# Simulation - 2D Composite Plate Heat Conduction

**Introduction to Computer Physics - Software Project**
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# Contents

# 1 The Concept

The simulation consists of 3 main elements:

- Large rectangular region (outer plate)
- Small rectangular region (inner plate)
- Small hot spot (local heating)

**The setup** of these elements is structured as follows: The large rectangle encloses the smaller rectangle, and together they form the composite plate. On this composite plate, there will be a hot spot where heat is introduced. The two plates consist of 2 different materials (e.g., Material A, Material B), each with different thermal conductivity.

**The visualization** will display a 2D heatmap (e.g., color map of $T(x, y, t)$) where the user can observe how the heat wave propagates and how the pattern changes when it encounters the smaller rectangle (Material B).

**The simulation** can be influenced by the user by making the following changes to the simulation elements: (a) changing the materials (A, B), (b) changing the intensity of the heat input, and (c) changing the position of the local heating.

# 2 The Simulation

## 2.1 Definition: Geometry

We simulate a **2D plate** with a **rectangular inclusion** and a **local heating region** within the 2D plate. Names are defined as follows:

- **2D plate** := main-area (Material A)
- **rectangular inclusion** := inclusion-area (Material B)
- **local heating region** := hotspot

### 2.1.1 Coordinate System

- Coordinates: $x$ in horizontal direction, $y$ in vertical direction.
- Simulation domain: $\Omega = [0, L_x] \times [0, L_y]$
- Example values: $L_x = 0.1m$, $L_y = 0.1m$

Since we simulate in 2D, the plate is assumed to be thin in the z-direction, allowing the temperature variation across the thickness to be neglected. This is the classical 2D approximation in heat conduction (Plane Wall Model) Wikipedia, 2025e.

### 2.1.2 Rectangular Inclusion (sec-area)

Inside the simulation area lies the smaller rectangle $\Omega_{inc}$. This consists of a different material and is defined as: $\Omega_{inc} = [x_1, x_2] \times [y_1, y_2]$ with for example:

- $x_1 = 0.04m$
- $x_2 = 0.06m$
- $y_1 = 0.04m$
- $y_2 = 0.06m$

Thus, we have for the domains:

- **main-area** (Material A): $\Omega_A = \frac{\Omega}{\Omega_{inc}}$
- **sec-area** (Material B): $\Omega_B = \Omega_{inc}$

### 2.1.3 Local Heating Region (hotspot)

A point source is numerically difficult to represent, therefore a small but finite heating area $\Omega_h$ around the point $(x_h, y_h)$ is simulated. Thus, for the simulation we have:

- Center of the heating region: $(x_h, y_h)$
- Heating area as a smaller square: $\Omega_h = [x_h - \Delta_h, x_h + \Delta_h] \times [y_h - \Delta_h, y_h + \Delta_h]$
- Example: $(x_h, y_h) = (0.02m, 0.05m)$
- Example: $\Delta_h = 0.0025m$ (5mm x 5mm square)

Numerically, this corresponds to a few grid points where a volumetric heat generation term $\dot{q}(x, y, t)$ is non-zero.

## 2.2 Materials & Parameters

A selection of 10 different materials will be available.

Table 2.1: Thermophysical properties of selected materials

| **Material** | **Thermal conductivity $k$ [W/(m·K)]** | **Heat capacity $c_p$ [J/(kg*K)]** | **Density $\rho$ [kg/m$^3$]** |
|---|---|---|---|
| Diamond | 1000 | 506 | 3500 |
| Silver | 426.77 | 236 | 10500 |
| Copper | 397.48 | 385 | 8940 |
| Gold | 317.98 | 128 | 19300 |
| Aluminium | 225.94 | 921 | 2698 |
| Bronze | 54.392 | 377 | 8750 |
| Basalt | 2.55 | 627–950 | 2700–3000 |
| Water | 0.6 | 4181 | 997.05 |
| Fiberglass | 0.176 | 1130 | 1230 |
| Air | 0.0025 | 1004 | 1.29 |

The material values were taken from the following sources Matmake, 2025; Thermstest, 2025; Wikipedia, 2025f. Initially, a fixed setup will be used, later expandable with additional materials.

- Main (Material A): Basalt (poor thermal conductivity)
- Inclusion (Material B): Aluminium (good thermal conductivity)

## 2.3 Thermal Diffusivity

For heat transport, thermal diffusivity is important. It can be viewed as the time derivative of a material's temperature and describes the rate at which heat propagation "decays/smooths out" in a material. This allows two materials and their thermal conductivity to be compared effectively. The following formula describes thermal diffusivity Wikipedia, 2025g:

$$\alpha = \frac{k}{\rho \cdot c_p} \tag{2.1}$$

Taking the two materials from 2.2, we obtain with the values from Table 2.1 the following calculations:

$$\alpha_A \approx \frac{2.55 W/(mK)}{3000 kg/m^3 \cdot 950 J/(kg \cdot K)} \approx 8.95 \times 10^{-7} m^2/s \tag{2.2}$$

$$\alpha_B \approx \frac{225 W/(mK)}{2700 kg/m^3 \cdot 920 J/(kg \cdot K)} \approx 1.027 \times 10^{-4} m^2/s \tag{2.3}$$

$$\alpha_B > \alpha_A \tag{2.4}$$

Thus, the heat propagation velocity in aluminium is many times higher than in basalt, which will also be visible in the simulation. The simulation then stores for each cell:

$$k_{i,j}, \rho_{i,j}, c_{p_{i,j}} \tag{2.5}$$

# 3 Partial Differential Equation (PDE) & Boundary/Initial Conditions

## 3.1 Derivation of the 2D Heat Conduction Equation

The derivation of the heat conduction equation is based on *Fourier's Law* and local energy conservation. For an isotropic medium with constant thermal conductivity $k$, density $\rho$, and heat capacity $c_p$, the following applies:

### Step 1: Fourier's Law

The heat flux vector is proportional to the negative temperature gradient:

$$\mathbf{q}(x, y, t) = -k \nabla T(x, y, t), \tag{3.1}$$

where $\nabla T = \left( \frac{\partial T}{\partial x}, \frac{\partial T}{\partial y} \right)$ is the temperature gradient.

### Step 2: Energy Conservation

The temporal change of internal energy per volume equals the divergence of the heat flux plus a volumetric heat source $\dot{q}_V(x, y, t)$:

$$\rho c_p \frac{\partial T}{\partial t} = -\nabla \cdot \mathbf{q} + \dot{q}_V(x, y, t). \tag{3.2}$$

### Step 3: Substituting Fourier's Law

Substituting $\mathbf{q} = -k \nabla T$, we obtain:

$$\rho c_p \frac{\partial T}{\partial t} = \nabla \cdot (k \nabla T) + \dot{q}_V(x, y, t). \tag{3.3}$$

### Step 4: Simplification for Constant $k$

For constant $k$, the divergence term reduces to:

$$\rho c_p \frac{\partial T}{\partial t} = k\nabla^2 T + \dot{q}_V(x, y, t), \tag{3.4}$$

with the Laplace operator in 2D:

$$\nabla^2 T = \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2}. \tag{3.5}$$

### Step 5: Final Form of the 2D Heat Conduction Equation

Division by $\rho c_p$ yields the standard form:

$$\frac{\partial T}{\partial t} = \alpha \left( \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right) + \frac{\dot{q}_V(x, y, t)}{\rho c_p}, \tag{3.6}$$

where the thermal diffusivity is defined as

$$\alpha = \frac{k}{\rho c_p}. \tag{3.7}$$

Wikipedia, 2025d.

## 3.2 Heat Source (Hotspot)

We model $\dot{q}(x, y, t)$ as:

$$\dot{q}(x, y, t) = \begin{cases} q_0 & \text{for } (x, y) \in \Omega_h \text{ and } 0 < t < t_{\text{heat}} \\ 0 & \text{otherwise} \end{cases} \tag{3.8}$$

Where $q_0[W/m^3]$ is the constant heat generation rate in the “hotspot region” and $t_{heat}$ is the duration of heat supply. Physically, this could represent, for example, a laser heating a small area or an embedded chip producing waste heat.

## 3.3 Initial Conditions

For a unique solution, initial and boundary conditions must be specified. We start with a uniform temperature, e.g., the ambient temperature $T_{amb}$:

$$T(x, y, 0) = T_0 = T_{amb} \tag{3.9}$$

e.g., $T_{amb} = 293K$ (20°C).

## 3.4 Boundary Conditions (Outer Edges)

### 3.4.1 Dirichlet Boundary Condition

For simplicity, the **Dirichlet boundary condition** is used initially. The plate is in contact with a heat reservoir at $T_{amb}$ at the boundaries:

$$T(x, y, t) = T_{amb} \quad \text{for } (x, y) \in \delta\Omega, t > 0 \tag{3.10}$$

**Physical Meaning** The temperature at the boundary is fixed and independent of the internal behavior.

**Example** The plate lies in a perfect material that always maintains the constant temperature $T_{amb}$.

**Usage** Simplified "unrealistic" simulation. The focus is on heat propagation in the materials, not a realistic model.

### 3.4.2 Robin Boundary Condition (Convective)

For a realistic simulation where the surroundings of the plate also play a role, the convective boundary condition can be used:

$$-k\delta_n T = h(T - T_{amb}) \tag{3.11}$$

with:

- $h$: Heat transfer coefficient $[W/(m^2 \cdot K)]$
- $T_{amb}$: Ambient temperature

**Physical Meaning** The heat flux at the boundary is proportional (dependent) to the temperature difference between the plate and the surroundings.

**Example** The plate is cooled from outside by a material; this temperature is influenced by the plate itself.

**Usage** Realistic simulation where the temperature at the boundary is not fixed but determined by exchange with the surroundings. One wants to simultaneously simulate how heat propagation on the plate behaves when the plate is in different environments.

## 3.5 Addendum: Thermal Energy

In addition to the temperature distribution $T(x, y, t)$, the simulation can also effectively show how the total energy of the system changes, depending on which boundary condition applies and what materials the plate consists of. The formula for **thermal energy** $E(t)$ can be derived using the already derived *heat conduction equation* and the principle of energy conservation as follows:

### Internal Energy and Energy Density

The thermal energy of a substance is defined as ChemieSchule, 2025:

$$E = c \cdot m \cdot T\,,$$

where

- $c$: specific heat capacity $[J/(kg \cdot K)]$
- $m$: mass $[kg]$
- $T$: temperature $[K]$

With $m = \rho \cdot V$ (mass = density * volume), for a volume element $dV$:

$$dE = \rho\, c_p\, T\, dV$$

where

- $\rho$: density $[kg/m^3]$
- $c_p$: specific heat capacity at constant pressure $[J/(kg\,K)]$
- $T$: temperature $[K]$

For the fields in our simulation, therefore (energy per volume):

$$e(x, y, t) = \rho(x, y) c_p(x, y) T(x, y, t)$$

For the total volume $\Omega$ of the plate, the total energy is obtained as an integral:

$$E(t) = \int_\Omega \rho(x, y) c_p(x, y) T(x, y, t) e\, dA \tag{3.12}$$

Since we have a 2D plate, we write for the volume: $dV = e\, dA$, where $e$ is a constant plate thickness and $dA = dx \cdot dy$. (To show relative changes, $e = 1.0$ is set, corresponding to energy per meter of plate thickness.)

### Local → Global Energy Balance

To obtain the global energy balance, the formula for local energy conservation (see 3.1) is integrated over the entire volume $\Omega$:

$$\rho c_p \frac{\partial T}{\partial t} = \nabla \cdot (k \nabla T) + \dot{q}_V(x, y, t)$$
$$\int_\Omega \rho c_p \frac{\partial T}{\partial t} dV = \int_\Omega \nabla \cdot (k \nabla T) dV + \int_\Omega \dot{q}_V dV$$

The left side is the time derivative of the total energy:

$$\frac{dE}{dt} = \int_\Omega \rho c_p \frac{\partial T}{\partial t} dV \,.$$

For the divergence term on the right side, Gauss's integral theorem is used (volume integral → surface integral) Wikipedia, 2025c:

$$\int_\Omega \nabla \cdot (k \nabla T) dV = \oint_{\partial\Omega} k \nabla T \cdot \vec{n} dA \,,$$

where $\vec{n}$ = outward normal vector on the boundary surface $\partial\Omega$, yielding the **global energy balance** of the plate:

$$\frac{dE}{dt} = \oint_{\partial\Omega} k \nabla T \cdot \vec{n} dA + \oint_\Omega \dot{q}_V dV \tag{3.13}$$

- The surface integral describes the heat flux power across the boundary,
- the volume integral describes the power input through volume sources.

### Global Energy Balance (Robin)

For Robin boundary conditions, the heat flux at the boundary is given as:

$$-k \nabla T \cdot \vec{n} = h(T - T_{amb})$$

Solving and substituting into the energy balance term (3.13):

$$k \nabla T \cdot \vec{n} = -h(T - T_{amb}) \oint_{\partial\Omega} k \nabla T \cdot \vec{n} dA = \oint_{\partial\Omega} (-h(T - T_{amb})) dA$$

We obtain for the **global energy balance (Robin)**:

$$\frac{dE}{dt} = -\oint_{\partial\Omega} h(T - T_{amb}) dA + \oint_\Omega \dot{q}_V dV \tag{3.14}$$

which simply expressed is $\frac{dE}{dt} = Q_{in}(t) - Q_{out}(t)$.

# 4 Numerical Solution with Finite Differences (FTCS)

For the numerical solution of the 2D heat conduction, the **explicit finite difference scheme** (Forward Time - Centered Space) is used and extended to the variables $k(x,y), \rho(x,y), c_p(x,y)$ (material values). FTCS is a finite difference method (FDM). FDM approximates the derivatives in the PDE using finite difference expressions derived from Taylor series expansions and converts the PDE into a system of linear algebraic equations that can be efficiently solved with iterative algorithms Haque et al., 2025; Wikipedia, 2025b.

## 4.1 Grid in Space and Time

A regular grid is used for:

1. Spatial discretization:

$$x_i = i\Delta x, \;\; i = 0, ..., N_x \tag{4.1}$$
$$y_j = j\Delta y, \;\; j = 0, ..., N_y \tag{4.2}$$

   with

$$\Delta x = \frac{L_x}{N_x}, \;\; \Delta y = \frac{L_y}{N_y} \tag{4.3}$$

2. Time discretization:

$$t^n = n\Delta t, \;\; n = 0, 1, 2, ... \tag{4.4}$$

And we approximate:

$$T^n_{i,j} \approx T(x_i, y_j, t^n) \tag{4.5}$$

Example values are: $N_x = N_y = 100 \Rightarrow \Delta x = \Delta y = 10^{-3} m$ (1 mm grid) and $\Delta t$ is chosen based on the stability condition (see 4.4). For each grid point (i,j), the material values are stored ($k_{i,j} = k_A$ or $k_B$ and the corresponding values $\rho_{i,j}, c_{p_{i,j}}$):

$$(k_{i,j}, c_{p_{i,j}}, \rho_{i,j}) = \begin{cases} (k_A, c_{p,A}, \rho_A), & (x_i, y_i) \in \Omega_A, \\ (k_B, c_{p,B}, \rho_B), & (x_i, y_i) \in \Omega_B \end{cases} \tag{4.6}$$

And correspondingly for the hotspot (see 3.2):

$$\dot{q}^n_{i,j} \approx \dot{q}(x_i, y_i, t^n) \tag{4.7}$$

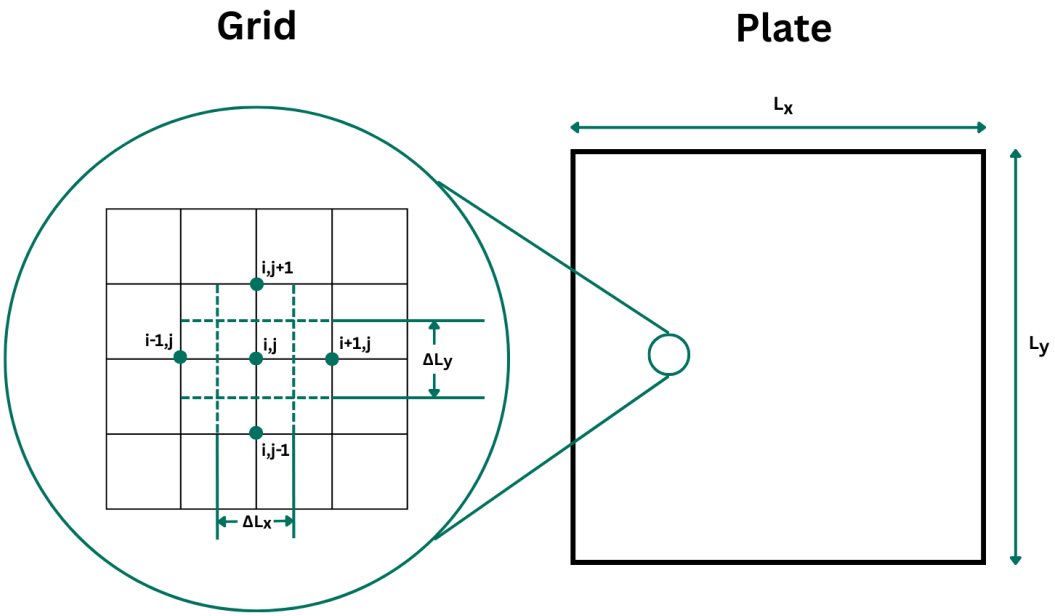


Figure 4.1: The grid on the plate

## 4.2 Discretization of $\nabla \cdot (k\nabla T)$

The operator describes a form that is also meaningful for different k in neighboring cells for 2D:

$$\nabla \cdot (k\nabla T) = \frac{\partial}{\partial x}(k\frac{\partial T}{\partial x}) + \frac{\partial}{\partial y}(k\frac{\partial T}{\partial y}) \tag{4.8}$$

To account for the spatially varying conductivity, conductivities at cell boundaries are defined as average values. Thus, the arithmetic mean for the four edges at a point is given by:

$$k_{i+\frac{1}{2},j} = \frac{1}{2}(k_{i+1,j} + k_{i,j}), \quad k_{i-\frac{1}{2},j} = \frac{1}{2}(k_{i-1,j} + k_{i,j}), \tag{4.9}$$

$$k_{i,j+\frac{1}{2}} = \frac{1}{2}(k_{i,j+1} + k_{i,j}), \quad k_{i,j-\frac{1}{2}} = \frac{1}{2}(k_{i,j-1} + k_{i,j}). \tag{4.10}$$

With central differences, the divergence at point $(i, j)$ becomes:

$$[\nabla \cdot (k\nabla T)]^n_{i,j} \approx \frac{1}{\Delta x}(k_{i+\frac{1}{2},j}\frac{T^n_{i+1,j} - T^n_{i,j}}{\Delta x} - k_{i-\frac{1}{2},j}\frac{T^n_{i,j} - T^n_{i-1,j}}{\Delta x}) + \frac{1}{\Delta y}(k_{i,j+\frac{1}{2}}\frac{T^n_{i,j+1} - T^n_{i,j}}{\Delta y} - k_{i,j-\frac{1}{2}}\frac{T^n_{i,j} - T^n_{i,j-1}}{\Delta y}) \tag{4.11}$$

## 4.3 Explicit Time-Stepping Method FTCS (Time Discretization)

The PDE (see 3.1 (Formula (3.7)) reads:

$$\frac{\partial T}{\partial t} = \alpha(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2}) + \frac{\dot{q}_V(x,y,t)}{\rho c_p} \tag{4.12}$$

$$\tag{4.13}$$

After rearranging and simplified representation (considering constant k) we obtain:

$$\rho_{i,j} c_{p_{i,j}} \frac{\partial T}{\partial t} = \nabla \cdot (k \nabla T) + \dot{q} \tag{4.14}$$

The discrete time derivative is approximated with a forward step:

$$\left.\frac{\partial T}{\partial t}\right|_{i,j}^{n} \approx \frac{T_{i,j}^{n+1} - T_{i,j}^{n}}{\Delta t} \tag{4.15}$$

Substituting into (4.15):

$$\rho_{i,j} c_{p_{i,j}} \frac{T_{i,j}^{n+1} - T_{i,j}^{n}}{\Delta t} = [\nabla \cdot (k \nabla T)]_{i,j}^{n} + \dot{q}_{i,j}^{n} \tag{4.16}$$

And we obtain the **update formula** (for interior points without boundary condition):

$$T_{i,j}^{n+1} = T_{i,j}^{n} + \frac{\Delta t}{\rho_{i,j} c_{p_{i,j}}}([\nabla \cdot (k \nabla T)]_{i,j}^{n} + \dot{q}_{i,j}^{n}\ , \tag{4.17}$$

with $[\nabla \cdot (k \nabla T)]_{i,j}^{n}$ from (4.11).

### Implementation of the Dirichlet Boundary Condition

The Dirichlet boundary condition (see 3.4.1) is implemented on the grid by

$$T_{i,j}^{n} = T_{amb} \quad \text{for} \quad i = 0, i = N_x \text{ or } j = 0, j = N_y, \forall n \tag{4.18}$$

and in the numerical implementation is explicitly set after each time step and not updated by (4.17).

### Implementation of the Robin Boundary Condition

It is assumed that the plate is coupled to the surroundings at temperature $T_{amb}$ through convection with heat transfer coefficient $h$. For all points on the outer boundary:

$$-k_{i,j} \nabla T_{i,j}^{n} \cdot \vec{n} = h(T_{i,j}^{n} - T_{amb}), \quad \text{for} \quad i = 0, i = N_x \text{ or } j = 0, j = N_y, \forall n, \tag{4.19}$$

alternatively expressed:

$$-k(x,y) \nabla T(x,y,t) \cdot \vec{n} = h(T(x,y,t) - T_{amb}), \quad (x,y) \in \partial\Omega, t > 0. \tag{4.20}$$

For each boundary side, the normal is explicitly:

- Left boundary: $x = 0$, normal $\vec{n} = (-1, 0)$
- Right boundary: $x = L_x$, normal $\vec{n} = (+1, 0)$
- Lower boundary: $y = 0$, normal $\vec{n} = (0, -1)$
- Upper boundary: $y = L_y$, normal $\vec{n} = (0, +1)$

Thus, e.g., the right boundary is given by:

$$-k(x,y)\left.\frac{\partial T}{\partial x}\right|_{x=L_x} = h\big(T(L_x, y, t) - T_{amb}\big). \tag{4.21}$$

**Example Discretization at the Right Boundary $x = L_x$ ($i = N_x$)**

Considering the boundary node $(i = N_x, j)$ and using a one-sided difference inward (1st order) for the partial derivative $\partial T/\partial x$, we obtain:

$$\left.\frac{\partial T}{\partial x}\right|_{x=L_x} \approx \frac{T^n_{N_x,j} - T^n_{N_x-1,j}}{\Delta x}. \tag{4.22}$$

Thus, the discrete form of the Robin boundary condition reads:

$$-k_{N_x,j}\,\frac{T^n_{N_x,j} - T^n_{N_x-1,j}}{\Delta x} = h\big(T^n_{N_x,j} - T_{amb}\big). \tag{4.23}$$

This is a linear relationship between the boundary temperature $T^n_{N_x,j}$ and the interior value $T^n_{N_x-1,j}$. Rearranging for the boundary temperature yields the **update formula** (right boundary with Robin boundary condition):

$$\begin{aligned} -k_{N_x,j}T^n_{N_x,j} + k_{N_x,j}T^n_{N_x-1,j} &= h\Delta x\, T^n_{N_x,j} - h\Delta x\, T_{amb}, \\ (k_{N_x,j} + h\Delta x)\, T^n_{N_x,j} &= k_{N_x,j}T^n_{N_x-1,j} + h\Delta x\, T_{amb}, \end{aligned}$$

thus finally

$$T^n_{N_x,j} = \frac{k_{N_x,j}}{k_{N_x,j} + h\Delta x}\, T^n_{N_x-1,j} + \frac{h\Delta x}{k_{N_x,j} + h\Delta x}\, T_{amb}. \tag{4.24}$$

Analogously, we obtain for the remaining sides:

- **Left boundary** ($x = 0$, $i = 0$):

$$T^n_{0,j} = \frac{k_{0,j}}{k_{0,j} + h\Delta x}T^n_{1,j} + \frac{h\Delta x}{k_{0,j} + h\Delta x}T_{amb}. \tag{4.25}$$

- **Lower boundary** ($y = 0$, $j = 0$):

$$T^n_{i,0} = \frac{k_{i,0}}{k_{i,0} + h\Delta y}T^n_{i,1} + \frac{h\Delta y}{k_{i,0} + h\Delta y}T_{amb}. \tag{4.26}$$

- **Upper boundary** ($y = L_y$, $j = N_y$):

$$T^n_{i,N_y} = \frac{k_{i,N_y}}{k_{i,N_y} + h\Delta y}T^n_{i,N_y-1} + \frac{h\Delta y}{k_{i,N_y} + h\Delta y}T_{amb}. \tag{4.27}$$

## 4.4 Stability Condition (CFL)

The “Courant-Friedrichs-Lewy number” indicates how many cells the flow may propagate in one time step Wikipedia, 2025a. For the explicit FTCS method, the step size $\Delta t$ is thus constrained by the stability condition. For the local thermal diffusivity

$$\alpha_{i,j} = \frac{k_{i,j}}{\rho_{i,j} c_{p_{i,j}}} \tag{4.28}$$

we choose

$$\Delta t \leq \frac{1}{2}(\alpha_{max}(\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2}))^{-1}, \quad \alpha_{max} = \max_{i,j} \alpha_{i,j}, \tag{4.29}$$

to ensure numerical stability. Note: The Robin boundary condition can slightly affect the effective stability, but within this framework, the above condition remains a good guideline.

## 4.5 Energy on the Finite Difference Grid

The discrete formula for energy $E^n$ on the grid is based on the derivation of the **global energy balance** (see 3.5) and the definition of the grid (see 4.1): The grid is defined as:

$$x_i = i\Delta x, \quad i = 0, ..., N_x, \quad y_j = j\Delta y, \quad j = 0, ..., N_y$$

Adding a plate thickness $e$, we obtain for each grid element as a small volume:

$$\Delta V = e\Delta x \Delta y \tag{4.30}$$

The discrete approximation of the total energy at time step $t^n$ is thus:

$$E^n \approx \sum_{i=0}^{N_x} \sum_{j=0}^{N_y} \rho_{i,j} c_{p_{i,j}} T_{i,j}^n \Delta V \tag{4.31}$$

With the simple assumption $e = 1$ (energy per meter of plate thickness), we obtain:

$$E^n \approx \sum_{i=0}^{N_x} \sum_{j=0}^{N_y} \rho_{i,j} c_{p_{i,j}} T_{i,j}^n \Delta x \Delta y \tag{4.32}$$

Finally, we define the energy difference from the initial energy:

$$\Delta E^n = E^n - E^0. \tag{4.33}$$

# 5 Example Calculation: Manual Computation

In this chapter, a concrete example is worked through, where I manually execute the FTCS time steps on a simplified grid with Robin boundary conditions (convective heat transfer).

## 5.1 Model Setup

### Geometry and Grid

We choose a greatly simplified $5 \times 5$ grid (i.e., $N_x = N_y = 4$) on a square plate:

- Plate size: $L_x = L_y = 0.04m$
- Grid spacing: $\Delta x = \Delta y = 0.01m = 1cm$
- Indices: $i, j \in \{0, 1, 2, 3, 4\}$

### Material Distribution

- **Base (Basalt):** All points except the center point (2,2)
- **Inclusion (Aluminium):** Only the center point (2,2)

Material parameters (Table 2.1): with $\alpha = \frac{k}{\rho c_p}$ (thermal diffusivity).

Table 5.1: Thermophysical properties of the selected materials

| **Material** | $k$ **[W/(m*K)]** | $c_p$ **[J/(kg*K)]** | $\rho$ **[kg/m$^3$]** | $\alpha$ **[m$^2$/s]** |
|---|---|---|---|---|
| Basalt (Bst) | 2.55 | 950 | 3000 | $8.95\times10^{-7}$ |
| Aluminium (Al) | 225.94 | 921 | 2698 | $9.10\times10^{-5}$ |

### Robin Boundary Condition Parameters

- Ambient temperature: $T_{amb} = 293K$ (20°C)
- Heat transfer coefficient: $h = 25W/(m^2 \cdot K)$ (typical for free convection in air)

### Initial Condition and Hotspot

- Initial temperature: $T_{i,j}^0 = 293K$ for all points
- Hotspot at (1,2): $\dot{q}_{1,2} = 10^6 W/m^3$

### Time Step

From the stability condition (Eq. 4.29) with $\alpha_{max} = 9.10 \times 10^{-5} m^2/s$:

$$\Delta t \leq \frac{1}{2} \cdot (9.10 \times 10^{-5} \cdot \frac{2}{(0.01)^2})^{-1} \approx 0.275s \tag{5.1}$$

We choose conservatively: $\Delta t = 0.1s$

## 5.2 Grid Sketch

```
         i=0      i=1      i=2      i=3      i=4

j=4    [R_E]---[R_t]---[R_t]---[R_t]---[R_E]    (top boundary)
         |        |        |        |        |
j=3    [R_l]---[Inn]---[Inn]---[Inn]---[R_r]
         |        |        |        |        |
j=2    [R_l]---[H,I]---[Alu]---[Inn]---[R_r]    (H = Hotspot, Alu = Aluminium)
         |        |        |        |        |
j=1    [R_l]---[Inn]---[Inn]---[Inn]---[R_r]
         |        |        |        |        |
j=0    [R_E]---[R_b]---[R_b]---[R_b]---[R_E]    (bottom boundary)
```

Legend:

- R_E = Corner point (Robin)
- R_l, R_r, R_t, R_b = Boundary points left/right/top/bottom
- Inn = Interior point (Basalt)
- Alu = Aluminium inclusion
- H,I = Hotspot (interior point with heat source)

## 5.3 Robin Boundary Condition

### General Form (from Chapter 4, Eq. 4.24-4.27)

The Robin boundary condition couples the boundary temperature to the interior neighbor:

$$-k\frac{\partial T}{\partial n} = h(T - T_{amb})$$

### Discrete Formulas for Each Boundary

- Right boundary (i=4):

$$T_{4,j}^n = \frac{k_{4,j}}{k_{4,j} + h\Delta x} T_{3,j}^n + \frac{h\Delta x}{k_{4,j} + h\Delta x} T_{amb} \tag{5.2}$$

- Left boundary (i=0):

$$T_{0,j}^n = \frac{k_{0,j}}{k_{0,j} + h\Delta x} T_{1,j}^n + \frac{h\Delta x}{k_{0,j} + h\Delta x} T_{amb} \tag{5.3}$$

- Upper boundary (j=4):

$$T_{i,4}^n = \frac{k_{i,4}}{k_{i,4} + h\Delta y} T_{i,3}^n + \frac{h\Delta y}{k_{i,4} + h\Delta y} T_{amb} \tag{5.4}$$

- Lower boundary (j=0):

$$T_{i,0}^n = \frac{k_{i,0}}{k_{i,0} + h\Delta y} T_{i,1}^n + \frac{h\Delta y}{k_{i,0} + h\Delta y} T_{amb} \tag{5.5}$$

### Calculation of Coefficients for Basalt Boundary

With $k = 2.55 W/(m \cdot K)$, $h = 25 W/(m^2 \cdot K)$, $\Delta x = \Delta y = 0.01 m$:

$$h\Delta x = 25 \cdot 0.01 = 0.25 W/(m \cdot K) \tag{5.6}$$

$$k + h\Delta x = 2.55 + 0.25 = 2.80 W/(m \cdot K) \tag{5.7}$$

thus the **coefficients are:**

$$\beta_k = \frac{k}{k + h\Delta x} = \frac{2.55}{2.80} = 0.9107 \tag{5.8}$$

$$\beta_h = \frac{h\Delta x}{k + h\Delta x} = \frac{0.25}{2.80} = 0.0893 \tag{5.9}$$

*Check:* $\beta_k + \beta_h = 0.9107 + 0.0893 = 1$

#### Boundary Formula (simplified for Basalt)

$$T^n_{boundary} = 0.9107 \cdot T^n_{interior} + 0.0893 \cdot 293 \tag{5.10}$$
$$T^n_{boundary} = 0.9107 \cdot T^n_{interior} + 26.165K \tag{5.11}$$

## 5.4 Time Step n=0→n=1

#### Step 1: Initial State ($t^0$)

All temperatures: $T^0_{i,j} = 293\text{K}$

#### Step 2: Update of Interior Points

- **P(1,2)** Hotspot in Basalt
- **P(0,2)** Boundary point $T^0_{0,2} = 293$
- **P(2,2)** Aluminium $T^0_{2,2} = 293$
- **P(1,1)** Basalt $T^0_{1,1} = 293$
- **P(1,3)** Basalt $T^0_{1,3} = 293$

**Edge conductivities:**

$$k_{1+\frac{1}{2},2} = \frac{1}{2}(k_{2,2} + k_{1,2}) = \frac{1}{2}(226 + 2.55) = 114.275W/(m \cdot K)$$
$$k_{1-\frac{1}{2},2} = \frac{1}{2}(k_{0,2} + k_{1,2}) = \frac{1}{2}(2.55 + 2.55) = 2.55W/(m \cdot K)$$
$$k_{1,2+\frac{1}{2}} = \frac{1}{2}(k_{1,3} + k_{1,2}) = \frac{1}{2}(2.55 + 2.55) = 2.55W/(m \cdot K)$$
$$k_{1,2-\frac{1}{2}} = \frac{1}{2}(k_{1,1} + k_{1,2}) = \frac{1}{2}(2.55 + 2.55) = 2.55W/(m \cdot K)$$

**Divergence term:** Since all $T^0 = 293K$, all temperature differences are zero:

$$[\nabla \cdot (k\nabla T)]^0_{1,2} = 0$$

**Update formula (Eq. 4.17):**

$$T^1_{1,2} = T^0_{1,2} + \frac{\Delta t}{\rho_{1,2} c_{p_{1,2}}}([\nabla \cdot (k\nabla T)]^0_{1,2} + \dot{q}^0_{1,2})$$
$$T^1_{1,2} = 293 + \frac{0.1}{3000 \cdot 950}(0 + 10^6)$$
$$T^1_{1,2} = 293 + \frac{10^5}{2.85 \times 10^6} = 293.035K$$

**Point (2,2) - Aluminium inclusion:** No heat source, all neighboring temperatures equal:

$$T_{2,2}^1 = 293 + \frac{0.1}{2700 \cdot 920}(0 + 0) = 293K$$

**All other interior points:** Without heat source and with equal neighboring temperatures:

$$T_{i,j}^1 = 293K \text{ for all other interior points}$$

#### Step 3: Update of Boundary Points (Eq. 5.11)

**Left boundary (i=0), e.g., point (0,2):**

$$\begin{aligned} T_{0,2}^1 &= 0.9107 \cdot T_{1,2}^1 + 26.165 \\ T_{0,2}^1 &= 0.9107 \cdot 293.035 + 26.165 \\ T_{0,2}^1 &= 293.032K \end{aligned}$$

Since the other interior neighbors are still at 293K:

$$T_{boundary}^1 = 0.9107 * 293 + 26.165 = 293.000K$$

## 5.5 Time Step n=1 $\rightarrow$ n=2

#### Starting Point after $t^1$

| Point | Temperature $T^1$ [K] | Material |
|---|---|---|
| (1,2) | 293.035 | Basalt + Hotspot |
| (0,2) | 293.032 | Basalt (Boundary) |
| (2,2) | 293.000 | Aluminium |
| All others | 293.000 | - |

#### Update of the Aluminium Point (2,2)

**Neighbors:**

- (1,2): $T_{1,2}^1 = 293.035$K (Hotspot)
- (3,2): $T_{3,2}^1 = 293.000$K
- (2,1): $T_{2,1}^1 = 293.000$K
- (2,3): $T_{2,3}^1 = 293.000$K

**Edge conductivities (all neighbors are Basalt):**

$$k_{2\pm\frac{1}{2},2} = k_{2,2\pm\frac{1}{2}} = \frac{1}{2}(226 + 2.55) = 114.275\,W/(m \cdot K)$$

**Divergence term:**

$$\begin{aligned}[\nabla \cdot (k\nabla T)]^1_{2,2} = &\frac{1}{(\Delta x)^2}\Big[k_{2+\frac{1}{2},2}(T^1_{3,2} - T^1_{2,2}) - k_{2-\frac{1}{2},2}(T^1_{2,2} - T^1_{1,2})\Big] \\ &+ \frac{1}{(\Delta y)^2}\Big[k_{2,2+\frac{1}{2}}(T^1_{2,3} - T^1_{2,2}) - k_{2,2-\frac{1}{2}}(T^1_{2,2} - T^1_{2,1})\Big]\end{aligned}$$

**x-direction:**

$$\begin{aligned}&\frac{1}{(0.01)^2}\Big[114.275(293 - 293) - 114.275(293 - 293.035)\Big] \\ &= 10^4\Big[0 - 114.275 \cdot (-0.035)\Big] = 10^4 \cdot 4.0 = 40000\,W/m^3\end{aligned}$$

**y-direction:**

$$\frac{1}{(0.01)^2}\Big[114.275 \cdot 0 - 114.275 \cdot 0\Big] = 0$$

**Total:**

$$[\nabla \cdot (k\nabla T)]^1_{2,2} = 40000\,W/m^3$$

**Update:**

$$\begin{aligned}T^2_{2,2} &= 293 + \frac{0.1}{2700 \cdot 920} \cdot 40000 \\ T^2_{2,2} &= 293 + \frac{4000}{2.484 \times 10^6} = 293 + 0.00161 \\ T^2_{2,2} &= 293.0016\,K\end{aligned}$$

### Update of the Hotspot Point (1,2)

**Neighbors:**

- (0,2): $T^1_{0,2} = 293.032\text{K}$ (Robin boundary!)
- (2,2): $T^1_{2,2} = 293.000\text{K}$
- (1,1): $T^1_{1,1} = 293.000\text{K}$
- (1,3): $T^1_{1,3} = 293.000\text{K}$

**Divergence term:**

**x-direction:**

$$\frac{1}{(0.01)^2}\Big[114.275(293-293.035)-2.55(293.035-293.032)\Big]$$
$$=10^4\Big[114.275\cdot(-0.035)-2.55\cdot 0.003\Big]$$
$$=10^4\Big[-4.0-0.00765\Big]=-40076.5\,W/m^3$$

**y-direction:**

$$\frac{1}{(0.01)^2}\Big[2.55(293-293.035)-2.55(293.035-293)\Big]$$
$$=10^4\Big[2.55\cdot(-0.035)-2.55\cdot 0.035\Big]$$
$$=10^4\Big[-0.0893-0.0893\Big]=-1786\,W/m^3$$

**Total:**

$$[\nabla\cdot(k\nabla T)]^1_{1,2}=-40076.5-1786=-41862.5\,W/m^3$$

**Update:**

$$T^2_{1,2}=293.035+\frac{0.1}{3000\cdot 950}(-41862.5+10^6)$$
$$T^2_{1,2}=293.035+\frac{0.1\cdot 958137.5}{2.85\times 10^6}$$
$$T^2_{1,2}=293.035+0.0336=293.069\,K$$

#### Update of the Robin Boundary Points

**Point (0,2) – Left boundary next to hotspot:**

$$T^2_{0,2}=0.9107\cdot T^2_{1,2}+26.165$$
$$T^2_{0,2}=0.9107\cdot 293.069+26.165=266.90+26.165$$
$$T^2_{0,2}=293.063\,K$$

## 5.6 Energy Balance with Robin Boundary Condition

#### Global Energy Balance (Eq. 3.14)

$$\frac{dE}{dt}=-\oint_{\partial\Omega}h(T-T_{amb})\,dA+\int_\Omega \dot{q}_V\,dV \tag{5.12}$$

### Discrete Calculation for n=1

**Heat input (Hotspot):**

$$Q_{in} = \dot{q} \cdot \Delta V \cdot \Delta t = 10^6 \cdot (0.01)^2 \cdot 1 \cdot 0.1 = 10\,J$$

(with plate thickness $e = 1\text{m}$)

**Heat loss across the boundary:**
The heat flow across a boundary segment of length $\Delta x$ (or $\Delta y$) and thickness $e = 1\text{m}$:

$$\dot{Q}_{out,segment} = h \cdot (T_{boundary} - T_{amb}) \cdot \Delta x \cdot e$$

**For point (0,2) after time step 1:**

$$\dot{Q}_{out,(0,2)} = 25 \cdot (293.032 - 293) \cdot 0.01 \cdot 1 = 25 \cdot 0.032 \cdot 0.01 = 0.008\,W$$

**Over $\Delta t = 0.1$s:**

$$Q_{out,(0,2)} = 0.008 \cdot 0.1 = 0.0008\,J$$

**Total boundary loss (all 16 boundary points):**
Since only (0,2) has a noticeably elevated temperature:

$$Q_{out,total} \approx 0.0008\,J$$

### Net Energy Change

$$\Delta E^1 \approx Q_{in} - Q_{out} = 10 - 0.0008 \approx 10\,J$$

### Verification via Temperature Change

The energy in the hotspot point:

$$\Delta E_{1,2} = \rho c_p \Delta T \cdot \Delta V = 3000 \cdot 950 \cdot 0.035 \cdot 10^{-4} \cdot 1 = 9.975\,J$$

*The energy balance is consistent!*

Table 5.2: Comparison of boundary conditions

| **Property** | **Dirichlet** | **Robin ($h = 25$)** |
|---|---|---|
| Boundary temperature $T^0$ | fixed 293 K | fixed 293 K |
| Boundary temperature $T^1_{0,2}$ | fixed 293 K | **293.032 K** |
| Boundary temperature $T^2_{0,2}$ | fixed 293 K | **293.063 K** |
| Heat flux at boundary | maximum (forced) | **proportional to $\Delta T$** |
| Physical meaning | Perfect heat reservoir | Convective cooling |

## 5.7 Comparison: Robin vs. Dirichlet

#### Interpretation of Robin Coefficients

$$\beta_k = \frac{k}{k + h\Delta x} = 0.9107$$

- $\beta_k \approx 1$: The boundary nearly follows the interior temperature (weak cooling)
- $\beta_k \approx 0$: The boundary stays close to $T_{amb}$ (strong cooling, approaches Dirichlet)

For stronger cooling (e.g., $h = 500\,W/(m^2 \cdot K)$):

$$\beta_k = \frac{2.55}{2.55 + 5} = 0.338$$

The boundary would then remain much closer to $T_{amb}$.

## 5.8 Summary of Results

#### Temperature Evolution

Table 5.3: Temperature evolution over time steps

| **Time step n** | $T_{1,2}$ **(Hotspot)** | $T_{2,2}$ **(Alu)** | $T_{0,2}$ **(Robin boundary)** |
|---|---|---|---|
| 0 | 293.000 K | 293.000 K | 293.000 K |
| 1 | 293.035 K | 293.000 K | 293.032 K |
| 2 | 293.069 K | 293.002 K | 293.063 K |

#### Energy Balance

#### Physical Insights

1. **Robin boundary responds to internal heating:** The boundary temperature rises with the interior temperature ($T_{0,2}$ follows $T_{1,2}$).

Table 5.4: Energy balance per time step

| **Time step** | $Q_{in}$ **[J]** | $Q_{out}$ **[J]** | $\Delta E$ **[J]** |
|---|---|---|---|
| $0 \to 1$ | 10.0 | ≈0.001 | ≈10.0 |
| $1 \to 2$ | 10.0 | ≈0.003 | ≈10.0 |

2. **Heat loss is initially minimal:** For small temperature differences ($\Delta T \approx 0.03$K), the convective heat flux is negligible.
3. **Long-term behavior:** In steady state, an equilibrium will be established where $Q_{in} = Q_{out}$.
4. **Material contrast is effective:** The high edge conductivity to aluminium (114.275 W/(m·K)) ensures rapid heat transport to the inclusion.

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