i-1,j} + T_{i+1,j} + T_{i,j+1} + T_{i,j-1}\right)
  \]
- solve a system of ODEs

A Steady-State Model

- heat sources: consider additional source term \(F_{ij}\) due to
  - external heating
  - radiation
- \(F_{ij} = f_i h_x h_y (f_i\text{ heat flux per area})\)
- equilibrium with source term requires \(q_{ij} + F_{ij} = 0:\)
  \[
  q_{ij} h_x h_y = -k_y h_y (2T_i - T_{i-1,j} - T_{i+1,j})
  \]
  \[
  -k_y h_y (2T_j - T_{j-1,i} - T_{j+1,i})
  \]
- again, Linear System of Equations

Boundary Conditions

- temperature known in boundary layer cells; for example
  \[
  q_{ij}^{\text{left}} = k_y (T_i - T_{0,j}) h_y = k_y (T_i - T(x_0)) h_y
  \]
  with \(T(x_0)\) not an unknown!
  (models a heated/cooled wall with constant temperature \(T(x_0)\) at the left boundary)
- temperature flux known in boundary layer cells; e.g. \(q_{ij}^{\text{left}} = 0:\)
  \[
  f_i h_x h_y = -k_y h_y (T_i - T_{0,j})
  \]
  \[
  -k_y h_y (2T_j - T_{j-1,i} - T_{j+1,i})
  \]
  models an isolated wall at the left boundary.

Part II: A Continuous Model – The Heat Equation

From Discrete to Continuous

Derivation of the Heat Equation

Variants of the Heat Equation

Boundary and Initial Conditions

Part II

A Continuous Model – The Heat Equation

From Discrete to Continuous (2)

- replace \(k_y\) by \(k/h_y\), \(k_x\) by \(k/h_x\), and get:
  \[
  f_i = \frac{k}{h_x} (2T_i - T_{i-1,j} - T_{i+1,j})
  \]
  \[
  \frac{k}{h_y} (2T_j - T_{j-1,i} - T_{j+1,i})
  \]
- consider arbitrarily small cells: \(h_x, h_y \to 0:\)
  \[
  f_i = -k \left( \frac{\partial^2 T}{\partial x^2} \right)_{ij} - k \left( \frac{\partial^2 T}{\partial y^2} \right)_{ij}
  \]
- leads to a partial differential equation (PDE):
  \[
  -k \left( \frac{\partial^2 T(x,y)}{\partial x^2} + \frac{\partial^2 T(x,y)}{\partial y^2} \right) = f(x,y)
  \]
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Derivation of the Heat Equation

- finite volume model, but with arbitrary control volume $D$
- change of heat energy (per time) is a result of
  - transfer of heat energy across $D$'s surface,
  - heat sources and sinks in $D$ (external influences)
- resulting integral equation:
  \[
  \frac{\partial}{\partial t} \int_D \rho c T \, dV = \int_D q \, dV + \int_{\partial D} k \nabla T \cdot \vec{n} \, dS
  \]
- density $\rho$, specific heat $c$, and heat conductivity $k$ are material parameters
- heat sources and sinks are modelled in term $q$

Derivation of the Heat Equation (2)

- according to theorem of Gauß:
  \[
  \int_{\partial D} k \nabla T \cdot \vec{n} \, dS = \int_D k \Delta T \, dV
  \]
- leads to integral equation for any domain $D$:
  \[
  \int_D \rho c T_1 - q - k \Delta T \, dV = 0
  \]
- hence, the integrand has to be identically 0:
  \[
  T_1 = \kappa \Delta T + \frac{q}{\rho c} \quad \kappa := \frac{k}{\rho c}
  \]
- $\kappa > 0$ is called the thermal diffusion coefficient (since the Laplace operator models a (heat) diffusion process)

Variants of the Heat Equation

Different scenarios:
- vanishing external influence, $q = 0$:
  \[
  T_1 = \kappa \Delta T
  \]
- alternative notation
  \[
  \frac{\partial T}{\partial t} = \kappa \left( \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2} \right)
  \]
- equilibrium solution, $T_1 = 0$:
  \[
  0 = \kappa \Delta T + \frac{q}{\rho c} \implies -\Delta T = \frac{q}{\kappa \rho c}
  \]

“Poisson’s Equation”

Boundary Conditions

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:
  \[
  \frac{\partial T}{\partial n}(x, y, z) = \varphi(x, y, z)
  \]
- special case: insulation
  \[
  \frac{\partial T}{\partial n}(x, y, z) = 0
  \]

Part III: Discretization: Finite Difference and Finite Volume Methods

Part III

Discretization: Finite Difference and Finite Volume Methods

From Continuous Back To Discrete Models

Continuous Models:
- result from a limit process ($h \to 0$) from discrete model (wire mesh, finite volume)
- opposite route $\to$ discretisation

Discretisation methods:
- Finite Differences:
  “replace derivative by difference quotients”
- Finite Volumes:
  compute fluxes on boundary of control volumes and examine conservation laws

The Model Problem

- 2D Poisson Equation:
  \[
  \frac{\partial^2}{\partial x^2} u(x, y) + \frac{\partial^2}{\partial y^2} u(x, y) = f(x, y)
  \]
  on the unit square $\Omega = (0, 1)^2$
- with Dirichlet boundary conditions:
  \[
  u(x, y) = g(x, y) \quad \text{on } \partial \Omega
  \]
Finite Difference Discretisation

- replace partial derivative (at each mesh point) by difference quotient:
  \[ \frac{\partial^2 u}{\partial x^2}(x_i, y_j) \approx \frac{u(x_{i+1}, y_j) - 2u(x_i, y_j) + u(x_{i-1}, y_j)}{h_x^2} \]
  \[ \frac{\partial^2 u}{\partial y^2}(x_i, y_j) \approx \frac{u(x_{i}, y_{j+1}) - 2u(x_i, y_j) + u(x_{i}, y_{j-1})}{h_y^2} \]

- leads to Linear System of Equations (\( h := h_x = h_y \)):
  \[ \frac{1}{h_x^2}(u_{i+1,j} + u_{i,j+1} - 4u_{i,j}) + u_{i,j-1} = f(x_i, y_j) \quad x_j \in (0, 1]^2 \]
  \[ u(x_i) = g(x_i) \quad x_i \in \partial \Omega \]

Resulting Linear System of Equations

- matrix-vector notation of the system:
  \[ A_h x_0 = f_0 \]
- \( x_0 \) a vector of all unknowns \( u \)
- requires numbering of the unknowns
- using row-wise numbering, e.g.:
  \[ x_0 = (u_1, \ldots, u_{1,n}, u_{2,1}, \ldots, u_{2,n}, \ldots, u_{n,1}, \ldots, u_{n,n}) \]

Resulting Linear System of Equations (2)

- \( A_0 \) is a sparse matrix (only 5 diagonals are non-zero)
- \( A_0 \) is block-tridiagonal:
  \[ A_0 = \begin{pmatrix} B_h & I \\ \vdots & \ddots & \ddots \\ I & \vdots & B_h \end{pmatrix} \]
  \[ B_h = \text{tridiag}(1, -4, 1), \text{ where } I \text{ is the unit matrix} \]

Meshes for Finite Difference Discretisation

- regular, Cartesian mesh; analogous to the wire-mesh model:

- compute approximate value of \( u \) for each mesh point:
  \[ u_i \approx u(x_i) \quad u_{jk} \approx u(x_{jk}) \]

Finite Volume Method – Meshes

- domain \( \Omega \) subdivided into grid cells/elements \( \Omega_{ij} \):

- \( u \) constant in \( \Omega_{ij} \), i.e., \( u(x, y) = u_{ij} \)

Finite Volume Discretisation

- integrate over grid cells \( \Omega_{ij} \):
  \[ \int_{\Omega_{ij}} \frac{\partial^2 u}{\partial x^2}(x, y) \, dx \, dy = \frac{1}{h_x^2} \left[ 1 \begin{array}{c} 1 \\ -2 \\ 1 \end{array} \right] \]
  \[ \int_{\Omega_{ij}} \frac{\partial^2 u}{\partial y^2}(x, y) \, dx \, dy = \frac{1}{h_y^2} \left[ 1 \begin{array}{c} 1 \\ -4 \\ 1 \end{array} \right] \]

- integration by parts:
  \[ \int_{\Omega_{ij}} \frac{\partial u}{\partial x}(x, y) \, dx \, dy = \int_{y_i,j} \left[ \frac{\partial u}{\partial x}(x, y) \right]_{y_i,j}^{y_{i+1},j} \, dy \]
  \[ \int_{\Omega_{ij}} \frac{\partial u}{\partial y}(x, y) \, dx \, dy = \int_{x_i,j} \left[ \frac{\partial u}{\partial y}(x, y) \right]_{x_i,j}^{x_{i+1},j} \, dx \]

Finite Volume Discretisation (2)

- remember: \( u \) constant in \( \Omega_{ij} \), i.e., \( u(x, y) = u_{ij} \)
- thus approximation of derivatives on edges:
  \[ \frac{\partial u}{\partial x}_{i,j} = \frac{u_{i+1,j} - u_{i,j}}{h_x} \quad \frac{\partial u}{\partial x}_{i,j} = \frac{u_{i,j} - u_{i,j-1}}{h_x} \]
  \[ \frac{\partial u}{\partial y}_{i,j} = \frac{u_{i+1,j} - u_{i,j}}{h_y} \quad \frac{\partial u}{\partial y}_{i,j} = \frac{u_{i,j} - u_{i,j-1}}{h_y} \]

- again leads to Linear System of Equations:
  \[ \frac{1}{h_x} (u_{i+1,j} - 2u_{i,j} + u_{i,j-1}) h_y + \frac{1}{h_y} (u_{i+1,j} - 2u_{i,j} + u_{i,j+1}) h_x = f_{ij} h_x h_y \]
Finite Volume Discretisation – More General . . .

- typical formulation for first-order PDEs:
  \[
  \iiint \frac{\partial u}{\partial t} \frac{\partial F(u(x,y))}{\partial x} + \frac{\partial G(u(x,y))}{\partial y} \, dx \, dy = \ldots
  \]

- and analogously:
  \[
  \iiint \left[ \frac{\partial F(u(x,y))}{\partial x} \, dx \, dy \right] = \left[ F(u(x,y)) \right]_{x_i - \frac{1}{2}}^{x_i + \frac{1}{2}}
  \]
  \[
  \ddot{\iiint} \left[ \frac{\partial G(u(x,y))}{\partial y} \, dx \, dy \right] = \left[ G(u(x,y)) \right]_{y_j - \frac{1}{2}}^{y_j + \frac{1}{2}}
  \]

- for Poisson Equation: \( F(u) = \frac{\partial^2 u}{\partial x^2} \), etc.