Lecture 04 - Finite Differences for Modelling Heat Conduction

June 17, 2025

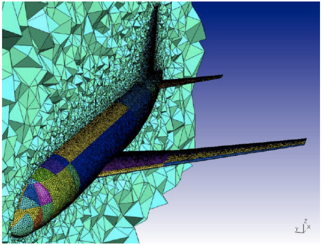
Outline

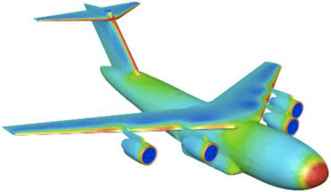
Finite Differences for Modelling Heat Conduction

This lecture covers an application of solving linear systems. Partial differential equations (PDEs) involve multivariable functions and (partial) derivatives. They describe numerous phenomena:

- Electromagnetism,
- Fluid flow,
- Sound propagation,
- Financial problems,
- Solid mechanics (engineering),
- Quantum mechanics,
- . . .

Finite Differences for Modelling Heat Conduction





The numerical solution of PDEs are a common source of sparse linear systems (e.g., finite difference/finite volume/finite element methods). This lecture introduces finite differences for a PDE describing heat conduction.

Finite Differences for Modelling Heat Conduction

Setup:

1. Suppose that we want to approximate the (unknown) **temperature function**, $T(x, y, z)$ (where x, y, z are spatial coordinates) in some 3-D solid object, **at equilibrium** (i.e. T does not vary with respect to time).
2. Suppose further that we have a given (known) **heat source function**, $f(x, y, z)$.

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Then the heat distribution may be modelled using the **Poisson equation**:

$$\begin{aligned} f + \left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2} \right) &\underbrace{=}_{\text{at equilibrium}} 0 \\ \Leftrightarrow -\left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2} \right) &= f \\ \Leftrightarrow -\Delta T &= f. \end{aligned}$$

The differential operator

$$\Delta = \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right)$$

is called the **Laplacian operator**.

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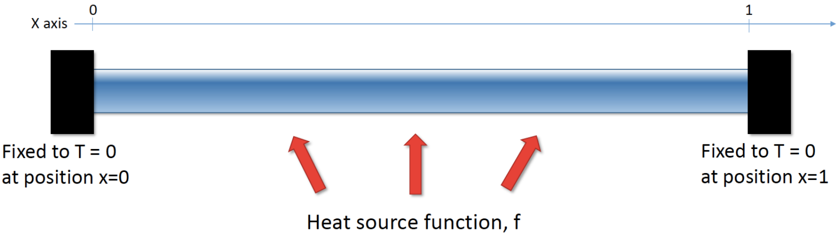
1D Example Boundary conditions are also necessary to fully define the problem. Consider a 1D example where

$$
\begin{aligned}
-\frac{\partial^2 T}{\partial x^2} &= f \quad \text{on } (0,1), && (1)\\
T(0) &= 0, && (2)\\
T(1) &= 0. && (3)
\end{aligned}
$$

Lines (2) and (3) are the boundary conditions. In this case the temperature T is zero at both $x = 0$ and $x = 1$. The figure below shows the domain pictorially.



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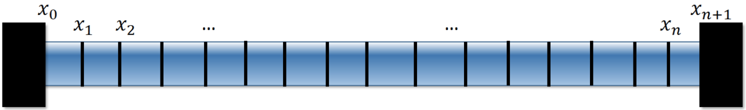
We want to find an approximate numerical solution, given the source f and the boundary temperatures. Our approach here is to first discretize (subdivide) the material into finite subintervals. Then approximate the spatial derivatives with finite differences. **Discretizing** the domain is done by chopping the length of the 1D bar into chunks. That is, define discrete points on the bar $0 = x_0 < x_1 < x_2 < \cdots < x_n < x_{n+1} = 1$, which are referred to as **gridpoints** x_i.



We let T_i denote the numerical approximation of the exact solution $T(x_i)$ for $i = 0, \ldots, n$.

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Here we assume evenly spaced intervals. Define the grid spacing h as

$$\begin{aligned} h = x_i - x_{i-1} &= \frac{1}{n+1}, \\ &= \frac{\text{domain length}}{\#\text{ of intervals}}. \end{aligned}$$

Due to the boundary conditions we know $T_0 = 0$ and $T_{n+1} = 0$. Therefore, the unknowns we must solve for are the n temperature values $T_1, T_2, \ldots, T_n$ (i.e., at non-boundary gridpoints). These gridpoints are referred to as the **active** gridpoints.

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Now that the discrete domain is defined we discretize the partial derivatives. Recall, **finite differences** are one approach to obtain discrete approximations of derivatives. For example,

$$\frac{\partial T}{\partial x}(x_i) \approx \frac{T(x_i) - T(x_{i-1})}{x_i - x_{i-1}} \approx \frac{T_i - T_{i-1}}{h}. \tag{4}$$

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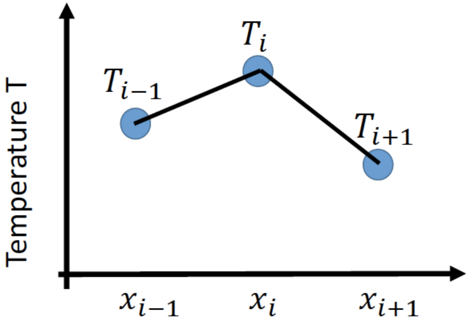
We will use the **centered finite difference** approximation of $\frac{\partial^2 T}{\partial x^2}$, specifically

$$\begin{aligned}\frac{\partial^2 T}{\partial x^2}(x_i) & \\ \approx & \frac{\frac{T_{i+1}-T_i}{h} - \frac{T_i - T_{i-1}}{h}}{h} \\ = & \frac{T_{i+1} - 2T_i + T_{i-1}}{h^2}\end{aligned} \tag{5}$$



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It can be seen from (5), and the above figure, that T_i depends on its neighbours T_{i+1} and T_{i-1}. The resulting relationships between gridpoints determines T_i, for $i = 1, 2, \ldots, n$. Each gridpoint $i = 1, 2, \ldots, n$ gives one equation relating its value to its two neighbours:

$$-\left(\frac{T_{i+1} - 2T_i + T_{i-1}}{h^2}\right) = f_i, \qquad \text{for} \qquad i = 1, \ldots, n. \qquad (6)$$

Equation (6) is our **discrete** equation approximating the **continuous** equation $-\frac{\partial^2 T}{\partial x^2} = f$.
The general form of the matrix equation from (6) is

$$\frac{1}{h^2}\begin{bmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2 & -1 \\ & & & -1 & 2 \end{bmatrix}\begin{bmatrix} T_1 \\ T_2 \\ \vdots \\ T_{n-1} \\ T_n \end{bmatrix} = \begin{bmatrix} f_1 \\ f_2 \\ \vdots \\ f_{n-1} \\ f_n \end{bmatrix}.$$

How The Boundary Conditions Determine The First And Last Rows

$$
\begin{aligned}
f_1 &= -\left(\frac{T_2 - 2T_1 + \underbrace{T_0}_{=0}}{h^2}\right) \\
&= \frac{2T_1 - T_2}{h^2} \\
f_n &= -\left(\frac{\underbrace{T_{n+1}}_{=0} - 2T_n + T_{n-1}}{h^2}\right) \\
&= \frac{-T_{n-1} + 2T_n}{h^2}
\end{aligned}
$$

What can we say about the matrix structure? It is a banded matrix, but more specifically symmetric and tridiagonal.

Finite Differences for Modelling Heat Conduction

Heat Conduction in 2D Plate Consider the 2D domain of a square plate with zero temperature boundaries. We want to determine the heat distribution $T(x, y)$ on the interior given a heat source function $f(x, y)$. Figure 1 shows an example of the 2D plate and a heat distribution for an example f.

Finite Differences for Modelling Heat Conduction

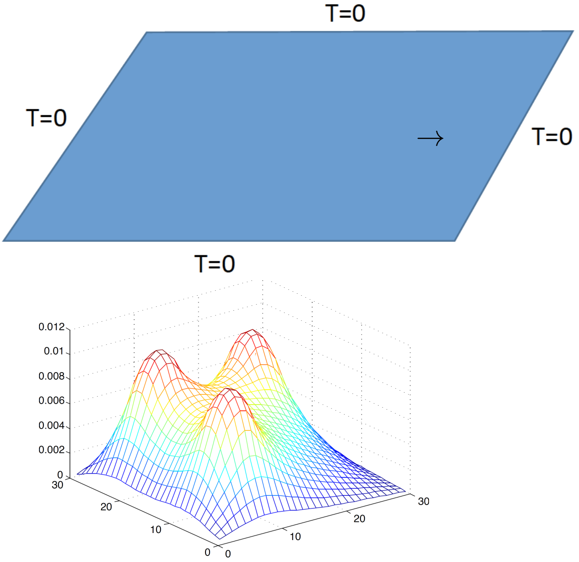

Figure: Two-dimensional plate domain (left) and heat distribution (right).

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Gridpoints are now indexed by i, j so that (x_i, y_j) defines a discrete location on the 2D plate. The inset shows an example grid. The approximate temperature at (x_i, y_j) is denoted $T_{i,j}$ such that $T_{i,j} \approx T(x_i, y_j)$. We now need to approximate the 2D continuous Poisson equation

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

at each gridpoint.

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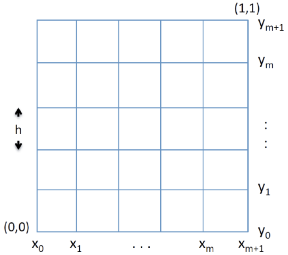
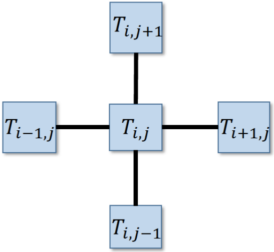
The discrete Poisson equation in 2D is obtained by approximating the 2[nd] derivative in each axis separately, then summing them together. That is,



$$
\begin{aligned}
-\left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2}\right) &= f \\
-\left(\frac{T_{i+1,j} - 2T_{i,j} + T_{i-1,j}}{h^2} + \frac{T_{i,j+1} - 2T_{i,j} + T_{i,j-1}}{h^2}\right) &= f_{i,j} \\
\frac{4T_{i,j} - T_{i-1,j} - T_{i+1,j} - T_{i,j-1} - T_{i,j+1}}{h^2} &= f_{i,j} \quad (7)
\end{aligned}
$$

Finite Differences for Modelling Heat Conduction

The finite difference **stencil** is a convenient visual notation for (7) centered at each gridpoint (see Figure 2). The nonzeros in the stencil will be the nonzeros in a row of the matrix.



$$\rightarrow \begin{bmatrix} 0 & -\frac{1}{h^2} & 0 \\ -\frac{1}{h^2} & +\frac{4}{h^2} & -\frac{1}{h^2} \\ 0 & -\frac{1}{h^2} & 0 \end{bmatrix}$$

Figure: The finite difference stencil for the left hand side of (7), i.e., the **negative** of the 2D discrete Laplacian.

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To put (7) into matrix form we need to "flatten" the indices from 2D (i, j) to 1D (k). The 2D computational domain is indexed from 0 to $m + 1$ in each dimension (see Figure 3 left). Since the boundary values are known to be 0, we only need to solve for unknowns $T_{i,j}$ for all $i, j \in [1, m]$ (a total of m^2 unknowns). How do we index the unknowns into a 1D array? A natural rowwise ordering numbers gridpoints along the x-axis first, then along the y-axis (see Figure 3 right).

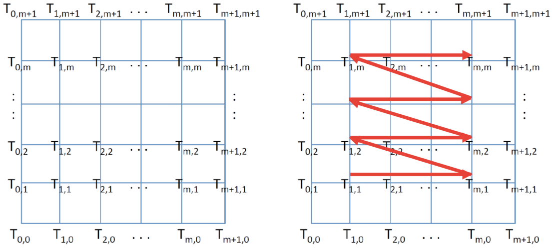

Figure: Two-dimensional indexing (left) for a discrete plate and a possible 1D ordering/flattening (right).

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Specifically,

$$
\begin{aligned}
T_{1,1} &\rightarrow T_1, \\
T_{2,1} &\rightarrow T_2, \\
&\vdots \\
T_{m,1} &\rightarrow T_m, \\
T_{1,2} &\rightarrow T_{m+1}, \\
T_{2,2} &\rightarrow T_{m+2}, \\
&\vdots \\
T_{m,m} &\rightarrow T_{m^2}.
\end{aligned}
$$

That is, we convert from 2D indices (i, j) to 1D indices k using $k = i + (j - 1) \times m$.

Finite Differences for Modelling Heat Conduction

The general form of the Laplacian matrix in 2D with this natural rowwise ordering is given in Figure 4.

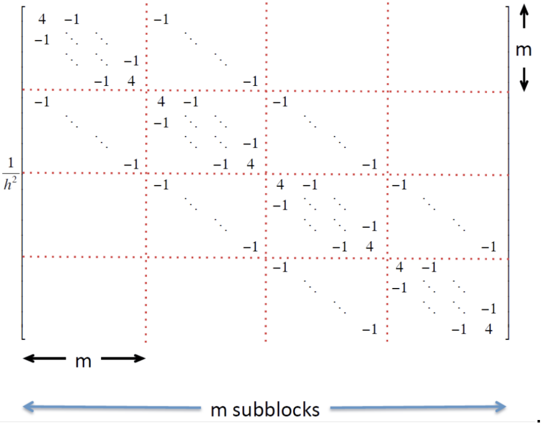

Figure: General matrix structure for discrete Laplacian with natural rowwise ordering.

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Notice that their are 5 bands:

- 1 diagonal band,
- 2 bands immediately above/below the diagonal,
- 2 bands separated horizontally by m entries.

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Explanation:

- Let (i, j) be arbitrary, $1 \leq i \leq m, 1 \leq j \leq m$.
- Consider the equation

$$\frac{1}{h^2}\left(4T_{i,j} - T_{i-1,j} - T_{i+1,j} - T_{i,j-1} - T_{i,j+1}\right) = f_{i,j}.$$

- The 4 coefficient appears on the diagonal, since i, j on the LHS agrees with i, j on the RHS.
- The $-T_{i-1,j}$ term contributes
  - nothing, if $i = 1$, by boundary conditions, and
  - -1 immediately to the left of the diagonal, otherwise.
- The $-T_{i+1,j}$ term contributes
  - nothing, if $i = m$, by boundary conditions, and
  - -1 immediately to the right of the diagonal, otherwise.
- The $-T_{i,j-1}$ term contributes
  - nothing, if $j = 1$, by boundary conditions, and
  - -1, m positions to the left of the diagonal, otherwise.
- The $-T_{i,j+1}$ term contributes
  - nothing, if $j = m$, by boundary conditions, and
  - -1, m positions to the right of the diagonal, otherwise.

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Remarks:

1. The 2-D setup quickly becomes more complicated than the 1-D setup.
2. Adding more dimensions would further increase the complexity.
3. If we relax our assumption about not allowing changes in temperature over time, then we would need to add a time dimension. E.g. adding a time dimension to the 1-D setup would make it 2-D to start. We would have to be careful to clearly define our boundary conditions in this case.

Finite Differences for Modelling Heat Conduction

Other types of PDE problems, discretizations, and geometries give rise to different matrix structures and properties. For example, a triangular mesh can be used with a finite volume discretization to study the flow around an airfoil (see Figure 5).

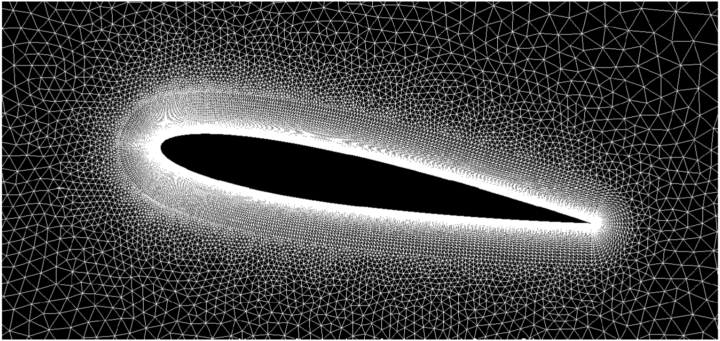

Figure: Example discretization using triangles for an airfoil.

Finite Differences for Modelling Heat Conduction

This lecture only considered modelling heat in an equilibrium using the Poisson equation. The time-dependent heat equation considers non-equilibrium situations, i.e., how temperature evolves over time. The finite difference equations are similar and lead to another linear system to solve.