Scientific Computing I

Module 5: Heat Transfer – Discrete and Continuous Models

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Part I: Discrete Models

Part I

Discrete Models

Motivation: Heat Transfer

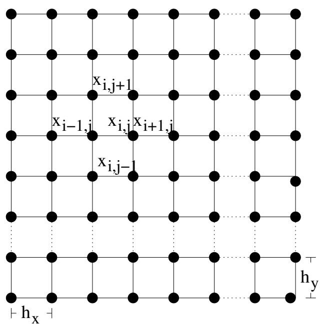
- objective: compute the temperature distribution of some object
- under certain prerequisites:
  - temperature at object boundaries given
  - heat sources
  - material parameters
- observation from physical experiments:

$$q \approx k \cdot \delta T$$

heat flux proportional to temperature differences

A Wiremesh Model

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



A Wiremesh Model (2)

- 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: $k\left(x_{i-1,j} - x_{i,j}\right)$
  - from the right: $k\left(x_{i+1,j} - x_{i,j}\right)$
  - from below: $k\left(x_{i,j-1} - x_{i,j}\right)$
  - from above: $k\left(x_{i,j+1} - x_{i,j}\right)$
- 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 $x_{i,j}$.

A Wiremesh Model (3)

- 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

$$x_{i,0} = x_{i,1} \quad \Leftrightarrow \quad x_{i,1} - x_{i,0} = 0$$

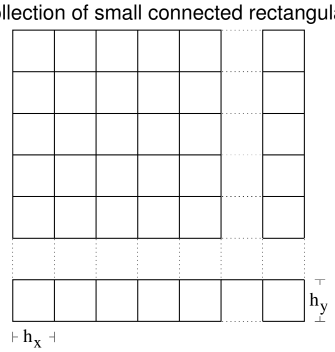
  models an isolated wall at the lower boundary.
- heat sources: temperature given at a certain position i, j:

$$x_{i,j} = T_s.$$

- task: solve Linear System of Equations

A Finite Volume Model

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



- 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 $(T_1 - T_0)$ between the adjacent cells
  - length h of the edge
- e.g.: heat flux across the left edge:

$$q_{i,j}^{(\text{left})} = k_x \left(T_{i,j} - T_{i-1,j}\right) h_y$$

  note: heat flux **out of** the cell (and $k_x > 0$)
- heat flux across all edges determines change of heat energy:

$$\begin{aligned} q_{ij} &= k_x \left(T_{ij} - T_{i-1,j}\right) h_y + k_x \left(T_{ij} - T_{i+1,j}\right) h_y \\ &+ k_y \left(T_{ij} - T_{i,j-1}\right) h_x + k_y \left(T_{ij} - T_{i,j+1}\right) h_x \end{aligned}$$

A Steady-State Model

- heat sources: consider additional source term $F_{i,j}$ due to
  - external heating
  - radiation
- $F_{i,j} = f_{i,j} h_x h_y$ ($f_{i,j}$ heat flux per area)
- equilibrium with source term requires $q_{i,j} + F_{i,j} = 0$:

$$\begin{aligned} f_{i,j} h_x h_y &= -k_x h_y \left(2T_{i,j} - T_{i-1,j} - T_{i+1,j}\right) \\ & \quad -k_y h_x \left(2T_{i,j} - T_{i,j-1} - T_{i,j+1}\right) \end{aligned}$$

- again, Linear System of Equations

Towards a Time Dependent Model

- idea: set up an ODE for each cell
- simplification: no external heat sources or sinks, i.e. $f_{i,j} = 0$
- change of temperature per time is proportional to heat flux $q_{i,j}(t)$ into the cell (no longer 0):

$$\begin{aligned} \frac{d}{dt} T_{i,j}(t) &= -c \cdot q_{i,j}(t) \\ &= \frac{\kappa_x}{h_x} \left(-2T_{ij}(t) + T_{i-1,j}(t) + T_{i+1,j}(t)\right) \\ &+ \frac{\kappa_y}{h_y} \left(-2T_{ij}(t) + T_{i,j-1}(t) + T_{i,j+1}(t)\right) \end{aligned}$$

- solve a system of ODEs

Boundary Conditions

(Finite Volume Models)

- temperature known in boundary layer cells; for example

$$q_{1,j}^{(\text{left})} = k_x \left(T_{1,j} - T_{0,j}\right) h_y = k_x \left(T_{1,j} - T(x_{0,j})\right) h_y$$

  with $T_{0,j} = T(x_{0,j})$ not an unknown!
  (models a heated/cooled wall with constant temperature $T(x_{0,j})$ at the left boundary)
- temperature flux known in boundary layer cells; e.g. $q_{1,j}^{(\text{left})} = 0$:

$$\begin{aligned} f_{1,j} h_x h_y &= -k_x h_y \left(T_{1,j} - T_{2,j}\right) \\ & \quad -k_y h_x \left(2T_{1,j} - T_{1,j-1} - T_{1,j+1}\right) \end{aligned}$$

  models an isolated wall at the left boundary.

Part II: A Continuous Model – The Heat Equation

Part II

A Continuous Model – The Heat Equation

From Discrete to Continuous

- remember the discrete model:

$$\begin{aligned} f_{i,j} &= -\frac{k_x}{h_x} \left(2T_{i,j} - T_{i-1,j} - T_{i+1,j}\right) \\ & \quad -\frac{k_y}{h_y} \left(2T_{i,j} - T_{i,j-1} - T_{i,j+1}\right) \end{aligned}$$

- assumption: heat flux across edges is proportional to temperature *difference*

$$q_{i,j}^{(\text{left})} = k_x \left(T_{i,j} - T_{i-1,j}\right) h_y$$

- in reality: heat flux proportional to temperature *gradient*

$$q_{i,j}^{(\text{left})} \approx k h_y \frac{T_{i,j} - T_{i-1,j}}{h_x}$$

From Discrete to Continuous (2)

- replace k_x by k/h_x, k_y by k/h_y, and get:

$$\begin{aligned} f_{i,j} &= -\frac{k}{h_x^2} \left(2T_{i,j} - T_{i-1,j} - T_{i+1,j}\right) \\ & \quad -\frac{k}{h_y^2} \left(2T_{i,j} - T_{i,j-1} - T_{i,j+1}\right) \end{aligned}$$

- consider arbitrarily small cells: $h_x, h_y \to 0$:

$$f_{i,j} = -k \left(\frac{\partial^2 T}{\partial x^2}\right)_{i,j} - k \left(\frac{\partial^2 T}{\partial y^2}\right)_{i,j}$$

- leads to a *partial differential equation* (PDE):

$$-k \left(\frac{\partial^2 T(x,y)}{\partial x^2} + \frac{\partial^2 T(x,y)}{\partial y^2}\right) = f(x,y)$$

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 ρ, 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:

$$\int_D \rho c T_t - q - k \Delta T\, dV = 0$$

- hence, the integrand has to be identically 0:

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

- $\kappa > 0$ is called the *thermal diffusion coefficient* (since the Laplace operator models a (heat) diffusion process)

Variants of the Heat Equation

Different scenarios:
- vanishing external influence, $q = 0$:

$$T_t = \kappa \Delta T$$

alternative notation

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

- equilibrium solution, $T_t = 0$:

$$0 = \kappa \Delta T + \frac{q}{\rho c} \quad \longrightarrow \quad -\Delta T = \frac{q}{\kappa \rho c}$$

"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

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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:

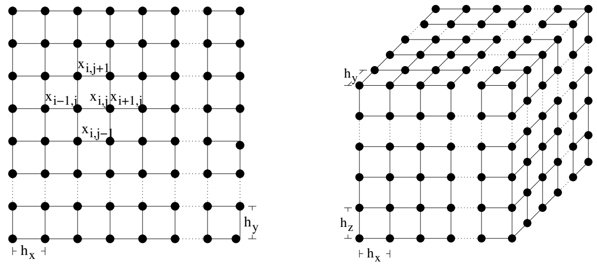
$$\frac{\partial^2}{\partial x^2}u(x,y) + \frac{\partial^2}{\partial y^2}u(x,y) = f(x,y)$$

on the unit square $\Omega = (0,1)^2$
- with Dirichlet boundary conditions:

$$u(x,y) = g(x,y) \qquad \text{on } \partial\Omega$$

Meshes for Finite Difference Discretisation

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



- compute approximate value of u for each mesh point:

$$u_{ij} \approx u(x_{ij}) \qquad u_{ijk} \approx u(x_{ijk})$$

Finite Difference Discretisation

- replace partial derivative (at each mesh point) by difference quotient:

$$\frac{\partial^2 u}{\partial x^2}(x_{i,j}) \approx \frac{u(x_{i+1,j}) - 2u(x_{i,j}) + u(x_{i-1,j})}{h_x^2}$$

$$\frac{\partial^2 u}{\partial y^2}(x_{i,j}) \approx \frac{u(x_{i,j+1}) - 2u(x_{i,j}) + u(x_{i,j-1})}{h_y^2}$$

- leads to Linear System of Equations ($h := h_x = h_y$):

$$\frac{1}{h^2}\left(u_{i+1,j} + u_{i,j+1} - 4u_{i,j} + u_{i,j-1} + u_{i-1,j}\right) = f(x_{i,j}) \quad x_{i,j} \in (0,1)^2$$

$$u(x_{i,j}) = g(x_{i,j}) \quad x_{i,j} \in \partial\Omega$$

Resulting Linear System of Equations

- matrix-vector notation of the system:

$$A_h x_h = f_h$$

- x_h a vector of all unknowns u_{ij}
  $\Rightarrow$ requires *numbering* of the unknowns
- using row-wise numbering, e.g.:
  $x_h = (u_{1,1}, \ldots, u_{1,n}, u_{2,1}, \ldots, u_{2,n}, \ldots, u_{n,1}, \ldots, u_{n,n})$

Resulting Linear System of Equations (2)

- A_h is a sparse matrix (only 5 diagonals are non-zero)
- A_h is block-tridiagonal:

$$A_h = \frac{1}{h^2}\begin{pmatrix} B_h & I & & \\ I & \ddots & \ddots & \\ & \ddots & \ddots & I \\ & & I & B_h \end{pmatrix}$$

- $B_h = \text{tridiag}(1, -4, 1)$, where I is the unit matrix

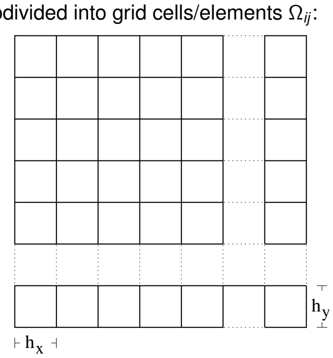
Notation: Discretisation Stencils

- idea: illustrate the matrix structure via a so-called **discretisation stencil**
- represents one row of the matrix
- matrix elements ordered according to their "geometrical" orientation
- discretisation stencil for Poisson equations:

$$\text{1D: } \frac{1}{h^2}\begin{bmatrix} 1 & -2 & 1 \end{bmatrix} \qquad \text{2D: } \frac{1}{h^2}\begin{bmatrix} & 1 & \\ 1 & -4 & 1 \\ & 1 & \end{bmatrix}$$

Finite Volume Methods – Meshes

- domain Ω subdivided into grid cells/elements Ω_{ij}:



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

Finite Volume Discretisation

- integrate over grid cells Ω_{ij}:

$$\int_{\Omega_{ij}} \frac{\partial^2 u}{\partial x^2}(x,y) + \frac{\partial^2 u}{\partial y^2}(x,y)\,dx\,dy = \underbrace{\int_{\Omega_{ij}} f(x,y)\,dx\,dy}_{:= f_{ij} h_x h_y}$$

- integration by parts:

$$\int_{\Omega_{ij}} \frac{\partial^2 u}{\partial x^2}(x,y)\,dx\,dy = \int_{y_{j-\frac{1}{2}}}^{y_{j+\frac{1}{2}}} \left(\frac{\partial u}{\partial x}(x,y)\Big|_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \right) dy$$

$$\int_{\Omega_{ij}} \frac{\partial^2 u}{\partial y^2}(x,y)\,dx\,dy = \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \left(\frac{\partial u}{\partial y}(x,y)\Big|_{y_{j-\frac{1}{2}}}^{y_{j+\frac{1}{2}}} \right) dx$$

Finite Volume Discretisation (2)

- remember: u constant in Ω_{ij}, i.e., $u(x, y) = u_{ij}$
- thus approximation of derivatives on edges:

$$\frac{\partial u}{\partial x}\Big|_{x_{i+\frac{1}{2}}} = \frac{u_{i+1,j} - u_{ij}}{h_x} \qquad \frac{\partial u}{\partial x}\Big|_{x_{i-\frac{1}{2}}} = \frac{u_{ij} - u_{i-1,j}}{h_x}$$

$$\frac{\partial u}{\partial y}\Big|_{y_{j+\frac{1}{2}}} = \frac{u_{i,j+1} - u_{ij}}{h_y} \qquad \frac{\partial u}{\partial y}\Big|_{y_{j-\frac{1}{2}}} = \frac{u_{ij} - u_{i,j-1}}{h_y}$$

- again leads to Linear System of Equations:

$$\frac{1}{h_x}\left(u_{i+1,j} - 2u_{i,j} + u_{i-1,j}\right)h_y + \frac{1}{h_y}\left(u_{i,j+1} - 2u_{i,j} + u_{i,j-1}\right)h_x = f_{ij} h_x h_y$$

Finite Volume Discretisation – More General …

- typical formulation for first-order PDEs:

$$\int_{\Omega_{ij}} \frac{\partial u}{\partial t} + \frac{\partial F(u(x,y))}{\partial x} + \frac{\partial G(u(x,y))}{\partial y}\, \mathrm{dx\,dy} \quad = \quad \ldots$$

- and analogously:

$$\int_{\Omega_{ij}} \frac{\partial F(u(x,y))}{\partial x}\, \mathrm{dx\,dy} \quad = \quad \int_{y_{j-\frac{1}{2}}}^{y_{j+\frac{1}{2}}} F(u(x,y))\Big|_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \mathrm{dy}$$

$$\int_{\Omega_{ij}} \frac{\partial G(u(x,y))}{\partial y}\, \mathrm{dx\,dy} \quad = \quad \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} G(u(x,y))\Big|_{y_{j-\frac{1}{2}}}^{y_{j+\frac{1}{2}}} \mathrm{dx}$$

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