

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

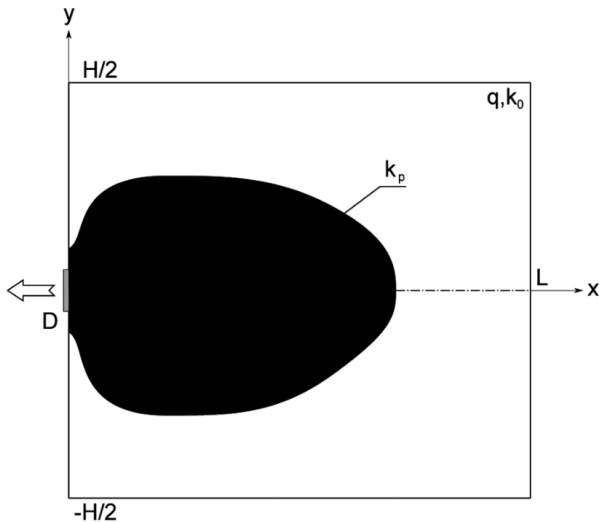
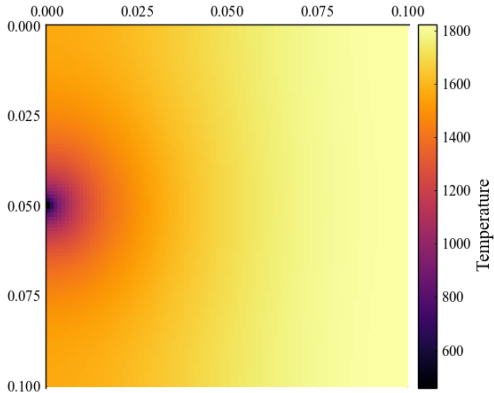


Figure 1: Finite-size volume generating heat ( $q, k_0$ ) cooled thanks to a high-conductivity structure ( $k_p$ ) with an arbitrary shape. [4]



**Figure 2:** Heatmap for a  $0.1\text{m} \times 0.1\text{m}$  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  $100 \times 100$  uniform control volumes.



# The Heat Equation

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

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

where  $\nabla$  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 continuously differentiable vector field defined on a neighborhood of  $\mathcal{V}$ , then*

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

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

## Discretization of Heat Equation

$$\int_{V_i} \frac{\partial T}{\partial t} d\mathbf{x} = \int_{V_i} \nabla \cdot (k(\mathbf{x}) \nabla T) d\mathbf{x} \stackrel{(2)}{=} \int_{\partial V_i} k(\mathbf{x}) \nabla T \cdot \hat{\mathbf{n}} ds \quad (3)$$

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For a control volume  $V_i$  we'll label the North boundary as  $\partial V_N$ , the South boundary as  $\partial V_S$ , the East boundary as  $\partial V_E$ , and the West boundary as  $\partial V_W$ .

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Additionally, let  $\Delta x$  be the length of the North and South boundaries, and  $\Delta y$  the length of the East and West boundaries.

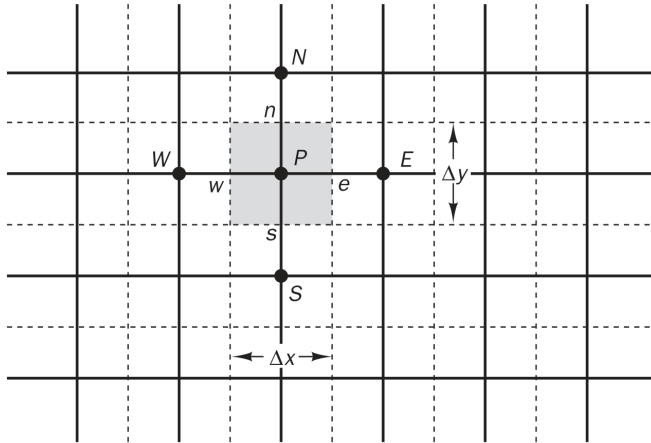


Figure 3: Portion of two-dimensional grid using in the Finite Volume Method for a control volume  $V_P$ . [7, p. 129]

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$$\begin{aligned}\implies \Delta x \Delta y \frac{dT_i}{dt} &= \left( k_N \frac{T_N - T_i}{\|\mathbf{x}_N - \mathbf{x}_i\|} + k_S \frac{T_S - T_i}{\|\mathbf{x}_S - \mathbf{x}_i\|} \right) \Delta x \\ &+ \left( k_E \frac{T_E - T_i}{\|\mathbf{x}_E - \mathbf{x}_i\|} + k_W \frac{T_W - T_i}{\|\mathbf{x}_W - \mathbf{x}_i\|} \right) \Delta y\end{aligned}$$

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An optimization problem (in standard form) has the form

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

where

- ▶  $\mathbf{x} = (x_1, \dots, x_n)$  are the optimization variables,
- ▶  $f_0 : \mathbb{R}^n \rightarrow \mathbb{R}$  is the objective function,
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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.

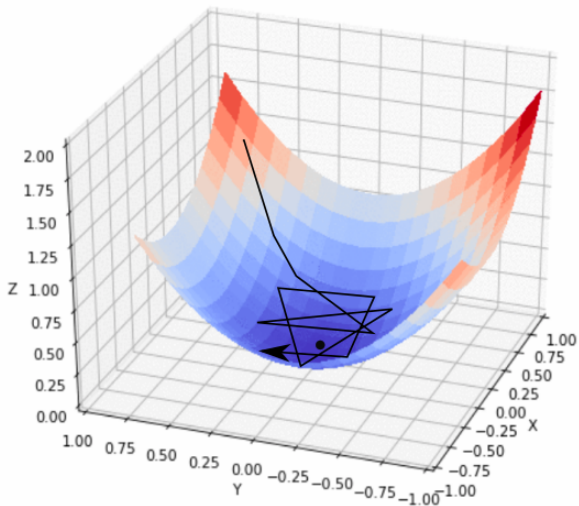


Figure 4: A gradient descent algorithm in action. [3]

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(Convex problems have a lot of properties we can take advantage of that make the optimization problem easier to solve. Most notably, for a convex optimization problem, all local optima are global optima.)

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 stabilizes 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  $i = 0, 1, \dots, m$ .
- 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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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)

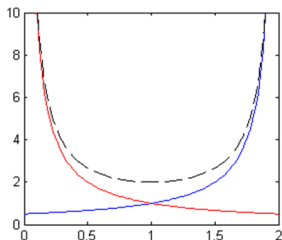
Essentially the algorithm is creating *convex* approximations to the objective and constraint functions:

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

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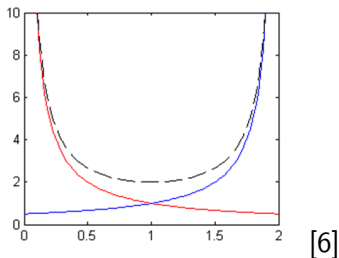
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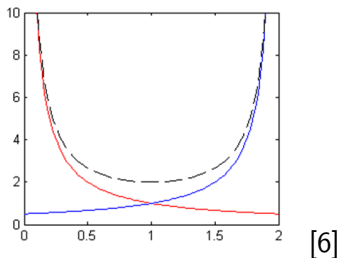


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For our implementation of the SIMP method, the MMA algorithm was employed within the NLOpt optimization package in Julia.

# Solid Isotropic Material with Penalization (SIMP)

Solid Isotropic Material with Penalization (SIMP) is a method based on topology optimization that can be used to solve the VP Heat Conduction Problem.

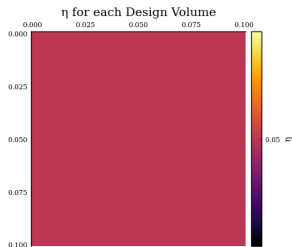
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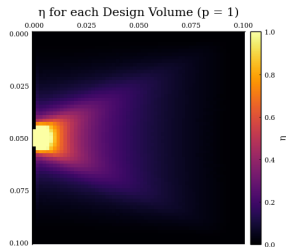
In each step of the SIMP method we increase or decrease the proportion of high-conductivity material used in our object by a small quantity.

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.

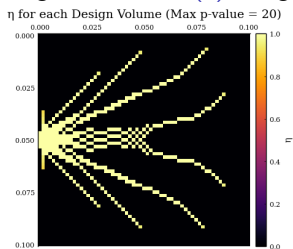
# Solid Isotropic Material with Penalization (SIMP)



(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:

$$k_0 = 1 \frac{\text{W}}{\text{m}^2 \text{K}} \quad \text{and} \quad k_+ = 100 \frac{\text{W}}{\text{m}^2 \text{K}}$$

- ▶ All structures have a square aspect ratio with  $L = H = 0.1\text{m}$
- ▶ The heat-sink is located on the middle of the west side of the structure
- ▶ The heat-sink has Dirichlet boundary conditions:  $T_S = 0^\circ\text{C}$
- ▶ 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  $\Omega$  that has conductivity  $k_0$ .
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$$\begin{array}{ll} \text{minimize} & f(T) \\ \text{subject to} & \nabla \cdot (k \nabla T) + q = 0 \\ & \mathbf{x} \in \Omega \end{array} \quad \text{for } \Omega_+ \quad (5)$$

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

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

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:

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

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Inequality (6) imposes a cap on the maximum volume ( $V$ ) of  $\Omega_+$  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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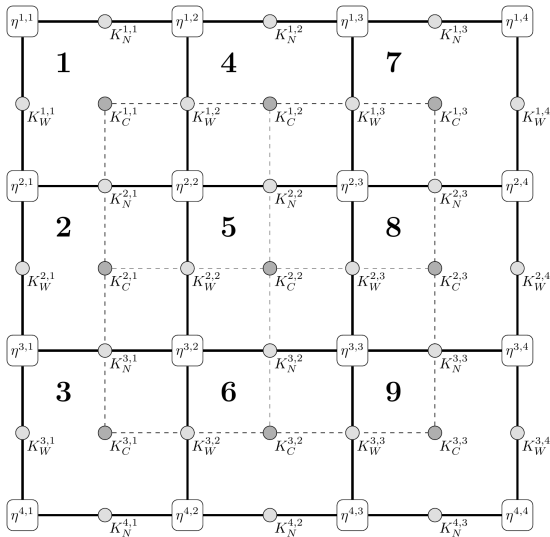
# Penalization Process

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The SIMP method has a clever way of getting around this particular issue of discrete variables: create a continuous function that allows for a “mix” of the two conductive materials.

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

$\eta$  is called the *design parameter* and  $p$  the *penalization parameter*.



**Figure 6:** Overlaid Temperature (—) and Design (---) grids with  $4 \times 4$  Design Element ( $\eta^{i,j}$ ) and  $3 \times 3$  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!)

$$\nabla \cdot (k \nabla T) + q = 0 \quad (8)$$

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

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

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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:

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

$$k_W^{i,j} = \frac{k^{i,j} + k^{i+1,j}}{2} \quad k_N^{i,j} = \frac{k^{i,j} + k^{i,j+1}}{2} \quad (11)$$

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$$K_C^{i,j} = K_W^{i,j} + K_W^{i,j+1} + K_N^{i,j} + K_N^{i+1,j} \quad (12)$$

## Discretized Optimization Problem

$$\mathbf{KT} = \Delta x \Delta y \mathbf{Q}. \quad (13)$$

# Discretized Optimization Problem

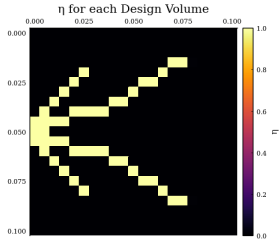
$$\mathbf{KT} = \Delta x \Delta y \mathbf{Q}. \quad (13)$$

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

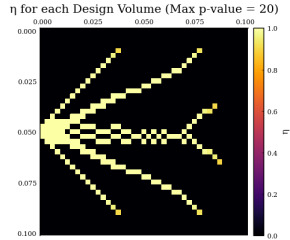
$$\begin{aligned} &\text{minimize} && f_{av}(\mathbf{T}) = \frac{1}{N_T} \mathbf{1}^T \mathbf{T} \\ &\text{subject to} && \mathbf{KT} = \Delta x \Delta y \mathbf{Q} \\ & && \mathbf{1}^T \boldsymbol{\eta} - N_T \bar{\phi} \leq 0 \\ & && \mathbf{k} = k_0 \mathbf{1} + (k_+ - k_0) \boldsymbol{\eta}^p \\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

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

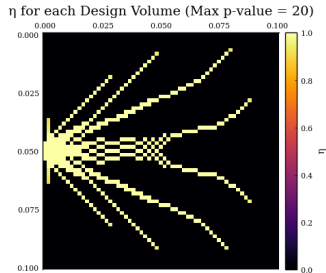
# Numerical Experiments



(a)  $20 \times 20$  control volumes



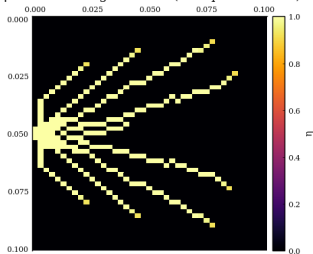
(b)  $40 \times 40$  control volumes



(c)  $60 \times 60$  control volumes

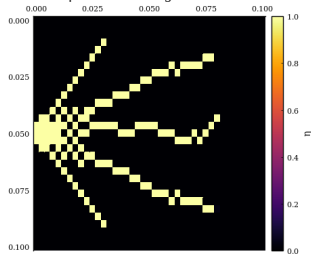
# Non-Square Grids

$\eta$  for each Design Volume (Max p-value = 20)



(a)  $50 \times 40$  control volumes

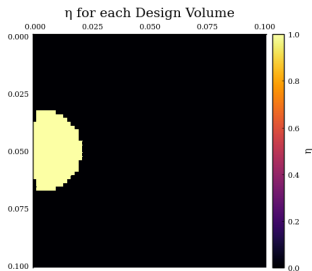
$\eta$  for each Design Volume



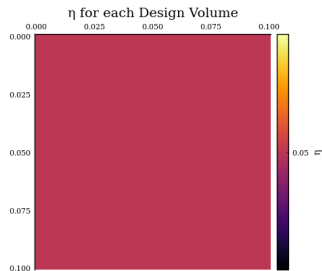
(b)  $30 \times 40$  control volumes



# Higher Initial Penalization



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



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

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

# Minimum Average Temperature Convergence

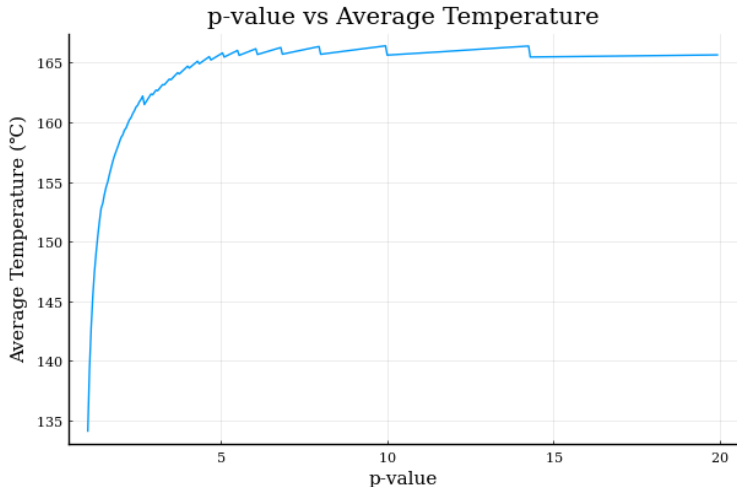
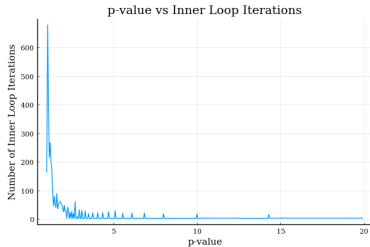
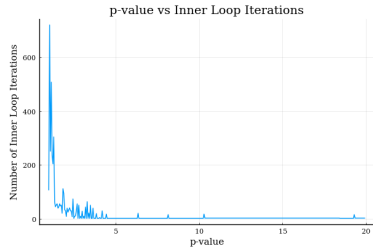


Figure 10:  $p$ -value plotted against Average Temperature Evaluation for  $60 \times 60$  control volumes with a maximum  $p$ -value of 20.



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



(b)  $p$ -value plotted against the number of inner loop iterations for  $50 \times 40$  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

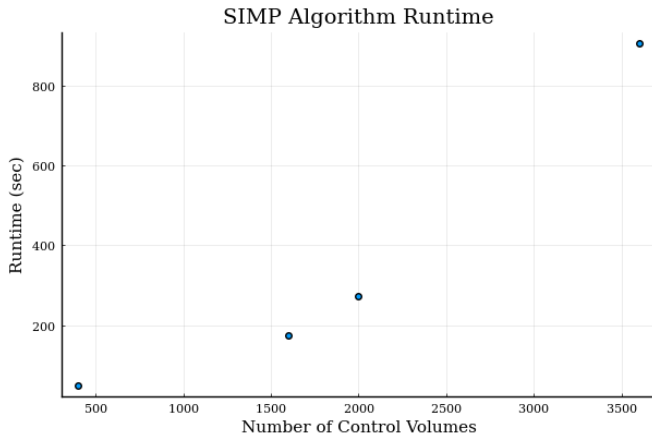


Figure 12: Plot of runtime for SIMP algorithm for various numbers of control volumes.

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# Questions?

