Topological Optimization Using the SIMP Method

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Outline

- The Volume-to-Point (VP) Heat Conduction Problem
- The Heat Equation
- The Finite Volume Method (FVM)
  - FVM Discretization of Heat Equation
- Optimization
  - The Method of Moving Asymptotes (MMA)
- Solid Isotropic Material with Penalization (SIMP)
- Numerical Experiments

The Volume-to-Point (VP) Heat Conduction Problem

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Suppose that we have a finite amount of high-conductivity (k_+) material available.

Our goal is to determine the optimal distribution of the k_+ material through the given volume such that *the average temperature is minimized*.

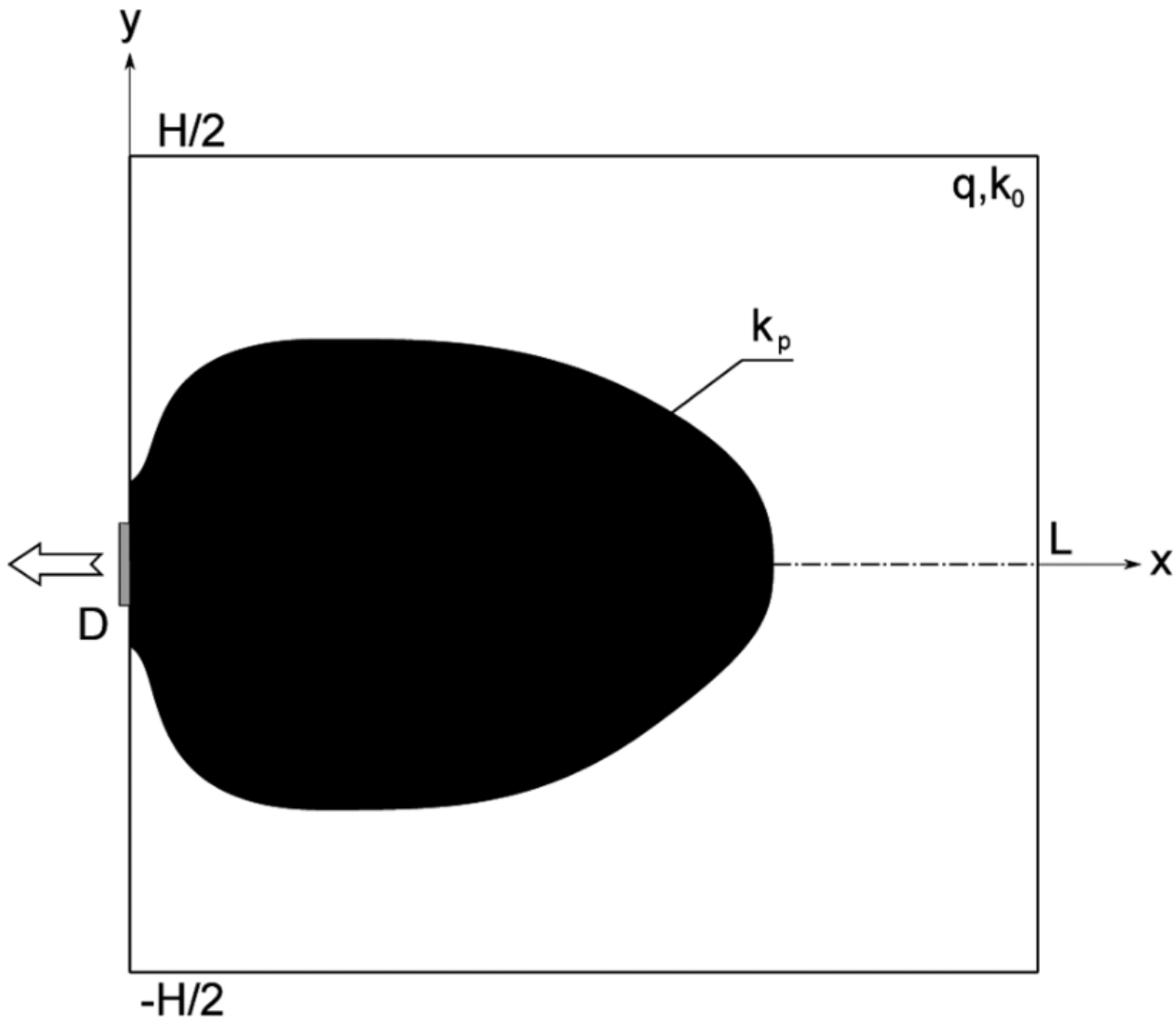

Figure 1: Finite-size volume generating heat (q, k_0) cooled thanks to a high-conductivity structure (k_p) with an arbitrary shape. [4]

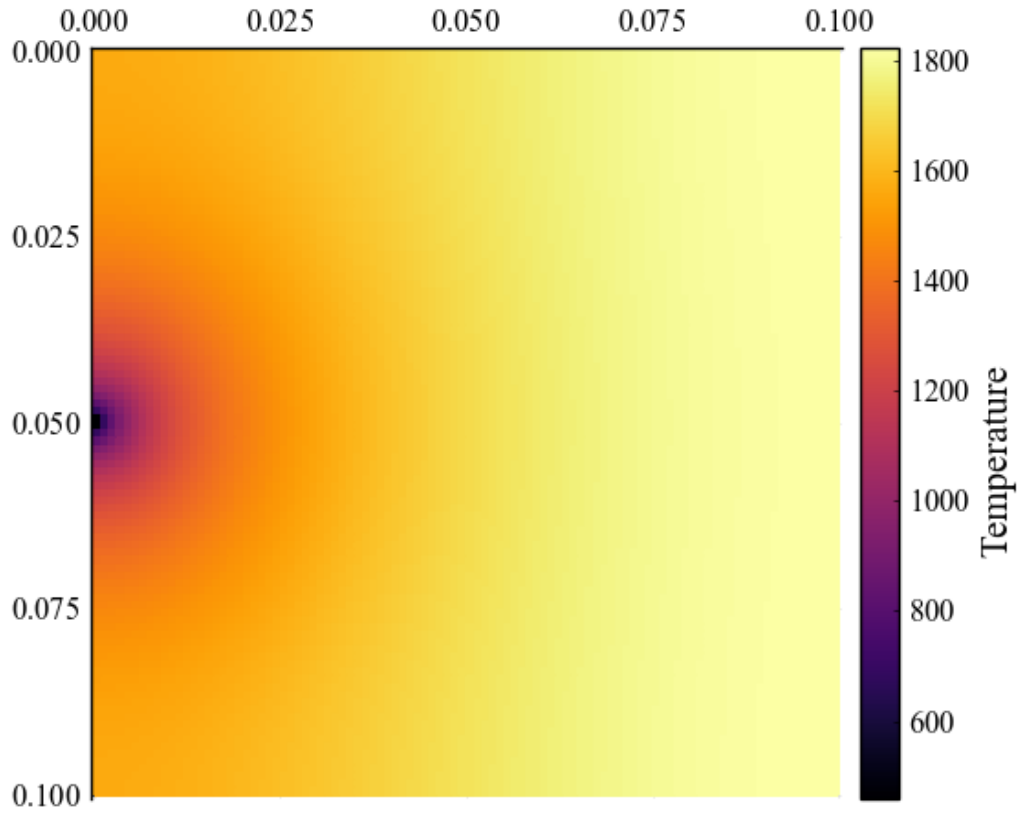

Figure 2: Heatmap for a 0.1m $\times$ 0.1m object with uniform heat generation and a heat sink at the center of its west boundary. This map was produced via the Finite Volume Method using 100×100 uniform control volumes.

The Heat Equation

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Physical principles demand that such a temperature function must satisfy the equation

$$\frac{\partial T}{\partial t} = \nabla \cdot \left(k(\mathbf{x}) \nabla T \right), \tag{1}$$

where ∇ is the gradient operator and the function k represents the thermal diffusivity at a point in our object.

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The main idea of FVM is to integrate the heat equation over each control volume and then use the Divergence Theorem to convert volume integrals into surface integrals involving the fluxes across the boundaries of the control volumes.

Theorem (The Divergence Theorem)

Suppose that $\mathcal{V}$ is a compact subset of $\mathbb{R}^n$ that has a piecewise smooth boundary $\mathcal{S}$ (i.e. $\partial\mathcal{V} = \mathcal{S}$) with outward pointing normal vectors. If $\mathbf{F}$ is a continously differentiable vector field defined on a neighborhood of $\mathcal{V}$, then

$$\iiint_{\mathcal{V}} (\nabla \cdot \mathbf{F}) \, \mathrm{d}\mathcal{V} = \oiint_{\mathcal{S}} (\mathbf{F} \cdot \hat{\mathbf{n}}) \, \mathrm{d}\mathcal{S} \tag{2}$$

where $\hat{\mathbf{n}}$ is the outwards pointing normal vector to the boundary.

Discretization of Heat Equation

$$\int_{V_i} \frac{\partial T}{\partial t}\,\mathrm{d}\mathbf{x} = \int_{V_i} \nabla \cdot \big(k(\mathbf{x})\nabla T\big)\,\mathrm{d}\mathbf{x} \underset{(2)}{=} \int_{\partial V_i} k(\mathbf{x})\nabla T \cdot \hat{\mathbf{n}}\,\mathrm{d}s \qquad (3)$$

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Additionally, let Δx be the length of the North and South boundaries, and Δy the length of the East and West boundaries.

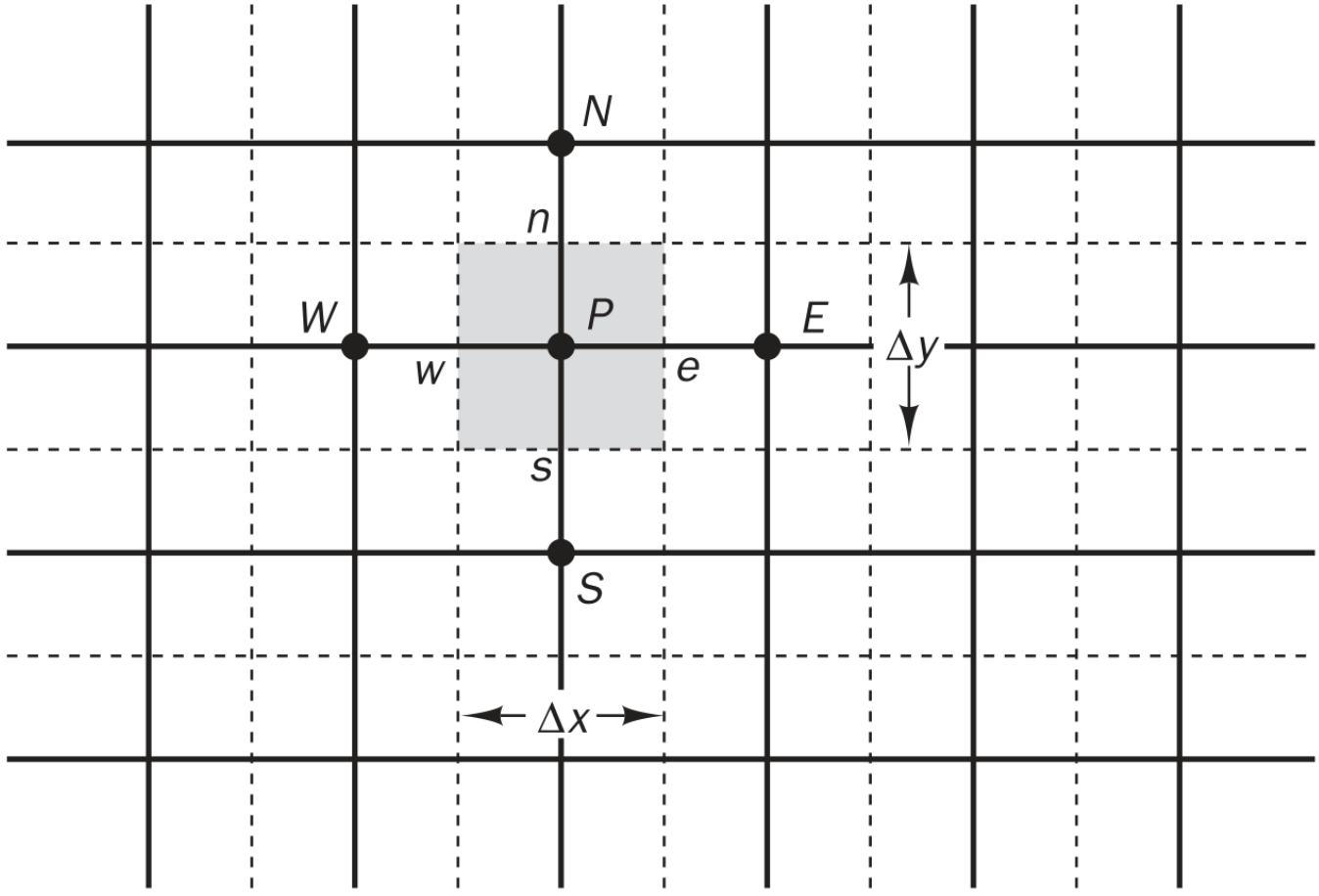

Figure 3: Portion of two-dimensional grid using in the Finite Volume Method for a control volume V_P. [7, p. 129]

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$$\begin{aligned}\int_{\partial V_i} k(\mathbf{x})\nabla T\cdot\hat{\mathbf{n}}\,\mathrm{d}s \quad = \quad & \int_{\partial V_N} k(\mathbf{x})\nabla T\cdot\hat{\mathbf{n}}_N\,\mathrm{d}s + \int_{\partial V_S} k(\mathbf{x})\nabla T\cdot\hat{\mathbf{n}}_S\,\mathrm{d}s \\ & + \int_{\partial V_E} k(\mathbf{x})\nabla T\cdot\hat{\mathbf{n}}_E\,\mathrm{d}s + \int_{\partial V_W} k(\mathbf{x})\nabla T\cdot\hat{\mathbf{n}}_W\,\mathrm{d}s\end{aligned}$$

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$$\int_{V_i} \frac{\partial T}{\partial t}\,\mathrm{d}\mathbf{x} \approx k_N \frac{T_N - T_i}{\|\mathbf{x}_N - \mathbf{x}_i\|}\Delta x + k_S \frac{T_S - T_i}{\|\mathbf{x}_S - \mathbf{x}_i\|}\Delta x$$

$$+ k_E \frac{T_E - T_i}{\|\mathbf{x}_E - \mathbf{x}_i\|}\Delta y + k_W \frac{T_W - T_i}{\|\mathbf{x}_W - \mathbf{x}_i\|}\Delta y$$

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$$\Longrightarrow \Delta x\Delta y\frac{\mathrm{d}T_i}{\mathrm{d}t} = \left(k_N\frac{T_N-T_i}{\|\mathbf{x}_N-\mathbf{x}_i\|} + k_S\frac{T_S-T_i}{\|\mathbf{x}_S-\mathbf{x}_i\|}\right)\Delta x$$

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The Optimization Problem

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Definition

An optimization problem (in standard form) has the form

$$\begin{array}{ll} \text{minimize} & f_0(\mathbf{x}) \\ \text{subject to} & f_i(\mathbf{x}) \leq 0, \quad i = 1, \ldots, m \\ & h_i(\mathbf{x}) = 0, \quad i = 1, \ldots, p \end{array} \tag{4}$$

where

- $\mathbf{x} = (x_1, \ldots, x_n)$ are the optimization variables,
- $f_0 : \mathbb{R}^n \to \mathbb{R}$ is the objective function,
- $f_i : \mathbb{R}^n \to \mathbb{R}$ are the inequality constraint functions, and
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In our VP problem we are concerned with minimizing the function $f_{av}(T)$, the average temperature, subject to an inequality constraint on the maximum volume of conductive material.

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The main differentiating factor between methods is how the descent direction is determined.

For example, the Gradient Descent algorithm chooses $\Delta x = -\nabla f(x)$ as the descent direction, while the Conjugate Gradient method requires that descent directions be conjugate to one another.

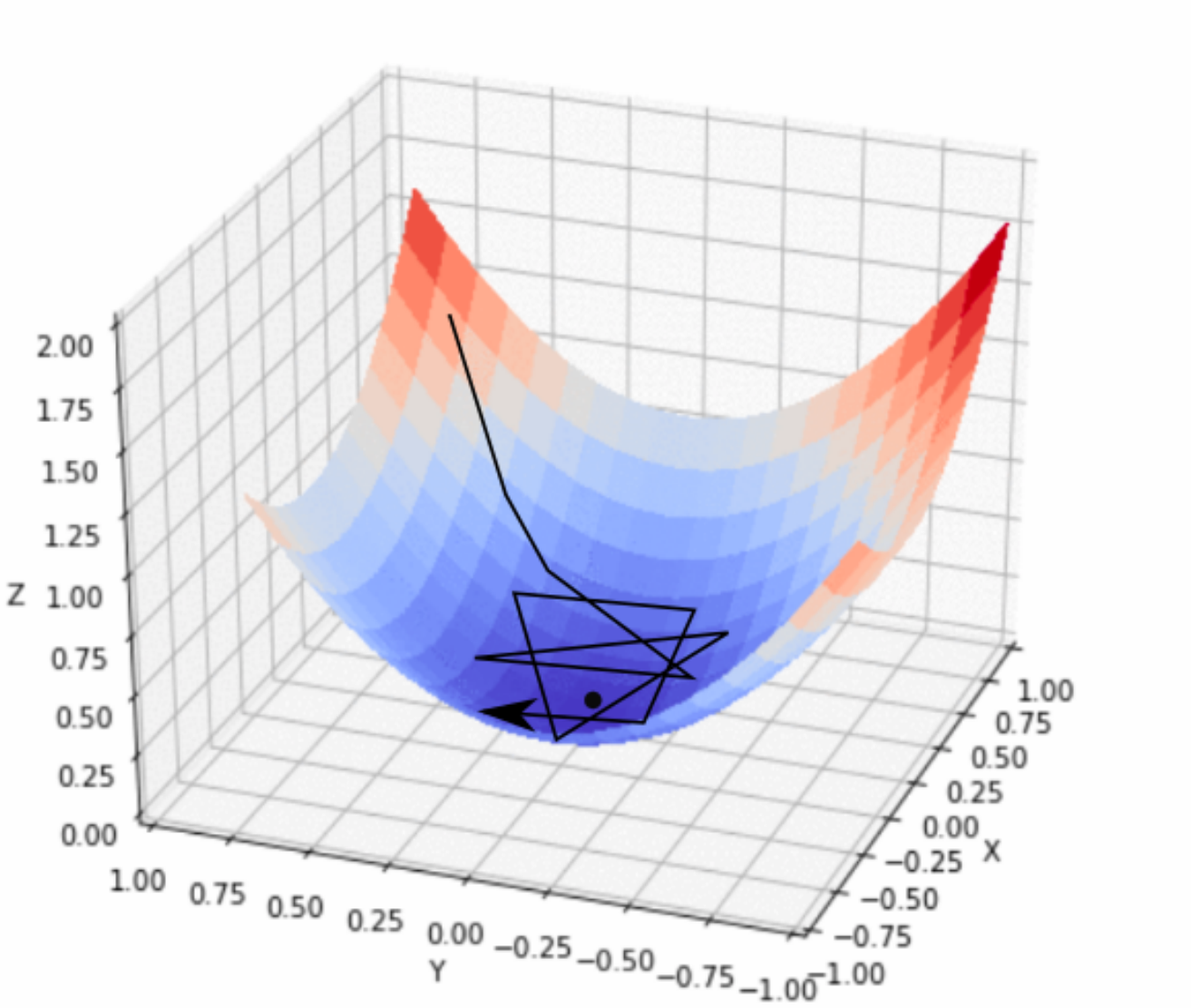

Figure 4: A gradient descent algorithm in action. [3]

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Hence, we will employ a more complicated optimization algorithm.

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These parameters act as asymptotes for the subproblem and moving the asymptotes between iterations stablizes the convergence of the entire process.

The Method of Moving Asymptotes (MMA)

Step 0: Choose a starting point $\mathbf{x}^{(0)}$, and let the iteration index $k = 0$.

Step 1: Given an iterate $\mathbf{x}^{(k)}$, calculate $f_i(\mathbf{x}^{(k)})$ and the gradients $\nabla f_i(\mathbf{x}^{(k)})$ for $i = 0, 1, \ldots, m$.

Step 2: Generate a subproblem $P^{(k)}$ by replacing the functions f_i by approximating functions $f_i^{(k)}$, based on calculations from Step 1.

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Step 3: Solve $P^{(k)}$ and let the optimal solution of this subproblem be the next iteration point $\mathbf{x}^{(k+1)}$. Let $k = k + 1$ and go to Step 1.

Each $f_i^{(k)}$ is obtained by a linearization of f_i in variables of the type

$$\frac{1}{x_j - L_j} \quad \text{or} \quad \frac{1}{U_j - x_j}$$

dependent on the signs of the derivatives of f_i at $\mathbf{x}^{(k)}$. The values of L_j and U_j are normally changed between iterations and are referred to as moving asymptotes.

The Method of Moving Asymptotes (MMA)

Essentially the algorithm is creating *convex* approximations to the objective and constraint functions:

$$f_i^{(k)}(\mathbf{x}) = r_i^{(k)} + \sum_{j=1}^{n} \left(\frac{p_{ij}^{(k)}}{U_j^{(k)} - x_j} + \frac{q_{ij}^{(k)}}{x_j - L_j^{(k)}} \right)$$

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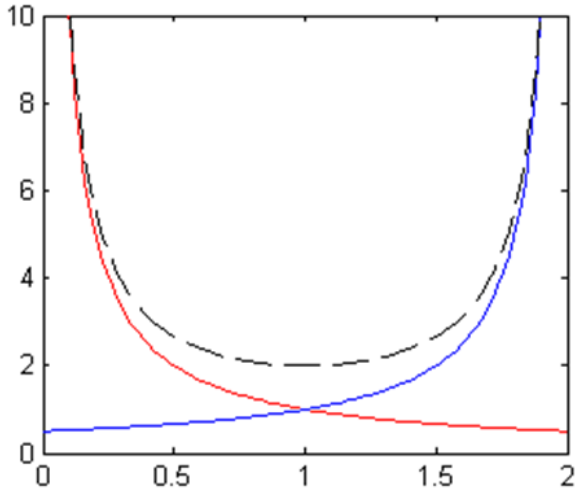

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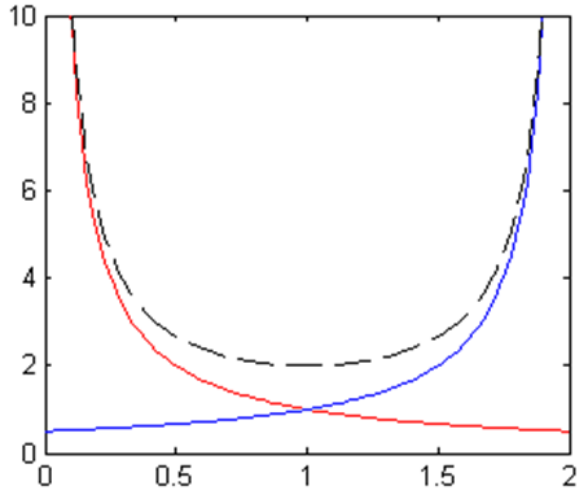

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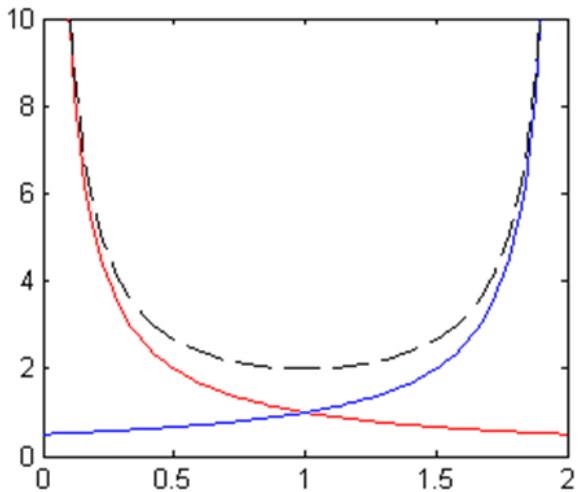

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For our implementation of the SIMP method, the MMA algorithm was employed within the NLopt optimization package in Julia.

Solid Isotropic Material with Penalization (SIMP)

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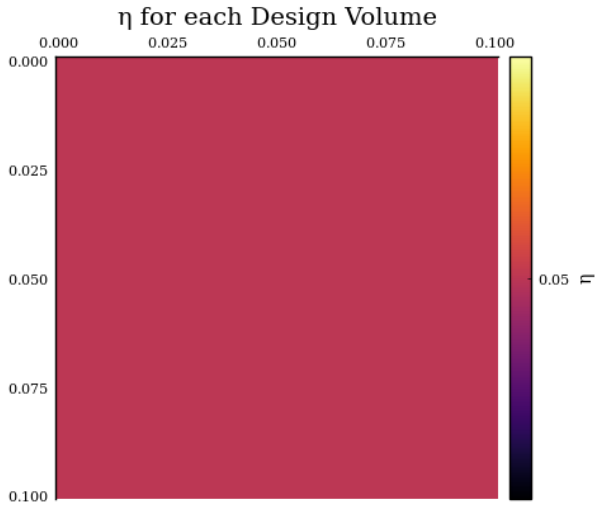
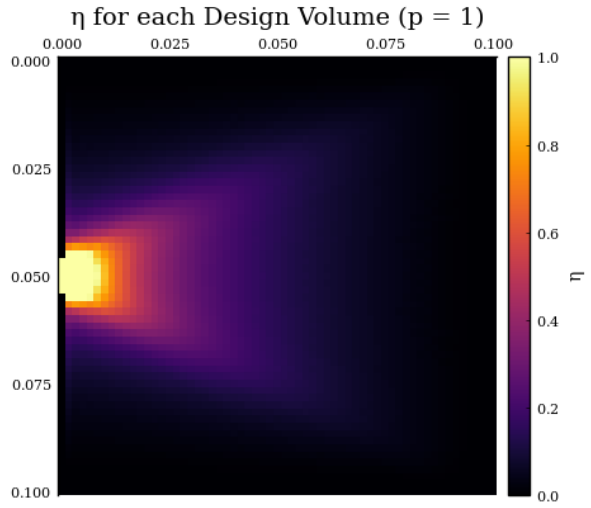
In each step of the SIMP method we increase or decrease the proportion of high-conductivity material used in our object by a small quantity.

This allows us to apply methods designed for continuous optimization problems to the discrete VP problem as it transforms the binary 1—0 problem into a sequence of continuous problems.

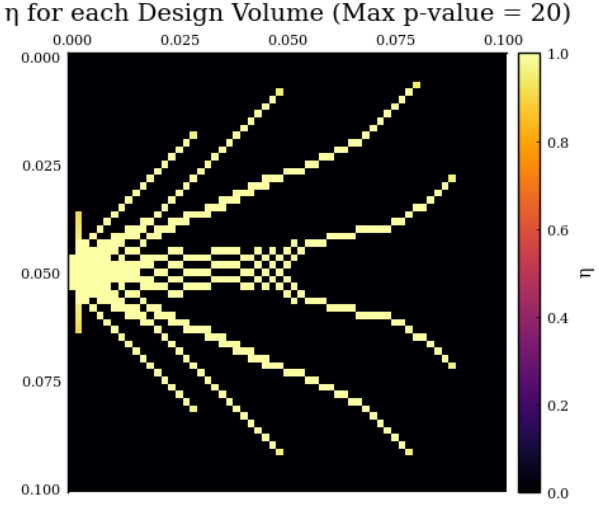
Solid Isotropic Material with Penalization (SIMP)



(a) Initial Design



(b) Design After 1 Outer-Loop



(c) Final Design

Preliminary Parameters

First of all, the energy differential equation driving the heat-flux inside the finite-volume requires:

1. All calculations are run under steady-state conditions. That is, we seek a stable solution where quantities are independent of time.
2. All heat produced in the volume is evacuated through the heat sink.
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We also set the following conditions:

- Thermal conductivities depend only on the material, and therefore are constant:
$$k_0 = 1 \frac{\mathrm{W}}{\mathrm{m}^2\,\mathrm{K}} \qquad \text{and} \qquad k_+ = 100 \frac{\mathrm{W}}{\mathrm{m}^2\,\mathrm{K}}$$
- All structures have a square aspect ratio with $L = H = 0.1\mathrm{m}$
- The heat-sink is located on the middle of the west side of the structure
- The heat-sink has Dirichlet boundary conditions: $T_S = 0°\mathrm{C}$
- All other boundaries are adiabatic (Neumann boundary conditions): $\nabla T \cdot \mathbf{n} = 0$

Notation

We use the following notation to describe the sets involved in the VP-problem:

- $\mathbf{x} \in \Omega =$ two-dimensional spatial field

  We set $\Omega = \Omega_0 \cup \Omega_+$ where
  - $\Omega_0 =$ portion of Ω that has conductivity k_0.
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  - $\Omega_+ =$ portion of Ω with conductivity k_+. This is the portion of the space with high-conductivity material.

Using the above established notation, we develop the following optimization problem:

$$\begin{array}{lll} \text{minimize} & f(T) & \text{for } \Omega_+ \\ \text{subject to} & \nabla \cdot (k \nabla T) + q = 0 & \\ & \mathbf{x} \in \Omega & \end{array} \tag{5}$$

Notation

We use the following notation to describe the sets involved in the VP-problem:

- $\mathbf{x} \in \Omega =$ two-dimensional spatial field

  We set $\Omega = \Omega_0 \cup \Omega_+$ where
  - $\Omega_0 =$ portion of Ω that has conductivity k_0.
  - $\Omega_+ =$ portion of Ω with conductivity k_+. This is the portion of the space with high-conductivity material.

Using the above established notation, we develop the following optimization problem:

$$\begin{array}{lll} \text{minimize} & f(T) & \text{for } \Omega_+ \\ \text{subject to} & \nabla \cdot (k \nabla T) + q = 0 & \\ & \mathbf{x} \in \Omega & \end{array} \tag{5}$$

The objective function $f(T)$ varies depending on desired design outcomes. Some possible objective functions include average temperature (used in our implementation), temperature variance, and maximum temperature.

Porosity Constraint

We impose a constraint upon this problem to limit the quantity of k_+ material available:

$$\int_{\Omega_+} \mathrm{d}\mathbf{x} = \int_{\Omega} \delta_+ \, \mathrm{d}\mathbf{x} \leq V \quad \text{where} \quad \begin{cases} \delta_+ = 0 & \text{if } \mathbf{x} \in \Omega_0 \\ \delta_+ = 1 & \text{if } \mathbf{x} \in \Omega_+ \end{cases} \tag{6}$$

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Inequality (6) imposes a cap on the maximum volume (V) of Ω_+ and hence limits the available amount of high-conductivity material that can be applied to the domain.

If we did not have this constraint, the optimal solution would be to set $\Omega_+ = \Omega$, making the entire domain have high conductivity material.

Penalization Process

The problem of whether to place high conductivity material in a particular location or not is discrete in nature. This is unfortunate as continuous optimization problems are generally easier to solve.

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$$k(\eta) = k_0 + (k_+ - k_0)\,\eta^p \qquad \text{with} \qquad 0 \leq \eta \leq 1 \qquad \text{and} \qquad p \geq 1. \tag{7}$$

η is called the *design parameter* and p the *penalization parameter*.

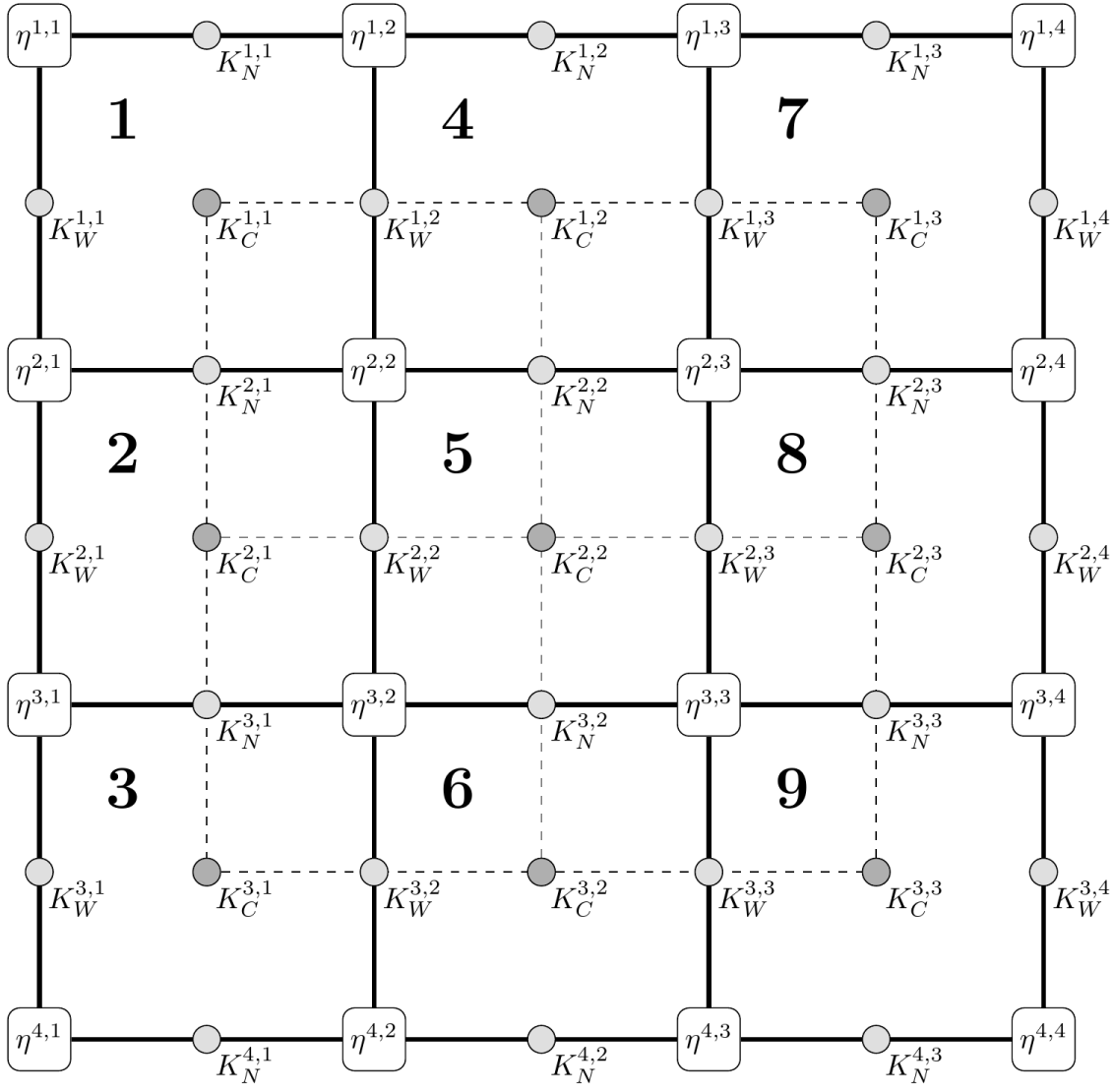

Figure 6: Overlayed Temperature (—) and Design (– – –) grids with 4×4 Design Element ($\eta^{i,j}$) and 3×3 Temperature Control Volume ($K_C^{i,j}$) Nodes. $K_N^{i,j}$ and $K_W^{i,j}$ indicate nodes at the North and West boundaries, respectively, of each Temperature Control Volume. Each Temperature control volume is numbered beginning in the upper left and continuing column-by-column, left-to-right.

Discretization (Again!)

$$\nabla \cdot (k \nabla T) + q = 0 \tag{8}$$

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For temperature control volume (i, j), the finite volume method discretizes (8) into the following linear equation

$$K_C^{i,j} T^{i,j} = K_W^{i,j} T^{i,j-1} + K_W^{i,j+1} T^{i,j+1} + K_N^{i,j} T^{i-1,j} + K_N^{i+1,j} T^{i+1,j} + \Delta x \Delta y Q^{i,j} \tag{9}$$

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The K_W and K_N coefficients are dependent on the thermal conductivity and cross-sectional area of their corresponding faces:

$$K_W^{i,j} = \frac{k_W^{i,j} \Delta y}{\Delta x} \quad \text{and} \quad K_N^{i,j} = \frac{k_N^{i,j} \Delta x}{\Delta y} \tag{10}$$

$$k_W^{i,j} = \frac{k^{i,j} + k^{i+1,j}}{2} \qquad k_N^{i,j} = \frac{k^{i,j} + k^{i,j+1}}{2} \tag{11}$$

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$$K_C^{i,j} = K_W^{i,j} + K_W^{i,j+1} + K_N^{i,j} + K_N^{i+1,j} \tag{12}$$

Discretized Optimization Problem

$$\mathbf{KT} = \Delta x \Delta y \mathbf{Q}. \tag{13}$$

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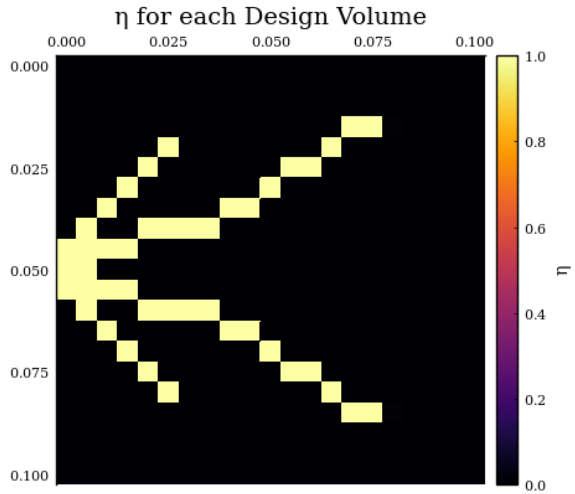
Rearranging what we have done into matrix equations, we can get the following discretized formulation of the average temperature optimization problem:

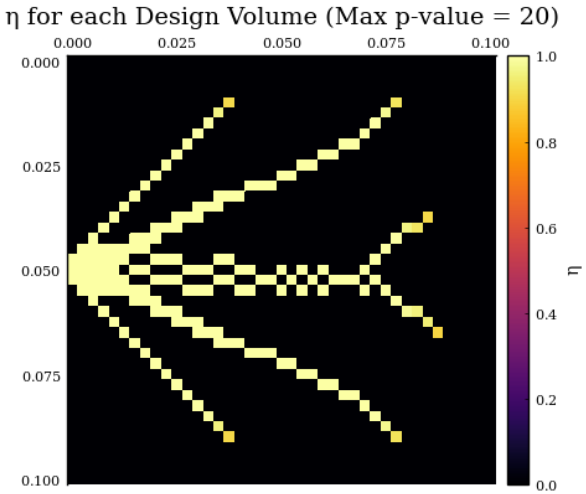
$$\begin{array}{ll} \text{minimize} & f_{av}(\mathbf{T}) = \frac{1}{N_T}\mathbf{1}^T\mathbf{T} \\ \text{subject to} & \mathbf{KT} = \Delta x \Delta y \mathbf{Q} \\ & \mathbf{1}^T\boldsymbol{\eta} - N_T\overline{\phi} \leq 0 \\ & \mathbf{k} = k_0\mathbf{1} + (k_+ - k_0)\boldsymbol{\eta}^p \\ & 0 \leq \boldsymbol{\eta} \leq 1 \text{ and } p \geq 1 \end{array} \tag{14}$$

where N_T represents the number of temperature control volumes and $\overline{\phi}$ represents the maximum porosity (the cap on the amount of high-conductivity material).

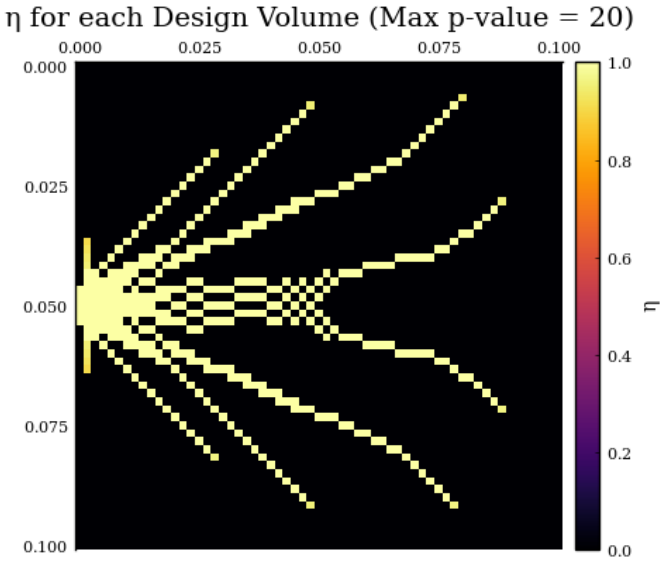
Numerical Experiments



(a) 20×20 control volumes

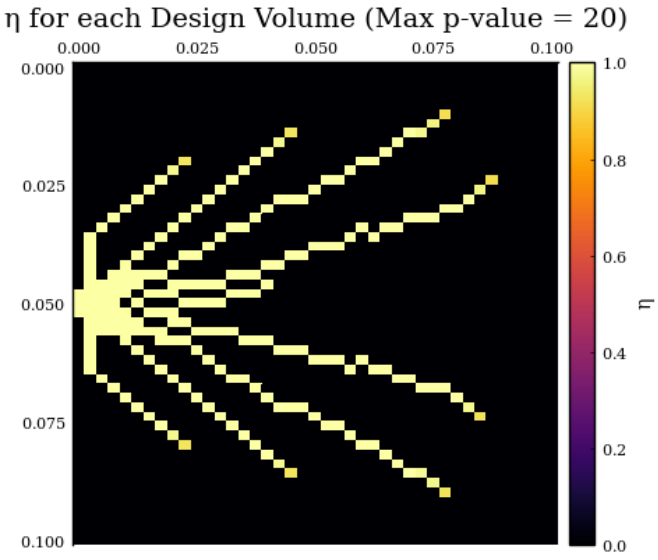


(b) 40×40 control volumes

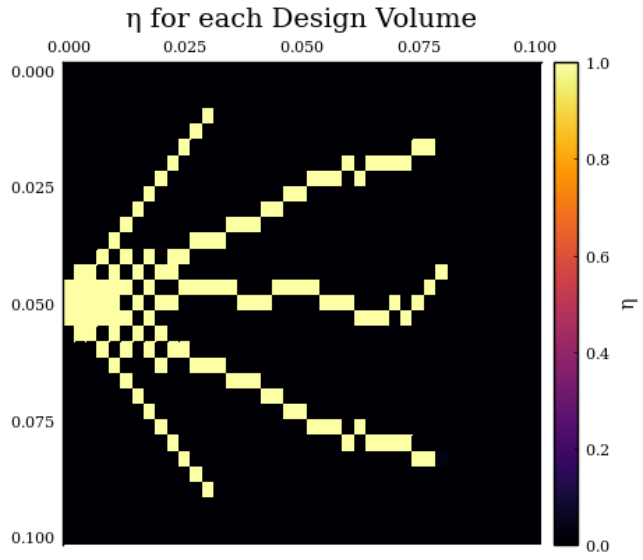


(c) 60×60 control volumes

Non-Square Grids

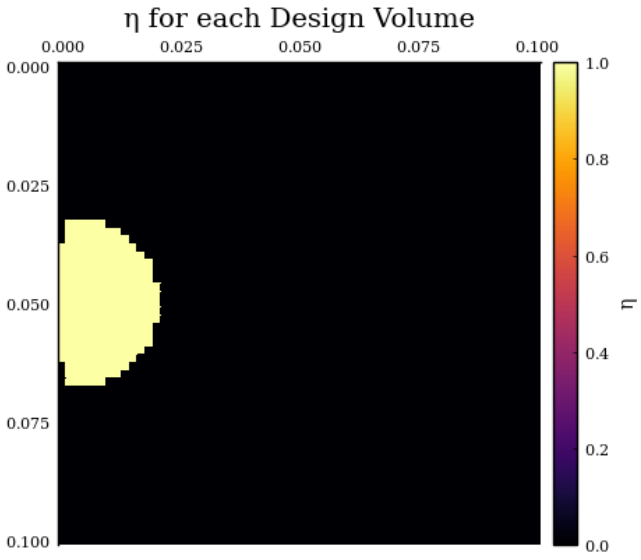


(a) 50×40 control volumes

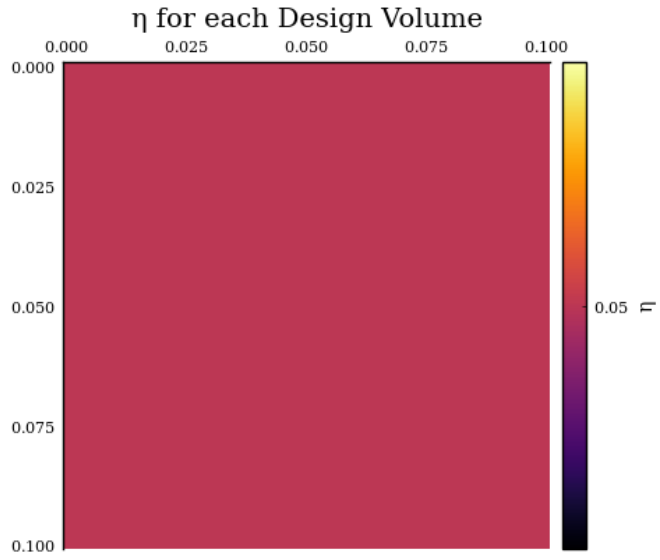


(b) 30×40 control volumes

Higher Initial Penalization



(a) 60×60 Control Volumes with Initial $p = 5$.



(b) 60×60 Control Volumes with Initial $p = 19$.

Figure 9: Design outputs for initial p-values greater than 1.

Minimum Average Temperature Convergence

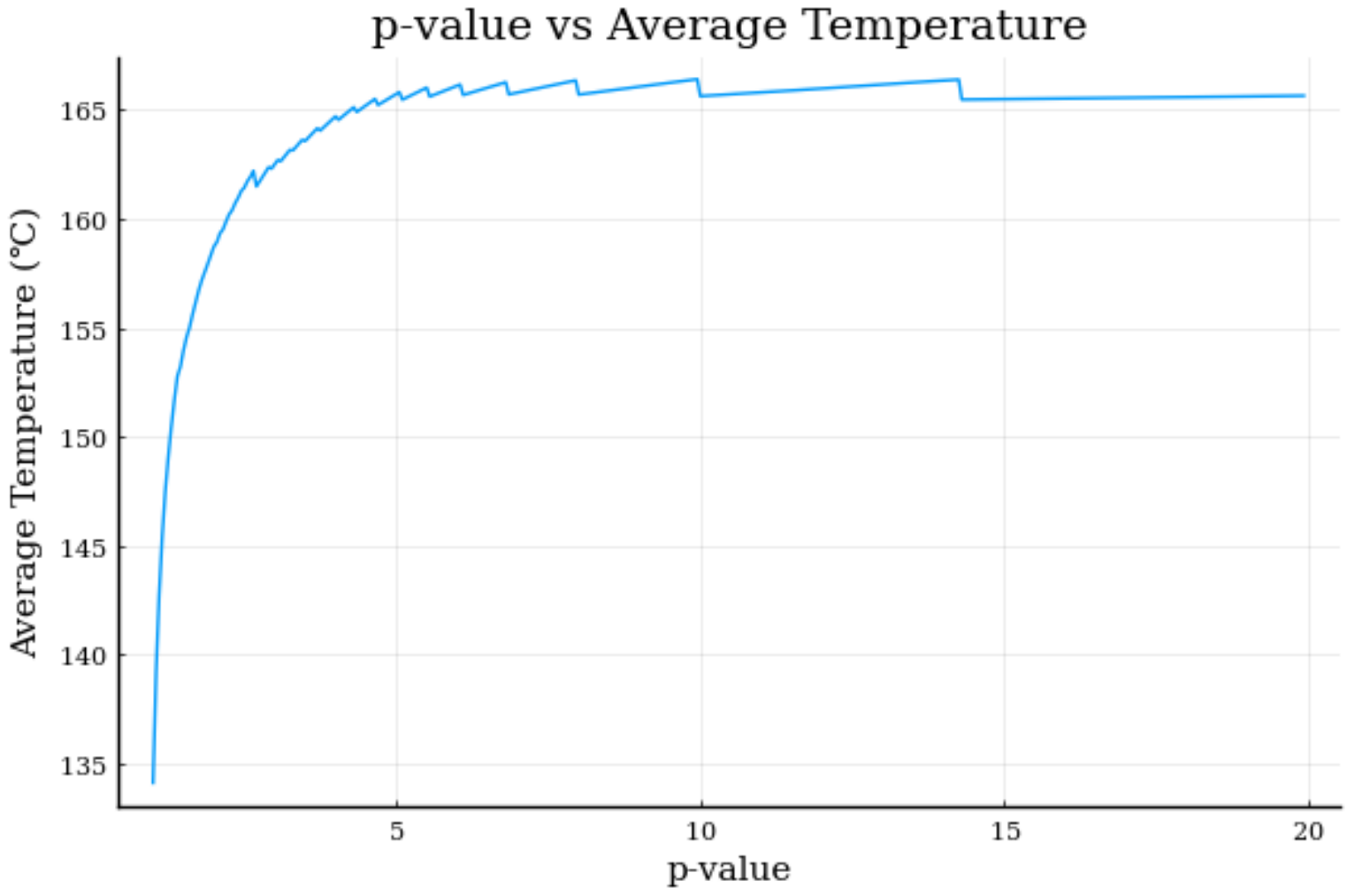
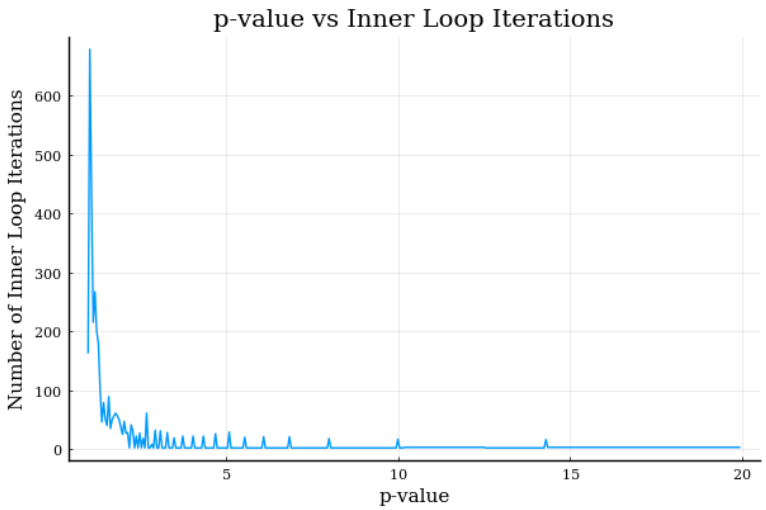
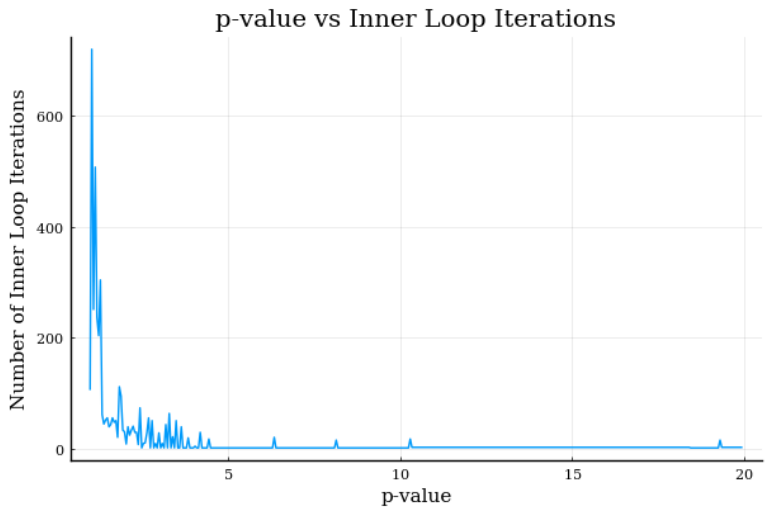


Figure 10: p-value plotted against Average Temperature Evaluation for 60×60 control volumes with a maximum p-value of 20.



(a) p-value plotted against the number of inner loop iterations for 60×60 control volumes with a maximum p-value of 20.



(b) p-value plotted against the number of inner loop iterations for 50×40 control volumes with a maximum p-value of 20.

Figure 11: p-value vs. Number of Inner Loop Iterations for Square and Rectangular Control Volumes

Algorithm Runtime

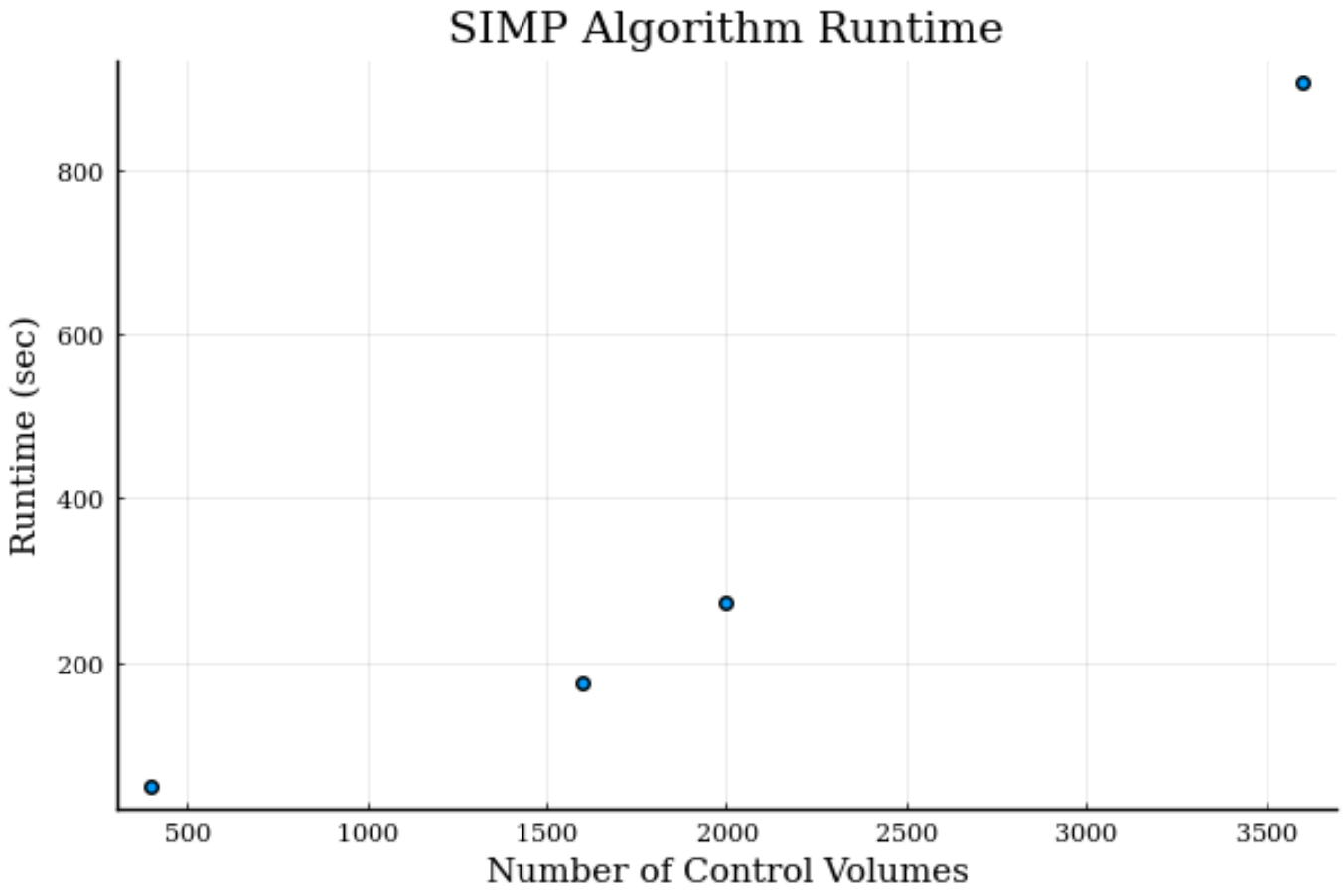


Figure 12: Plot of runtime for SIMP algorithm for various numbers of control volumes.

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Questions?