MODELING AND OPTIMIZING SOLIDIFICATION PROCESSES

MASTER THESIS

by

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Thank you God for bearing me in this way.

Abstract

The design of metal parts is done, or at least improved, in many cases by the so called structural optimization methods. These attempt to find an "optimal design" in terms of maximal stiffness, minimal mass, etc. But often such an optimal design can present difficulties when trying to produce it, say in a casting process.

The goal of this thesis is two folded: first, to describe some models for the solidification and second to explore the possibility of applying the known optimization methods used in structural problems, in particular the topological derivative, for the solidification models. In other words improve the design of a part in order to be easier to produce.

Contents

List of symbols

u	Temperature
f_s	Solid fraction
q	(Heat, energy) Flux
n	normal
$\mathcal{J}$	Objective functional w.r.t. domain Ω
J	Objective functional w.r.t. solution u
j	Objective functional w.r.t. ball radius ϵ
ϱ	Energy density
ρ_m	Density of metal
ρ_s	Density of sand
c_m	Heat capacity of metal
c_s	Heat capacity of sand
λ	Latent heat
k	Thermal conductivity
k_m	Heat conductivity of metal
k_s	Heat conductivity of sand
u_S	Solid temperature. Just solid metal under this temperature
u_L	Liquid temperature. Just liquid metal above this temperature
α_0	Conductivity of sand (in Helmholtz equation).
β_0	Constant for sand (in Helmholtz equation).
α_1	Conductivity of metal (in Helmholtz equation).
β_1	Constant for metal (in Helmholtz equation).
μ	Crystal grow constant
V	Hilbert Space
H^1	Sobolev space W_2^k
$H^1_{0,D}$	Functions with compact support and Dirichlet conditions in H^1

Chapter 1

Introduction

The procedures for the design of structures or machine parts have evolved from the beginning of the industrial era. Designing a part is now a process involving not only humans but also computers and algorithms. The design of a bridge, for example, able to support a given load but at the same time using as few material as possible is a task that can be solved with the help of structural optimization algorithms.

When using such algorithms it is possible to find structures with optimal mechanical properties with respect to compliance, mass, eigenfrequencies, etc.

Nevertheless, it could happen that an "optimal" design in a mechanical sense is a very bad design from the point of view of production. In other words, it could be difficult or even impossible to produce. It is easy to imagine that if a design represents a very complicated shape with many details its production will require more care. But even more simple shapes could present severe difficulties in its production. In figure 1 a simple cross shape is presented and defects called *porosities* appear in the center.

Many parts are produced by a casting technology which involves the solidification of liquid metal. This is a complicated process that puts strong requirements on the material and the design.

The aim of the thesis is to use the models for solidification to optimize

Figure 1.1: Porosities

the topology of an original design.

In the first part (chapter 2) we introduce one of the most popular process for the production of metal pieces, the casting process. We will see the dynamics involved in the process, how the heat is transfered and what is expected from a good cast.

The central part of the casting is the solidification. Several models for solidification exist, from a macroscopical point of view using only energy considerations to microscopical models where the formation and grow of solid particles are modeled. The solidification process is modeled using the heat transfer equation, which is numerically solved using finite elements.

In the second part, presented in chapter 3, we will explore possible optimization methods, in particular the *topological gradient* see [1], [7], [8]. Finding the expression of the topological gradient for a particular problem is not a trivial mathematical exercise. The casting process, being a very complicated process is no exception. We will be forced to adapt our model and adjust the objective function to be able to use the already computed topological gradient for the Helmholtz equation, in [1].

Coupling the optimization with the models for solidification in order to improve an initial design will represent the last part of the thesis.

Chapter 2

Solidification of Metals

In this chapter we describe one of the process used in the production of metal parts. Afterwards we will mention the main physical aspects of the process with the purpose of introducing a model in the form of equation for the solidification. At the end, numerical methods will be proposed for the solution of the equation and some results from a C++ program will be shown.

2.1 Casting Processes

For the production of complicated pieces, machining (drilling, milling, welding, etc.) is no longer a feasible option. The task could become very difficult, if not impossible, and the desired mechanical properties weakened.

An old alternative for the production of complicated shapes is,

- Create a copy of the object you want to produce using a different material, easy to work with, like wood, wax or clay.
- Use the copy to make a mold; usually a sand mold.
- Pour liquid metal in the mold and fill it.
- Wait for the metal to cool down, or help it.

- Remove the mold.

If sufficient care is taken in the process and enough experience is present in the manufacturers, the final result will be a solid metal reproduction of the original shape. This is the casting process.

The study of castings involve very complicated mechanical and physical processes. The metal is an alloy, which means that several components are present and in different states. You can have materials, impurities and gases in the initial fluid melt. The dynamics of the filling are quit complicated and even if a good model for this is founded, the presence of non-located gases, impurities and bubbles make the task even more hard.

During the cooling and solidification other problems appear, inner flows trough a dendrite labyrinth of solid metal. Nuclei particles and impurities diving in the flow. Tensile stress in liquid, surface contraction, vapor release. This continues until the melt is all solid.

Still with all the metal solidified, contraction continues and resistance of the mold is present. In this process many times the piece cracks, or worst, collapses. But even if no visible defect is apparent, inner voids, cracks or residual stresses could exist there.

The reader interested in more information about castings is referred to [2].

2.1.1 Solidification Dynamics

How does a liquid metal is transformed in solid? In the school we learned that water is liquid if its temperature is above zero degrees, and solid (ice) if its temperature is below zero. While the temperature is zero we suppose to have a mixture of ice and water with the corresponding liberation of latent heat according to the quantity of mass we want to solidify.

In practice and specially for alloys, even when there is a melting temperature, liquid metal does not transform suddenly in solid when passing this

temperature. The liquid can in fact cool down below its melting temperature for a while. The phenomenon is called *undercooling*.

The first solid particles appear in regions of liquid metal at temperatures below the melting point. This are called nucleus and are formed around foreign particles or in the wall of the mould. The process is called *nucleation* and several models exist for it, see [11].

After a nucleus is created a solid, some times called crystal, grows around it. Models also exist for this grow. In metals however, the solid metal grows in form of dendrites in complicated shapes. The grow is usually modeled as dependent on the temperature and its derivative.

2.1.2 Heat Transfer in Castings

The process for a liquid metal to lose its heat and transform in solid is slow and passes through different stages, see [2]. The flow of heat varies in different parts of the mould

1. liquid metal
2. solid metal
3. interface between metal and mould
4. mould
5. surroundings.

Liquid metal Here the temperature varies more or less randomly due to convection. When the mould is filled, the forced convection produces turbulent flow and mixing. Here we have a heat transfer model but the heat is transported in a relative fast way, with the consequence of smooth temperature gradients. For that reason in some cases the gradient of temperature in the liquid metal is neglected.

Solid metal For metals with low thermal conductivity the heat flow can be modeled by the standard heat diffusion equation

$$\dot{u} = k_m \Delta u$$

with boundary conditions

$$u|_{\Gamma_W} = u_W \qquad \text{in the wall of the mould}$$

$$u|_{\Gamma_F} = u_F \qquad \text{in the solidification front}$$

The solidification front grows proportional and in the direction of the gradient of temperature.

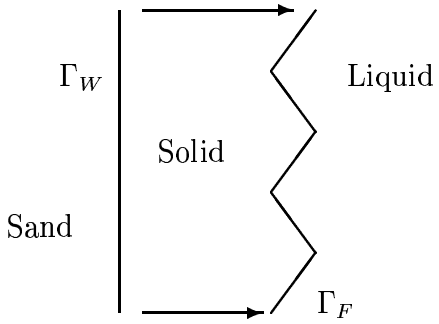

Figure 2.1: Solidification Front

Interface (Cast-Mould) While the metal is liquid there are relative many contact points between mould and metal. In this case the conduction of heat is high (this creates high nucleation rates at the boundary). But as soon as the metal solidifies, and specially when there is contraction, the contact points are reduced, or disappear, and an *air gap* is created between metal and mould. This gap reduces significatively the conduction of heat. Assuming homogeneous contraction, the size of the gap can even be estimated. In [2] we find the estimation

$$d \sim D(k_m(u_{freezing} - u) + k_s(u_{interface} - u_o))$$

Here D is the dimension of the mould. The estimation is crude, because the expansion is by no means homogeneous, but it gives a point of reference. The estimation of a *heat transfer coefficient* for the interface has been longly studied, and for high temperature castings even radiation becomes an important way for conduction.

Mould Here there is no question or problem. The diffusion of heat can be modeled with the same equation

$$\dot{u} = k_s \Delta u.$$

However is important to notice that in all the cases $k_s << k_m$. This keeps the cast hot and reduces the heat lose.

Surroundings In most instances this is also negligible. For normal sand moulds the environment temperature of the mould does not alter the solidification, and in fact the outside temperature of the mould increases barely. This is, of course, not always true, specially for thin-walled moulds. Where the cast can be sensitive to the outside temperature.

The heat conduction in the mould is usually slow. This is sometimes not desirable, and some means are used to increase the heat transfer. Cooling systems or simply the place of a block of metal in the mould is used normally. Fins that are in fact in contact with the cast are also in use. The optimal size and position of these fins represents an interesting problem.

2.1.3 Solid Formation

When the temperature falls below the freezing point, the change to solid is not instantaneous. In liquid the molecules vibrate and move changing its position which could be rather random. For the solid, the molecules align themselves to form an ordered grid or array in more or less packed rows. This is what is called a *crystal*.

Assuming that cooling down a liquid material produces always a crystal is not true. In the production of glass, the material cools and loses thermal motion, but the atoms are incapable to rearrange in a lattice. The glass is a *supercooled* liquid and it can remain as a liquid forever. Interesting to say that glass is not a crystal but an amorphous material, as some may belive. For metal this phenomenon exist also but not that dramatic. Clean liquid metals can be frozen to temperatures of hundreds grads below its freezing point if clean containers are used, see [2]. However in real castings there is no clean metal or containers. The presence of impurities and alloys tends to increase the nucleation and reduce the undercooling.

After a nuclei is created, the solid grows around it. For clean materials this grow is quite homogeneous creating cells. For metal castings the velocity of grow is rather high and the solid grows in tree-like form (dendrites). The grows continues until the cells come in contact with other growing cells. When the cell stops growing its called a *grain*. The solid metal is then formed for several grains. The properties of the cast will depend strongly on the final structure of grains.

2.1.4 Good Castings

How can one decide if the cast process is good or bad?

It has been recognized that, as a general rule, the presence of large grains in the solid is a disadvantage. The finer grain size bring some practical consequences, see [2].

- Improved resistance to hot tearing during solidification.
- Improved resistance to cracking when welding.
- Reduced scattering of ultrasonic waves and X-rays, allowing better non-destructive inspection.
- Improved resistance to grain boundary corrosion.
- Higher tensile yield and ultimate strengths.

- Higher toughness.
- Improved fatigue resistance.

Although not all the benefits appears in all the castings, the general rule is that small grains are better.

Is it possible to control the process to reduce the size of the grains?

The size of the grains depends on the nucleation rate and on the grow. Clearly the ideal case would be a high nucleation rate together with a slow grain grow. Many times this is achieved adding inoculants to the melt. For gray iron, for example, the inoculants include ferrosilicon, calcium, silicide and graphite. This helps to undercool the melt in the vicinity of the particles and promotes nucleation. If during the solidification interval the liberation of latent heat increases the temperature in some point, the effect of the inoculants can be affected. This should be avoided if possible.

If during the solidification part of the liquid metal is completely surrounded by solid metal a *hot spot* is created. The cast contracts when solidifies. A hot spot could be then cause of inner voids, porosities or stress concentration. Hot spots, figure 2.2, are avoided in practice by control of the cooling process.

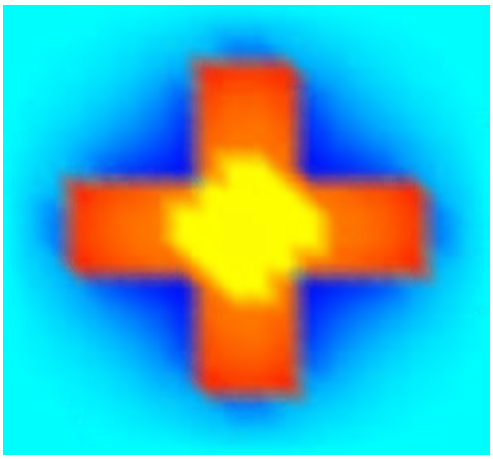

Figure 2.2: Liquid metal surrounded by solid forms a “hot spot”.

Using of metal fins incrusted in the cast before the pouring of liquid metal or using pipes with cool fluid flowing are used to help the cooling. The geometry of the cast is known to affect the presence of hot spots. Junctions are used, T-junctions and L-junctions, for example.

2.2 Heat Conduction with Phase Change

When temperature in a body is different in distinct parts, there is a tendency in the temperature distribution to the equilibrium. Namely the hotter parts gives energy and increases the temperature of the cooler parts. This can be described as a flow of energy *heat* in the body. The transference of heat is caused by three means. (i) convection, when heat is transfered with moving masses, always fluids. (ii) conduction, where energy is transfered through the body and (iii) radiation, where the energy is transfered via electromagnetic radiation. Here we consider only conduction in isotropic media, this means that the properties are not depended upon given directions. The classical reference for heat conduction in solids is Carslaw [3].

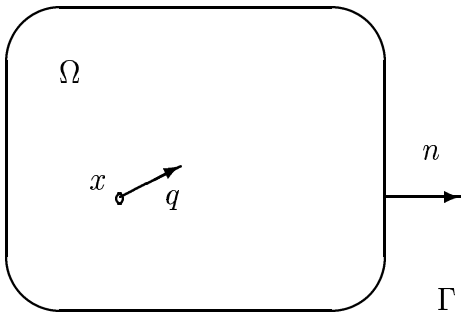

Figure 2.3: Domain for Heat Conduction.

The theory for heat conduction rest upon the Fourier's law. It states that the flow of heat in a point is proportional to the gradient of temperature, and in the opposite direction. Let $\Omega \in \mathbb{R}^n$ where $n \in 2, 3$ represent an object,

and let $u : \Omega \times \mathbb{R} \to \mathbb{R}$ describe its temperature. The flow $q : \Omega \times \mathbb{R} \to \mathbb{R}^n$ is given by,

$$q(x,t) = -k\nabla(u(x,t)). \tag{2.1}$$

Where k is called the *thermal conductivity* of the material.

To find the equation of heat transfer with phase change the continuity equation, assuming no energy sources will be required,

$$\frac{\partial \varrho}{\partial t} + \nabla \cdot q = 0. \tag{2.2}$$

The energy density ϱ is related with the temperature of the body, but when the temperature of substance goes below its freezing point (or above its melting point), estimation of the energy requires more than only the temperature. During the transformation of phase heat is released (or absorbed). This kind of heat is called *latent heat*, and it is defined as the amount of heat required to change the phase of a unit of mass. We can think in the latent heat as some energy hidden in the solid. In this way we need to consider an extra term for the energy in our continuity equation.

In order to measure this energy we have to include an extra variable f_s in our model, the *solid fraction*. The solid fraction describes locally the percentage of solid in a point. This means that, in the model, we don't restrict our material to be only solid or liquid, but we allowed the material to be in some kind of intermediate phase with some fraction of solid and some of liquid. This is called in some works the *mushy region*.

The density of energy is given by $\varrho = \rho(cu - \lambda f_s)$ where,

ρ density of the material,
c specific heat,
u the temperature,
λ the latent heat and
f_s is the solid fraction.

Substituting ϱ and 2.1 in 2.2, see [10] the energy equation becomes

$$\rho c \frac{\partial u}{\partial t} = \nabla \cdot (k\nabla u) + \rho\lambda \frac{\partial f_s}{\partial t} \qquad \text{in } \Omega. \tag{2.3}$$

Equation (2.3) describes only what is happening inside of the body. It is necessary to specify what is going on in the boundary. The typical conditions used on the boundary are the following:

Given temperature in the boundary. The temperature on the boundary surface $\Gamma_T \subset \Gamma$ is prescribed as function of time and space.

If the flux normal to the boundary of the body is defined as

$$q_n = -k\frac{\partial u}{\partial n}$$

then another conditions are common.

Isolated boundary or prescribed flux. If the boundary represents an insulator, then the flux through the boundary $\Gamma_F \subset \Gamma$ is considered as zero. In other cases a prescribed flux can be considered.

Newton's Law of cooling. If the object is considered to be in an ambient temperature u_s then the flux through $\Gamma_S \subset \Gamma$ can be considered to be proportional to the difference between this and the temperature of the object on the boundary.

Then the common boundary conditions are:

$u = u^*$	on Γ_T	prescribed temperature
$q_n = q_F^*$	on Γ_F	prescribed flow
$q_n = \alpha(u - u_s)$	on Γ_S	Newton's Law.

There are two variables in our model, the temperature u and the solid fraction f_s, it is expected to have more relations. These should relate the solid fraction with the temperature. In a general way the solid fraction can be represented as a function of time, temperature and even the solid fraction it self or more variables and relations can be included.

2.2.1 Models for the Solid Fraction

In the so called micro-models or macro-micro models, the solid fraction is computed using models for the nucleation and the grow of crystals. In [4], for example, it is assumed that the crystals are spheres of equal radius $R(t)$

and that the number of nuclei is $N(t)$. With this assumption the solid fraction would be,

$$f_s = \frac{4}{3}\pi R^3(t)N(t).$$

With the further assumption of constant nucleation and crystal grow rate related with undercooling via

$$R = r_0 + \int_0^t \mu(u_e - u(t))^2 dt,$$

where r_0 is the critical radius, μ is the growth constant and u_e the *eutectic temperature*, i.e. $u_e - u(t)$ is the undercooling, the expression for f_s is

$$f_s(t) = 1 - e^{-\frac{4}{3}N\pi R^3(t)}.$$

More sophisticated micro models and macro-micro models exist.

In the macro models, the solid fraction is calculated using the mushy region, as an average of the micro models. The models assume that the solid fraction satisfy

$$\frac{\partial f_s}{\partial t} = \Phi(u, f_s).$$

The choice of Φ varies. A simpler possibility, see [5] would be

$$f_s(u) = \begin{cases} 1 & u < u_S \\ \dfrac{u_L - u}{a(u_s - u) + (u_L - u_S)} & u_S < u < u_L \\ 0 & u > u_L \end{cases} \tag{2.4}$$

where $a \in [0, 1]$ is a parameter that can be adjusted to simulate different solidification problems.

The question of what models are better is not easy to answer. Beyond the matter of simplicity and speed. For solidification problems is more common the use of macro models. The temperature distributions are better approximate for them. It is claimed, on the other side, that micro and macro-micro models offer satisfactory information about the undercooling, grain size, grain density, etc.

2.3 Numerical Method

For the solution of the heat conduction equation (2.3), the use of finite elements is common, see [9].

Let $\Omega \in \mathbb{R}^d$, and $Q = \Omega \times [0, T]$. The initial boundary value problem is

$$\rho c \frac{\partial u}{\partial t} = \nabla \cdot (k \nabla u) + \rho \lambda \frac{\partial f_s}{\partial t} \qquad \text{in } \Omega. \tag{2.5}$$

where the expression for the solid fraction, from 2.4, can be written as

$$\frac{\partial f_s}{\partial t} = \Phi(u),$$

with boundary conditions

$$\begin{aligned} u &= u^* && \text{on } \Gamma_T \\ q_n &= q_F^* && \text{on } \Gamma_F \\ q_n &= \alpha(u - u_s) && \text{on } \Gamma_S \end{aligned}$$

and initial condition

$$u(x, 0) = u_0(x).$$

The variation of the solid fraction as a function of time can be transformed using the relation

$$\frac{\partial f_s}{\partial t} = \frac{df_s}{du} \cdot \frac{\partial u}{\partial t}.$$

Using this relation in (2.5) we get

$$\left(\rho c - \rho \lambda \frac{df_s}{du} \right) \frac{\partial u}{\partial t} = \nabla \cdot (k \nabla u) \qquad \text{in } \Omega. \tag{2.6}$$

The solid fraction f_s increases when the temperature u is decreased. This means that df_s/du is negative in (2.6) and that $\partial u/\partial t$ is smaller, i.e. the temperature decreases slowly during the solidification.

As we see, the effect of the solid fraction can be considered as an increase in the parameter ρc of the heat equation. In order to simplify the following equations let's define

$$C_u = \rho c - \rho \lambda \frac{df_s}{du}.$$

For this problem is common to use first weak formulation and the Galerkin discretization in space. From there a system of ordinary differential equations is obtained, but the time variable is still continuous. Thereafter some integration method in time can be applied to get an approximation of the solution.

2.3.1 Finite Elements

The weak formulation in space consist in finding $u : [0, T) \to V$ such that

$$\int_\Omega \left(C_u \frac{\partial u}{\partial t} - \nabla \cdot (k \nabla u) \right) \eta(x) dx = 0 \qquad \forall \eta \in V = H^1_{0,D}(\Omega) \tag{2.7}$$

In abstract form the problem is a variational equation.

Find $u : [0, T) \to V$ such that

$$\langle C_u \frac{\partial u}{\partial t}, \eta \rangle + a(u, \eta) = \phi(\eta) \qquad \forall \eta \in V \tag{2.8}$$

with the scalar inner product

$$\langle C_u \frac{\partial u}{\partial t}, \eta \rangle = \int_\Omega C_u \frac{\partial u}{\partial t} \eta \tag{2.9}$$

the bilinear form

$$a(u, \eta) = \int_\Omega \nabla u \cdot \nabla k \eta + \int_{\Gamma_S} \alpha u \eta, \tag{2.10}$$

and the linear form

$$\phi(\eta) = - \int_{\Gamma_F} q^*_F \eta + \int_{\Gamma_S} \alpha u_s \eta. \tag{2.11}$$

For the space discretization we use a finite element subspace $V_h \subset V$.

The Galerkin discretization is:

Find $u_h : [0, T) \to V_h$ such that

$$\langle C_u \dot{u}_h, \eta_h \rangle + a(u_h, \eta_h) = \phi(\eta_h) \qquad \forall \eta_h \in V_h \tag{2.12}$$

We proceed now to choose a basis $\{\varphi_1, \varphi_2, ..., \varphi_N\}$ for V_h and expand the solution with respect to the basis.

$$u_h(x,t) = \sum_{i=1}^{N} u_i(t)\varphi_i(x)$$

Using (2.9), (2.10) and (2.11) the mass matrix, stiffness matrix and force vector are defined as

$$M_{ij} = \langle C_u \varphi_i, \varphi_j \rangle$$

$$K_{ij} = a(\varphi_i, \varphi_j)$$

$$F_i = \phi(\varphi_i).$$

2.3.2 Time Integration

The Galerkin discretization (2.12) is represented, using the previous analysis, as a system of ordinary differential equations.

$$M\frac{\partial u}{\partial t} + Ku = F, \qquad u(0) = u_0 \tag{2.13}$$

To approximate a solution for this kind of system we use a simple time integration approach, discretizing the time interval using a time step τ and integrating (2.13) on a single interval $(t, t+\tau)$. We obtain,

$$M\left(u(t+\tau) - u(t)\right) + \int_t^{t+\tau} Ku(s)ds = \int_t^{t+\tau} F(s)ds$$

The idea now is to use integration rules to approximate the integrals. A family of approximations for a real integral using a parameter $\alpha \in [0,1]$ is

$$\int_a^b f(x)dx \approx \alpha f(b) + (1-\alpha)f(a).$$

Using it we get the expression

$$\left(M + \alpha K\right) u(t+\tau) = \left(M - (1-\alpha)K\right) u(t) + \left(\alpha F(t+\tau) + (1-\alpha)F(t)\right).$$

The elements in the right hand side are known and we call them b. Making $A = M + \alpha K$ and $x = u(t + \tau)$, we get a problem of the form

$$Ax = b \tag{2.14}$$

Solving it, means to find the temperature distribution in the next time step.

If $\alpha = 0$ the method is called *explicit Euler*, for $\alpha = 1$ *fully implicit Euler* and for $\alpha = 0.5$ *trapezoidal rule* which is an implicit method too.

2.4 Implementation

In section 2.3 a numerical method was suggested for the solution of the heat conduction with phase change equation. To get numerical results a program was written in C++.

Hexahedral elements are used for the FEM analysis. The global matrices are constructed computing the element contributions using the nodal functions in the base element

$$\begin{array}{cc} \varphi_0(x,y,z) = xyz & \varphi_1(x,y,z) = (1-x)yz \\ \varphi_2(x,y,z) = x(1-y)z & \varphi_3(x,y,z) = (1-x)(1-y)z \\ \varphi_4(x,y,z) = xy(1-z) & \varphi_5(x,y,z) = (1-x)y(1-z) \\ \varphi_6(x,y,z) = x(1-y)(1-z) & \varphi_7(x,y,z) = (1-x)(1-y)(1-z) \end{array}$$

The scheme of the program is

1. Define mesh points.
2. Set kind of material in the points.
3. Set initial temperature according to the material.
4. Recompute material (liquid $\rightarrow$ mushy $\rightarrow$ solid)
5. Compute matrix A and vector b from mesh and actual profile u_k.
6. Use conjugate gradient to solve $Au_{k+1} = b$ and find u_{k+1}

7. Set $u_k = u_{k+1}$.

8. Terminate program or return to step 4.

9. Render result.

First we define the mesh, i.e. the coordinates of the points. This is done making a uniform partition of the sides of the cube.

To each point a number should be assigned representing the kind of material (sand, liquid metal, mushy metal or solid metal). Liquid metal is assigned to the desired shape and sand to the rest of the points. The material will change when the time runs.

An initial temperature is prescribed.

Given a temperature profile u_k the next profile u_{k+1} will be calculated solving the linear system (2.14). In each time step the matrix A and the vector b are computed using the grid which has information about the material in the points. The system is solved using the conjugate gradient method and the new profile is founded. Then the material is recomputed if necessary, to see if there are liquid points transformed in mushy or mushy points transformed in solid. The steps are repeated until some conditions are fulfilled. For example until the maximal temperature is below the solid temperature or a maximal number of steps is achieved.

There is a short description of the program and the classes used in appendix A.

2.5 Example

We consider a cube geometry for the sand mould. The cavity where the metal will be represented is a cross shape, see figure 2.5. A resolution of 20 points in each side is used.

The initial temperaure in the metal is 1200° and in the sand ambient temperature of 20°. The parameters, including the modified parameters for the mushy region, were approximated from MAGMASOFT material database.

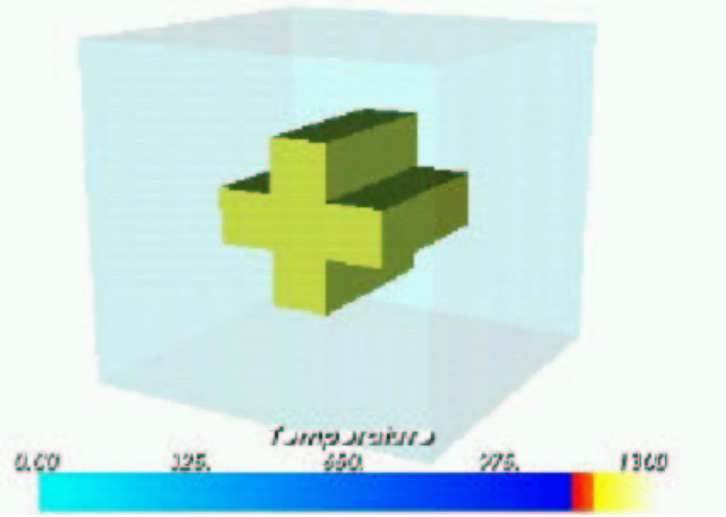

Figure 2.4: Cross shape used for the implementation.

Parameter	Value
Thermal conductivity	
(metal)	30.0
(sand)	1.0
Heat capacity $\times$ density	
(metal)	5.6E5
(sand)	1.6E6
(mushy)	1.5E8
Mushy interval (Celsius)	$1140° - 1170°$

To visualize data in space is not always easy. In figure 2.5 the temperature at the surface is rendered.

A typical way to showing scalar data in a three dimensional domain is the use of plane sections. In this way we can visualize the interior of the domain. In figure 2.6 we have three plane sections for the temperature.

The program generates data files with information about the maximal temperature and the average temperature. This information will be required for the optimization.

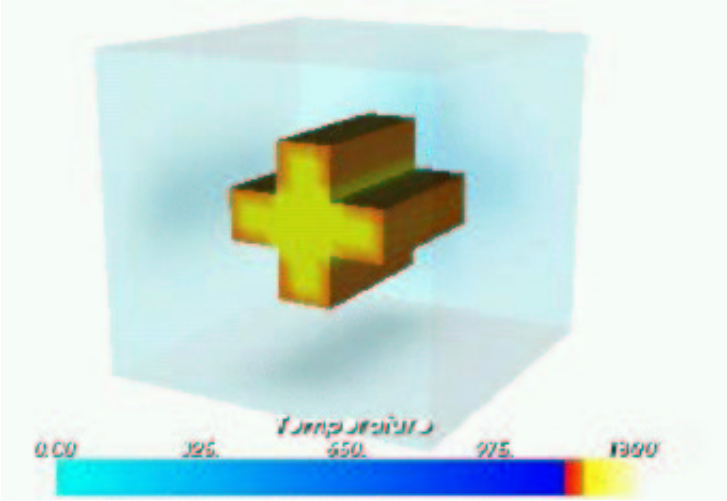

Figure 2.5: Surface temperature after 10 seconds.

As we have seen, castings represents a hard problem to model. By making some simplifications to the problem, neglecting chemical reactions, fluid flow, convection and radiation, we have arrived to a simplified model for the solidification process. Equations for the phase change problem is based on the heat conduction equation, but an extra term is included, the solid fraction. At this point a decision is made. If one is interested in the simulation of the grain structure, then a micro or macro-micro model should be used by considering nucleation and crystal grow. In our case we are interested in the temperature profile. We have described a numerical method to solve the heat conduction with phase change using finite elements. Code in C++ was written and results presented.

In the next chapter we will describe an optimization problem, describe possible solution method for it and use the theory and code developed in this chapter to perform an optimization.

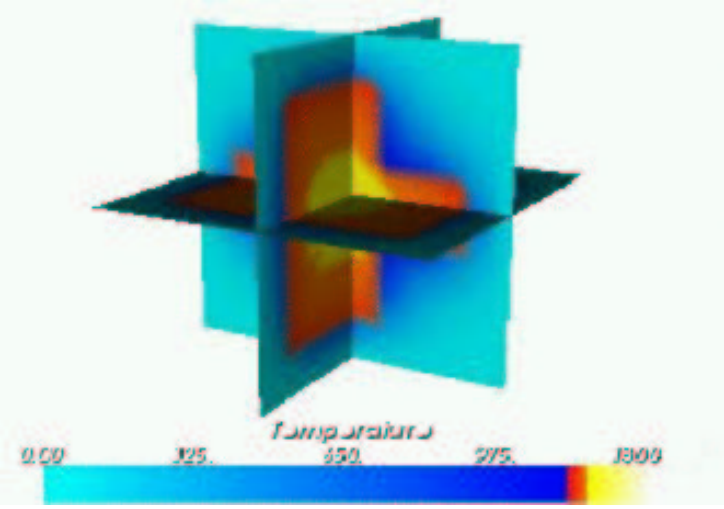

Figure 2.6: Plane sections showing temperature after 14 seconds.

Chapter 3

Optimization of the Casting Process

In section 2.1.4 we presented the characteristics of a good cast. But how can we recognize the quality of the cast using the temperature profile?

Roughly speaking the ideal case would be a uniform cooling down process. Having constant temperature everywhere is absolutely impossible. However this suggest us a functional to minimize. Namely, we can use the deviation from the uniform temperature as an objective function.

$$\mathcal{J} = \int_Q |u(x,t) - u_a(t)|^2, \tag{3.1}$$

where $u_a(t)$ represents the average temperature at time t, i.e.

$$u_a(t) = \frac{1}{|\Omega|} \int_\Omega u(x,t)dx.$$

3.1 Problem Statement

An optimization problem requires an objective function and some constraints. The problem we are considering could be stated as follows.

$$\min_\Omega \mathcal{J}(\Omega), \text{ where } \mathcal{J}(\Omega) = J_\Omega(u_\Omega), \text{ s.t. } Au_\Omega = f \tag{3.2}$$

The constraint $Au_\Omega = f$ means that u_Ω is the solution of some PDE. In our case the heat equation with phase change (2.5).

With boundary conditions and initial condition given in section 2.3.

In other words the problem is to find an optimal domain Ω for which our functional $\mathcal{J}$ is minimized.

Problems of this kind fall in the category of *shape optimization* or *topology optimization* depending if the changes in topology of the domain are allowed.

3.2 Shape Derivative

A possibility to find an optimum for (3.2) is to use the so called *shape derivative*, back to Hadamard . Here deformations of the original domain Ω of the form $(Id + \theta)(\Omega)$ are considered with Id identity and θ a vector field, both from $\mathbb{R}^d$ to $\mathbb{R}^d$.

The shape derivative is then a continuous linear form $J'(\Omega)$ such that

$$\mathcal{J}((Id + \theta)(\Omega)) = \mathcal{J}(\Omega) + \mathcal{J}'(\Omega)(\theta) + o(\theta) \qquad \lim_{\theta \to 0} \frac{|o(\theta)|}{\|\theta\|} = 0,$$

$\mathcal{J}'(\Omega)$ is the Fréchet derivative at 0.

For the computation of the shape derivative it is required usually the adjoint state. The main drawback of the shape optimization method is that the domains obtained belong always to the class of homotopy of Ω, i.e. only the boundary can be altered and the topology remains the same.

3.3 Topological Gradient

Using shape optimization is possible to change the boundary of the domain during the optimization process, nevertheless the topology remains constant. A proposed method for allowing topological changes is the use of *Topological Gradient* see [7]. The topological gradient has been computed and used with success for some specific PDE problems.

The idea behind the method is to try to estimate or approximate the effect on the objective functional produced by making a small ε-hole in the domain. It has been used also when trying to approximate the effect of other imperfections like cracks or holes of different shapes.

The topological gradient is defined when we attempt to perform an asymptotical expansion for the objective functional. If Ω is the original domain, and $\Omega_\epsilon := \Omega - B_\epsilon(x)$, then the topological gradient $g(x)$ for $x \in \Omega$ is defined in the following way,

$$j(\Omega_\epsilon) = j(\Omega) + f(\epsilon)g(x) + o(f(\epsilon)) \tag{3.3}$$

where

$$\lim_{\epsilon \to 0} \frac{R(f(\epsilon))}{o(\epsilon)} = 0$$

If we assume that the functional j depends explicitly on the solution u_ϵ of the problem and only implicitly on Ω_ϵ i.e. $j(\Omega_\epsilon) = J(u_\epsilon)$ then the expansion can be written as

$$J(u_\epsilon) = J(u_0) + \left\langle \frac{\partial J(u_0)}{\partial u}, u_\epsilon - u_0 \right\rangle + o(f(\epsilon)) \tag{3.4}$$

The computation of the topological gradient is done for several operators using the *Domain Truncation Method*. For this method let $R > \epsilon$ such that $B_R \in \Omega$. Defining the annulus $A = B_R - B_\epsilon$ the original problem is separated in two problems, one inside A and the other one outside. Using the Lagrangian

$$\mathcal{L}(u, \lambda) = J(u) + a_\epsilon(u, \lambda) - l(\lambda) \quad \forall \lambda \in V$$

and the solution of the adjoint operator

$$a_\epsilon(\eta, p_\epsilon) = -\left\langle \frac{\partial J(u_0)}{\partial u}, \eta \right\rangle \qquad \forall \eta \in V$$

the sensitivity in (3.4) is related to the Dirichlet-Neumann operator on the boundary of A. Finding the Fréchet derivative of the Dirichlet-Neumann operator means, many times, to find analytical solutions in A or good simple approximations. Even for simple problems, like Poisson, the computation of the gradient is by no means an easy task.

3.4 Insertion of inhomogeneities.

Our goal is to find an optimal shape or topology for the object we want to cast. One can think in the object as a cavity in the mould. In this way the domain of definition Ω is fixed (the cubic mould) but the modifications in the shape can be represented as changing the material from metal to sand.

This problem is called *insertion of inhomogeneities* and it is used in problems related with finding small defects or cracks, see [1].

In [1] Amstutz, Dominguez and Samet derive the sensitivity analysis with respect to the insertion of inhomogeneities for the Helmholtz equation.

$$\nabla \cdot (\alpha_\epsilon \nabla u_\epsilon) + \beta_\epsilon u_\epsilon = 0. \tag{3.5}$$

This problem seems to be very different to our equation (2.5). We will see that this is really not completely the case.

When performing a time integration, our model can be seen as consisting of the solution of a sequence of static heat conduction problems in each time step. Using (2.6) the temperature distribution for time $u(t+\tau)$ depends on the previous time step $u(t)$ via

$$C_u \frac{u(t+\tau) - u(t)}{\tau} = \nabla \cdot (k \nabla u(t+\tau)) \qquad \text{in } \Omega,$$

This can be transformed in

$$\nabla \cdot (k \nabla u(t+\tau)) - C_u \frac{u(t+\tau)}{\tau} = C_u \frac{u(t)}{\tau} \qquad \text{in } \Omega,$$

With the substitution,

$$\beta_\epsilon = -\frac{C_u}{\tau} \ , \ \alpha_\epsilon = k_\epsilon \text{ and } f = C_u \frac{u(t)}{\tau}$$

we arrive to the equation

$$\nabla \cdot (\alpha_\epsilon \nabla u_\epsilon) + \beta_\epsilon u_\epsilon \ = \ f \quad \text{in } \Omega. \tag{3.6}$$

3.5 Topological derivative for our problem

In [1] the topological asymptotic expansion is developed for the problem

$$\nabla \cdot (\alpha_\epsilon \nabla u_\epsilon) + \beta_\epsilon u_\epsilon = 0 \quad \text{in } \Omega, \tag{3.7}$$

using the cost function

$$j(\epsilon) = J(u_\epsilon) = \int_\Omega \alpha_\epsilon |u(x,t) - u_a(t)|^2. \tag{3.8}$$

In these expressions α_ϵ represents the different properties of the material i.e. the inhomogeneities. For our problem it represents the conductivity of the material in the given position.

The asymptotical expansion depends on the shape of the inhomogeneity. In the case of a ball ω we have, see [1],

$$j(\epsilon) - j(0) \sim \tag{3.9}$$

$$\epsilon^d |\omega| \left\{ \frac{d\alpha_0(\alpha_1 - \alpha_0)}{(d-1)\alpha_0 + \alpha_1} \nabla u_0(0) \cdot \nabla p_0(0) - (\beta_1 - \beta_0) u_0(0) p_0(0) + \frac{\delta_J}{|\omega|} \right\}$$

where, for the cost function (3.8)

$$\frac{\delta_J}{|\omega|} = (\alpha_1 - \alpha_0)|u_0(0) - u_a(0)|^2$$

$\alpha_\epsilon \in \{\alpha_0, \alpha_1\}$ and $\beta_\epsilon \in \{\beta_0, \beta_1\}$ represent the material properties depending on the position either sand or metal. In our case α_0, β_0 represents the sand.

It seems that our problem is different, the equation and even the functional. We explain now that this don't affect the given topological gradient (3.9).

From (3.6) the equation we want to consider, is

$$\nabla \cdot (\alpha_\epsilon \nabla u_\epsilon) + \beta_\epsilon u_\epsilon = f \quad \text{in } \Omega.$$

The difference between (3.7) and (3.6) is the term f in the right hand side and it deserves more attention.

If we see the problem in its variational form

$$a_\epsilon(u_\epsilon, \eta) = l(\eta) \qquad \forall \eta \in V$$

the bilinear form a_ϵ corresponds with the bilinear form of (3.7) but not the linear form l. In order to use the topological gradient (3.9), it is required for the linear form l that its variation vanishes, i.e. $\delta l = 0$. This is the case if $f = 0$. Set l' the functional for the equation with $f = 0$, then

$$l_\epsilon(\eta) = l'_\epsilon(\eta) + \int_\Omega f\eta.$$

For every time step f is independent of ϵ. In other words, the insertion of inhomogeneities does not alter f but the temperature in the next step. Then we have,

$$\delta l' = 0 \Rightarrow \delta l = 0$$

There is still something to be done, because the objective function seems different. In the first place our objective function (3.1) is defined in time. This is not a problem. We can measure the deviations from uniform temperature in every time step with integrals of the form

$$\int_\Omega |u(x) - u_a|^2.$$

Remember that our domain is now the complete mould, metal and sand. We need to define our objective function in the sand too. We are really not (directly) interested in the temperature of the sand, so we can define a desired temperature profile using the temperature of the sand in the previous step $u(x,t)$ and the average temperature of the metal u_a.

$$u_d(x) = \begin{cases} u_a & x \text{ is a metal point} \\ u(x,t) & x \text{ is a sand point} \end{cases} \tag{3.10}$$

As we have seen the cost functional

$$j(\epsilon) = \int_\Omega \alpha_\epsilon |u(x,t) - u_a(t)|^2.$$

is not so restrictive.

Now we are in a good position to use the topological gradient in our example.

3.6 Numerical Results

We will apply the model described in the previous chapter here too. As we have seen it would be possible to calculate the topological gradient for our model, but only for a single time step.

The question now is to decide in which step should we apply it in order to get better results. An idea could be to apply the gradient in each time step, from the beginning. This sound like a good idea, however it means to solve quite many problems, one in each step. In our example we will try to find the "worst" time step t_w where the difference between maximal temperature and mean temperature in the metal is maximal, i.e. when

$$D := \max\{u(x, t_m) | x \in \Omega, t_m \in [0, T)\} - \frac{1}{|\Omega|} \int_\Omega u(x, t_m)) dx$$

is maximal.

Our hope is that by reducing the maximal point in the curve we will reduce all the points in the curve and with that the objective function.

In figure 3.6 we have the curve showing the deviations of the maximal from the mean temperature.

There is a maximal point after around 37 seconds. We can also see that this maximum is not global, the curve continues to grow after step 90. But at this point most of the metal is already solid. The difference is created because the boundary of the object is cooling down faster and the center of the cast remains in the mushy state.

The topological gradient is computed in the step 37. The topological gradient is computed in our discretized domain and the points with very negative gradient. In our example we remove points whose topological gradient is negative and less than 20% of the minimal (negative) gradient.

The time integration is executed repeatedly and material is removed in each step. The resulting curves showing the deviation from the maximal to the average temperature for different volumes and the pictures showing the removed material are presented in the following figures.

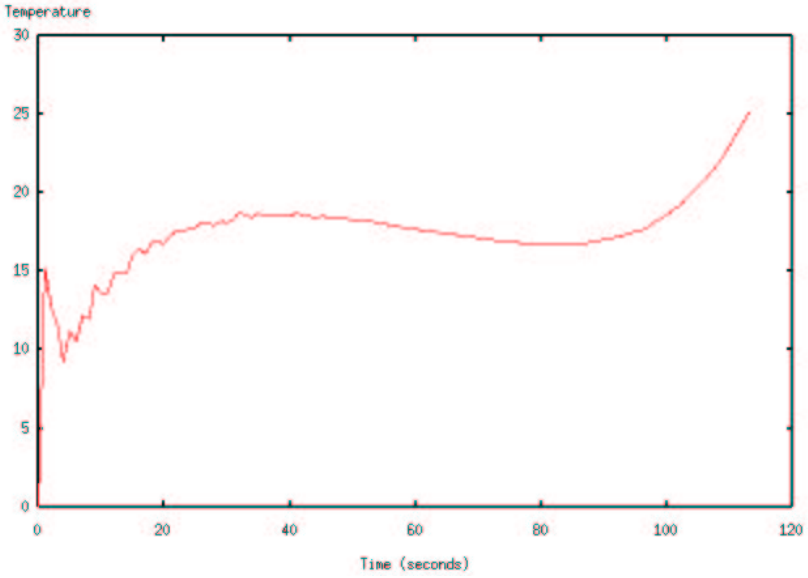

Figure 3.1: Deviation from maximal and mean temperatures in time.

The total improvements can be computed integrating the curves, in figure 3.7. The improvement is shown for the first iterations in figure 3.9.

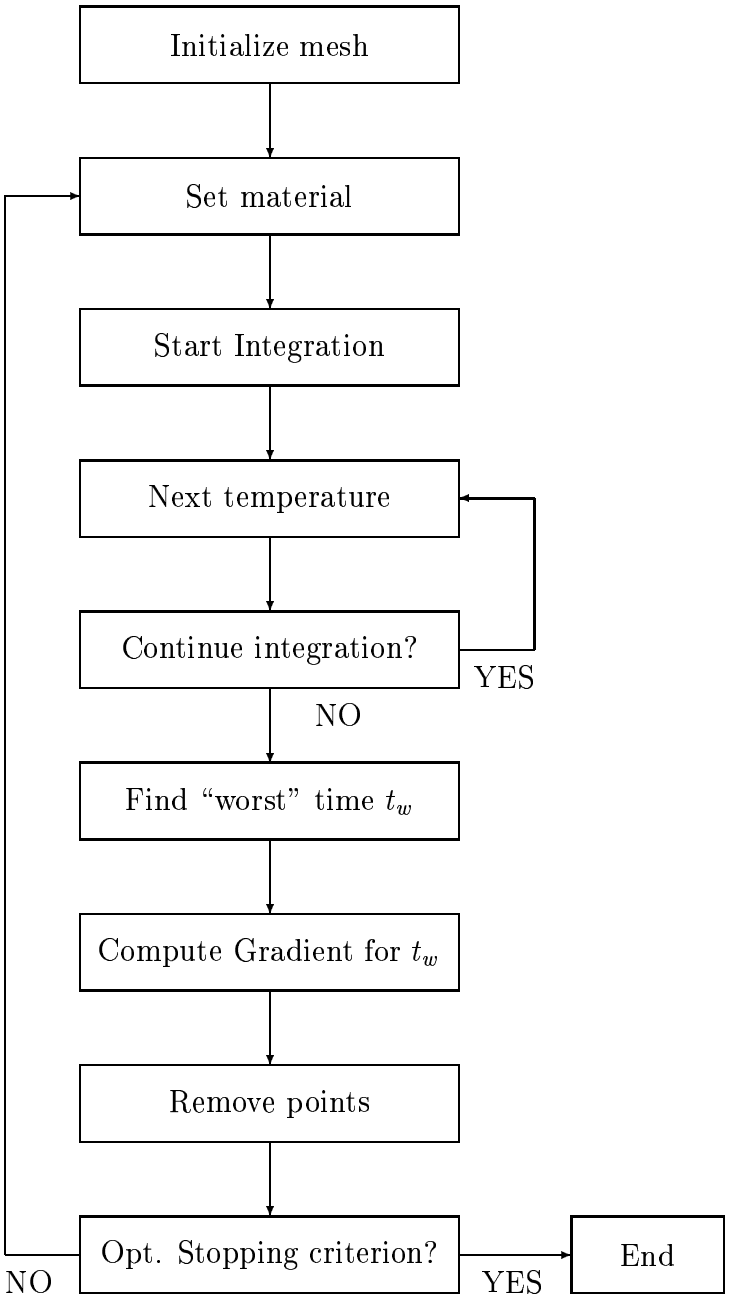

Figure 3.2: Diagram of the Algorithm

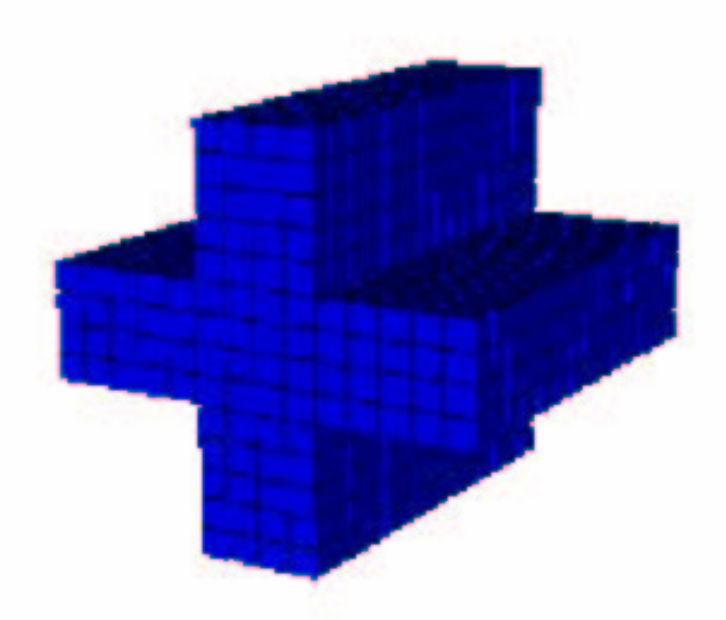

Figure 3.3: Original Domain.

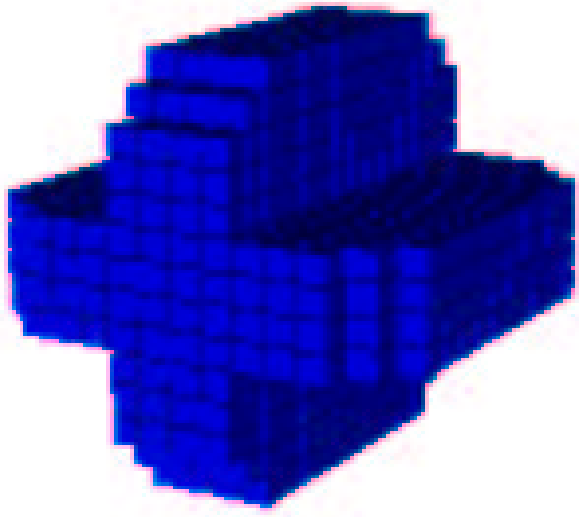

Figure 3.4: 8 % of material removed.

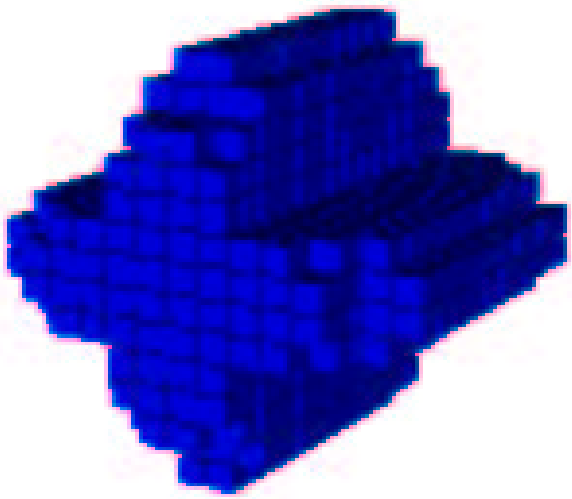

Figure 3.5: 17 % of material removed.

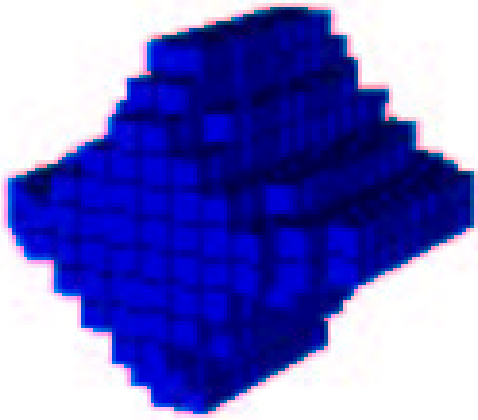

Figure 3.6: 22 % of material removed.

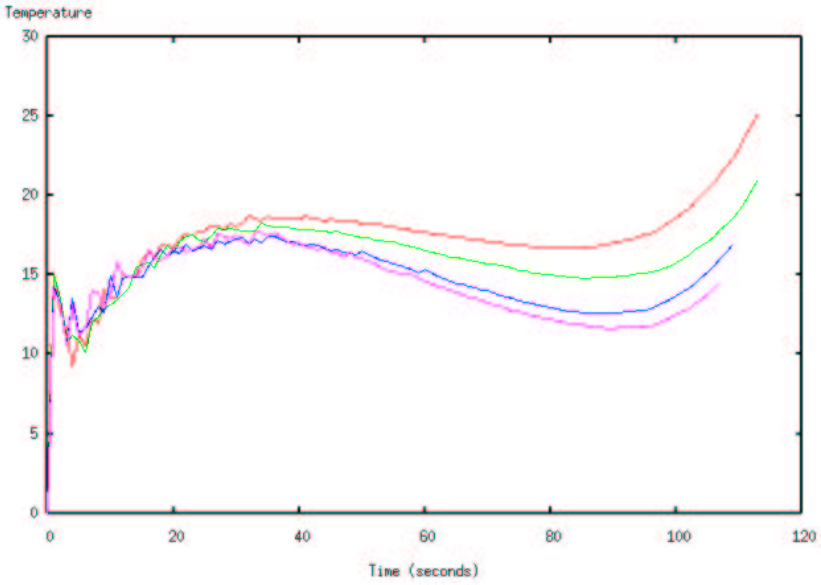

Figure 3.7: Reduction in the temperature difference.

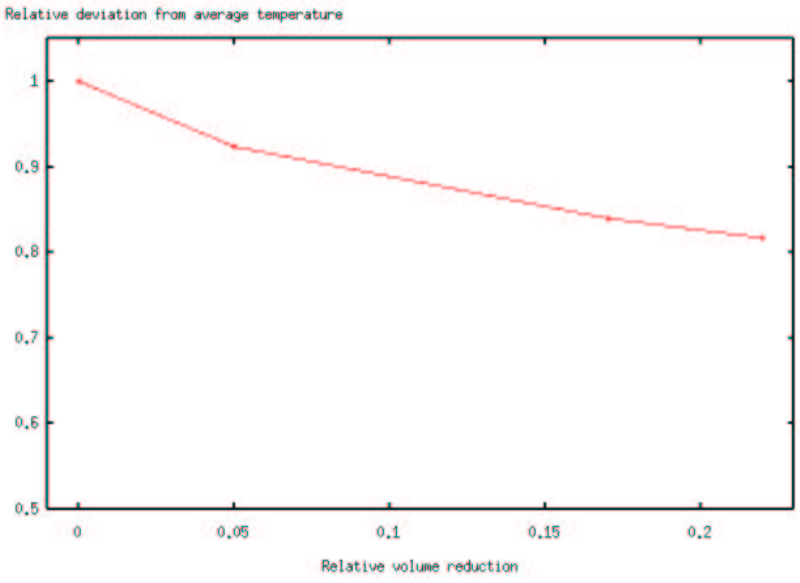

Figure 3.8: Relative deviation related to material removed.

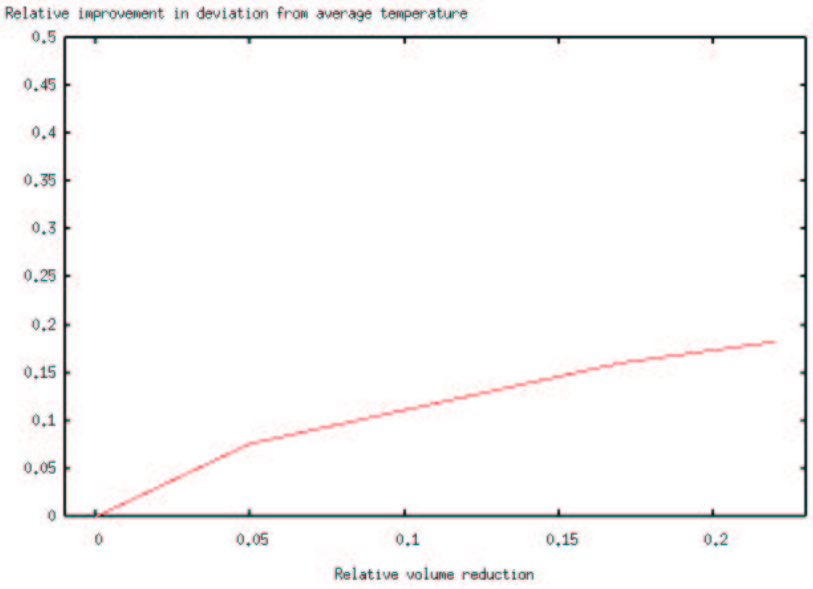

Figure 3.9: Relative improvement related to material removed.

Chapter 4

Conclusions

As we have seen casting processes involve complicated physical phenomena. There exist several possibilities to model them, many based mainly on solidification problems, but nucleation and crystallization plays a fundamental role in others. In this thesis we have assumed a simplified model considering the solidification as a heat conduction with phase change. Code in C++ was implemented and results of numerical test presented.

The main problem was to optimize the shape or topology of some initial design for a cast. We have consider an objective function related with the deviations from the average temperature. The topological gradient approach was used, nevertheless not for the full solidification model, but for a single time step using the pre-calculated gradient for the Helmholtz equation with inhomogeneities.

The results of the program shows the reduction in the temperature deviations when changing the shape of the material via reducing the volume. It seems that a ball is the optimal shape. However there is no geometrical or physical restrictions in our approach. This kind of analysis can be coupled with a structural optimization algorithm, in order to get a part with good mechanical properties too. Future work could be related with the computation of the topological gradient for the full model, and perhaps new objective functions related just with the temperature or even with the crystal size.

Appendix A

Description of the Code

The code developed for this thesis is written in C++. For the visualization and data storage it uses classes from VTK (visualization tool kit), see [13].

The initialization of the mesh and initial conditions is done using VTK objects. Here we define the points of the mesh and decide which points represents metal or sand. In this part is possible to read metal points from a file if required. Afterwards the initial temperature is set according to the material.

The procedure *MakeGlobalMatrices* computes the global mass and stiffness matrices M and K, and returns the matrices $A = M + \alpha K$ and $B = M - (1 - \alpha)K$. The product of the matrix B and the previous temperature profile u_k gives the vector b. Now we have the system on (2.14)

$$Ax = b.$$

This system is solved using a conjugate gradient solver. The class *CG-Solver* is defined using the matrix A and gives an approximation for x when multiplying it for b. Here we can compute the next temperature state given the previous profile. The integration will be continued until the maximal temperature is below a certain limit or until a maximal number of steps is reached.

The procedures *getVectorFromGrid* and *setVectorInGrid* are used to get the temperatures from the grid in a vector or from the vector in the grid.

The function *topologicalDerivative* computes the topological derivative for each point in our discretization and stores the result in a vector. It compute the minimal topological derivative too. For computing the topological derivative we need to specify the time step.

A.1 VTK classes

- vtkArray: Array class for VTK.
- vtkGlyph3D: Filter class. It takes an input source, i.e. cube, and place a scaled copy in each point of a data set (structured grid).
- vtkIdList: List of indices. This is in fact a list of integers.
- vtkLookupTable: A table of colors to be used when scalar values need to be plotted.
- vtkPoints, vtkPointData: Classes to store points and data in them.
- vtkPolyData: Class to store polygonal data. Used to describe any kind of object with nodes, edges and faces.
- vtkPolyDataMapper, vtkActor, vtkRenderer, vtkRenderWindow, vtkRenderWindowInteractor: VTK objects to control the visualization pipeline. Better explained in [13].
- vtkScalarBarActor: Class to create a color bar below a picture. It relates scalar values, like temperatures, and colors.
- vtkStructuredGrid: A three dimensional mesh with regular topology but able to manage irregular geometry. Most used for finite difference or hexahedral finite elements. It has information about the coordinates of it's nodes and can store data in the nodes and/or in the elements.

- vtkStructuredGridGeometryFilter: Filter class used to extract a geometry from a structured grid. We have use it to extract cutting planes and present the temperature inside the domain.

- vtkSourceCube: Class to generate a cube geometry.

  This is just a short description of the classes. We refer the reader to the VTK book in the bibliography or to the VTK homepage www.vtk.org for more information.

A.2 Linear Algebra Classes

- vector: Class to store vector. Its elements are doubles and it provides addition operations.

- sparsematrix: Class to store and manipulate sparse matrices. It provides allocation, assignment and vector multiplication.

- CGSolver: Conjugate gradient solver for $Ax = b$, *CGSolver* approximate the vector x given a matrix A and a vector b.

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Herewith I assure that I made the work on hand independently and only with the aid of the itemized sources.

Héctor Flores Cantú

Kaiserslautern, November 19, 2004.