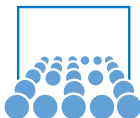


Scientific Computing I

Module 5: Heat Transfer – Discrete and Continuous Models

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Part I: Discrete Models

Motivation: Heat Transfer

Wiremesh Model

A Finite Volume Model

Time Dependent Model

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

Motivation: Heat Transfer

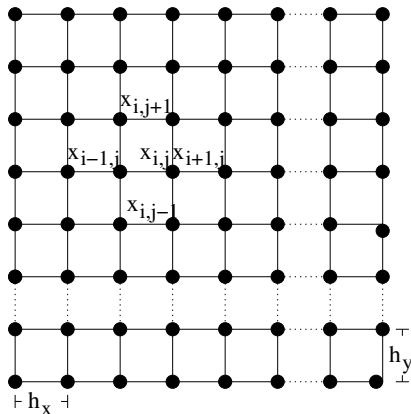
- objective: compute the temperature distribution of some object
- under certain prerequisites:
 - temperature at object boundaries given
 - heat sources
 - material parameters
- observation from physical experiments:

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

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

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- incoming temperature fluxes at point i,j via the four wires:
 - from the left: $k (x_{i-1,j} - x_{i,j})$
 - from the right: $k (x_{i+1,j} - x_{i,j})$
 - from below: $k (x_{i,j-1} - x_{i,j})$
 - from above: $k (x_{i,j+1} - x_{i,j})$

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 - from below: $k (x_{i,j-1} - x_{i,j})$
 - from above: $k (x_{i,j+1} - x_{i,j})$
- equation for steady state: sum over all fluxes = zero:

$$x_{i,j} = \frac{1}{4} (x_{i-1,j} + x_{i+1,j} + x_{i,j-1} + x_{i,j+1})$$

for all temperatures $x_{i,j}$.

A Wiremesh Model (3)

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models a heated/cooled wall with constant temperature T_j at the left boundary.

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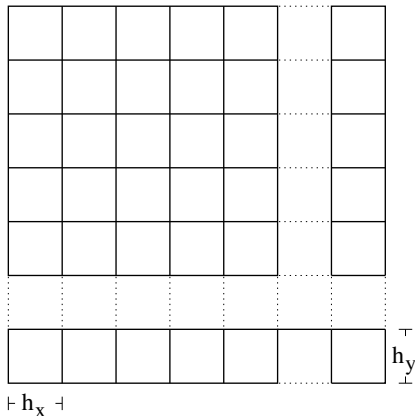
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$$x_{i,j} = T_s.$$

- 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
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note: heat flux **out of** the cell (and $k_x > 0$)

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- heat flux across all edges determines change of heat energy:

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

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 $q_{i,j} + F_{i,j} = 0$:

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

- 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):

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

- solve a system of ODEs

Boundary Conditions

(Finite Volume Models)

- temperature known in boundary layer cells; for example

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

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)

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- temperature flux known in boundary layer cells; e.g. $q_{1,j}^{(\text{left})} = 0$:

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

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

- remember the discrete model:

$$f_{i,j} = -\frac{k_x}{h_x} (2T_{i,j} - T_{i-1,j} - T_{i+1,j}) \\ -\frac{k_y}{h_y} (2T_{i,j} - T_{i,j-1} - T_{i,j+1})$$

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

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

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

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

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

From Discrete to Continuous (2)

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

$$f_{i,j} = -\frac{k}{h_x^2} (2T_{i,j} - T_{i-1,j} - T_{i+1,j}) - \frac{k}{h_y^2} (2T_{i,j} - T_{i,j-1} - T_{i,j+1})$$

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

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

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- 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)

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- 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 :

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

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- 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

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

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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

Finite Difference Methods

- Meshes for Finite Difference Discretisation
- Finite Difference Discretisation
- Resulting Linear System of Equations
- Discretisation Stencils

Finite Volume Methods

- Finite Volume Meshes
- Finite Volume Discretisation

From Continuous Back To Discrete Models

Continuous Models:

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

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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:

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

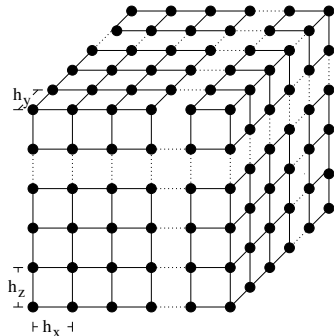
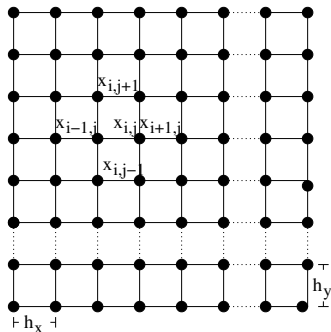
on the unit square $\Omega = (0, 1)^2$

- with Dirichlet boundary conditions:

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

Meshes for Finite Difference Discretisation

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



- compute approximate value of u for each mesh point:

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

Finite Difference Discretisation

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

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

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

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

$$\begin{aligned} \frac{1}{h^2} (u_{i+1,j} + u_{i,j+1} - 4u_{i,j} \\ + u_{i,j-1} + u_{i-1,j}) &= f(x_{i,j}) \quad x_{i,j} \in (0, 1)^2 \\ u(x_{i,j}) &= g(x_{i,j}) \quad x_{i,j} \in \partial\Omega \end{aligned}$$

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}
⇒ requires *numbering* of the unknowns
- using row-wise numbering, e.g.:
 $x_h = (u_{1,1}, \dots, u_{1,n}, u_{2,1}, \dots, u_{2,n}, \dots, u_{n,1}, \dots, u_{n,n})$

Resulting Linear System of Equations (2)

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

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

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

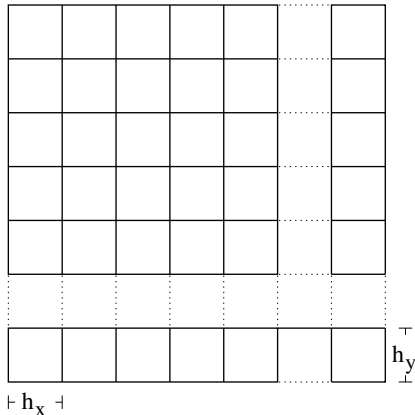
Notation: Discretisation Stencils

- 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:

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

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:

$$\begin{aligned} \left. \frac{\partial u}{\partial x} \right|_{x_{i+\frac{1}{2}}} &= \frac{u_{i+1,j} - u_{ij}}{h_x} & \left. \frac{\partial u}{\partial x} \right|_{x_{i-\frac{1}{2}}} &= \frac{u_{ij} - u_{i-1,j}}{h_x} \\ \left. \frac{\partial u}{\partial y} \right|_{y_{j+\frac{1}{2}}} &= \frac{u_{i,j+1} - u_{ij}}{h_y} & \left. \frac{\partial u}{\partial y} \right|_{y_{j-\frac{1}{2}}} &= \frac{u_{ij} - u_{i,j-1}}{h_y} \end{aligned}$$

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- again leads to Linear System of Equations:

$$\begin{aligned} &\frac{1}{h_x} (u_{i+1,j} - 2u_{i,j} + u_{i-1,j}) h_y \\ &+ \frac{1}{h_y} (u_{i,j+1} - 2u_{i,j} + u_{i,j-1}) h_x = f_{ij} h_x h_y \end{aligned}$$

Finite Volume Discretisation – More General ...

- typical formulation for first-order PDEs:

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

- and analogously:

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

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

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

