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
- 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
  \[ x_{i,0} = x_{i,1} \Leftrightarrow x_{i,1} - x_{i,0} = 0 \]
  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
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:

\[
q^{(\text{left})}_{i,j} = k_x (T_{i,j} - T_{i-1,j}) \, h_y
\]

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

\[
q_{ij} = k_x (T_{ij} - T_{i-1,j}) \, h_y + k_x (T_{ij} - T_{i+1,j}) \, h_y \\
+ k_y (T_{ij} - T_{i,j-1}) \, h_x + k_y (T_{ij} - T_{i,j+1}) \, h_x
\]
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 $q_{i,j} + F_{i,j} = 0$

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

- 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):

\[
\frac{d}{dt} T_{i,j}(t) = -c \cdot q_{i,j}(t)
\]

\[
= \frac{\kappa_x}{h_x} (-2T_{ij}(t) + T_{i-1,j}(t) + T_{i+1,j}(t))
\]

\[
+ \frac{\kappa_y}{h_y} (-2T_{ij}(t) + T_{i,j-1}(t) + T_{i,j+1}(t))
\]

• 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)

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

\[
\begin{align*}
    f_{1,j} h_x h_y &= -k_x h_y (T_{1,j} - T_{2,j}) \\
                    &- k_y h_x (2T_{1,j} - T_{1,j-1} - T_{1,j+1})
\end{align*}
\]

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

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

- in reality: heat flux proportional to temperature gradient

\[
q_{i,j}^{(\text{left})} \approx kh_y \frac{T_{i,j} - T_{i-1,j}}{h_x}
\]
From Discrete to Continuous (2)

• replace \( k_x \) by \( k/h_x \), \( k_y \) by \( k/h_y \), and get:

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

• 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 $\rho$, 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 \( D \):

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

- 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, $T_t = 0$:

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

“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
Part III: Discretization: Finite Difference and Finite Volume Methods

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 \((h \to 0)\) 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:

\[ u(x, y) = g(x, y) \quad \text{on} \ \partial \Omega \]
Meshes for Finite Difference Discretisation

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

\[ u_{ij} \approx u(x_{ij}) \quad u_{ijk} \approx u(x_{ijk}) \]
Finite Difference Discretisation

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

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

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

- 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:

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

- $B_h = \text{tridiag}(1, -4, 1)$, 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:

\[
\begin{align*}
1D: \quad & \frac{1}{h^2} \begin{bmatrix} 1 & -2 & 1 \end{bmatrix} \\
2D: \quad & \frac{1}{h^2} \begin{bmatrix} 1 & 1 \\ 1 & -4 & 1 \end{bmatrix}
\end{align*}
\]
Finite Volume Methods – Meshes

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

- consider **cell averages** $u_{ij}$ for each cell $\Omega_{ij}$, i.e., $u(x, y) \approx u_{ij}$
Finite Volume Discretisation

- integrate over grid cells $\Omega_{ij}$:

$$\int_{\Omega_{ij}} \frac{\partial^2 u}{\partial x^2} (x, y) + \frac{\partial^2 u}{\partial y^2} (x, y) \, dx \, dy = \int_{\Omega_{ij}} f(x, y) \, dx \, dy$$

- integration by parts:

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

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

$$:= f_{ij} h_x h_y$$
Finite Volume Discretisation (2)

- remember: \( u(x, y) = u_{ij} \) in each \( \Omega_{ij} \)
- thus approximation of derivatives on edges:
  \[ \frac{\partial u}{\partial x} \bigg|_{x_i + \frac{1}{2}} \approx \frac{u_{i+1,j} - u_{ij}}{h_x} \]
  \[ \frac{\partial u}{\partial x} \bigg|_{x_i - \frac{1}{2}} \approx \frac{u_{ij} - u_{i-1,j}}{h_x} \]
  \[ \frac{\partial u}{\partial y} \bigg|_{y_j + \frac{1}{2}} \approx \frac{u_{i,j+1} - u_{ij}}{h_y} \]
  \[ \frac{\partial u}{\partial y} \bigg|_{y_j - \frac{1}{2}} \approx \frac{u_{ij} - u_{i,j-1}}{h_y} \]

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

More detailed computation for first term:
\[
\int_{y_j - \frac{1}{2}}^{y_j + \frac{1}{2}} \left( \frac{\partial u}{\partial x}(x, y) \bigg|_{x_i + \frac{1}{2}} \right) \, dy = \int_{y_j - \frac{1}{2}}^{y_j + \frac{1}{2}} \left( \frac{u_{i+1,j} - u_{ij}}{h_x} - \frac{u_{ij} - u_{i-1,j}}{h_x} \right) \, dy = \frac{h_y}{h_x} (u_{i+1,j} - 2u_{ij} + u_{i-1,j})
\]
Finite Volume Discretisation – More General . . .

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

- and analogously:
  \[ \int_{\Omega_{ij}} \frac{\partial F(u(x, y))}{\partial x} \, dx \, dy = \int_{y_{j-\frac{1}{2}}}^{y_{j+\frac{1}{2}}} F(u(x, y)) \bigg|^{x_{i+\frac{1}{2}}}_{x_{i-\frac{1}{2}}} \, dy \]
  \[ \int_{\Omega_{ij}} \frac{\partial G(u(x, y))}{\partial y} \, dx \, dy = \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} G(u(x, y)) \bigg|^{y_{j+\frac{1}{2}}}_{y_{j-\frac{1}{2}}} \, dx \]

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