A HEAT-TRANSFER OPTIMIZATION PROBLEM

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By

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Abstract

Discretization is an important tool to transfer optimization problems that include differentiations and integrals into standard optimization problems with a finite number of variables and a finite number of constraints. Recently, Betts and Campbell proposed a heat-transfer optimization problem that includes the heat partial differential equation as one of its constraints, and the objective function includes integrals of the temperature function squared. Using discretization methods, this problem can be converted to a convex quadratic optimization problem, which can be solved by standard interior point method solvers in polynomial time.

The discretized model of the one dimensional problem is further analyzed, and some of its variants are studied. Extensive numerical testing is performed to demonstrate the power of the "discretize then optimize". Then the heat transfer optimization problem is generalized to two dimensions, and the discretized model and computational comparisons for this variant are included.

Flexibility of discretization methods allow us to apply the same "discretize then optimize" methodology to solve optimization problems that include differential and integral functions as constraints or objectives.

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Notation

$\mathcal{P}$: heated object

$\mathcal{P}^0$: boundary region of $\mathcal{P}$

m: space dimension

$\mathbf{x}$: vector $(x^1, x^2, \ldots, x^m)^T$ in $m-$dimensional space that illustrates the position of the points in a heated object

x^k: kth component of the space vector $\mathbf{x}$

x: first component of the space vector $\mathbf{x}$ in 1D and 2D models

y: second component of the space vector $\mathbf{x}$ in 2D model

t: time variable

T: end of time period

$f(\mathbf{x}, t)$: temperature at point $\mathbf{x} \in \mathcal{P}$ and time t

$g(\mathbf{x}, t)$: lower-bound function for the temperature profile

$u(\mathbf{x}, t)$: temperature at the boundary region, $\mathcal{P}^0$, at time t

q_0: weight corresponding to the temperature of the boundary point $u_0(t)$ in the 1D problem

q_ℓ: weight corresponding to the temperature of the boundary point $u_\ell(t)$ in the 1D problem

$\partial^2 f/\partial^2\mathbf{x}$: second order partial differential of f with respect to $\mathbf{x}$

ℓ_x: length of a heated object in $x-$axis

ℓ_y: length of a heated object in $y-$axis

ℓ: length of one dimensional bar, that is, $\ell_x = \ell$ in 1D

n_x: number of discretization points in $x-$axis

n_y: number of discretization points in $y-$axis

x_i: location of the ith point of a heated object in $x-$axis

y_j: location of the jth point of a heated object in $y-$axis

t_s: $(s-1)-$th point in a discretized time interval

$\mathbf{u}$: vector of all variables $u(\mathbf{x}, t)$'s in a discretized model

$\mathbf{f}$: vector of all variables $f(\mathbf{x}, t)$'s in the discretized model

I_k: $k \times k$ identity matrix

$\mathbf{e}_k$: kth unit vector

Preface

Optimization problems that include partial differential equations and integrals arise in many areas. Some of these problems, which include time variables can be solved using optimal control methods. Another approach to solve these problems is to approximate the involved functions and convert the problems to traditional optimization problems. Discretization methods can be used to approximate the differential and integral expressions. The resulting optimization problems typically have a large number of variables and constraints. The coefficient matrices are usually large and sparse. Today, advances in mathematical algorithms, software, and computer technology allows us to handle such large problems.

An example of optimization problems that include integrals and partial differential equations constraint is the heat transfer optimization problem, which is introduced by Betts and Campbell [3]. To make optimal control methods applicable for this problem, they carefully chose the objective functions and the constraints. Their first step to solve the problem is to discretize the functions in space. Then Hamiltonian systems and adjoint variables [2] are used to derive explicitly the optimality conditions. The obtained problem was solved with SOCS[1] [4]. This approach is called "optimize then discretize". As they observed, this method does not converge for even very small number of discretization points. They suggested in their paper that the "discretize then optimize" approach would work much better for this problem.

The "discretized then optimize" methodology for the Betts-Campbell's heat transfer optimization problem is elaborated more in this thesis. This

[1]Sparse Optimal Control Software (SOCS) is a sequential optimal control optimization package.

method allows us to convert the heat transfer optimization problem into a standard convex quadratic problem with linear constraints. The large size of the coefficient matrices motivated Biegler and Kameswaran to compactify the problem [7]. However, our computational results show that the compact model is actually numerically more difficult to solve than the original discretized model. Some of the assumptions and earlier work on this problem are also studied and evaluated in more details. The constraint qualification [10] that has been investigated for this problem is not necessary. The constraint qualification for interior point methods is not needed for linearly constrained convex quadratic problems.

The heat transfer optimization problem can be generalized to two dimensions. In this work, the optimization model for the two-dimensional problem is introduced, and then the problem is converted to the model variant for which the best computational results are obtained in the one-dimensional case. The two-dimensional problem is also solvable with standard interior point solvers, but due to the increasing size of the coefficient matrices, the discretization can not be as fine as in the case of the one-dimensional problem.

"Discretize then optimize" approach is a general powerful method, and can be applied to a large class of problems. Some possible variants and generalizations are introduced at the end of the thesis. These problems can be solved by the "discretize then optimize" strategy that is the subject of future research.

Chapter 1

Heat Transfer Problem

1.1 Introduction

Heat transfer is one of the important transient forms in many problems in mechanical and chemical engineering. In general, the internal transfer of energy by the flow of heat is called heat transfer [5]. Thermal energy is transported in three different modes: conduction, convection, and radiation.

Heat conduction is the mechanism of internal energy exchange from one body to another, or from one part of a body to another. In this thesis, by heat transfer we mean heat conduction through a solid, smooth, isolated object. This transfer occurs because of temperature differences in different parts of the object. The temperature difference is due to heating or cooling of the boundaries. More specifically, the temperature at the boundaries is accessible to be changed, and this provides us a control for the temperature of the other parts of the body. We are seeking optimal changes in the boundaries, so that every part of the object remains as hot (or cool) as desired, and the energy needed to maintain that stays at minimum.

1.2 Heat Equation

Consider an $m-$dimensional object $\mathcal{P}$. Let $\mathbf{x} = (x^1, \cdots, x^m)^T$ be a vector of the $m-$dimensional space. $\mathbf{x} \in \mathcal{P}$ indicates that the point positioned at $\mathbf{x}$, belongs to this object:

$$\mathcal{P} = \{\mathbf{x} \in \mathbb{R}^m \mid \mathbf{x} \in \text{ “the object” } \}.$$

Assume that this object is heat-isolated from its surroundings except for some specified parts of its boundaries $\mathcal{P}^0$, where

$$\mathcal{P}^0 \subseteq \mathcal{P} \subseteq \mathbb{R}^m.$$

Although the object $\mathcal{P}$ could have any shape, to keep the problem as simple as possible and to prevent complication of different shapes and heat flows through the body, we assume that the object is just a solid bar, which is smooth on the outside, and the rate of heat flow is the same through its body. We are interested in observing the temperature of this bar through a time period, say $[0, T]$, while we want certain constraints to be satisfied. Denote the temperature at each point $\mathbf{x}$ of this bar and each time t by $f(\mathbf{x}, t)$.

Since the bar is solid, heat transfer through this bar is by means of conduction. Heat conduction means that the heat equation

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

is satisfied [5], where f is the temperature function, t is time, and κ is the thermal diffusivity, a material constant. Hence, we have to satisfy the heat equation constraint for the bar,

$$\frac{\partial f(\mathbf{x}, t)}{\partial t} = \sum_{i=1}^{m} \frac{\partial^2 f(\mathbf{x}, t)}{\partial^2 x^i}, \tag{1.1}$$

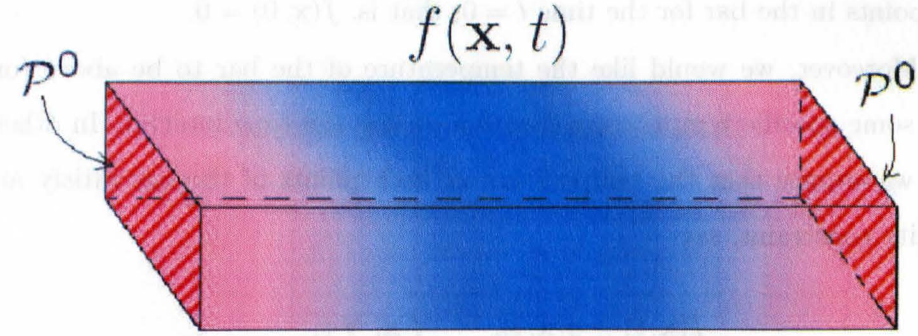

Figure 1.1: A bar heated at its ends.

for all $\mathbf{x} \in \mathcal{P}$ and $t \in [0, T]$, where $\mathcal{P}$ is the observed object, and T is the final time when the observation is done. By $\partial^2 f/\partial^2\mathbf{x}$ we mean the second-order partial differentiation of f with respect to $\mathbf{x}$. In the case when with this partial differential equation (PDE) we are given initial conditions and also boundary conditions, the problem is a classic heat transfer problem, which is well studied in the literature [6]. In one dimension, this PDE can be solved by separation of variables, which will provide us with an analytical solution, and hence the temperature function $f(\mathbf{x}, t)$ is known.

Assume now that boundary conditions are not given. We consider the temperature on the boundaries to be the control variables. The boundary points of the bar are where the bar is connected to a heating/cooling device. The rest of the bar has no connection to the heat source devices, and there is no heat transfer to the environment through any other parts of the bar. Now, according to the heat equation (1.1) and the given initial conditions, the temperature at each points of the bar is a function of time. To avoid unnecessary complications, we assume that the initial condition is zero for all of the points in the bar for the time $t = 0$, that is, $f(\mathbf{x}, 0) = 0$.

Moreover, we would like the temperature of the bar to be above (or below) some specific temperature function during the time interval. In other words, we require that the temperature at each points of the bar satisfy an inequality constraint, say

$$f(\mathbf{x}, t) \geq g(\mathbf{x}, t), \qquad \forall\, \mathbf{x},\ \forall\, t,$$

where $g(\mathbf{x}, t)$ is a given function in time and space. However, by setting only lower-bound condition, many answers might satisfy the constraints. For example, we can heat up the bar to a very high temperature, and then we are sure that the lower bound is satisfied. Note that excessive heat might cause deformations in the bar, might change its physical properties, or even make the bar to melt down. In practice, it is reasonable to seek a temperature profile that is not higher than what is necessary. This goal, usually arises from economical restrictions, as well as natural and engineering limitations.

To satisfy these limitation and to prevent overheating, we should set an appropriate objective function that lowers the temperature, and then try to minimize this function. There are many candidates for the objective function. It can be the total consumed energy to heat or cool down the bar. Minimizing this function will minimize the total cost, while keeping the bar above the lower bound profile, and hence, the obtained temperature, is the lowest possible. Another choice for the objective function can be the sum of the absolute values of all the temperature overshooting in time and space. This will give us a measurement of the energy, that is transferring through the bar. By minimizing this objective, like minimizing the consumed energy, we minimize the total energy throughout the bar. Furthermore, the objective function can be chosen as the worst overshooting of the temperature profile of the bar compared to the lower bound profile. In this case, we are trying to obtain the temperature of the bar as close to the lower bound profile as possible. The temperature of the bar is an approximation of the temperature profile, while satisfying the heat equation and also the initial conditions.

In all the cases, what we are looking for are the values of the control variables, that is, the temperature values at the boundary. By knowing them, we know the heating/cooling pattern at the boundary.

1.3 The Optimization Model of the Problem

First, as the objective function, we choose the sum of all the temperature values squared, over time and space. Since time and the space are continuous intervals, the objective is the integral of the temperature function over time and all spatial coordinates.[1] The objective is

$$\int_0^T \int_{\mathbf{x}\in\mathcal{P}} f^2(\mathbf{x},t)d\mathbf{x}dt + \int_0^T \int_{\mathbf{x}\in\mathcal{P}} u^2(\mathbf{x},t)d\mathbf{x}dt,$$

where $u(\mathbf{x},t)$ is the temperature function at the boundary points of the object, and $\mathbf{x} \in \mathcal{P}^0$. The boundary points of $\mathcal{P}$ are the control points in this problem.

The heat equation constraints, (1.1), is a second order partial differential equation in time and space. The initial setting for this partial differential equation for simplicity is assumed to be zero for all points at time 0:

$$f(\mathbf{x},0) = 0, \qquad \forall\, \mathbf{x} \in \mathcal{P}.$$

Moreover, the temperature profile should satisfy a lower bound inequality.

[1] As it is shown later, this choice will lead to a convex quadratic optimization problem.

Therefore we have

$$f(\mathbf{x},t) \geq g(\mathbf{x},t), \qquad \forall\, \mathbf{x} \in \mathcal{P}.$$

Now, having all the constraints and the objective, we can formulate the optimization model of this problem

$$\min_{f(\mathbf{x},t),u(\mathbf{x},t)} \quad \psi(\mathbf{x},t) = \int_0^T \int_{\mathbf{x}\in\mathcal{P}} f^2(\mathbf{x},t)d\mathbf{x}dt + \int_0^T \int_{\mathbf{x}\in\mathcal{P}} u^2(\mathbf{x},t)d\mathbf{x}dt$$

$$\begin{aligned}
\text{s.t.} \quad & \frac{\partial f(\mathbf{x},t)}{\partial t} = \sum_{i=1}^{m} \frac{\partial^2 f(\mathbf{x},t)}{\partial^2 x^i}, && \forall\, \mathbf{x} = (x^1,\ldots,x^m) \in \mathcal{P} \\
& f(\mathbf{x},t) \geq g(\mathbf{x},t), && \forall\, \mathbf{x} \in \mathcal{P} \\
& f(\mathbf{x},0) = 0, && \forall\, \mathbf{x} \in \mathcal{P} \\
& f(\mathbf{x},t) = u(\mathbf{x},t), && \forall\, \mathbf{x} \in \mathcal{P}^0 \\
& && \forall\, t \in [0,T].
\end{aligned}$$

The above model is a general model for this heat transfer problem, where the lower bound function $g(\mathbf{x},t)$ can be any function. Further, there is no restriction on the dimension of the heated object, or the shape of it, although that surely affects the numerical results. There are variety of choices for the objective function and, to use the methodology studied in this work, even the partial differential equation does not have to be the heat equation. The boundary constraints and initial conditions can be different too, and yet, the same solving strategy is applicable for all of these models.

Chapter 2

The One-Dimensional Case

2.1 The One-Dimensional Model

The optimization model that we specified in Section 1.3 is rather general. For detailed study and numerical experiments, we need to be more specific about the heated object and the constraints. First, to keep the model simple and to facilitate numerical experiments, we assume that the bar is one dimensional, $n = 1$. In other words, we assume a very thin, but long bar that can be considered as a one dimensional object. This is a bar with length ℓ_{x^1} and almost no width or height, that is, $\mathcal{P} = [0, \ell_{x^1}]$.

This assumptions simplify the problem we are interested in, significantly. The points in the bar have only one coordinate, $\mathbf{x} = (x^1)$. For simplicity in notation, let us denote $x := x^1$ and $\ell := \ell_{x^1}$ in the one dimensional case. Therefore, the temperature function, $f(\mathbf{x}, t)$, depends only on two coordinates, x and t. The boundary points of this bar are just the two endpoints of it, namely $x = 0$ and $x = \ell$. The temperature at these two points are the control variables at each given time point. Let us denote them by $u_0(t) = f(0, t)$

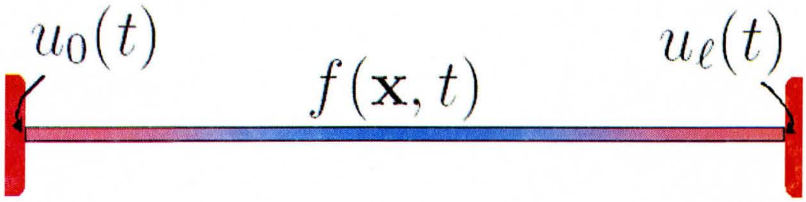

Figure 2.1: One-dimensional bar which is heated at both ends.

and $u_\ell(t) = f(\ell, t)$, respectively.

The heat equation simplifies to two terms

$$\frac{\partial f(x,t)}{\partial t} = \frac{\partial^2 f(x,t)}{\partial^2 x}. \tag{2.1}$$

The initial conditions for this partial differential equation are

$$f(x, 0) = 0, \qquad \forall\, x \in \mathcal{P} = [0, \ell].$$

The goal is to find $u_0(t)$ and $u_\ell(t)$ so that the following objective function obtains its minimum:

$$\int_0^T \int_x f^2(x,t)\,dx\,dt + \int_0^T \left[q_0 u_0^2(t) + q_\ell u_\ell^2(t)\right] dt.$$

The first part of the objective is the integral of the temperature squared over time and space for internal points of the bar. The integral of the temperature of the two boundary points, has been separately formulated in the second term, where the constants q_0 and q_ℓ are two fixed weight numbers corresponding to the endpoints $x = 0$ and $x = \ell$, respectively. Thus, we have the one-dimensional heat transfer optimization problem, where $\mathcal{P} = [0, \ell]$, is

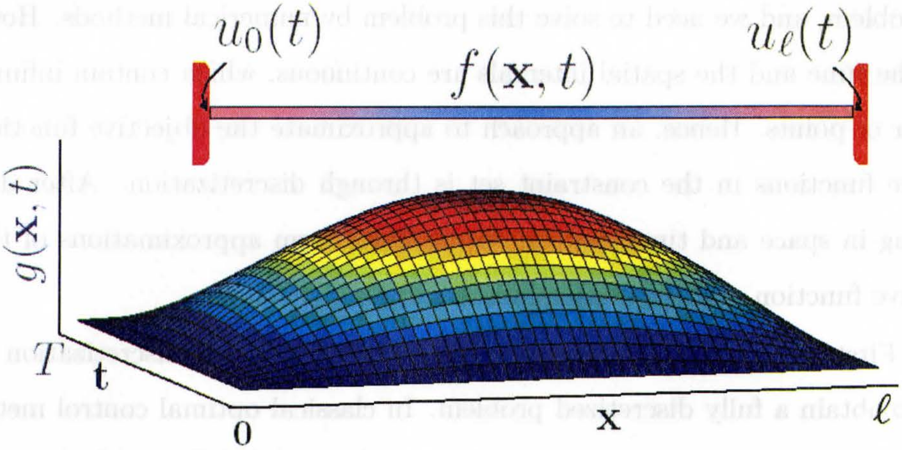

Figure 2.2: The 1D bar with the lower bound temperature profile.

$$\begin{aligned}
\min_{u_0(t),u_\ell(t)} \quad & \psi(x,t) = \int_0^T \int_0^\ell f^2(x,t)dxdt + \int_0^T \left[q_0 u_0^2(t) + q_\ell u_\ell^2(t)\right] dt \\
\text{s.t.} \quad & \frac{\partial f(x,t)}{\partial t} = \frac{\partial^2 f(x,t)}{\partial^2 x}, && \forall\, x \in [0,\ell], \forall\, t \in [0,T] \\
& f(x,t) \geq g(x,t), && \forall\, x \in [0,\ell], \forall\, t \in [0,T] \\
& f(x,0) = 0, && \forall\, x \in [0,\ell], \forall\, t \in [0,T] \\
& f(x,t) = u(x,t), && \forall\, x \in \mathcal{P}^0, \;\; \forall\, t \in [0,T]
\end{aligned}$$

The heat equation is a PDE that is well studied in the applied mathematics literature [6]. An analytical solution can be obtained for this equation when the initial and the boundary conditions are given. However, in the current case, we do not have the boundary conditions as given data. Moreover, there is a temperature lower bound constraint, which has to be satisfied for this problem. Therefore, there is no appropriate analytical method to solve this problem, and we need to solve this problem by numerical methods. However, the time and the spatial intervals are continuous, which contain infinite number of points. Hence, an approach to approximate the objective function and the functions in the constraint set is through discretization. After discretizing in space and time, we can obtain finite term approximations of the objective function and the constraints.

First we apply discretization in space and afterwards discretization in time to obtain a fully discretized problem. In classical optimal control methods, which concern optimization problems with partial differential equation constraints, one can write the continuous optimality conditions first and then either discretize them or discretize a functional analytic method for solving the necessary conditions. However, the optimal control approach does not work for this problem. Betts and Campbell showed in their report [3] that the numerical results from optimal control are not satisfying. They have also chosen a specific lower-bound function and objective function carefully, to ensure applicability of optimal control methods. On the contrary to discretization methods, optimal control methods are highly sensitive to the choice of these functions.

2.2 Spatial Discretization

As a first step in discretization, we discretize the problem in space. The length of the bar is ℓ. Without loss of generality, let the far left point of the bar be at position 0, and the right end of the bar be at position ℓ. Although in general many discretization methods [12] can be applied here, for simplicity, we take n_x to be the number of equally spaced spatial discretization points, while taking equal steps of size $\delta = \ell/n_x$. Denote $x_i = i\delta$, $i = 0, 1, \ldots, n_x$, to be the ith discretization point. Therefore we have $f(x_0, t) = f(0, t) = u_0(t)$, and $f(x_{n_x}, t) = f(\ell, t) = u_\ell(t)$.

Now we should approximate the objective function and the constraints using these n_x points. For the objective function, we use the trapezoidal method [1] to approximate the space dependent integral:

$$
\begin{aligned}
\int_0^\ell f^2(x,t)dx &\approx \delta \sum_{i=0}^{n_x-1} \frac{f^2(x_i,t) + f^2(x_{i+1},t)}{2} \\
&= \frac{\delta}{2}\left[f^2(x_0,t) + f^2(x_{n_x},t) + \sum_{k=1}^{n_x-1} 2f^2(x_i,t)\right] \\
&= \frac{\delta}{2}\left[u_0^2(t) + u_\ell^2(t)\right] + \delta \sum_{i=1}^{n_x-1} f^2(x_i,t).
\end{aligned}
$$

Assume that the weight numbers of the endpoints, $q_0 = q_\ell$, are equal to each other, and denote the common value by q. Now substituting the above approximation in the objective function and reordering the terms with u_0 and u_ℓ gives us

$$
\begin{aligned}
\psi(x,t) &= \int_0^T \int_0^\ell f^2(x,t)dxdt + q\int_0^T \left[u_0^2(t) + u_\ell^2(t)\right] dt \\
&\approx \int_0^T \frac{\delta}{2}\left[u_0^2(t) + u_\ell^2(t)\right] dt + \int_0^T \delta \sum_{i=1}^{n_x-1} f^2(x_i,t)dt \\
&\qquad + q\int_0^T \left[u_0^2(t) + u_\ell^2(t)\right] dt \\
&= \delta \int_0^T \sum_{i=1}^{n_x-1} f^2(x_i,t)dt + \left(\frac{\delta}{2} + q\right)\int_0^T \left[u_0^2(t) + u_\ell^2(t)\right] dt. \qquad (2.2)
\end{aligned}
$$

In the constraints, the partial differential equations (2.1) are of the second order in space and the first order in time. To approximate the spatial dependencies in the PDEs, among all possible approximation methods [1], we choose the second-order finite difference method. For the inner points we have

$$\frac{\partial f(x_i,t)}{\partial t} = \frac{f(x_{i-1},t) - 2f(x_i,t) + f(x_{i+1},t)}{\delta^2},$$

where $i = 2, \ldots, n_x - 2$. The approximations that include the endpoints are

$$\begin{aligned}\frac{\partial f(x_1,t)}{\partial t} &= \frac{u_0 - 2f(x_1,t) + f(x_2,t)}{\delta^2}\\ \frac{\partial f(x_{n_x-1},t)}{\partial t} &= \frac{f(x_{n_x-2},t) - 2f(x_{n_x-1},t) + u_\ell}{\delta^2}.\end{aligned}$$

Now we have a system of ordinary differential equations.

In the lower-bound constraint, we only consider the value of the functions at the discretized spatial points, $x_0, \ldots, x_{n_x}$. Thus, we have

$$\begin{aligned}&0 \le f(x_i,t) - g(x_i,t), && i = 1, \ldots, n_x - 1\\ &0 \le u_0(t) - g(0,t),\\ &0 \le u_\ell(t) - g(\ell,t).\end{aligned}$$

Therefore, the spatially-discretized heat transfer optimization problem is

$$\min_{u_0(t),u_\ell(t)} \quad \delta \int_0^T \sum_{i=1}^{n_x-1} f^2(x_i,t)dt + \left(\frac{\delta}{2} + q\right) \int_0^T \left[u_0^2(t) + u_\ell^2(t)\right] dt \tag{2.3}$$

$$\begin{aligned}\text{s.t.} \quad \frac{\partial f(x_1,t)}{\partial t} &= \frac{u_0(t) - 2f(x_1,t) + f(x_2,t)}{\delta^2}\\ \frac{\partial f(x_i,t)}{\partial t} &= \frac{f(x_{i-1},t) - 2f(x_i,t) + f(x_{i+1},t)}{\delta^2} \quad i = 2, \ldots, n_x - 2\\ \frac{\partial f(x_{n_x-1},t)}{\partial t} &= \frac{f(x_{n_x-2},t) - 2f(x_{n_x-1},t) + u_\ell(t)}{\delta^2}\\ f(x_i,t) &\ge g(x_i,t)\\ u_0(t) &\ge g(0,t)\\ u_\ell(t) &\ge g(\ell,t)\end{aligned}$$

$$
\begin{aligned}
&f(x_0, t) = u_0(t) \\
&f(x_n, t) = u_\ell(t) \\
&f(x_i, 0) = 0 \qquad\qquad i = 0, \ldots, n_x,
\end{aligned}
$$

for all $t \in [0, T]$.

2.3 Time Discretization

Now we can proceed to discretize this problem in time. Again, among all possible distribution of the discretization points, we take N equally distributed discretization points in the time interval $[0, T]$. Since we are taking steps with equal lengths, the step size is $h = T/N$. Denote the temperature function for these points by $f(x_i, t_s) = f\big(x_i, (s-1)h\big)$, $u_0(t_s) = u\big((s-1)h\big)$, and $u_\ell(t_s) = u_\ell\big((s-1)h\big)$.

To approximate the time-dependent integrals in the objective function, we use the rectangular rule [1]. (That is assuming the value of the function in an interval is the function value at the far left point of the interval). Therefore the objective function (2.3) is approximated as

$$\psi(x,t) \approx h\delta \sum_{s=1}^{N} \sum_{i=1}^{n_x - 1} f^2(x_i, t_s) + h\left(\frac{\delta}{2} + q\right) \sum_{s=1}^{N} \left[u_0^2(t_s) + u_\ell^2(t_s)\right]. \quad (2.4)$$

There are only quadratic terms in this function with positive coefficients, hence a convex quadratic function.

For the ordinary differential equations, we use the first order finite difference method. The approximated heat equation in time and space is

$$\frac{f(x_1,t_{s+1})-f(x_1,t_s)}{h}=\frac{u(t_s)-2f(x_1,t_s)+f(x_2,t_s)}{\delta^2}, \qquad s=1,\ldots,N$$

$$\frac{f(x_i,t_{s+1})-f(x_i,t_s)}{h}=\frac{f(x_{i-1},t_s)-2f(x_i,t_s)+f(x_{i+1},t_s)}{\delta^2}, \qquad s=1,\ldots,N$$

$$i=2,\ldots,n_x-1$$

$$\frac{f(x_{n_x},t_{s+1})-f(x_{n_x},t_s)}{h}=\frac{f(x_{n_x-2},t)-2f(x_{n_x-1},t)+u_\ell(t)}{\delta^2}, \quad s=1,\ldots,N.$$

So we obtain a rather large $(n_x+1)\times N$ system of linear equations. The lower bound functions and the initial condition functions are also approximated by taking the function value only at the discretized points. Therefore, the fully discretized optimization problem is

$$\min_{u_0,u_\ell} \quad h\delta\sum_{s=1}^{N}\sum_{i=1}^{n_x-1} f^2(x_i,t_s)+h\left(\frac{\delta}{2}+q\right)\sum_{s=1}^{N}\left[u_0^2(t_s)+u_\ell^2(t_s)\right] \tag{2.5}$$

$$\begin{aligned}
\text{s.t.} \quad & \frac{f(x_1,t_{s+1})-f(x_1,t_s)}{h}=\frac{u(t_s)-2f(x_1,t_s)+f(x_2,t_s)}{\delta^2} \\
& \frac{f(x_i,t_{s+1})-f(x_i,t_s)}{h}=\frac{f(x_{i-1},t_s)-2f(x_i,t_s)+f(x_{i+1},t_s)}{\delta^2} \\
& \qquad\qquad\qquad\qquad i=2,\ldots,n_x-1 \\
& \frac{f(x_{n_x},t_{s+1})-f(x_{n_x},t_s)}{h}=\frac{f(x_{n_x-2},t)-2f(x_{n_x-1},t)+u_\ell(t)}{\delta^2} \\
& u_0(t_s)-g(0,t_s)\geq 0 \\
& u_\ell(t_s)-g(n_x,t_s)\geq 0 \\
& f(x_i,t_s)-g(x_i,t_s)\geq 0 \qquad\qquad i=1,\ldots,n_x-1 \\
& f(x_i,t_1)=0 \qquad\qquad i=1,\ldots,n_x-1 \\
& u_0(t_1)=0 \\
& u_\ell(t_1)=0,
\end{aligned}$$

for all $s = 1, \ldots, N$.

Since we have a convex quadratic objective function here, and all of the constraints are linear, the resulting problem is a convex quadratic optimization problem. This class of problems can be solved in polynomial time by using interior point methods [11]. Moreover, since the problem is convex, the achieved optimum is guaranteed to be the global minimum for this problem.

2.4 A More Specific Example

To obtain numerical results, we need to specify the functions that are involved in the optimization model. We consider this problem with a specified lower bound constraint, and time and space intervals, and analyze the results further. The specified functions and intervals that we use here have been introduced by Betts and Campbell [3]. They chose these functions to ensure that optimal control methods are applicable as well.

Assume that the length of the bar is π. We are observing the temperature of this one dimensional bar during the time period $[0, 5]$. We also require that the temperature satisfy the lower-bound constraint

$$f(x,t) \geq g(x,t) = c\left[\sin(x)\sin\left(\frac{\pi t}{5}\right) - a\right] - b, \tag{2.6}$$

with $a = 0.5$, $b = 0.2$, and $c = 1$. Thus, we have

$$g(x,t) = \sin(x)\sin\left(\frac{\pi t}{5}\right) - 0.7.$$

By these assumptions, we have $\ell = \pi$, $T = 5$, $u_\ell(t) = u_\pi(t)$, and $\delta = \pi/n_x$. Thereby, the optimization problem is

$$\min_{u_0(t), u_\pi(t)} \quad \psi(x,t) = \int_0^5 \int_0^\pi f^2(x,t)dxdt + q\int_0^5 \left[u_0^2(t) + u_\pi^2(t)\right]dt$$

$$
\begin{aligned}
\text{s.t.} \quad & \frac{\partial f(x,t)}{\partial t} = \frac{\partial^2 f(x,t)}{\partial^2 x} && \forall\, x \in [0,\pi], \forall\, t \in [0,5] \\
& f(x,t) \geq \sin(x) \sin\left(\frac{\pi t}{5}\right) - 0.7 && \forall\, x \in [0,\pi], \forall\, t \in [0,5] \\
& f(x,0) = 0 && \forall\, x \in [0,\pi], \forall\, t \in [0,5] \\
& f(0,t) = u_0(t) && \forall\, t \in [0,5] \\
& f(\pi,t) = u_\pi(t) && \forall\, t \in [0,5].
\end{aligned}
$$

The solution strategy is exactly the same for this problem as outlined in Sections 2.2 and 2.3. After discretizing in space, we use the second-order difference method to approximate the partial differential equation. The integral in the objective function is approximated by the trapezoidal method. The rest of the functions are just discretized to their values at the selected points in space.

After space discretization, Betts and Campbell introduced a new variable τ for time [3]. This new variable might have improved the results in optimal control methods, but it seems that it is merely scaling when using discretization method. Regardless, in the one dimensional case, we use this new variable too, to follow the Betts and Campbell's model. Denote $\tau = t/\delta^2$. The time interval and the derivatives in terms of τ are

$$
\begin{aligned}
& 0 \leq t \leq 5 && \rightarrow && 0 \leq \tau \leq 5\delta^{-2} && \rightarrow && \tau \in [0, T'] = [0, 5\delta^{-2}] \\
\Rightarrow \quad & \partial\tau = \frac{\partial t}{\delta^2} && \rightarrow && \partial\tau = \delta^{-2}\partial t.
\end{aligned}
$$

By the above expression, the semi-discretized objective function (2.3) can be written in terms of τ as

$$\begin{aligned}\psi(x,t) &= \delta \int_0^5 \sum_{i=1}^{n_x-1} f^2(x_i,t)dt + \left(\frac{\delta}{2}+q\right)\int_0^5 \left[u_0^2(t)+u_\pi^2(t)\right]dt\\ &= \delta^3 \int_0^{5\delta^{-2}} \sum_{i=1}^{n_x-1} f^2(x_i,\tau)d\tau + \left(\delta^2\frac{\delta}{2}+q\right)\int_0^{5\delta^{-2}} \left[u_0^2(\tau)+u_\pi^2(\tau)\right]d\tau.\end{aligned}$$

This change of variable allow us to eliminate the denominator of the equality constraints. The ordinary differential equations of the internal points of the bar in terms of τ are as follows

$$\begin{aligned}\frac{\partial f(x_i,\tau)}{\partial \tau} &= \frac{\partial f(x_i,\tau)}{\partial t}\frac{\partial t}{\partial \tau}\\ \Rightarrow \frac{\partial f(x_i,\tau)}{\partial \tau} &= f(x_{i-1},\tau) - 2f(x_i,\tau) + f(x_{i+1},\tau).\end{aligned}$$

Noting that $t = \delta^{-2}\tau$, the lower bound function and the the rest of the constraints can be written in terms of τ as well. Hence, the optimization problem has the form

$$\min_{u_0(\tau),u_\pi(\tau)} \quad \delta^3 \int_0^{5\delta^{-2}} \sum_{i=1}^{n_x-1} f^2(x_i,\tau)d\tau + \left(\frac{\delta^3}{2}+q\right)\int_0^{5\delta^{-2}} \left[u_0^2(\tau)+u_\pi^2(\tau)\right]d\tau$$

$$\begin{aligned}\text{s.t.}\quad \frac{\partial f(x_1,\tau)}{\partial \tau} &= u_0(\tau) - 2f(x_1,\tau) + f(x_2,\tau)\\ \frac{\partial f(x_i,\tau)}{\partial \tau} &= f(x_{i-1},\tau) - 2f(x_i,\tau) + f(x_{i+1},\tau) \qquad i = 2,\ldots,n_x-2\\ \frac{\partial f(x_{n_x-1},\tau)}{\partial \tau} &= f(x_{n_x-2},\tau) - 2f(x_{n_x-1},\tau) + u_\pi(\tau)\end{aligned}$$

$$\begin{aligned}f(x_i,\tau) &\geq \sin(i\delta)\sin\left(\frac{\pi\delta^{-2}\tau}{5}\right) - 0.7 \qquad i = 1,\ldots,n_x-1\\ u_0(\tau) &\geq -0.7\\ u_\pi(\tau) &\geq -0.7\end{aligned}$$

$$
\begin{aligned}
&f(x_0, \tau) = u_0(\tau) \\
&f(x_n, \tau) = u_\pi(\tau) \\
&f(x_i, 0) = 0 && i = 0, \ldots, n_x \\
&\quad 0 \leq \tau \leq 5\delta^{-2}.
\end{aligned}
$$

Before continuing to discretize the problem in time, let us simplify it further. Note that the bar and the temperature along the bar are symmetric [7]. Taking advantage of this symmetry, the problem can be simplified further. Biegler and Kameswaran simplified the model using this symmetry [7]. Thus, we can solve the problem only for one half of the bar, and then the temperature of the other half would be symmetric to the solution that we have obtained for the first half. Since both ends of the bar and every point with equal distance from the nearest endpoint have the same temperature, we have

$$
\begin{aligned}
u_0(\tau) &= u_\pi(\tau) = u(\tau), \\
f(x_i, \tau) &= f(x_{n-i}, \tau).
\end{aligned}
$$

Assume that the number of space discretizing points, n_x, is even. Then the number of points in space reduces to $\frac{n_x}{2}$, where $x_{\frac{n_x}{2}}$ denotes the middle point of the bar. The sum over the temperature of all points in the objective function reduces to

$$
2 \sum_{i=1}^{\frac{n_x}{2}-1} f^2(x_i, \tau) + f^2(x_{\frac{n_x}{2}}, \tau).
$$

Also, the equality constraint for the $(\frac{n_x}{2} - 1)$-th point in space simplifies too, since $f\big(x_{\frac{n_x}{2}-1}, t\big) = f\big(x_{\frac{n_x}{2}+1}, t\big)$.

By this simplification, the number of the ordinary differential equation constraints, the boundary, and the initial conditions reduce to half. The optimization model of the problem for the points in the first half of the bar is

$$
\begin{aligned}
\min_{u(\tau)} \quad & \delta^3 \int_0^{5\delta^{-2}} \left[2 \sum_{i=1}^{\frac{n_x}{2}-1} f^2(x_i,\tau) + f^2(x_{\frac{n_x}{2}},\tau) \right] d\tau \\
& \qquad\qquad +2\delta^2 \left(\frac{\delta}{2} + q \right) \int_0^{5\delta^{-2}} \left[u_0^2(\tau) + u_\pi^2(\tau) \right] d\tau \\
\text{s.t.} \quad & \frac{\partial f(x_1,\tau)}{\partial \tau} = u_0(\tau) - 2f(x_1,\tau) + f(x_2,\tau) \\
& \frac{\partial f(x_i,\tau)}{\partial \tau} = f(x_{i-1},\tau) - 2f(x_I,\tau) + f(x_{i+1},\tau), \quad i = 2,\ldots,\frac{n_x}{2}-1 \\
& \frac{\partial f(x_{\frac{n_x}{2}},\tau)}{\partial \tau} = 2f(x_{\frac{n_x}{2}-1},\tau) - 2f(x_{\frac{n_x}{2}},\tau) \\
& f(x_i,\tau) \geq \sin(i\delta)\sin\left(\frac{\pi\delta^{-2}\tau}{5}\right) - 0.7, \qquad i = 1,\ldots,\frac{n_x}{2} \\
& u_0(\tau) \geq -0.7 \\
& f(x_0,\tau) = u(\tau) \\
& f(x_i,0) = 0 \qquad i = 0,\ldots,\frac{n_x}{2} \\
& 0 \leq \tau \leq 5\delta^{-2}.
\end{aligned}
$$

Now we can discretize the simplified problem in time too. As described in the previous sections, let the time discretization number be N. Then the time step size is $h = T'/N = 5\delta^{-2}/N$, where $T' = 5\delta^{-2}$. To approximate the integrals in the objective function, we use the rectangular method, as in (2.5). The equality constraints are approximated by a first order finite difference method, as described in Section 2.3. The approximation of the rest of the constraints is straightforward. Note that the lower bound constraints are now bounding the value of the function at some points and therefore yield only lower bounds for some variables. Therefore, by substituting the new function in (2.7) and considering the fact that the number of the spatial points are reduced to half, we have the fully discretized model of the heat transfer optimization problem as

$$
\begin{aligned}
\min_{u(\tau)} \quad & h\delta^3 \sum_{s=1}^{N} \left(2 \sum_{i=1}^{\frac{n_x}{2}-1} f^2(x_i, \tau) + f^2(x_{\frac{n_x}{2}}, \tau) \right) + 2h\delta^2 \left(q + \frac{\delta}{2} \right) \sum_{s=1}^{N} u^2(t_s) \\
\text{s.t.} \quad & \frac{f(x_1, t_{s+1}) - f(x_1, t_s)}{h} = u(t_s) - 2f(x_1, t_s) + f(x_2, t_s) \qquad \forall\ s \\
& \frac{f(x_i, t_{s+1}) - f(x_i, t_s)}{h} = f(x_{i-1}, t_s) - 2f(x_i, t_s) + f(x_{i+1}, t_s) \\
& \qquad\qquad i = 2, \ldots, \frac{n_x}{2} - 1, \quad \forall\ s \\
& \frac{f(x_{\frac{n_x}{2}}, t_{s+1}) - f(x_{\frac{n_x}{2}}, t_s)}{h} = 2f(x_{\frac{n_x}{2}-1}, t_s) - 2f(x_{\frac{n_x}{2}}, t_s) \qquad \forall\ s
\end{aligned}
$$

$$
\begin{aligned}
& f(x_i, t_s) \geq \sin(i\delta) \sin\left(\frac{\pi\delta^2 (s-1)h}{5} \right) - 0.7 \qquad i = 1, \ldots, \frac{n_x}{2}, \quad \forall\ s \\
& u(t_s) \geq -0.7 \qquad \forall\ s
\end{aligned}
$$

$$
\begin{aligned}
& f(x_0, t_s) = u(t_s), \qquad \forall\ s \\
& f(x_i, 0) = 0 \qquad i = 0, \ldots, \frac{n_x}{2}, \quad \forall\ s,
\end{aligned}
$$

where $\forall\ s$ means $s = 1, \ldots, N$.

This discrete problem is an approximation of the original continuous problem. An upper bound for the error that has been made by this approximation can be easily computed from the known errors of the trapezoidal method, rectangular method, and finite difference methods. Calculating the total error for this problem shows that the order of the error in space is $1/n_x^2$, and the order of the error in time is $1/N$.

2.5 Matrix Form

Now that we have the problem with finite number of constraints and variables, we write it in matrix form, so that we can apply standard optimization solvers to solve the problem numerically. For this purpose, we write all the variables in a vector form. To keep consistency with the previous notation, we introduce two vectors of variables at this point. They can be merged together easily when necessary. Let vectors $\mathbf{u}$ and $\mathbf{f}$ be

$$\mathbf{u}^T = \Big[u(t_1), \ \ldots, \ u(t_N)\Big]_{1\times N} \tag{2.7}$$

and

$$\mathbf{f}^T = \Big[\mathbf{f}_1^T, \ \mathbf{f}_2^T, \ \cdots, \ \mathbf{f}_{\frac{n_x}{2}}^T\Big]_{1\times N\frac{n_x}{2}}, \tag{2.8}$$

where

$$\mathbf{f}_i^T = \Big[f(x_i,t_1), \ \cdots, \ f(x_i,t_N)\Big]_{1\times N}, \qquad i = 1,\ldots,\frac{n_x}{2}.$$

By having the vectors of the variables, we can derive the appropriate objective and constraints matrices. Denote I_N to be the $N\times N$ identity matrix and consider the following diagonal matrices H and Q

$$H = 4h\delta^2\left(q+\frac{\delta}{2}\right)I_N, \qquad Q = \begin{bmatrix} 4h\delta^3 I_N & & \\ & \ddots & \\ & & 2h\delta^3 I_N \end{bmatrix}_{\frac{n_x}{2}N\times\frac{n_x}{2}N}.$$

It is easy to see that the objective function can be written as

$$\psi(\mathbf{x},t) = \frac{1}{2}\mathbf{f}^T Q\mathbf{f} + \frac{1}{2}\mathbf{u}^T H\mathbf{u}.$$

This objective function is clearly in the form of a convex quadratic function, where the coefficient matrices are diagonal. Now consider the discretized heat equation constraints for $s = 1, \dots, N$ as

$$
\begin{aligned}
f(x_1, t_{s+1}) + (2h-1)f(x_1, t_s) - hu(t_s) - hf(x_2, t_s) &= 0, && \forall\ s \\
f(x_i, t_{s+1}) + (2h-1)f(x_i, t_s) - hf(x_{i-1}, t_s) - hf(x_{i+1}, t_s) &= 0, && \forall\ s \\
& && i = 2, \dots, \frac{n_x}{2} - 1 \\
f(x_{\frac{n_x}{2}}, t_{s+1}) + (2h-1)f(x_{\frac{n_x}{2}}, t_s) - 2hf(x_{\frac{n_x}{2}-1}, t_s) &= 0, && \forall\ s.
\end{aligned}
$$

These $\frac{n_x}{2} \times N$ set of equations can be written in matrix form as

$$
\begin{aligned}
L\mathbf{u} + G\mathbf{f}_1 + L\mathbf{f}_2 &= \mathbf{0} \\
L\mathbf{f}_{i-1} + G\mathbf{f}_i + L\mathbf{f}_{i+1} &= \mathbf{0} \\
2L\mathbf{f}_{\frac{n_x}{2}-1} + G\mathbf{f}_{\frac{n_x}{2}} &= \mathbf{0},
\end{aligned}
$$

where the matrices L and G are defined as

$$
L = \begin{bmatrix} 0 & & & \\ -h & 0 & & \\ & \ddots & \ddots & \\ & & -h & 0 \end{bmatrix}_{N \times N} \quad \text{and} \quad G = \begin{bmatrix} 1 & & & \\ 2h-1 & \ddots & & \\ & \ddots & \ddots & \\ & & 2h-1 & 1 \end{bmatrix}_{N \times N} \tag{2.9}
$$

The equality constraints in this problem are the constraints deducted from the heat equation and the initial condition constraints. We write them in a matrix form by using the matrices

$$A = \begin{bmatrix} G & L & & & \\ L & G & L & & \\ & \ddots & \ddots & \ddots & \\ & & L & G & L \\ & & & 2L & G \end{bmatrix}_{\frac{n_x}{2}N \times \frac{n_x}{2}N} \quad \text{and} \quad B = \begin{bmatrix} L \\ \mathbf{0} \\ \vdots \\ \mathbf{0} \end{bmatrix}_{\frac{n_x}{2}N \times N}.$$

The first row of G has the only nonzero number in each block of $[G \quad L]$ or $[L \quad G \quad L]$ and represents the initial conditions of the bar. Hence, using these large, but very sparse and nicely structured matrices, the initial conditions and the heat equation constraints can be given as

$$A\mathbf{f} + B\mathbf{u} = \mathbf{0}.$$

To write the inequality constraints, let us introduce the constant vectors $\mathbf{d}_i$ corresponding to each internal spatial point x_i, defined as follows

$$\mathbf{d}_i = \begin{bmatrix} 0.7 - \sin(i\delta)\sin\left(\frac{\pi\delta^2 h}{5} \times 0\right) \\ 0.7 - \sin(i\delta)\sin\left(\frac{\pi\delta^2 h}{5} \times 1\right) \\ \vdots \\ 0.7 - \sin(i\delta)\sin\left(\frac{\pi\delta^2 h}{5} \times (N-1)\right) \end{bmatrix}_{N\times 1} \qquad i = 1, \ldots, \frac{n_x}{2}.$$

Now let us define vector $\mathbf{d}$ as

$$\mathbf{d}^T = \left[\mathbf{d}_1^T,\ \mathbf{d}_2^T,\ \ldots,\ \mathbf{d}_{\frac{n_x}{2}}^T\right]_{1\times\frac{n_x}{2}N}. \tag{2.10}$$

Moreover, suppose that the boundaries lower bound vector $\mathbf{c}$ is defined as $\mathbf{c}^T = \Big[0.7, \ \ldots, \ 0.7\Big]_{1\times N}$. Then, the inequality constraints can be written as

$$\mathbf{f} + \mathbf{d} \geq \mathbf{0},$$

$$\mathbf{u} + \mathbf{c} \geq \mathbf{0}.$$

Now the discretized optimization problem is in matrix form as

$$\begin{aligned} \min_{\mathbf{u},\mathbf{f}} \qquad & \psi = \frac{1}{2}\mathbf{f}^T Q \mathbf{f} + \frac{1}{2}\mathbf{u}^T H \mathbf{u} \\ \text{s.t.} \qquad & A\mathbf{f} + B\mathbf{u} = \mathbf{0}, \\ & \mathbf{f} + \mathbf{d} \geq \mathbf{0}, \\ & \mathbf{u} + \mathbf{c} \geq \mathbf{0}. \end{aligned}$$

This formulation shows clearly that the objective function is convex quadratic. Also, all the constraints are linear, and therefore the problem is a convex quadratic optimization problem. It guarantees that once an optimum solution is found, it is the global optimum for this problem. Moreover, we have shown how discretization can be used to transfer the original nonlinear problem into a convex quadratic problem with a very sparse matrix structure. This problem can be solved using quadratic or general nonlinear optimization packages in polynomial time using interior point methods [11].

Chapter 3

Computational Experiments

3.1 Sparse Model

As it was shown in Chapter 2, the nonlinear, one-dimensional heat transfer problem can be converted to the following convex quadratic problem, when we use discretization in both space and time. The problem is now fully discretized with finite number of variables and constraints.

$$\begin{aligned} \min_{\mathbf{u},\mathbf{f}} \quad & \frac{1}{2}\mathbf{f}^T Q \mathbf{f} + \frac{1}{2}\mathbf{u}^T H \mathbf{u} \\ \text{s.t.} \quad & A\mathbf{f} + B\mathbf{u} = \mathbf{0}, \\ & \mathbf{f} + \mathbf{d} \geq \mathbf{0}, \\ & \mathbf{u} + \mathbf{c} \geq \mathbf{0}. \end{aligned} \tag{3.1}$$

Betts and Campbell noticed that, in the solution of this problem, the only spatial point at which the inequalities are active, is the middle point $x_{\frac{n_x}{2}}$, where n_x is an even number [3]. Thus, we can eliminate the inequality constraints for the rest of the points and only keep

$$\mathbf{f}_{\frac{n_x}{2}} + \mathbf{d}_{\frac{n_x}{2}} \geq \mathbf{0},$$

in the constraint set. By $\mathbf{f}_{\frac{n_x}{2}}$ we mean the corresponding variables of the spatial point $\frac{n_x}{2}$, which is the $(\frac{n_x}{2})$-th block of size $(N \times 1)$ from the vector $\mathbf{f}$, whereas there are N variables for each spatial point due to the N discretization points in time. Similarly, by $\mathbf{d}_{\frac{n_x}{2}}$ we refer to the corresponding rows of the vector $\mathbf{d}$, the lower bound function, which give us the appropriate inequalities for the $(\frac{n_x}{2})$-th point. Hence, the further simplified heat transfer problem for the given symmetric temperature profile function is

$$\begin{aligned} \min_{\mathbf{u},\mathbf{f}} \quad & \frac{1}{2}\mathbf{f}^T Q \mathbf{f} + \frac{1}{2}\mathbf{u}^T H \mathbf{u} \\ \text{s.t.} \quad & A\mathbf{f} + B\mathbf{u} = \mathbf{0}, \\ & \mathbf{f}_{\frac{n_x}{2}} + \mathbf{d}_{\frac{n_x}{2}} \geq \mathbf{0}. \end{aligned} \tag{3.2}$$

A good nonlinear or quadratic optimization package should be able to solve this problem [11]. We used the package MOSEK to solve this problem efficiently. Note that all the coefficient matrices in this problem are large in size, but also sparse and structured. In particular, the objective coefficient matrices H and Q are only diagonal matrices of size $(N \times N)$ and $(\frac{n_x}{2}N \times \frac{n_x}{2}N)$, where n_x is the number of discretization points in space, and N is the number of discretization points in time. Further, the constraint coefficient matrices A and B are structured, sparse matrices of size $(\frac{n_x}{2}N \times \frac{n_x}{2}N)$ and $(\frac{n_x}{2}N \times N)$. The matrices A and B are almost diagonal with four nonzero diagonals in the matrix A, and one nonzero diagonal in the matrix B. Because of the sparsity of the coefficient matrices, we refer to model (3.1) as the "sparse full model", and we call model (3.2), which has only the inequality constraints for one spatial point, as the "sparse model".

$$A = \left[\begin{array}{c|c|c|c|c}
\begin{matrix}1&&\\2h\text{-}1&1&\\&\ddots&\ddots\\&2h\text{-}1&1\end{matrix} & \begin{matrix}0&&\\-h&0&\\&\ddots&\ddots\\&-h&0\end{matrix} & & & \\ \hline
\begin{matrix}0&&\\-h&0&\\&\ddots&\ddots\\&-h&0\end{matrix} & \begin{matrix}1&&\\2h\text{-}1&1&\\&\ddots&\ddots\\&2h\text{-}1&1\end{matrix} & \begin{matrix}0&&\\-h&0&\\&\ddots&\ddots\\&-h&0\end{matrix} & & \\ \hline
 & \ddots & \ddots & \ddots & \\
 & & \begin{matrix}0&&\\-h&0&\\&\ddots&\ddots\\&-h&0\end{matrix} & \begin{matrix}1&&\\2h\text{-}1&1&\\&\ddots&\ddots\\&2h\text{-}1&1\end{matrix} & \begin{matrix}0&&\\-h&0&\\&\ddots&\ddots\\&-h&0\end{matrix} \\ \hline
 & & & \begin{matrix}0&&\\-2h&0&\\&\ddots&\ddots\\&-2h&0\end{matrix} & \begin{matrix}1&&\\2h\text{-}1&1&\\&\ddots&\ddots\\&2h\text{-}1&1\end{matrix}
\end{array}\right]_{\frac{n_x}{2}N \times \frac{n_x}{2}N}$$

Figure 3.1: The coefficient matrix of the equality constraints.

3.2 Compact Model

Although the matrices are sparse, their size grows rapidly as discretization in time or space becomes finer. To improve the problem formulation for large size matrices, Biegler and Kameswaran [7] suggested to convert the so called sparse model to a more compact model. In that model, the only variables are the control variable[1] $\mathbf{u}$, which are indeed the variables that we are looking for. In this case, the size of the problem does not depend on the number of the spatial discretization points, but only on the number of the time discretization points. To write the variables in terms of $\mathbf{u}$, we utilize the equality constraints. First, note that A is an invertible matrix.[2] Hence, we can write $\mathbf{f}$ in terms of

[1]The vector of the time discretized temperature function $u(t)$ at the boundary points.

[2]See Appendix A in Biegler and Kameswaran's paper [7]

$\mathbf{u}$ as

$$\mathbf{f} = -A^{-1}B\mathbf{u}.$$

Let us denote the matrix $A^{-1}B$ by W, where

$$W = [W_1, W_2, \ldots, W_{\frac{n_x}{2}}]^T = A^{-1}B.$$

The matrix W is of size $(\frac{n_x}{2}N \times N)$, and each W_k corresponds to each of the $\frac{n_x}{2}$ points in space, and has the size $(N \times N)$. Let us denote the objective coefficient matrices by R, where

$$R = H + B^T A^{-T} Q A^{-1} B = H + W^T Q W.$$

Now we can write a compactified heat transfer problem in terms of $\mathbf{u}$ as

$$\begin{aligned} \min_{\mathbf{u}} \quad & \frac{1}{2}\mathbf{u}^T R \mathbf{u} \\ \text{s.t.} \quad & W_{\frac{n_x}{2}}\mathbf{u} - \mathbf{c}_{\frac{n_x}{2}} \geq \mathbf{0}. \end{aligned} \tag{3.3}$$

Note that R, compared to Q and H, is a much smaller, but also a much denser matrix. The size of R is only related to the number of discretization points in time, that is, R is of size $(N \times N)$. For further reference, we call this model, "the compact model".

As all the matrix computations for this problem are done in MATLAB, to obtain the matrix $W = A^{-1}B$, one can simply use MATLAB's linear system solving function, "\". However, this operator might be demanding in time and memory. Biegler and Kameswaran introduced an alternative approach to calculate W by backward calculation of its blocks. That is, first calculating $W_{\frac{n_x}{2}}$, then $W_{\frac{n_x}{2}-1}$ and so on. This procedure can be found in Appendix A of their paper [7]. The label "compact model using the Biegler's procedure" refers to the compact model, where the inverse matrix is calculated using the Biegler and Kameswaran's procedure, while the results obtained using MATLAB functions are identified by "compact model using the MATLAB operator "\"".

3.3 Computational Results

All the numerical results in this thesis are produced on a Pentium 4 desktop computer, with 760 MB memory and 3.06 GHz CPU. The optimization solver is the quadratic optimization package of MOSEK, version 4.0. The MATLAB interface for this solver is used, and all the matrix preparations have been done in MATLAB version 7.01.

By "it." in the tables we mean the number of iterations that MOSEK takes to obtain a solution. The "CPU" label in the tables shows the CPU time returned by MOSEK, that is, excluded the time that MATLAB matrix setup needs. The word "total" is used to refer to the actual time needed to obtain the results, including both the preparation time in MATLAB and also the time that MOSEK needs to solve the problem. All the times reported in the tables are in seconds.

Table 3.1 represents results for the sparse model (3.2). The number of spatial discretization points is fixed to $n = 10$ in this table, and the number of time discretization points, N, grows from 1000 to 64000. Actually, time discretization can get as fine as 130000, and still MOSEK can solve the problem without difficulty, on the same computer. MOSEK can handle sparse matrices efficiently, and although the problem becomes quite large, the results are obtained rather quickly. Note that, for $N = 32000$, the size of the objective

N	objective	equality infeas.	it.	CPU	total
1000	4.7368855723e-001	2.40e-014	16	2	2
2000	4.7419864510e-001	4.16e-015	19	3	3
4000	4.7445343255e-001	1.21e-015	18	5	6
8000	4.7458076680e-001	1.66e-015	24	13	14
16000	4.7464441791e-001	5.63e-015	23	28	29
32000	4.7467624130e-001	1.05e-014	20	43	45
64000	4.7469215293e-001	2.02e-014	26	118	122

Table 3.1: Computational results with the sparse model, $n_x = 10$.

coefficient matrix is 192000×192000, and the size of the constraints coefficient matrix is 160000×192000. The number of variables is 192000 and the number of constraints is 160000. The total solution time for this problem is 45 seconds. The objective values reported in Table 3.1 suggest that the number of accurate digits are growing as the value of N grows, and for $N = 64000$ it seems that there is 4 digits accuracy.

Table 3.2 presents numerical results for the compact model (3.3). To calculate the matrix $A^{-1}B$, the "\" operator of MATLAB is used. The objective value in this model is similar to the objective value in the sparse model.

N	objective	equality infeas.	it.	CPU	total
500	4.7266656430e-001	1.90e-013	43	12	18
1000	4.7368855809e-001	5.25e-012	50	219	251
1500	4.7402870633e-001	2.78e-011	52	419	517
2000	4.7419865557e-001	1.02e-010	61	957	1178
2500	N. A.				

N. A.: Results not available due to memory shortage.

Table 3.2: Computational results with the compact model using the MATLAB operator "\", $n_x = 10$.

Moreover, the number of iterations that MOSEK needs to solve the problem in this model is higher than with the simplified sparse model. Solving this model seems to be much more demanding in time and memory. The time needed is going quickly to the order of minutes. Finally, it is the growing memory demand which presents the problem from solving even for $N = 2500$ by reporting the "out of memory" message. The matrix setup in MATLAB, which is required for this model, takes almost the same amount of time as solving the problem by the MOSEK.

Table 3.3 illustrates numerical results for the compact model. In this table, to calculate the matrix $A^{-1}B$ the procedure that Biegler and Kameswaran have suggested in the Appendix of their paper [7] is used. However, the results

N	objective	equality infeas.	it.	CPU	total
500	4.7266656835e-001	1.57e-013	42	12	26
1000	4.7368855821e-001	4.81e-012	50	228	325
1500	4.7403435006e-001	2.84e-011	46	378	1027
2000	N. A.				

N. A.: Results not available due to memory shortage.

Table 3.3: Computational results with the compact model using the Biegler's procedure, $n_x = 10$.

obtained by this procedure are hardly better than using the MATLAB solving operator. The number of iterations remains the same, if not higher, and the time required to solve the problem is even more. The time needed for matrix setup is also higher, since the difference of the total time and solved CPU time is higher. Also, the computer reported the "out of memory" error message even sooner, already for $N = 2000$.

The next three Tables 3.4, 3.5, and 3.6 show another set of results from the sparse model, the compact model using the solving operator "\", and the compact model using the Biegler procedure, respectively. In these tables, n_x is fixed to be 20 and the number of time discretization points, N, is varied. The conclusions deducted from these tables remain the same, as the ones deducted from the last three tables. The number of iterations, although increasing,

N	objective	equality infeas.	it.	CPU	total
1000	4.6714762881e-001	1.35e-014	17	4	6
2000	4.6765401066e-001	7.35e-015	17	5	7
4000	4.6790697824e-001	4.06e-015	22	12	13
8000	4.6803340715e-001	7.76e-015	20	21	23
16000	4.6809660769e-001	1.60e-014	23	45	48
32000	4.6812820490e-001	4.07e-014	29	141	147

Table 3.4: Computational results with the sparse model, $n_x = 20$.

is not monotonically increasing. The infeasibility of the equality constraints decreases at the first experiments and then increases again.

When using the MATLAB operator in the compact model for $n_x = 20$ as shown in Table 3.5, the results can be achieved up to $N = 1500$. Then the matrix preparation cause memory shortage. The results with the compact model compared to the sparse model also show that solving the compact model requires more time. The value of the infeasibility of the equality constraints are higher in compact model, which can imply that the solutions are not as accurate as in the sparse model. The same stays true for the compact model using the Biegler and Kameswaran's procedure. In this experiment, the results for this model are the weakest among the three.

In Table 3.7, the result for the sparse model are shown. In this table,

N	objective	equality infeas.	it.	CPU	total
500	4.6613290563e-001	1.34e-014	32	9	18
1000	4.6714762754e-001	1.62e-011	49	210	270
1500	4.6748531767e-001	3.69e-010	51	408	595
2000	N. A.				

N. A.: Results not available due to memory shortage.

Table 3.5: Computational results with the compact model using the MATLAB operator "\", $n_x = 20$.

N	objective	equality infeas.	it.	CPU	total
500	4.6613290561e-001	1.81e-014	32	9	34
1000	4.6714762759e-001	1.27e-011	51	217	422
1500	N. A.				

N. A.: Results not available due to memory shortage.

Table 3.6: Computational results with the compact model using the Biegler's procedure, $n_x = 20$.

n_x	objective	P. eq. inf.	D. eq. inf.	it.	CPU	total
10	4.7368855723e-001	2.40e-014	7.60e-014	16	1	2
20	4.6714762881e-001	1.35e-014	3.31e-014	17	3	3
30	4.6592989688e-001	1.08e-014	9.02e-015	17	5	5
40	4.6550888020e-001	8.74e-014	3.64e-012	14	5	6
50	4.6532183955e-001	1.36e-014	9.77e-004	16	7	8
60	4.6522725993e-001	1.15e-014	2.62e+005	16	9	10
500	IN.					

IN: The problem to be reported as primal infeasible.

Table 3.7: Computational results with the sparse model, $N = 1000$.

the number of time discretization points N is fixed to be 1000, and the number of the spatial discretization points, n_x, is changing.

For $n_x \leq 50$, the optimum solution obtained looks reliable since both the primal and dual infeasibility of the equality constraints, that MOSEK reports at the end, are in acceptable range. As soon as the number of spatial discretization points reaches 50, the dual infeasibility of the equality constraints makes a huge jump and keeps increasing rapidly afterwards. It seems numerical difficulties arise for finer spatial discretization in the sparse model. As it is shown in Table 3.8, these numerical difficulties occur in the form of primal

n_x	objective	P. eq. inf.	D. eq. inf.	it.	CPU	total
10	4.7368855437e-001	2.86e-015	9.60e-015	18	2	2
20	4.6714762758e-001	5.04e-015	1.49e-014	19	3	3
30	4.6592989652e-001	2.81e-015	9.79e-015	20	5	5
40	4.6550887632e-001	5.33e-015	7.28e-012	20	6	7
50	4.6532613567e-001	1.20e-014	9.77e-004	21	8	9
54	IN.					

IN: The problem to be reported as primal infeasible.

Table 3.8: Computational results with the sparse full model, $N = 1000$.

infeasibility in the sparse full model. This dual blow up might occur because of the discretization methods that has been applied on the objective function and the PDEs. The stability of the discretization methods depends on the number of discretization points in space and time, and the methods are not stable for every value of N and n.

Table 3.9 shows the numerical results when the number of time discretization points is fixed to $N = 5000$, and n is changing, and the same high dual equality infeasibility is reported by MOSEK for this problem. Although the dual infeasibility for the equality constraints stays in acceptable range for $n_x \leq 80$ in the sparse model. The numerical results for the sparse full model is shown in Table 3.10, and for this model MOSEK reports primal infeasibility for $n_x = 96$. Table 3.11 and Table 3.12 show the results for sparse model and sparse full model when N is fixed to 10000. Note how the solution become inaccurate in Table 3.11, when $n = 110$.

It seems that the feasibility of the problem depends on the ratio of the number of discretization points in space and time. Figure 3.2 illustrates the border line between the feasible and infeasible problems. A problem for which the number of time and spatial discretization points is below the borderline (solid curve) is reported to be infeasible while numerical results can be obtained for a problem for which the number of time and spatial discretization points lies above the borderline. The curve of the borderline can be estimated polynomially by $p(n) = 1.0585n^2 - 52.0142n + 622.9112$. Hence, to obtain numerical results for a problem with 500 spatial points, at least 241000 points in time are needed. The dashed curve in Figure 3.2 shows the plot of the polynomial $p'(n) = n^2 - 20n + 1000$. This polynomial is an approximation for the values on the borderline in the feasible side. $p'(n)$ can be used to es-

n_x	objective	P. eq. inf.	D. eq. inf.	it.	CPU	total
10	4.7450437095e-001	1.65e-015	5.65e-015	22	6	7
20	4.6795755398e-001	4.14e-015	4.40e-015	19	12	12
30	4.6673830621e-001	1.04e-014	9.46e-015	20	25	26
40	4.6631108973e-001	7.38e-014	2.08e-015	22	40	41
50	4.6611326563e-001	3.54e-014	4.22e-015	23	52	54
60	4.6600579261e-001	5.84e-014	1.12e-014	21	71	73
70	4.6594099396e-001	1.80e-014	8.05e-016	21	107	110
80	4.6589987601e-001	4.31e-014	1.12e-008	20	107	112
90	4.6587261800e-001	4.72e-014	4.00e+000	20	132	137
500	IN.					

IN: The problem to be reported as primal infeasible.

Table 3.9: Computational results with the sparse model, $N = 5000$.

n_x	objective	P. eq. inf.	D. eq. inf.	it.	CPU	total
10	4.7450437022e-001	4.52e-015	1.53e-014	25	6	7
20	4.6795755360e-001	7.04e-015	8.78e-015	24	11	12
30	4.6673830504e-001	7.59e-015	1.26e-014	24	23	25
40	4.6631108780e-001	1.06e-014	1.11e-014	28	39	41
50	4.6611326350e-001	1.65e-014	2.03e-015	30	53	55
60	4.6600579077e-001	7.63e-014	3.79e-015	26	69	72
70	4.6594099398e-001	1.04e-014	4.63e-015	31	115	119
80	4.6589987941e-001	3.19e-014	1.49e-008	30	115	120
96	IN.					

IN: The problem to be reported as primal infeasible.

Table 3.10: Computational results with the sparse full model, $N = 5000$.

n_x	objective	P. eq. inf.	D. eq. inf.	it.	CPU	total
10	4.7460622740e-001	4.27e-015	1.53e-015	23	12	14
20	4.6805868878e-001	1.09e-014	3.62e-015	21	24	26
30	4.6683926236e-001	2.00e-014	3.55e-015	22	81	83
40	4.6641196819e-001	3.73e-014	6.35e-016	23	92	96
50	4.6621410404e-001	4.27e-014	4.81e-016	23	146	150
60	4.6610659670e-001	6.61e-014	2.94e-016	25	268	276
70	4.6604176617e-001	1.47e-013	7.97e-015	26	469	476
80	4.6599968810e-001	6.33e-014	3.23e-015	27	363	373
90	4.6597083909e-001	2.28e-013	1.36e-015	27	544	557
100	4.6595021730e-001	9.11e-014	9.16e-016	24	664	678
110	6.5818993914e-001	5.42e-007	7.81e-003	87	1468	1483
5000	IN.					

IN: The problem to be reported as primal infeasible.

Table 3.11: Computational results with the sparse model, $N = 10000$.

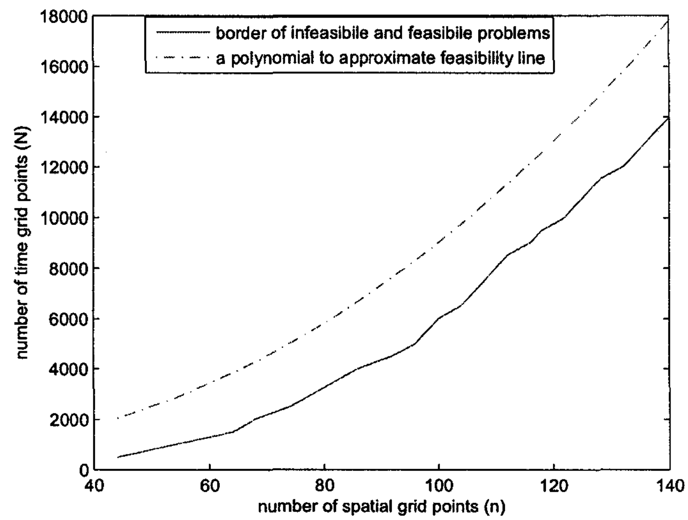

Figure 3.2: The plot of border line between the feasible and infeasible problems according to the number of time and spatial discretization points.

timate a proper number of time discretization points, N, for a chosen spatial discretization points, n, to obtain a good numerical results.

Table 3.13 shows numerical results for a set of problems in which the number of spatial discretization points and the number of time discretization points are obtained from the polynomial $p'(n)$ in Figure 3.2 (the dashed curve). As it can be seen from this table when N and n are both increasing, the number of accurate digits is also increasing more steadily, and the equality infeasibility for both primal and dual side stays in an acceptable range. This suggests that to obtain more stable results, changes should be applied on the pair (n, N).

Figures 3.3, 3.4, 3.5, 3.6, and 3.7 illustrate the obtained level curves of the temperature profile, $f(x, t)$, versus the lower bound constraint function, $g(x, t)$, at a fixed time. In Figures 3.3 to 3.7, the temperature function is

n_x	objective	P. eq. inf.	D. eq. inf.	it.	CPU	total
10	4.7460622746e-001	1.20e-014	3.99e-014	22	10	12
20	4.6805868731e-001	8.74e-015	1.06e-014	27	23	25
30	4.6683926048e-001	2.50e-014	1.28e-014	28	79	82
40	4.6641196894e-001	2.56e-014	8.67e-015	28	89	93
50	4.6621410259e-001	3.45e-014	2.74e-015	30	150	155
60	4.6610659722e-001	3.67e-014	1.14e-014	30	244	250
70	4.6604176649e-001	1.41e-013	1.37e-014	33	460	467
80	4.6599968737e-001	7.74e-014	3.13e-014	29	357	366
90	4.6597083939e-001	8.66e-014	2.50e-014	27	539	550
100	4.6595021647e-001	9.23e-014	1.54e-014	33	633	647
122	IN.					

IN: The problem to be reported as primal infeasible.

Table 3.12: Computational results with the sparse full model, $N = 10000$.

(n_x, N)	objective	P. eq. inf.	D. eq. inf.	it.	CPU	total
(10, 900)	4.7357870046e-001	3.39e-015	1.07e-014	17	2	3
(20, 1000)	4.6715023817e-001	2.03e-014	4.97e-014	17	3	3
(30, 1300)	4.6616516259e-001	3.94e-014	5.15e-014	19	5	7
(40, 1800)	4.6595364946e-001	2.53e-014	1.65e-014	17	11	11
(50, 2500)	4.6591256449e-001	1.28e-014	4.28e-015	17	19	20
(60, 3400)	4.6591180280e-001	1.03e-014	3.80e-015	21	39	41
(70, 4500)	4.6591937399e-001	3.33e-014	3.55e-015	20	65	69
(80, 5800)	4.6592739732e-001	4.08e-014	1.14e-013	20	124	128
(90, 7300)	4.6593415336e-001	1.25e-013	9.09e-013	22	262	271
(100, 9000)	4.6593950298e-001	1.77e-013	1.46e-011	22	636	648
(110, 10900)	N.A.					

N. A.: Results not available due to memory shortage.

Table 3.13: Computational results with the sparse full model for a set of selected points on $p'(n)$.

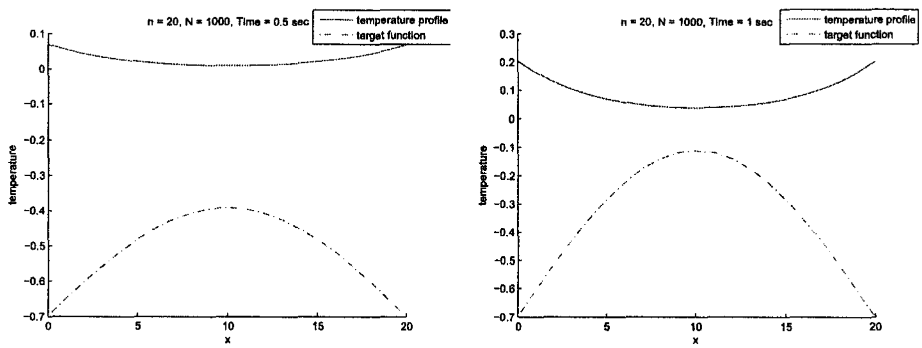

Figure 3.3: The obtained temperature profile and the lower bound function for time $t = 0.5$ and $t = 1$.

obtained for $n_x = 20$ and $N = 1000$. The function plotted in dashed line is $g(x, t)$, and the solid lined function is $f(x, t)$. The level curves of the figures are plotted every half a second, starting from $t = 0.5$, and the last figure shows their status at $t = 5$. The time period in which the problem is solved is $[0, 5]$. From the figures it is seen that the equality constraints are active only in the midpoint, that is $x = 10\delta$ for this problem since $n_x = 20$. The solution profile is clearly symmetric at each given time.

Figures 3.8 and 3.9 present the slack profile for the midpoint inequality constraint. For the first two figure, the setting is $N = 1000$ and $n_x = 10$, and for the next as it is $N = 1000$ and $n_x = 20$. As it can be seen from these figures, the inequality is potentially active during the time $1 \leq t \leq 4$. The more close up figure illustrates that the inequality is not active for the whole interval. It periodically becomes active and inactive.

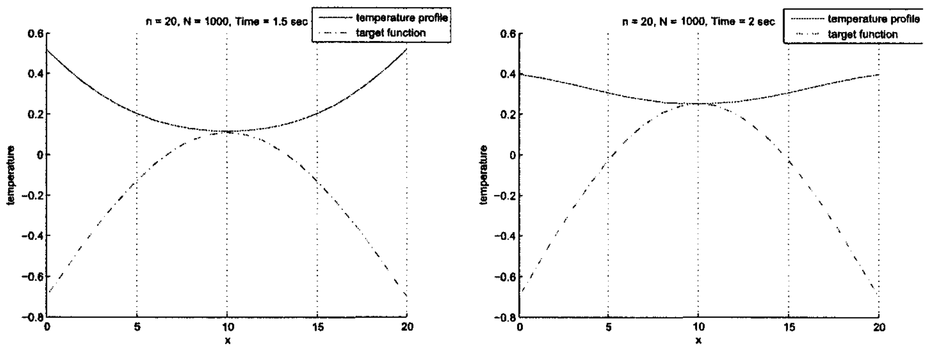

Figure 3.4: The obtained temperature profile and the lower bound function for time $t = 1.5$ and $t = 2$, the midpoint becomes active.

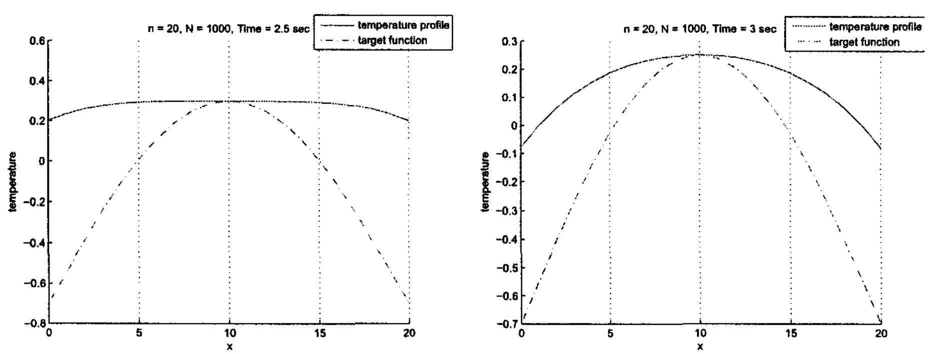

Figure 3.5: The obtained temperature profile and the lower bound function for time $t = 2.5$ and $t = 3$.

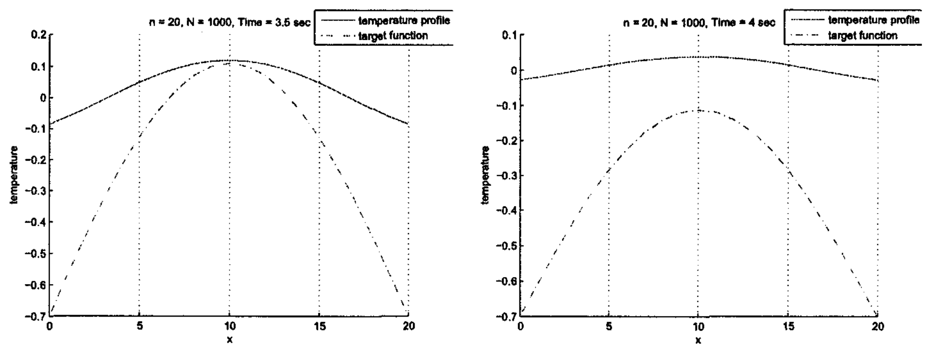

Figure 3.6: The obtained temperature profile and the lower bound function for time $t = 3.5$ and $t = 4$, none of the inequalities are active.

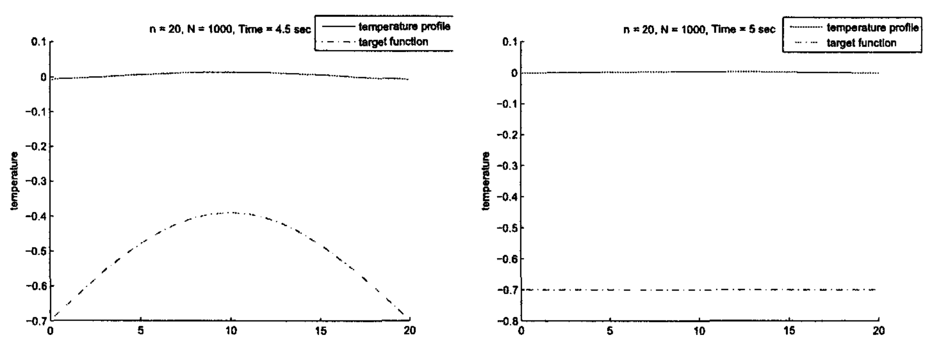

Figure 3.7: The obtained temperature profile and the lower bound function for time $t = 4.5$ and $t = 5$. The profiles taking the same shape as at the beginning state.

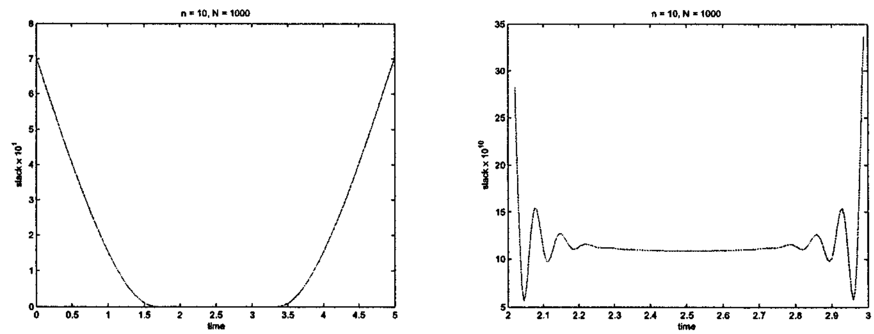

Figure 3.8: The slack variables for $n = 10$ and $N = 1000$.

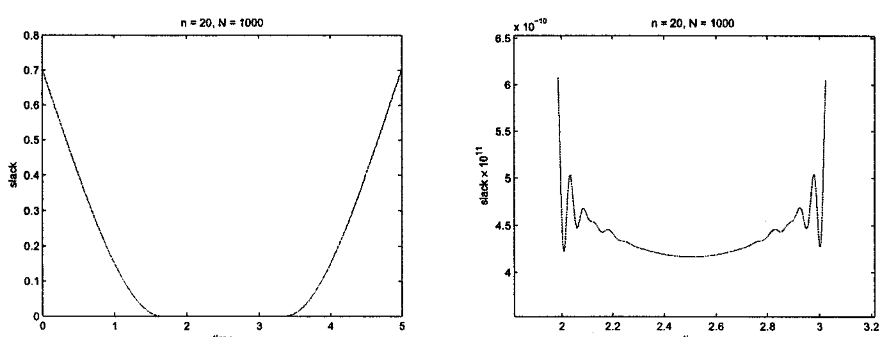

Figure 3.9: The slack variables for $n = 20$ and $N = 1000$.

Chapter 4

The Two Dimensional Case

4.1 The Two Dimensional Model

In Chapter 2, the heat transfer problem that we considered was simplified to a one-dimensional bar. We may generalize this problem to higher dimensions. Let us first go only one dimension higher, and assume that the heated object $\mathcal{P}$ is a two dimensional bar. For convenience, we denote the coordinates of each point $\mathbf{x}$ by their corresponding axis, namely $x = x^1$ and $y = x^2$. Accordingly, let the length of the bar in the x-axis be ℓ_x, and its length in the y-axis be ℓ_y. Assume that the endpoints of the bar on the x-axis are positioned at $x = 0$ and $x = \ell_x$. Similarly the endpoints on the y-axis are at $y = 0$ and $y = \ell_y$. Therefore, for each point $(x, y) \in \mathcal{P}$, we have $x \in [0, \ell_x]$ and $y \in [0, \ell_y]$.

Many sets of points of the bar can be assumed as boundary points. They can be the perimeter of this rectangular shaped bar, the lengths of it, the widths, or any other arbitrary set of points. However, to stay close to the chosen boundary points we used in case of the one dimensional bar, let us choose the boundary points, $\mathcal{P}^0$, to be the two endpoints of $\mathcal{P}$ on the x-axis,

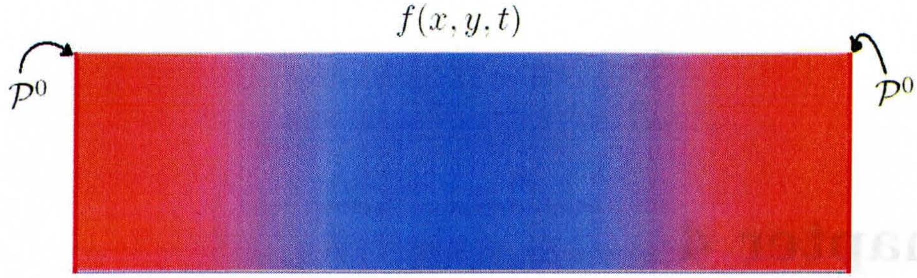

Figure 4.1: The three dimensional bar.

which are the two lines on either side of the bar, that is,

$$(x, y) \in \mathcal{P}^0 \iff x = 0 \text{ or } x = \ell_x, \quad \forall\, y \in [0, \ell_y].$$

Therefore $f(\mathbf{x}, t)$, the temperature function of the inner points of the bar, is a function of x, y, and t, while $u_0(\mathbf{x}, t)$ and $u_{\ell_x}(\mathbf{x}, t)$, the temperature of the each side of the bar, are functions of y and t. The time interval is assumed to be $[0, T]$.

$$f(0, y, t) = u_0(y, t), \qquad f(\ell_x, y, t) = u_{\ell_x}(y, t), \qquad \forall\ (x, y) \in \mathcal{P}^0. \tag{4.1}$$

Since the heat flow occurs through conduction, the heat equation has to be satisfied. Hence, one of the constraints is the 2D heat equation

$$\frac{\partial f(x,y,t)}{\partial t} = \frac{\partial^2 f(x,y,t)}{\partial x^2} + \frac{\partial^2 f(x,y,t)}{\partial y^2}. \tag{4.2}$$

Assume that the bar is smooth on its sides, and the rate of heat flow throughout the bar is the same. The heat equations should hold for all points of the bar at all times. Along with the heat PDE, we assume the initial conditions are given too. For simplicity, let the initial condition be zero for all points,

$$f(\mathbf{x}, 0) = 0, \qquad \forall\, \mathbf{x} = (x, y)^T \in \mathcal{P}.$$

The boundary conditions (4.1), are considered to be unknown at the time and they are the target of this problem. In finding these control variables our goal is to minimize energy usage, while the constraints are satisfied.

The lower bound that we want the temperature to satisfy can be chosen to be almost any continuously differentiable functions of x, y, and t. However, to be consistent with the one dimensional model, we choose a similar inequality constraint

$$g(x, y, t) = c_1 \left[\sin(x) \sin\left(\frac{\ell_x t}{T}\right) - a_1\right] + c_2 \left[\sin(y) \sin\left(\frac{\ell_y t}{T}\right) - a_2\right] - b,$$

with $c_1 = c_2 = 1$, $a_1 = a_2 = 0.5$, and $b = 0.2$. This lower bound function is a linear combination of the same function that is used in one dimension (2.6), so the lower bound function is

$$g(x, y, t) = \sin(x) \sin\left(\frac{\ell_x t}{T}\right) + \sin(y) \sin\left(\frac{\ell_y t}{T}\right) - 1.2.$$

Just as it was in the one-dimensional case, there are many choices for the objective function. We choose an objective function, that is similar to the objective function in the one dimensional case. Hence, we set the objective to be the sum of the temperatures squared at all points over time. Since time and space are both continuous, the objective is the integration of the squared of the temperature functions, $f(x, y, t)$, over time, the x-axis, and the y-axis in space. Therefore, our two dimensional heat transfer optimization problem is

$$
\begin{aligned}
\min \quad & \int_0^T \int_0^{\ell_y} \int_0^{\ell_x} f^2(x,y,t)dxdydt \\
& \qquad + \int_0^T \int_0^{\ell_y} \left[q_0 u_0^2(y,t) + q_{\ell_x} u_{l_x}^2(y,t) \right] dydt \\
\text{s.t.} \quad & \frac{\partial f(x,y,t)}{\partial t} = \frac{\partial^2 f(x,y,t)}{\partial^2 x} + \frac{\partial^2 f(x,y,t)}{\partial^2 y} \\
& f(x,y,t) \geq g(x,y,t) \\
& g(x,y,t) = \sin(x)\sin\left(\frac{\ell_x t}{T}\right) + \sin(y)\sin\left(\frac{\ell_y t}{T}\right) - 1.2 \\
& f(x,y,0) = 0 \\
& f(0,y,t) = u_0(y,t) \qquad f(\ell_x,y,t) = u_{\ell_x}(y,t) \\
& \quad 0 \leq t \leq T \qquad 0 \leq x \leq \ell_x \qquad 0 \leq y \leq \ell_y.
\end{aligned}
$$

To avoid unnecessary complications, let us fix the boundary weight coefficients to be $q = q_0 = q_{\ell_x} = 10^{-3}$. The solution strategy for this problem is not different from the one dimensional case. We discretize in time and space, and then approximate the PDEs, the objective function and the rest of the constraints.

4.2 Spatial Discretization

To solve this problem, we discretize the above model in space first. Let n_x and n_y be the number of discretization points in x and y, respectively. To be able to benefit from the symmetry of the problem later, we assume that n_x and n_y are both even numbers. For simplicity and consistency with the one dimensional problem, we take uniform steps in both directions. Therefore, the step sizes are

$$\delta x = \frac{\ell_x}{n_x}, \qquad \delta y = \frac{\ell_y}{n_y}.$$

Denote $x_i = i\delta x$ and $y_j = j\delta y$, for $i = 0, \dots, n_x$ and $j = 0, \dots, n_y$.

Now to approximate the integrals, we use the trapezoidal method [1] for space dependent integrals in the objective function. Here is the the approximation for the integration over x:

$$\begin{aligned}\int_0^{\ell_x} f^2(x,y,t)dx &\approx \frac{\delta x}{2}\sum_{i=0}^{n_x-1}\left[f^2(x_i,y,t)+f^2(x_{i+1},y,t)\right]\\ &= \delta x\sum_{i=1}^{n_x-1} f^2(x_i,y,t)+\frac{\delta x}{2}\left(u_0^2(y,t)+u_{\ell_x}^2(y,t)\right).\end{aligned}$$

Using the above approximation in the objective function, we obtain

$$\delta x\int_0^T\int_0^{\ell_y}\sum_{i=1}^{n_x-1} f^2(x_i,y,t)dydt+\left(q+\frac{\delta x}{2}\right)\int_0^T\int_0^{\ell_y}\left[u_0^2(y,t)+u_{\ell_x}^2(y,t)\right]dydt.$$

Now let us apply the trapezoidal rule on the two integrals over y. The space-discretized objective function is

$$\begin{aligned}&\delta x\int_0^T\left[\delta y\sum_{j=1}^{n_y-1}\sum_{i=1}^{n_x-1} f^2(x_i,y_j,t)+\frac{\delta y}{2}\sum_{i=1}^{n_x-1}\left[f^2(x_i,y_0,t)+f^2(x_i,y_{n_y},t)\right]\right]dt\\ &\quad+\delta y\left(q+\frac{\delta x}{2}\right)\int_0^T\left[\sum_{j=0}^{n_y-1}\left[u_0^2(y_j,t)+u_{\ell_x}^2(y_j,t)\right]\right.\\ &\quad\left.+\frac{1}{2}\left[u_0^2(y_0,t)+u_0^2(y_{n_y},t)+u_{\ell_x}^2(y_0,t)+u_{\ell_x}^2(y_{n_y},t)\right]\right]dt.\end{aligned}$$

After approximating the objective function, we can continue to approximate the partial differential equation that we have as a constraint. We use the second-order finite difference method once for x and once more for y, for the space dependencies. Applying the finite difference method twice we obtain

$$\begin{aligned}
\frac{\partial f(x_1,y_j,t)}{\partial t} &\approx \frac{u_0(y_j,t)-2f(x_1,y_j,t)+f(x_2,y_j,t)}{\delta x^2}+\\
&\qquad \frac{f(x_1,y_{j-1},t)-2f(x_1,y_j,t)+f(x_1,y_{j+1},t)}{\delta y^2},\\
\frac{\partial f(x_i,y_j,t)}{\partial t} &\approx \frac{f(x_{i-1},y_j,t)-2f(x_i,y_j,t)+f(x_{i+1},y_j,t)}{\delta x^2}+\\
&\qquad \frac{f(x_i,y_{j-1},t)-2f(x_i,y_j,t)+f(x_i,y_{j+1},t)}{\delta y^2},\\
&\qquad\qquad i=2,\ldots,n_x-2,\\
\frac{\partial f(x_{n_x-1},y_j,t)}{\partial t} &\approx \frac{f(x_{n_x-2},y_j,t)-2f(x_{n_x-1},y_j,t)+u_{\ell_x}(y_j,t)}{\delta x^2}+\\
&\qquad \frac{f(x_{n_x-1},y_{j-1},t)-2f(x_{n_x-1},y_j,t)+f(x_{n_x-1},y_{j+1},t)}{\delta y^2},\\
&\qquad\qquad j=1,\ldots,n_y-1.
\end{aligned}$$

Discretization for the rest of the constraints is fairly straightforward. The discretized inequality constraints are just a bound on the value of the function at the discretized points:

$$\begin{aligned}
&0\le u_0(y_j,t)-\sin(j\delta)\sin\left(\frac{\ell_y t}{T}\right)+1.2, && j=0,\ldots,n_y,\\
&0\le f(x_i,y_j,t)-\sin(i\delta)\sin\left(\frac{\ell_x t}{T}\right)-\sin(j\delta)\sin\left(\frac{\ell_y t}{T}\right)+1.2, &&\\
&\qquad\qquad i=1,\ldots,n_x-1, && j=0,\ldots,n_y,\\
&0\le u_{\ell_x}(y_j,t)-\sin(j\delta)\sin\left(\frac{\ell_y t}{T}\right)+1.2, && j=0,\ldots,n_y.
\end{aligned}$$

The initial condition is approximated by setting the initial state of each of the spatial points to be zero. Now the space discretized, two dimensional heat transfer problem is

$$
\begin{aligned}
\min_{f,u}\ & \delta x \delta y \int_0^T \left[\sum_{j=1}^{n_y-1} \sum_{i=1}^{n_x-1} f^2(x_i, y_j, t) + \frac{1}{2} \sum_{i=1}^{n_x-1} \left[f^2(x_i, y_0, t) + f^2(x_i, y_{n_y}, t) \right] \right] dt \\
& + \delta y \left(q + \frac{\delta x}{2} \right) \int_0^T \left[\sum_{j=0}^{n_y-1} \left[u_0^2(y_j, t) + u_{\ell_x}^2(y_j, t) \right] \right. \\
& \qquad \left. + \frac{1}{2} \left[u_0^2(y_0, t) + u_0^2(y_{n_y}, t) + u_{\ell_x}^2(y_0, t) + u_{\ell_x}^2(y_{n_y}, t) \right] \right] dt
\end{aligned}
$$

$$
\begin{aligned}
\text{s.t. } & \frac{\partial f(x_1, y_j, t)}{\partial t} = \frac{u_0(y_j, t) - 2f(x_1, y_j, t) + f(x_2, y_j, t)}{\delta x^2} + \\
& \qquad \frac{f(x_1, y_{j-1}, t) - 2f(x_1, y_j, t) + f(x_1, y_{j+1}, t)}{\delta y^2}, \\
& \frac{\partial f(x_i, y_j, t)}{\partial t} = \frac{f(x_{i-1}, y_j, t) - 2f(x_i, y_j, t) + f(x_{i+1}, y_j, t)}{\delta x^2} + \\
& \qquad \frac{f(x_i, y_{j-1}, t) - 2f(x_i, y_j, t) + f(x_i, y_{j+1}, t)}{\delta y^2}, \\
& \frac{\partial f(x_{n_x-1}, y_j, t)}{\partial t} = \frac{f(x_{n_x-2}, y_j, t) - 2f(x_{n_x-1}, y_j, t) + u_\pi(y_j, t)}{\delta x^2} + \\
& \qquad \frac{f(x_{n_x-1}, y_{j-1}, t) - 2f(x_{n_x-1}, y_j, t) + f(x_{n_x-1}, y_{j+1}, t)}{\delta y^2}, \\
& \qquad\qquad i = 2, \ldots, n_x - 2, \qquad j = 1, \ldots, n_y - 1, \\
& 0 \le u_0(y_j, t) - \sin(j\delta) \sin\left(\frac{\ell_y t}{T} \right) + 1.2, \\
& 0 \le f(x_i, y_j, t) - \sin(i\delta) \sin\left(\frac{\ell_x t}{T} \right) - \sin(j\delta) \sin\left(\frac{\ell_y t}{T} \right) + 1.2, \\
& 0 \le u_{\ell_x}(y_j, t) - \sin(j\delta) \sin\left(\frac{\ell_y t}{T} \right) + 1.2, \\
& \qquad\qquad i = 1, \ldots, n_x - 1, \qquad j = 0, \ldots, n_y, \\
& f(x_i, y_j, 0) = 0, \qquad i = 1, \ldots, n_x - 1, \qquad j = 0, \ldots, n_y, \\
& f(0, y, t) = u_0(y, t), \qquad f(\ell_x, y, t) = u_{\ell_x}(y, t), \\
& 0 \le t \le T.
\end{aligned}
$$

4.3 Time Discretization

Now let us discretize the problem in time. Suppose that the number of the grid points in time is N, and we are taking equal steps in time as well. Hence, the step size is $\delta t = T/N$, and let $f(\mathbf{x}, t_s) = f(\mathbf{x}, (s-1)\delta t)$. To approximate the time integral in the objective function, let us use the left hand side rectangular rule [1], as we did in one dimension. This approximation gives us a fully discretized objective function

$$\delta t \delta x \delta y \left[\sum_{s=1}^{N} \sum_{j=1}^{n_y-1} \sum_{i=1}^{n_x-1} f^2(x_i, y_j, t_s) + \frac{1}{2} \sum_{s=1}^{N} \sum_{i=1}^{n_x-1} \left(f^2(x_i, y_0, t_s) + f^2(x_i, y_{n_y}, t_s) \right) \right]$$
$$+ \delta t \delta y \left(q + \frac{\delta x}{2} \right) \left[\sum_{s=1}^{N} \sum_{j=1}^{n_y-1} \left[u_0^2(y_j, t_s) + u_{\ell_x}^2(y_j, t_s) \right] \right.$$
$$\left. + \frac{1}{2} \sum_{s=1}^{N} \left[u_0^2(y_0, t_s) + u_0^2(y_{n_y}, t_s) + u_{\ell_x}^2(y_0, t_s) + u_{\ell_x}^2(y_{n_y}, t_s) \right] \right]$$

To have the ordinary differential equations fully discretized, we use the first order finite difference approximation in time:

$$\frac{f(x_1, y_j, t_{s+1}) - f(x_1, y_j, t_s)}{\delta t} = \frac{u_0(y_j, t_s) - 2f(x_1, y_j, t_s) + f(x_2, y_j, t_s)}{\delta x^2}$$
$$+ \frac{f(x_1, y_{j-1}, t_s) - 2f(x_1, y_j, t_s) + f(x_1, y_{j+1}, t_s)}{\delta y^2},$$
$$j = 1, \ldots, n_y - 1, \quad s = 1, \ldots, N,$$

$$\frac{f(x_1, y_j, t_{s+1}) - f(x_1, y_j, t_s)}{\delta t} = \frac{f(x_{i-1}, y_j, t_s) - 2f(x_i, y_j, t_s) + f(x_{i+1}, y_j, t_s)}{\delta x^2}$$
$$+ \frac{f(x_i, y_{j-1}, t_s) - 2f(x_i, y_j, t_s) + f(x_i, y_{j+1}, t_s)}{\delta y^2},$$
$$i = 2, \ldots, n_x - 2, \quad j = 1, \ldots, n_y - 1, \quad s = 1 \ldots, N,$$

$$\frac{f(x_1,y_j,t_{s+1})-f(x_1,y_j,t_s)}{\delta t}=\frac{f(x_{n_x-2},y_j,t_s)-2f(x_{n_x-1},y_j,t_s)+u_{\ell_x}(y_j,t_s)}{\delta x^2}$$
$$+\frac{f(x_{n_x-1},y_{j-1},t_s)-2f(x_i,y_j,t_s)+f(x_{n_x-1},y_{j+1},t_s)}{\delta y^2},$$
$$j=1,\ldots,n_y-1,\quad s=1,\ldots,N.$$

The approximation of the rest of the functions in the constraints is just the value of those functions in the discretization points in time. Hence, the fully discretized two dimensional heat transfer optimization problem becomes

$$\begin{aligned}\min_{f,u}\quad \psi(\mathbf{x},t)=\delta t\delta x\delta y&\left[\sum_{s=1}^{N}\sum_{j=1}^{n_y-1}\sum_{i=1}^{n_x-1}f^2(x_i,y_j,t_s)\right.\\&\left.+\frac{1}{2}\sum_{s=1}^{N}\sum_{i=1}^{n_x-1}\left(f^2(x_i,y_0,t_s)+f^2(x_i,y_{n_y},t_s)\right)\right]\\&+\delta t\delta y\left(q+\frac{\delta x}{2}\right)\left[\sum_{s=1}^{N}\sum_{j=0}^{n_y-1}\left[u_0^2(y_j,t_s)+u_{\ell_x}^2(y_j,t_s)\right]\right.\\&\left.+\frac{1}{2}\sum_{s=1}^{N}\left[u_0^2(y_0,t_s)+u_0^2(y_{n_y},t_s)+u_{\ell_x}^2(y_0,t_s)+u_{\ell_x}^2(y_{n_y},t_s)\right]\right]\end{aligned}$$

$$\text{s.t}\quad \frac{f(x_1,y_j,t_{s+1})-f(x_1,y_j,t_s)}{\delta t}=\frac{u_0(y_j,t_s)-2f(x_1,y_j,t_s)+f(x_2,y_j,t_s)}{\delta x^2}$$
$$+\frac{f(x_1,y_{j-1},t_s)-2f(x_1,y_j,t_s)+f(x_1,y_{j+1},t_s)}{\delta y^2},$$
$$j=1,\ldots,n_y-1,\quad s=1,\ldots,N,$$

$$\frac{f(x_1,y_j,t_{s+1})-f(x_1,y_j,t_s)}{\delta t}=\frac{f(x_{i-1},y_j,t_s)-2f(x_i,y_j,t_s)+f(x_{i+1},y_j,t_s)}{\delta x^2}$$
$$+\frac{f(x_i,y_{j-1},t_s)-2f(x_i,y_j,t_s)+f(x_i,y_{j+1},t_s)}{\delta y^2},$$
$$i=2,\ldots,n_x-2,\quad j=1,\ldots,n_y-1,\quad s=1\ldots,N,$$

$$\begin{aligned}
\frac{f(x_1,y_j,t_{s+1})-f(x_1,y_j,t_s)}{\delta t} &= \frac{f(x_{n-2},y_j,t_s)-2f(x_{n-1},y_j,t_s)+u_{\ell_x}(y_j,t_s)}{\delta x^2}\\
&+\frac{f(x_{n-1},y_{j-1},t_s)-2f(x_i,y_j,t_s)+f(x_{n-1},y_{j+1},t_s)}{\delta y^2},\\
&\quad j=1,\ldots,n_y-1,\quad s=1,\ldots,N,
\end{aligned}$$

$$\begin{aligned}
u_0(y_j,t_s) &\geq \sin(j\delta)\sin\left(\frac{\ell_y t_s}{T}\right)-1.2, \qquad j=0,\ldots,n_y \qquad s=1,\ldots,N,\\
f(x_i,y_j,t_s) &\geq \sin(i\delta)\sin\left(\frac{\ell_x t_s}{T}\right)+\sin(j\delta)\sin\left(\frac{\ell_y t_s}{T}\right)-1.2,\\
&\qquad i=1,\ldots,n_x-1, \qquad j=0,\ldots,n_y \qquad s=1,\ldots,N,\\
u_{\ell_x}(y_j,t_s) &\geq \sin(j\delta)\sin\left(\frac{\ell_y t_s}{T}\right)-1.2, \qquad j=0,\ldots,n_y \qquad s=1,\ldots,N,
\end{aligned}$$

$$\begin{aligned}
&f(x_i,y_j,0)=0, && i=0,\ldots,n_x,\quad j=0,\ldots,n_y,\\
&f(0,y_j,t_s)=u_0(y_j,t_s), && j=0,...,n_y \quad s=1,...,N,\\
&f(\pi,y_j,t_s)=u_\pi(y_j,t_s), && j=0,...,n_y \quad s=1,...,N,\\
&0\leq t_s\leq 5, \qquad 0\leq x_i\leq \ell_x, \qquad 0\leq y_j\leq \ell_y.
\end{aligned}$$

As it can be seen from the above model, our heat transfer optimization problem is converted to a convex quadratic optimization problem. The objective function is a convex quadratic function and all the constraints are linear.

Now to simplify the problem and avoid too long formulas, let us assume that $n_x = n_y = n$ and so $\delta x = \delta y = \delta$. Also, denote $\delta t = h$ and then simplify the set of equality constraints further. After reordering the terms in the equality constraints we have

$$\begin{aligned}
\delta^2\Big(f(x_1,y_j,t_{s+1})-f(x_1,y_j,t_s)\Big) &= h\Big(u_0(y_j,t_s)-4f(x_1,y_j,t_s)+f(x_2,y_j,t_s)\\
&\quad + f(x_1,y_{j-1},t_s)+f(x_1,y_{j+1},t_s)\Big),\\
&\qquad j=1,\ldots,n-1,\quad s=1,\ldots,N-1,
\end{aligned}$$

$$\delta^2\Big(f(x_1,y_j,t_{s+1}) - f(x_1,y_j,t_s)\Big) = h\Big(f(x_{i-1},y_j,t_s) - 4f(x_i,y_j,t_s) \\ +f(x_{i+1},y_j,t_s) + f(x_i,y_{j-1},t_s) + f(x_i,y_{j+1},t_s)\Big), \\ i = 2,\dots,n-2, \quad j = 1,\dots,n-1, \quad s = 1\dots,N-1,$$

$$\delta^2\Big(f(x_1,y_j,t_{s+1}) - f(x_1,y_j,t_s)\Big) = h\Big(x_{n-2},y_j,t_s) - 4f(x_{n-1},y_j,t_s) \\ +u_{\ell_x}(y_j,t_s) + f(x_{n-1},y_{j-1},t_s) + f(x_{n-1},y_{j+1},t_s)\Big), \\ j = 1,\dots,n-1, \quad s = 1,\dots,N-1.$$

4.4 Matrix Form

Let us write the problem in a matrix form and then analyze the properties of its coefficients matrices further. First let us consider the variables in vector format. Let vector $\mathbf{u}$ be the vector of boundary variables, and let $\mathbf{f}$ be the vector of the temperature variables in space and time. Denote

$$\mathbf{u}^T = \Big[\mathbf{u}_0^T,\ \mathbf{u}_\ell^T\Big]_{1\times 2(n+1)N},$$

$$\mathbf{u}_0^T = \Big[\mathbf{u}_{00},\ \dots,\ \mathbf{u}_{0n}\Big]_{1\times(n+1)N}, \qquad \mathbf{u}_{0j}^T = \Big[u_0(y_j,t_1),\ \dots,\ u_0(y_j,t_N)\Big]_{1\times N}$$

$$\mathbf{u}_\ell^T = \Big[\mathbf{u}_{\ell 0},\ \dots,\ \mathbf{u}_{\ell n}\Big]_{1\times(n+1)N}, \qquad \mathbf{u}_{\ell j}^T = \Big[u_\ell(y_j,t_1),\ \dots,\ u_\ell(y_j,t_N)\Big]_{1\times N}$$

and

$$\mathbf{f}^T = \Big[\mathbf{f}_1^T,\ \mathbf{f}_2^T,\ \dots,\ \mathbf{f}_{n-1}^T\Big]_{1\times(n-1)(n+1)N},$$

where

$$\mathbf{f}_i^T = \Big[\mathbf{f}_{i,0},\ \dots,\ \mathbf{f}_{i,n}\Big]_{1\times(n+1)N}, \qquad \forall\, i = 1,\dots,n.$$

$$\mathbf{f}_{i,j}^T = \Big[f(x_i, y_j, t_1), \ \ldots, \ f(x_i, y_j, t_N)\Big]_{1\times N}, \quad \forall\, i = 1, \ldots, n-1, \quad j = 0, \ldots, n.$$

Now let I_k be the $k \times k$ identity matrix. Then the objective can be written as

$$\psi(\mathbf{u}, \mathbf{f}) = \frac{1}{2}\mathbf{f}^T Q \mathbf{f} + \frac{1}{2}\mathbf{u}^T H \mathbf{u},$$

where Q and H are diagonal matrices of sizes $\big((n-1)(n+1)N \times (n-1)(n+1)N\big)$ and $\big(2(n+1)N \times 2(n+1)N\big)$, respectively, and we have

$$H = 2h\delta\left(q + \frac{\delta}{2}\right)\begin{bmatrix} J_{(n+1)N} & \mathbf{0} \\ \mathbf{0} & J_{(n+1)N} \end{bmatrix}_{2(n+1)N\times 2(n+1)N}$$

and

$$Q = 2h\delta^2 \begin{bmatrix} J_{(n+1)N} & & \\ & \ddots & \\ & & J_{(n+1)N} \end{bmatrix}_{(n-1)(n+1)N\times(n-1)(n+1)N},$$

where

$$J_{(n+1)N} = \begin{bmatrix} \frac{1}{2}I_N & & & & \\ & I_N & & & \\ & & \ddots & & \\ & & & I_N & \\ & & & & \frac{1}{2}I_N \end{bmatrix}_{(n+1)N\times(n+1)N}.$$

To write the equality constraints in matrix form let us introduce the matrices L_j and G_j as

$$L_j = \begin{bmatrix} \mathbf{0} & & & & \\ h & \mathbf{0} & & & \\ & \ddots & \ddots & & \\ & & & h & \mathbf{0} \end{bmatrix}_{N\times N} \quad G_j = \begin{bmatrix} & 1 & & & \\ \delta^2 - 4h & & -\delta^2 & & \\ & & \ddots & & \ddots \\ & & & \delta^2 - 4h & & -\delta^2 \end{bmatrix}_{N\times N}$$

Also introduce the matrices L and G as

$$L = \begin{bmatrix} \mathbf{0} & L_j & \mathbf{0} & & & \\ & \mathbf{0} & L_j & \mathbf{0} & & \\ & & \ddots & \ddots & & \\ & & & \mathbf{0} & L_j & \mathbf{0} \end{bmatrix}_{(n-1)N\times(n+1)N}$$

and

$$G = \begin{bmatrix} L_j & G_j & L_j & & & \\ & L_j & G_j & L_j & & \\ & & \ddots & \ddots & \ddots & \\ & & & L_j & G_j & L_j \end{bmatrix}_{(n-1)N\times(n+1)N}.$$

Now the equality constraints are

$$\begin{aligned} L\mathbf{u}_0 + G\mathbf{f}_1 + L\mathbf{f}_2 &= \mathbf{0} \\ L\mathbf{f}_{i-1} + G\mathbf{f}_i + L\mathbf{f}_{i+1} &= \mathbf{0}, \qquad\qquad i = 2, \ldots, n-2 \\ L\mathbf{f}_{n-2} + G\mathbf{f}_{n-1} + L\mathbf{u}_\ell &= \mathbf{0}, \end{aligned}$$

or equivalently

$$A\mathbf{f} + B\mathbf{u} = \mathbf{0},$$

where the matrices A and B are of sizes $\big((n-1)(n-1)N \times (n-1)(n+1)N\big)$ and $\big((n-1)(n-1)N \times 2(n+1)N\big)$, respectively. Further, they have the following structures

$$A = \begin{bmatrix} G & L & & & \\ L & G & L & & \\ & \ddots & \ddots & \ddots & \\ & & L & G & L \\ & & & L & G \end{bmatrix}_{(n-1)(n-1)N \times (n-1)(n+1)N} \qquad B = \begin{bmatrix} L & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \\ \vdots & \\ \mathbf{0} & \mathbf{0} \\ \mathbf{0} & L \end{bmatrix}_{(n-1)(n-1)N \times 2(n+1)N}.$$

In all of the equations $\mathbf{0}$ denotes the zero matrix or vector of the appropriate size. Now let us introduce a set of the fixed vectors $\mathbf{d}_i$ to write the inequality constraints in vector form. Each $\mathbf{d}_i$ corresponds to the internal points x_i, and is defined as follows

$$\mathbf{d}_i^T = \left[\mathbf{d}_{i,0}^T,\ \mathbf{d}_{i,1}^T,\ \cdots,\ \mathbf{d}_{i,n}^T\right]_{1\times(n+1)N} \qquad i = 1, \ldots, n-1,$$

where $\mathbf{d}_{ij}$ for $j = 0, \ldots, n$ are defined as

$$\mathbf{d}_{i,j} = \begin{bmatrix} -\sin(i\delta)\sin\left(\frac{\ell_x \times 0}{T}\right) - \sin(j\delta)\sin\left(\frac{\ell_y \times 0}{T}\right) + 1.2 \\ -\sin(i\delta)\sin\left(\frac{\ell_x \times 1}{T}\right) - \sin(j\delta)\sin\left(\frac{\ell_y \times 1}{T}\right) + 1.2 \\ \vdots \\ -\sin(i\delta)\sin\left(\frac{\ell_x \times (N-1)}{T}\right) - \sin(j\delta)\sin\left(\frac{\ell_y \times (N-1)}{T}\right) + 1.2 \end{bmatrix}_{N \times 1}.$$

Now let us define the fixed vector $\mathbf{d}$ as

$$\mathbf{d}^T = \left[\mathbf{d}_1^T,\ \mathbf{d}_2^T,\ \ldots,\ \mathbf{d}_{n-1}^T\right]_{1\times(n-1)(n+1)N}. \tag{4.3}$$

For the inequalities on $\mathbf{u}$ let denote the fixed vector $\mathbf{c}$ as

$$\mathbf{c}^T = \left[\mathbf{c}_1^T,\ \mathbf{c}_2^T,\ \ldots,\ \mathbf{c}_n^T\right]_{1\times(n+1)N},$$

where $\mathbf{c}_j$ is defined for each point in $y-$axis as follows

$$\mathbf{c}_j = \begin{bmatrix} -\sin(j\delta)\sin\left(\frac{\ell_y \times 0}{T}\right) + 1.2 \\ -\sin(j\delta)\sin\left(\frac{\ell_y \times 1}{T}\right) + 1.2 \\ \vdots \\ -\sin(j\delta)\sin\left(\frac{\ell_y \times (N-1)}{T}\right) + 1.2 \end{bmatrix}_{N \times 1}, \qquad j = 0, \ldots, n.$$

Now the inequality constraints can be written as

$$\mathbf{f} + \mathbf{d} \geq \mathbf{0}$$
$$\mathbf{u} + \mathbf{c} \geq \mathbf{0}.$$

As a result, the two dimensional discretized heat transfer optimization problem can be written in matrix form as

$$\begin{aligned}
\min_{\mathbf{u},\mathbf{f}} \quad & \psi(\mathbf{u},\mathbf{f}) = \frac{1}{2}\mathbf{f}^T Q\mathbf{f} + \frac{1}{2}\mathbf{u}^T H\mathbf{u} \\
\text{s.t.} \quad & A\mathbf{f} + B\mathbf{u} = \mathbf{0}, \\
& \mathbf{f} + \mathbf{d} \geq \mathbf{0}, \\
& \mathbf{u} + \mathbf{c} \geq \mathbf{0}.
\end{aligned}$$

This is the formulation for a convex quadratic problem with linear constraints. This problem now can be solved with standard interior point method solvers, and the global optimality for the found optimum of this problem is guaranteed.

Chapter 5

Computational Experiments

In our computational experiments, we take the intervals in such a way that they are similar to the ones in the one dimensional case. Let $T = 5$, and so the time period of the process is $[0, 5]$. We assume that the bar is a square of length π, that is, $\ell_x = \ell_y = \pi$. Let us assume that the number of discretization points in the x-axis and the y-axis are equal, that is, $n_y = n_x = n$, and therefore $\delta = \delta x = \delta y = \pi/n$ and $h = \delta t = 5/N$. Note that the two dimensional model that is solved here is comparable with the "sparse full model" in the one dimensional case, as all the inequality constraints regardless of their activity are kept in the model, and the coefficient matrices of this problem are also large, sparse and structured.

The computer on which the two dimensional problem is solved is the same computer that is used for the one dimensional problem as described on page 29. The optimization solver package is MOSEK 3.0 and the setup of the matrices is done in MATLAB, as it was in the one dimensional case, see page 29 for details.

N	objective	P. eq. inf.	D. eq. inf.	it.	CPU	total
500	9.1175743063	2.37e-014	1.82e-013	23	41	43
1000	9.1326715839	1.11e-014	1.15e-013	24	85	86
1500	9.1376967275	2.06e-014	2.09e-013	23	133	135
2000	9.1402080785	1.83e-014	1.83e-013	25	222	227
3000	9.1427186178	5.89e-014	5.84e-013	25	356	361
4000	9.1439735405	3.57e-014	3.52e-013	27	542	552
4500	N.A.					

N.A.: Results not available due to memory shortage.

Table 5.1: Computational results for the 2D heat transfer problem, $n = 10$.

5.1 Computational Results

In Table 5.1, the number of the spatial discretization points is fixed to be $n = 10$, while the number of time discretization points, N is changing. Since in the two dimensional problem the size of the coefficient matrices is very large, the problem can not be solved for very fine discretization. The solver needs more memory to solve the two dimensional problem for $N \geq 4000$, and reports an error message for memory shortage.

Table 5.2 presents a comparison between the numerical results obtained

	2D Model			1D Model		
N	size	iter.	time	size	iter.	time
500	4.9005×10^9	23	43	4.95×10^7	15	1
1000	1.9602×10^{10}	24	86	1.98×10^8	18	3
1500	4.4105×10^{10}	23	135	4.455×10^8	20	6
2000	7.8408×10^{10}	25	227	7.92×10^8	22	6
3000	1.7642×10^{11}	25	361	1.7820×10^9	23	7
4000	3.1363×10^{11}	27	552	3.1680×10^9	26	12

Table 5.2: Comparison between the matrix size and number of iterations for the 1D and 2D models, $n = 10$.

for the one dimensional problem and the two dimensional problem, when the number of discretization points in space is fixed to $n = 10$. The required time to solve the two dimensional problem is much higher, and the number of iterations is higher too. As the number of discretization points in time, N, grows the size of the equality constraints coefficient matrices also grows linearly. Since no inequality constraint has been removed from the two dimensional optimization model, the corresponding data for the one dimensional problem is obtained from the sparse full model in which no inequality constraints has been removed.

n	objective	P. eq. inf.	D. eq. inf.	it.	CPU	total
10	9.0720825339	5.35e-014	4.77e-013	13	10	12
16	9.3497558433	4.46e-014	5.43e-013	18	216	224
20	9.3492693543	1.14e-014	1.27e-011	17	318	320
24	N.A.					

N.A.: Results not available due to memory shortage.

Table 5.3: Computational results for the 2D heat transfer problem, $N = 300$.

In the Table 5.3 the number of discretization point in time is fixed to $N = 300$, and the discretization in space becomes finer. Note that the size of the coefficient matrices in the two dimensional problem depends quadratically on the number of space discretization points, as shown on page 62. Therefore, the solver can not handle more than 22 points in each direction of the space, and the "out of memory" error message appears.

Table 5.4 compares the number of iterations, the solution time, and the size of the coefficient matrix for the equality constraints, in the one dimensional and the two dimensional problems. The data reported for both the problem classes are obtained from the sparse full model.

	2D Model			1D Model		
n	size	iter.	time	size	iter.	time
10	1.7642×10^9	13	12	1.782×10^7	15	1
16	1.1705×10^{10}	18	224	4.59×10^7	12	2
20	2.8656×10^{10}	17	320	7182×10^7	11	2

Table 5.4: A comparison between the matrix size and iteration for the 1D and 2D models, $N = 300$.

Chapter 6

Problem Generalizations and Conclusion

The one dimensional problem that was introduced in Chapter 1, can be modified in many different ways. Different variations of the objective function can be used as other measurements of energy, or any desired objective. The objective can be chosen in several ways so that the discretized objective function, and thus the problem becomes linear.

The constraints can be modified too. The partial differential equation constraint can be replaced by other differential equations for other problems. As long as the discretization of the partial differential parts does not make bilinear or nonlinear equations when the problem is discretized, the solving strategy remain the same, as it has been described in the previous chapters.

Moreover, additional requirements, such as the inequality constraint can be changed to some other functions and may include upper bounds, lower bounds, and equalities. More constraints can be added to the problem, which presumably might make the problem harder to solve.

Further, different discretization and approximation methods can be used on this problem to obtain more accurate solutions. The step sizes were assumed to be all equal for the problem solved in Chapter 3 and Chapter 5, which may not always be the best strategy. Various discretization schemes, mesh refinements may be applied [9].

In this chapter we discuss some modifications of the original problem.

6.1 Variants of the Objective Function

The objective function that we considered for the problem is the sum of temperature squared over all applicable points, or in other words, it is the 2-norm of the temperature function. Alternatively, other norms can be used as the objective function, such as 1-norm or the infinity-norm.

As an example for the objective function, let us minimize the overshooting of the optimal temperature function from the lower bound function. To evaluate the overshooting of $f(\mathbf{x},t)$ and $g(\mathbf{x},t)$ any norm can be used. Here is the objective function when the overshooting is evaluated using the 1-norm:

$$\min_{u_0(t),u_\ell(t),f(\mathbf{x},t)} \qquad \psi(\mathbf{x},t) = \int_t \int_\mathbf{x} [f(\mathbf{x},t) - g(\mathbf{x},t)]\, d\mathbf{x}dt.$$

Note that all the terms in this function are positive, because $g(\mathbf{x},t) \leq f(\mathbf{x},t)$.

Also some weights can be applied to the endpoints of the bar, say q_0 and q_ℓ for the point $x=0$ and $x=\ell$, respectively. Thus we have

$$\begin{aligned}
&\int_t \left(\int_\mathbf{x} [f(\mathbf{x},t) - g(\mathbf{x},t)]\, d\mathbf{x} + q_0 [u_0(t) - g(0,t)] + q_\ell [u_\ell(t) - g(\ell,t)] \right) dt \\
&= \int_t \left(\int_\mathbf{x} f(\mathbf{x},t) d\mathbf{x} + q_0 u_0(t) + q_\ell u_\ell(t) - \int_\mathbf{x} g(\mathbf{x},t) d\mathbf{x} \right) dt \\
&= \int_t \left(\int_\mathbf{x} f(\mathbf{x},t) d\mathbf{x} + q_0 u_0(t) + q_\ell u_\ell(t) \right) dt - \int_t \int_\mathbf{x} g(\mathbf{x},t) d\mathbf{x}dt.
\end{aligned}$$

The integral of the lower bound function, $g(\mathbf{x},t)$, is a given constant value, independent of the control variables and the resulting profile $f(\mathbf{x},t)$, so this constant value can be removed from the objective function, resulting

$$\min_{u_0(t),u_\ell(t),f(\mathbf{x},t)} \qquad \psi(\mathbf{x},t)\int_t\left(\int_{\mathbf{x}} f(\mathbf{x},t)d\mathbf{x} + q_0u_0(t) + q_ellu_\ell(t)\right)dt$$

The discretization for this problem is quite similar what was done for the original problem. The approximation of the objective function is just the sum of the function values in the discretized points. Now, if we consider that the spatial number of discretization points in space is $n_x = n$, and the number of time discretization points is N, the step sizes are $h = T/N$ and $\delta = \ell/n$. Then the discretized objective is

$$\min_{\mathbf{f},\mathbf{u}} \qquad \sum_{i=1}^{n-1}\sum_{s=1}^{N} f(x_i,t_s) + \sum_{s=1}^{N}[q_0u_0(t_s) + q_\ell u_\ell(t_s)].$$

Let us utilize the vector of variables $\mathbf{f}$ as defined in (2.8), and define $\mathbf{u}$ as

$$\mathbf{u}^T = \left[\mathbf{u}_0^T,\ \mathbf{u}_\ell^T\right]_{1\times 2N}, \tag{6.1}$$

where

$$\mathbf{u}_0^T = \left[\mathbf{u}_0(t_1),\ \ldots,\ \mathbf{u}_0(t_N)\right]_{1\times N} \qquad \text{and} \qquad \mathbf{u}_\ell^T = \left[\mathbf{u}_\ell(t_1),\ \ldots,\ \mathbf{u}_\ell(t_N)\right]_{1\times N}.$$

Thus the objective function can be written as

$$\min_{\mathbf{f},\mathbf{u}} \qquad \mathbf{e}_{(n-1)N}^T\mathbf{f} + \mathbf{j}^T\mathbf{u},$$

where

$$\mathbf{j}^T = \left[q_0\ \mathbf{e}_N^T,\ q_\ell\ \mathbf{e}_N^T\right]_{1\times 2N},$$

and $\mathbf{e}_k$ is the $(k \times 1)$ vector, which all of its coordinates equal to one.

The discretization of the constraints and is the same as described in Chapter 2. The objective function in this problem is linear, and since the discretized constraints are all linear[1], then the 1-norm overshooting problem is a linear optimization problem that can be solved by any linear optimization package, among those MOSEK's linear solver.

6.2 Variants of the Inequality Constraints

The inequality lower bound constraint can be modified in many ways. Also another constraint can be added to the problem. Assume that we add an upper-bound constraint

$$f(x,t) \leq b(x,t) = 0.5\left[\sin(x)\sin\left(\frac{\ell t}{T}\right)\right] + 0.1. \tag{6.2}$$

The two constraint are shown in Figure 6.1. The bounded heat transfer problem becomes

$$\min_{f(\mathbf{x},t),u(\mathbf{x},t)} \qquad \psi(\mathbf{x},t) = \int_t \int_{\mathbf{x}} f^2(\mathbf{x},t) d\mathbf{x} dt + \int_t \int_{\mathbf{x}} u^2(\mathbf{x},t) d\mathbf{x} dt$$

[1]See Section 2.3

$$
\begin{aligned}
\text{s.t.} \quad & \frac{\partial f(\mathbf{x},t)}{\partial t} = \frac{\partial^2 f(\mathbf{x},t)}{\partial \mathbf{x}^2}, \\
& f(\mathbf{x},t) \le -0.5 \left[\sin(x)\sin\left(\frac{\ell t}{T}\right)\right] - 0.1, \\
& f(\mathbf{x},t) \ge \sin(x)\sin\left(\frac{\ell t}{T}\right) - 0.7, \\
& f(\mathbf{x},0) = 0, \\
& f(0,t) = u_0(t), \\
& f(\ell,t) = u_\ell(t), \\
& \forall\, \mathbf{x} \in [0,\ell], \qquad \forall\, t \in [0,T].
\end{aligned}
$$

The discretization of this problem is similar to what we did in Chapter 2, and the obtained discretized problem is convex quadratic. Assume that the matrices and vectors are defined as in Section 2.5, and let $\mathbf{r}$ and $\mathbf{p}$ be the appropriate vectors for the upper bound function when it is discretized. Then the matrix form of the bounded heat transfer is

$$
\begin{aligned}
\min_{u} \quad & \psi = \frac{1}{2}\mathbf{f}^T Q \mathbf{f} + \frac{1}{2}\mathbf{u}^T H \mathbf{u} \\
\text{s.t.} \quad & A\mathbf{f} + B\mathbf{u} = 0, \\
& \mathbf{d} \le \mathbf{f} \le \mathbf{p}, \\
& \mathbf{c} \le \mathbf{u} \le \mathbf{r}.
\end{aligned}
$$

6.3 Variants of the of Partial Differential Equation Constraints

Many partial differential equation can be used instead of the heat equations (or be added) in an optimization problem to describe and optimize other physical

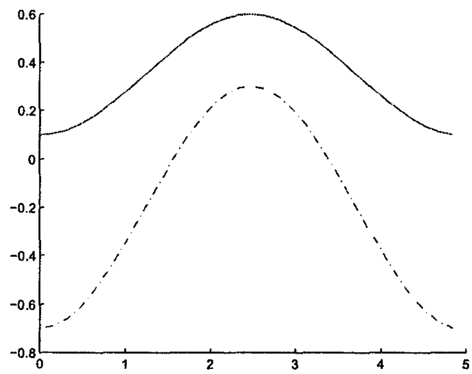

Figure 6.1: The upper bound constraint, solid, vs. the lower bound constraint, dashed

problems. Besides the heat equation $\partial f/\partial t - \partial^2 f/\partial^2 \mathbf{x} = 0$, many other basic PDEs can be used. Some examples of such PDEs are the linear transport equation,

$$\frac{\partial f}{\partial t} + \mathbf{b} \cdot \frac{\partial f}{\partial \mathbf{x}} = 0,$$

where $\mathbf{b}$ is a fixed vector, the Laplace's equation

$$\frac{\partial^2 f}{\partial^2 \mathbf{x}} = 0,$$

and the wave equation

$$\frac{\partial^2 f}{\partial^2 t} - \frac{\partial^2 f}{\partial^2 \mathbf{x}} = 0,$$

where appropriate constraints for these PDEs are added.problem to make sure of the controllability of these equations.

If there is no multiplication in the different parts in the substituted partial differential equation, then by using the same discretization methods the obtained set of equations remain linear. Therefore the same technique lead to analogous quadratic or linear optimization problems, when the objective function can be discretized to a linear or quadratic function.

6.4 Variants of the Discretization Methods

We used equally distributed mesh discretization, while many other methods could have been applied. Adaptive mesh refinement [9] is a good method, especially when the functions are not so smooth and have sudden bumps. Other approximations and discretizations can be applied too. In the approximation of the PDEs finite element methods, and also more accurate methods such as spectral methods can be employed. To evaluate the integration, Simpson's rule, Boole's rule, Gaussian quadrature, and many other numerical integration methods can be used [1] depending on the functions and the desired accuracy.

The error that is made in discretization methods highly affects the numerical results. When the discretization error is large, attempting to obtain higher accurate numerical results for the discrete problem does not necessarily lead to a more accurate solution for the original problem. Using a better and more accurate discretization methods, and consistency between the accuracy of discretization methods and the numerical optimization methods can help to obtain better solution for the original problem.

6.5 Conclusion

Optimization problems with partial differential equations and inequalities in their set of constraints can be solved using discretization methods. The discretization approach is powerful enough to handle more various functions in the constraints than optimal control methods. Various objective functions can be used, equality and inequality constraints can be added or modified in a problem, and still the same discretization method can result in optimization problems with analogous structure and characteristics.

In the case that the PDEs do not include multiplication of different partial differentiations and the functions in the inequality constraints are smooth, the described discretization method can simplify the constraints to a finite set of linear constraints. Whenever the objective function is discretized to a linear, quadratic, or nonlinear function, the problem becomes a linear, quadratic or nonlinear optimization problem, respectively.

The discretization method converted the nonlinear optimization model for the one-dimensional heat-transfer problem to a convex quadratic optimization problem for which the global optimality is guaranteed. Using the MOSEK solver this problem can be solved for fine discretization mesh points, while this problem can not be solved by optimal control methods properly [3]. When discretized, the problem has a large but sparse coefficient matrices. To improve the size of the matrices Biegler and Kameswaran [7] suggested to write all the temperature variables in terms of temperatures at the endpoints. Although this reduces the size of the problem significantly, the denser coefficient matrices and the predefined matrix operations affect the numerical results negatively. The results obtained for the compactified model are not as good as for the original large scale sparse model.

The one-dimensional heat-transfer optimization problem can be simplified further by removing the inactive inequalities from its constraint set [3]. The numerical results for both models show that some numerical difficulties occurs when solving the problem with finer spatial discretizations. The optimization packages tend to recognize the numerical difficulties in the original sparse model sooner than the more simplified model, by reporting primal infeasibility. However, some numerical issues can be detected in the dual solution of the more simplified model too. The instability occurs after reaching a certain number of discretization points in the space, when the number of time discretization points is fixed. This might be due to instability in the discretization methods which are applied to the objective function and the PDEs. The stability of the methods seems to depend on both the number of discretization points in time and space, and for a specified fineness in time, the number of spatial discretization points should be less than a certain number to achieve stability.

The problem can be generalized to the two dimensional heat transfer model. The strategy to solve the two dimensional problem stays the same as in the case of the one dimensional problem. However, the coefficient matrices are very large for the two dimensional case, and that causes numerical difficulties. Using better methods in memory management and better computers and optimization solvers can improve the numerical results.

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