Two-dimensional heat equation: finite difference, Crank-Nicholson scheme in Matlab®

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1 The heat equation

The heat absorbed by a mass m with specific heat c is proportional to its increase in temperature T. The absorbed heat is proportional to the temperature gradient and thermal conductivity of the material. For a given volume Ω bounded by a closed surface $\partial\Omega$ of density ρ and heat capacity c, we have that the variation of internal energy caused by heat transfer is given by

$$\frac{\partial}{\partial t}\oint_{\Omega} \rho c T \, d\Omega = \oint_{\partial\Omega} \lambda \nabla T \cdot \hat{\boldsymbol{n}} \, d(\partial\Omega)$$

by applying Gauss' theorem at RHS and assuming constant and uniform values of ρ, c and λ across the volume Ω, we get

$$\frac{\partial}{\partial t}\oint_{\Omega} T \, d\Omega = \frac{\lambda}{\rho c}\oint_{\Omega} \nabla^2 T \, d\Omega$$

where $\kappa = \lambda/(\rho c)$ is the volume's heat diffusivity. The heat equation is thus given by

$$\frac{\partial T}{\partial t} = \kappa \nabla^2 T$$

2 Space-time discretization

We discretize the two-dimensional parabolic problem

$$\frac{\partial T}{\partial t} = \kappa \nabla^2 T = \kappa \left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right) \tag{1}$$

with a second-order centered finite difference approximation of the second derivative in space and a Crank-Nicholson scheme for the integration in time. The Crank-Nicholson scheme is an unconditionally stable second-order time integration scheme. A uniform spatial grid is applied to the plate. The boundary nodes are not computed and their value is determined by a constant Dirichlet condition. These will be referred to as *ghost nodes* from now on. There are N^2 internal nodes are computed. We have

$$\begin{aligned}\frac{T_{i,j}^{n+1}-T_{i,j}^{n}}{\Delta t} =& \frac{\kappa}{2}\left(\frac{-T_{i-1,j}^{n+1}+2T_{i,j}^{n+1}-T_{i+1,j}^{n+1}}{\Delta x^2}+\frac{-T_{i-1,j}^{n}+2T_{i,j}^{n}-T_{i+1,j}^{n}}{\Delta x^2}+\right.\\ &\left.+\frac{-T_{i,j-1}^{n+1}+2T_{i,j}^{n+1}-T_{i,j+1}^{n+1}}{\Delta x^2}+\frac{-T_{i,j-1}^{n}+2T_{i,j}^{n}-T_{i,j+1}^{n}}{\Delta x^2}\right)\end{aligned}$$

$$\begin{aligned}\frac{T_{i,j}^{n+1}-T_{i,j}^{n}}{\Delta t} =& \frac{\kappa\Delta t}{2\Delta x^2}\left(-T_{i-1,j}^{n+1}+2T_{i,j}^{n+1}-T_{i+1,j}^{n+1}-T_{i-1,j}^{n}+2T_{i,j}^{n}-T_{i+1,j}^{n}+\right.\\ &\left.-T_{i,j-1}^{n+1}+2T_{i,j}^{n+1}-T_{i,j+1}^{n+1}-T_{i,j-1}^{n}+2T_{i,j}^{n}-T_{i,j+1}^{n}\right)\end{aligned} \tag{2}$$

with Δx and Δt being the grid step and the time step, respectively. We introduce the non-dimensional parameter $\alpha = \dfrac{\kappa\Delta t}{2\Delta x^2}$. By lexicographical ordering, the indices i and j referring to the position of each node may be expressed as the global index k, with $1 \leq k \leq N^2$.

$N(N-1)+1$	$N(N-1)+2$	$\cdots$	N^2-1	N^2
$N(N-2)+1$	$\cdots$	$\cdots$	$\cdots$	$N(N-1)$
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
$N+1$	$N+2$	$\cdots$	$2N-1$	$2N$
1	2	$\cdots$	$N-1$	N

Equation 2 can be rearranged as follows

$$-T_{k-N}^{n+1}-T_{k-1}^{n+1}+\frac{1+4\alpha}{\alpha}T_{k}^{n+1}-T_{k+1}^{n+1}-T_{k+N}^{n+1}=T_{k-N}^{n}+T_{k-1}^{n}+\frac{1-4\alpha}{\alpha}T_{k}^{n}+T_{k+1}^{n}+T_{k+N}^{n}$$

or, in matrix notation (by denoting $\beta_1 = \dfrac{1+4\alpha}{\alpha}$ and $\beta_2 = \dfrac{1-\alpha}{\alpha}$)

$$\underline{\underline{\boldsymbol{A}}}\cdot\underline{\boldsymbol{T}}^{n+1}=\underline{\underline{\boldsymbol{B}}}\cdot\underline{\boldsymbol{T}}^{n} \tag{3}$$

	Node(s)	boundary condition
SW	$k = 1$	$k - N,\ k - 1$
SE	$k = N$	$k - N,\ k + 1$
NW	$k = N(N-1) + 1$	$k + N,\ k - 1$
NE	$k = N^2$	$k + N,\ k + 1$
west	$N + 1 \xrightarrow{N} N(N-2) + 1$	$k - 1$
east	$2N \xrightarrow{N} N(N-1)$	$k + 1$
north	$N(N-1) + 2 \rightarrow N^2 - 1$	$k + N$
south	$2 \rightarrow N - 1$	$k - N$

Table 1: Internal weak nodes and boundary conditions.

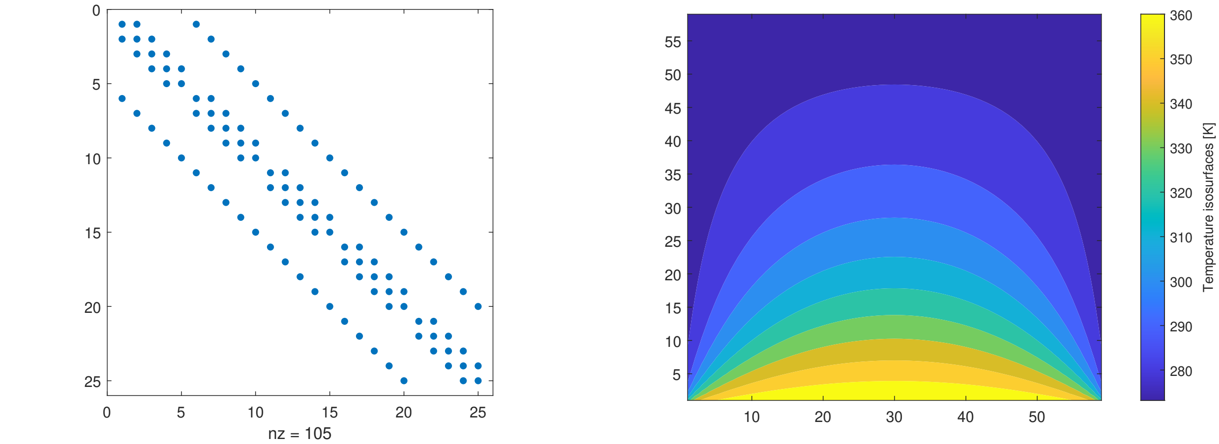
with $\underline{\underline{\boldsymbol{A}}}$ and $\underline{\underline{\boldsymbol{B}}}$ being two sparse pentadiagonal matrices. For instance, $\underline{\underline{\boldsymbol{A}}}$:

$$\underline{\underline{\boldsymbol{A}}} = \begin{bmatrix}
\beta_1 & -1 & \cdots & \cdots & \cdots & -1 & & & & & & & & & \\
-1 & \beta_1 & -1 & \cdots & \cdots & \cdots & -1 & & & & & & & & \\
 & -1 & \beta_1 & -1 & \cdots & \cdots & \cdots & -1 & & & & & & & \\
 & & -1 & \beta_1 & -1 & \cdots & \cdots & \cdots & -1 & & & & & & \\
 & & & \ddots & \ddots & \ddots & & & & \ddots & & & & & \\
-1 & \cdots & \cdots & \cdots & -1 & \beta_1 & -1 & \cdots & \cdots & \cdots & -1 & & & & \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
 & & & & -1 & \cdots & \cdots & \cdots & -1 & \beta_1 & -1 & \cdots & \cdots & \cdots & -1 \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
 & & & & & & & & & -1 & \cdots & \cdots & \cdots & -1 & \beta_1
\end{bmatrix} \tag{4}$$

3 Dirichlet boundary conditions

The constant boundary values ($T^{n+1}_{bound} = T^{n}_{bound}$) need to be included in the equations. All the weak internal nodes on the edges are linked to one boundary node, except the ones in the angles, which are influenced by adjacent boundary nodes lying on different edges. In order to take into account the boundary conditions, matrices $\underline{\underline{\boldsymbol{A}}}$ and $\underline{\underline{\boldsymbol{B}}}$ need to be slightly edited. The finite-difference, Crank-Nicholson scheme for the stencil computed for each node is expressed in matricial form by 3. For the nodes in the angles, two terms of equation 2 need to be substituted with the constant values defined by the Dirichlet boundary conditions (see table 1). For instance, the row describing the stencil of the southeast angle (internal weak node N) need to be modified as follows

$$\cancel{-T^{n+1}_{k-N}} - T^{n+1}_{k-1} + \beta_1 T^{n+1}_{k} \cancel{-T^{n+1}_{k+1}} - T^{n+1}_{k+N} = \cancel{T^{n}_{k-N}} + T^{n}_{k-1} + \beta_2 T^{n}_{k} \cancel{+T^{n}_{k+1}} + T^{n}_{k+N} + 2\left(T_{k-N} + T_{k+1}\right.$$



(a) Structure of the sparse, pentadiagonal, modified matrices $\underline{\underline{\boldsymbol{A}}}_{mod}$ and $\underline{\underline{\boldsymbol{B}}}_{mod}$ with $N^2 = 25$ nodes.

(b) Temperature distribution (in Kelvin) over an isotropic iron plate after 200 seconds (Dirichlet boundary conditions at bottom).

Figure 1

whereas all the rows relative to the nodes of the north edge need to be edited as follows:

$$-T_{k-N}^{n+1} - T_{k-1}^{n+1} + \beta_1 T_k^{n+1} - T_{k+1}^{n+1} \cancel{- T_{k+N}^{n+1}} = T_{k-N}^{n} + T_{k-1}^{n} + \beta_2 T_k^{n} + T_{k+1}^{n} \cancel{+ T_{k+N}^{n}} + {\color{red}+2T_{k+N}}$$

The best way to achieve the scheme is by setting to zero the off-diagonal terms of $\underline{\underline{\boldsymbol{A}}}$ and $\underline{\underline{\boldsymbol{B}}}$ (see table 1). By doing so, one obtains two sparse diagonal matrices similar to the ones in figure 1a.

Before solving the system 3 with the modified matrices, the code must include the Dirichlet boundary conditions. We denote the vector of boundary conditions $\underline{\boldsymbol{b}}$, which includes all the constant boundary values for the temperature that are expressed through the blue terms for the nodes in table .

Hence, one needs to solve the system:

$$\underline{\underline{\boldsymbol{A}}}_{mod} \cdot \underline{\boldsymbol{T}}^{n+1} = \underline{\underline{\boldsymbol{B}}}_{mod} \cdot \underline{\boldsymbol{T}}^{n} + \underline{\boldsymbol{b}} \tag{5}$$

Note that matrices $\underline{\underline{\boldsymbol{A}}}_{mod}$, $\underline{\underline{\boldsymbol{A}}}_{mod}$ and vector $\underline{\boldsymbol{b}}$ are constant for each time integration and do not need to be updated. The vector $\underline{\boldsymbol{T}}^{n+1}$ can be computed by solving the linear system

$$\underline{\boldsymbol{T}}^{n+1} = \underline{\underline{\boldsymbol{A}}}_{mod}^{-1} \left(\underline{\underline{\boldsymbol{B}}}_{mod} \cdot \underline{\boldsymbol{T}}^{n} + \underline{\boldsymbol{b}} \right) \tag{6}$$

for each iteration. Figure 1b shows the temperature distribution over a 1m^2 square, uniform and isotropic iron plate $\kappa \cong 11.72 \cdot 10^{-4}\text{m}^2/\text{s}$ after 200s. Plate thickness is assumed to be constant. The finite-difference discretization is achieved with $N = 51$ nodes. At the beginning of the simulation the temperature is uniform all over the plate $T_0 = 273.15$K. Dirichlet boundary conditions are set to $T0$ on the west, north and east edges, and to $T0 + 100$K on the south edge. Boundary conditions are kept constant throughout the simulation. $\Delta x = 2$cm, $\Delta t = 10^{-2}$s.

4 Neumann boundary condition at bottom edge

We wish to maintain a constant temperature gradient across the lower (bottom, *south*) boundary (*edge*) of the plate throughout the simulation, while keeping constant temperature values on the remaining edges. Dirichlet boundary conditions are thus defined on the left, top and right boundaries, while the value of the outer nodes of the south edge must adapt in order to satisfy the condition:

$$\nabla T \cdot \hat{\boldsymbol{n}} = 0 \Longleftrightarrow \frac{\partial T}{\partial n} = \frac{\partial T}{\partial y} = 0$$

across the bottom boundary. In order to do so, we can express the spatial derivative with a second order, forward finite difference scheme:

$$\Phi_{bound} = \left.\frac{\partial T}{\partial y}\right|_{bound} \cong \frac{-T_{k+N} + 4T_k - 3T_{outer}}{2\Delta x}$$

the value of T_{bound} can be introduced in first n equations in system 3, leading to

$$\begin{aligned} -T_{k-1}^{n+1} + \left(\beta_1 - \frac{4}{3}\right) T_k^{n+1} - T_{k+1}^{n+1} - T_{k+1}^{n+1} - \frac{2}{3} T_{k+N}^{n+1} = \\ = T_{k-1}^{n} + \left(\beta_1 + \frac{4}{3}\right) T_k^{n} + T_{k+1}^{n} + \frac{2}{3} T_{k+N}^{n} - \frac{4\Delta x}{3}\Phi_{bound} \end{aligned} \tag{7}$$

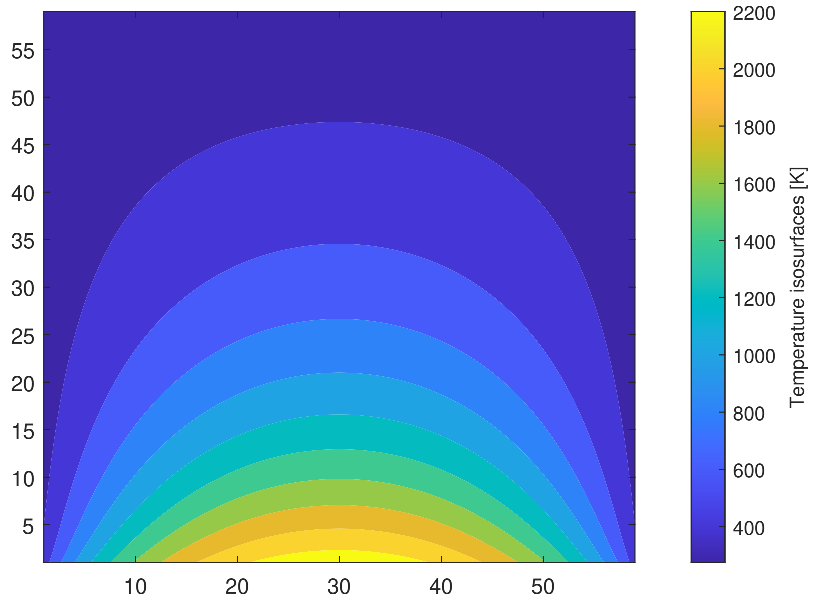


Figure 2: Temperature distribution over a square plate after 200 s. An uniform Neumann boundary condition is applied at the lower boundary. The temperature gradient at bottom is set to $100\mathrm{K}/\Delta x$. Note that the value of the temperature on the lower edge (external *ghost* nodes) is not a constraint of the problem.