Algorithms of Scientific Computing

Fast Poisson Solvers

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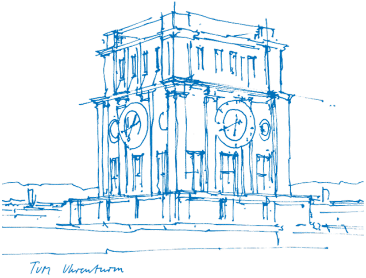


Part I

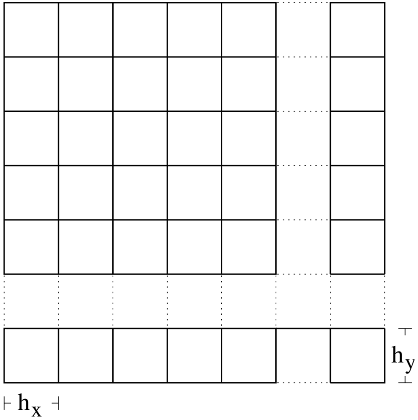
Excursion: Discrete Models for Heat Transfer and the Poisson Equation

Modelling of Heat Transfer

- objective: compute the temperature distribution of some object
- under certain prerequisites:
  - temperature T at object boundaries given
  - heat sources
  - material parameters $k, \dots$
- observation from physical experiments: $q \approx k \cdot \delta T$
  heat flow proportional to temperature differences

A Finite Volume Model

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



- examine the heat flow across the cell edges

Heat Flow Across the Cell Boundaries

- consider temperature T_{ij} in each cell
- Heat flow across a given edge is proportional to
  - temperature difference $\left(T_{ij} - T_{i-1,j}\right)$ between adjacent cells
  - length h of the edge
- e.g.: heat flow across the left edge:

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

  k_x depends on material
- heat flow across all edges determines change of heat energy:

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

Temperature change due to heat flow

- model assumption: conservation of energy, i.e.,

  in equilibrium, total heat flow equal to 0 for each cell

- or: consider additional source term F_{ij} due to
  - external heating
  - radiation
- $F_{ij} = f_{ij} h_x h_y$ (f_{ij} heat flow per area)
- equilibrium with source term requires $q_{ij} + F_{ij} = 0$:

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

Finite Volume Model

- divide by $h_x h_y$:

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

- again, system of linear equations
- how to treat boundaries?
  - prescribe temperature in a cell
    (e.g. boundary layer of cells)
  - prescribe heat flow across an edge;
    for example insulation at left edge:

$$
q_{ij}^{(\mathrm{left})} = 0
$$

From Discrete to Continuous

- system of equations derived from the discrete model:

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

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

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

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

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

From Discrete to Continuous (2)

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

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

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

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

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

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

Part II

Fast Poisson Solvers and the Sine Transform

- situation: solve a system of linear equations

$$-u_{i-1,j} - u_{i+1,j} + 4u_{ij} - u_{i,j-1} - u_{i,j+1} = f_{ij} \qquad \forall i, j$$

- or, simpler, for a 1D problem:

$$-u_{n-1} + 2u_n - u_{n+1} = f_n \quad \text{for } n = 1, \ldots, N-1$$

  with $u_0 = u_N = 0$
- consider very fine meshes, e.g. with 1000×1000 unknowns (in 2D)
- solution can be computed fast, $\mathcal{O}(N)$, in 1D (tri-diagonal system), but hard to solve efficiently in 2D (and even harder in 3D)

Applying the Sine Transform

Idea: apply discrete sine transfrom on u_n and f_n

$$u_n = 2 \sum_{k=1}^{N-1} U_k \sin \frac{\pi nk}{N}, \qquad f_n = 2 \sum_{k=1}^{N-1} F_k \sin \frac{\pi nk}{N} \tag{1}$$

into the system of equations

$$-u_{n-1} + 2u_n - u_{n+1} = f_n \quad \text{for } n = 1, \ldots, N-1$$

Why should that help?

- corresponding continuous problem is $-u''(x) = f(x)$
- is solved by $u(x) = \sin(x)$, if $f(x) = \sin(x)$ (with $u(x) = 0$ at both boundaries)
- sine modes are **eigenvectors** of the system matrix, and **eigenmodes** of the continuous solution

Applying the Sine Transform (2)

We insert the transformations

$$u_n = 2 \sum_{k=1}^{N-1} U_k \sin \frac{\pi nk}{N} \qquad \text{and} \qquad f_n = 2 \sum_{k=1}^{N-1} F_k \sin \frac{\pi nk}{N}$$

into the system of linear equations

$$\begin{aligned} -u_{n+1} + 2u_n - u_{n-1} = f_n \quad \text{for} \quad n = 1, \ldots, N-1 \\ u_0 = u_N = 0, \end{aligned}$$

and get, for $n = 1, \ldots, N-1$:

$$\begin{aligned} -2 \sum_{k=1}^{N-1} U_k \sin \frac{\pi(n+1)k}{N} + 4 \sum_{k=1}^{N-1} U_k \sin \frac{\pi nk}{N} - 2 \sum_{k=1}^{N-1} U_k \sin \frac{\pi(n-1)k}{N} \\ = 2 \sum_{k=1}^{N-1} F_k \sin \frac{\pi nk}{N} \end{aligned}$$

Applying the Sine Transform (3)

Use theorems of addition

$$\sin(A+B) = \sin(A)\cos(B) + \cos(A)\sin(B) \quad \text{and}$$
$$\sin(A-B) = \sin(A)\cos(B) - \cos(A)\sin(B)$$

applied to:

$$\sin\left(\frac{\pi(n+1)k}{N}\right) = \sin\left(\frac{\pi nk}{N} + \frac{\pi k}{N}\right) \quad \text{and}$$
$$\sin\left(\frac{\pi(n-1)k}{N}\right) = \sin\left(\frac{\pi nk}{N} - \frac{\pi k}{N}\right)$$

We have the situation

$$\sin(A+B) + \sin(A-B) = 2\sin(A)\cos(B)$$

or, particularly:

$$\sin\left(\frac{\pi(n+1)k}{N}\right) + \sin\left(\frac{\pi(n-1)k}{N}\right) = 2\sin\left(\frac{\pi nk}{N}\right)\cos\left(\frac{\pi k}{N}\right)$$

Applying the Sine Transform (4)

Use theorems of addition in the left-hand side:

$$-2\sum_{k=1}^{N-1}\left(U_k \sin\frac{\pi(n+1)k}{N} + U_k \sin\frac{\pi(n-1)k}{N}\right) + 4\sum_{k=1}^{N-1} U_k \sin\frac{\pi nk}{N}$$

$$-4\sum_{k=1}^{N-1} U_k \sin\frac{\pi nk}{N}\cos\frac{\pi k}{N} + 4\sum_{k=1}^{N-1} U_k \sin\frac{\pi nk}{N}$$

and obtain simplified system of equations:

$$-4\sum_{k=1}^{N-1} U_k \sin\frac{\pi nk}{N}\cos\frac{\pi k}{N} + 4\sum_{k=1}^{N-1} U_k \sin\frac{\pi nk}{N} = 2\sum_{k=1}^{N-1} F_k \sin\frac{\pi nk}{N}$$

$$\Leftrightarrow 2\sum_{k=1}^{N-1} U_k \sin\frac{\pi nk}{N}\left(1-\cos\frac{\pi k}{N}\right) = \sum_{k=1}^{N-1} F_k \sin\frac{\pi nk}{N}$$

Solution of the System of Equations

We transformed the system of equations into

$$2\sum_{k=1}^{N-1} U_k \sin\frac{\pi nk}{N}\left(1-\cos\frac{\pi k}{N}\right) = \sum_{k=1}^{N-1} F_k \sin\frac{\pi nk}{N}$$

All equations are satisfied, if

$$2U_k\left(1-\cos\frac{\pi k}{N}\right) = F_k \quad \text{for all } k = 1,\ldots,N-1$$

This is true, if we set

$$U_k = \frac{F_k}{2-2\cos\frac{\pi k}{N}} \quad \text{for all } k = 1,\ldots,N-1.$$

Fast Poisson Solver – Algorithm

1. Compute the coefficients F_k by a **Fast Sine Transform**:

$$F_k = \frac{1}{N} \sum_{n=1}^{N-1} f_n \sin \frac{\pi n k}{N}$$

2. Compute all coefficients U_k from the F_k as

$$U_k = \frac{F_k}{2 - 2\cos \frac{\pi k}{N}} \quad \text{for all } k = 1, \ldots, N-1.$$

3. Compute the u_n from the U_k by means of an Inverse **Fast Sine Transform**:

$$u_n = 2 \sum_{k=1}^{N-1} U_k \sin \frac{\pi n k}{N},$$

Fast Poisson Solver – Algorithm (2)

Computational Costs:

- the two Fast Sine Transforms require $\mathcal{O}(N \log N)$ operations
- step 2 needs only $\mathcal{O}(N)$ operations

$\Rightarrow$ **total computational effort is $\mathcal{O}(N \log N)$**

- thus: slower than solving the tridiagonal system of equations directly, which has effort $\mathcal{O}(N)$
- however: pays off in 2D and higher-dimensional settings!
(due to similar complexity)

When can the Algorithm be applied:

- boundary conditions need to be $u_0 = u_N = 0$
(otherwise: different transform required)
- requires rectangular/cuboid domain and Cartesian mesh
- requires uniform material parameters k