On the one dimensional Stefan problem

with some numerical analysis

Tobias Jonsson

Spring 2013
Thesis, 15hp
Bachelor of Mathematics, 180hp
Department of Mathematics and Mathematical Statistics

Sammanfattning

I den här uppsatsen presenteras Stefanproblemet med två olika randvillkor, ett konstant och ett tidsberoende. Det här problemet är ett klassiskt exempel på ett frirandsproblem där randen rör sig med tiden, inom partiella differentialekvationer. För det endimensionella fallet visas specifika egenskaper och det viktiga Stefanvillkoret härleds. Betydelsen av maximumprinciper och existensen av en unik lösning diskuteras. För att lösa problemet numeriskt, görs en analys i gränsvärdet $t \to 0$. Approximativa lösningar fås till Stefanproblemet, som visas grafiskt med tillhörande feluppskattningar.

Abstract

In this thesis we present the Stefan problem with two boundary conditions, one constant and one time-dependent. This problem is a classic example of a free boundary problem in partial differential equations, with a free boundary moving in time. Some properties are being proved for the one-dimensional case and the important Stefan condition is also derived. The importance of the maximum principle, and the existence of a unique solution are being discussed. To numerically solve this problem, an analysis when the time t goes to zero is being done. The approximative solutions are shown graphically with proper error estimates.

Contents

1 Introduction

A Stefan Problem is a specific type of boundary value problem for a partial differential equation concerning heat distribution in a phase changing medium. Since the evolving interface is a priori unknown, a part of the solution will be to determine the boundary. An example is the diffusion of heat in the melting of ice, and as the melting occurs the boundary of the ice will be changing position. The problem is by some authors denoted as a "free boundary value problem" due to the boundary of the domain is a priori unknown [1] [5] [6]. To distinct the case of a moving boundary (associated with a time-dependant problem) from the problem with stationary boundary a few authors denote the latter as a "moving boundary problem" [3]. To stick with the common notation, the term "free boundary problem" will be used in this thesis and denote both the time-dependant and the stationary boundary.

To achieve a unique solution for a Stefan Problem there needs to be two boundary condition, one to determine the a priori unknown boundary itself and one is as usual a suitable condition on the fixed boundary. The natural occurrence of a Stefan problem is mostly associated with the melting and solidification problems, however there also exist some Stefan-like problems, for instance the fluid flow in porous media or even shock waves in gas dynamics [12].

A precise formulation of a Stefan problem is not possible, however we can list some characteristic factors regarding this type of problems. To mention a few examples of common features we have: (1) The heat distribution and heat transfer is described by equations, (2) there exist a distinct interface (or phase change-boundary) between two phases (or more), which are distinguishable from each other, (3) the temperature of the interface is a priori known [6].

To facilitate the reading, a list of notations used throughout the text is given at the end of the thesis.

1.1 Objectives

The objectives of this thesis is to get a mathematical understanding of the problem with an unknown free boundary in one dimension. That includes to explain the mathematical model, derive the analytic solution and discuss the validity of the solution. For an even more explaining picture we would like to include two different kinds of boundary condition and also a numerical analysis, with simulated solutions. Due to the fact of numerical approximations, an error analysis is of course required.

1.2 Historical background

The first known paper about diffusion of heat in a medium with a change of phase state was published by the french mathematicians Gabriel Lamé and Benoît Paul Émile Clapeyron in 1831 [7]. The stated problem was to cool a liquid filling the halfspace $x > 0$ and determine the thickness of the generated solid crust, with a constant boundary condition at $x = 0$. They discovered that the thickness of the crust is proportional to the square root of the time, but no determination of the coefficient of proportionally was attached.

Almost 60 years later in 1889 was this question picked up and stated in a more general form by the Austrian physicist and mathematician Joseph Stefan [12]. Joseph Stefan published four papers describing mathematical models for real physical problems with a change of phase state. This was the first general study of this type of problem, since then free boundary problems are called Stefan problems. Of the four papers published it was the one about ice formation in the polar seas that has drawn the most attention, which can be found in [14]. The given mathematical solution was actually found earlier by the German physicist and mathematician Franz Ernst Neumann in 1860. It is called the Neumann solution [15].

1.3 Physical background

The melting of ice and solidification of water are two examples of something called a *phase transformation*, which is a discontinuous change of the properties in the substance. The different states of aggregation in the transition are called phases and they share the same physical properties (for instance density and chemical composition), therefore a phase is more specific then a state of matter. As a phase transition occurs, there will appear a *latent heat* which either is absorbed or released by the body/thermodynamic system without changing the temperature. *Heat* itself is a mechanism of energy transport between objects due to a difference in temperature. It is synonymous with heat flow and we say it is the flow of energy from a hotter body to a colder one. Temperature can be seen as a measure of an object's "willingness" or more precise probability to give up energy. Heat flow may be understood with statistical mechanics which uses probability theory applied on thermodynamics. For further reading, there exists a good and gentle introduction to thermodynamics and statistical physics [13]. In the case of heat conduction, i.e., heat transfer by direct contact, one might wonder at what rate the heat flows between a hot object and a cold one. To obtain an equation describing the heat distribution, consider any open and piece-wise smooth region Ω where $\Omega \subset \mathbb{R}^n$, with a boundary $\partial\Omega$. By natural assumption the rate of change of a total quantity should be equal to the net flux through the boundary $\partial\Omega$:

$$\frac{d}{dt}\int_\Omega u\,dV = -\int_{\partial\Omega} \mathbf{F}\cdot\boldsymbol{\nu}\,dS = \int_\Omega -\mathrm{div}\mathbf{F}\,dV, \tag{1.1}$$

where u is the density of some quantity (such as heat), $\boldsymbol{\nu}$ being the unit normal pointing inwards and $\mathbf{F}$ being the flux density. In the last equality of equation (1.1) we used Gauss's theorem under the condition that the flux function $\mathbf{F}$ defined on the domain Ω is continuously differentiable. Assuming that u and u_t

exist and are continuous, we can use Leibniz's rule for differentiation under the integral sign on the first integral in equation (1.1),

$$\int_\Omega \frac{\partial u}{\partial t}\, dV = \int_\Omega -\text{div}\mathbf{F}\, dV. \tag{1.2}$$

We present here a classical result:

Theorem 1.3.1. *Let f be any function such $f \in C(\Omega)$ where $\Omega \subset \mathbb{R}^n$,*

$$\textit{If } \int_V f\, dV(x) = 0, \quad \textit{for all test volumes } V \subset \Omega, \textit{then}$$

$$f \equiv 0 \quad \textit{on } \Omega. \tag{1.3}$$

Proof. Assume $f \not\equiv 0$, then at a point $x_0 \in \Omega$, $f(x_0) = \lambda > 0$ (The proof for the other case is similarly). But since f is continuous we have for any ϵ, for instance $\epsilon = \frac{\lambda}{2} > 0$, there is a $\delta > 0$ such that if

$$\begin{gathered} |x - x_0| < \delta, \quad x \in \Omega \\ \Rightarrow \\ |f(x) - f(x_0)| < \epsilon = \frac{\lambda}{2} \end{gathered} \tag{1.4}$$

which implies that

$$\frac{\lambda}{2} < f(x) < \frac{3\lambda}{2} \tag{1.5}$$

and by integrating the inequality above (1.5) over the test volume V

$$\int_V f(x)\, dx > \int_V \frac{\lambda}{2}\, dx = \frac{\lambda}{2} \times volume(V) > 0. \tag{1.6}$$

Therefore we can conclude that

$$\int_V f(x)\, dx > 0 \tag{1.7}$$

we must have a contradiction and thus is $f \equiv 0$. □

By writing equation (1.2) as

$$\int_\Omega \frac{\partial u}{\partial t} + \text{div}\mathbf{F}\, dV = 0 \tag{1.8}$$

we must conclude from Theorem 1.3.1 that

$$u_t = -\text{div}\, \mathbf{F}. \tag{1.9}$$

The flux density $\mathbf{F}$ is often proportional to the negative gradient of u (minus since the flow is from higher heat to lower heat):

$$\mathbf{F} = -\alpha \mathrm{D}u \ \ (\alpha > 0) \tag{1.10}$$

where α is the thermal diffusivity. Assuming that α is constant, we get by equation (1.10) and equation (1.9) the *heat equation*:

$$u_t = \alpha \operatorname{div}(\mathrm{D}u) = \alpha \Delta u. \tag{1.11}$$

2 One dimensional Stefan problem

We will now formulate the most simple form of a mathematical model describing phase transitions. The classical Stefan problem is a solidification and a melting problem, for example the transition between ice and water. To acquire a solution for the classical Stefan problem, the *heat equation* needs to be solved. As mentioned before, a boundary condition on the evolving boundary is needed to get a unique solution. It is called "the Stefan condition" and will be derived below. In this chapter we will follow the ideas from [2].

2.1 The Stefan condition

The evolving unknown interface is denoted as $x = s(t)$, where x is the position in space; $s(t)$ is the free boundary and t is the time. To derive the Stefan condition we need to make some assumptions. As the transitions occur there will be a small volume change, although here, we will ignore this property in favour for simplicity. By physical reason the temperature should be continuous at the interface $x = s(t)$ between the phases:

$$\lim_{x \to s(t)^+} u_S(x,t) = \lim_{x \to s(t)^-} u_L(x,t) = u_m \quad \text{for all } t. \tag{2.1}$$

The *phase-change temperature* between the two phases is assumed to be of constant value, u_m. At a fixed time $t = t_0$ consider a domain Ω with two different phases separated at $x = s(t_0)$, which can be seen in Figure 1. We assume plane symmetry to have the temperature u to depend on only t and x.

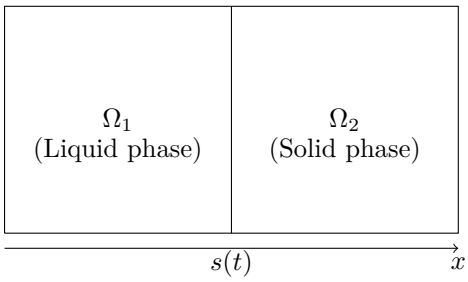

Figure 1: *Domain Ω separated into two phases at $x = s(t)$ which are $\Omega_1 = \Omega \cap \{x < s(t)\}$ and $\Omega_2 = \Omega \cap \{x > s(t)\}$.*

Assume the case of the interface evolving to the right, i.e, when the solid is melting. Thus we should expect that $u \geq u_m$ in the liquid phase and $u \leq u_m$ in the solid phase. At time $t = t_0$ consider a portion of the interface, for simplicity in the shape of a disk A with area S. Later at time $t_1 > t_0$ the position of the interface has changed to $s(t_1) > s(t_0)$. Meanwhile a cylinder of volume $S \times (s(t_1) - s(t_0))$ has melted and therefore released a quantity of heat Q:

$$Q = S(s(t_1) - s(t_0)) \times \rho l, \tag{2.2}$$

where l is the specific latent heat and ρ is the density. The heat flux

$$\boldsymbol{\phi}_L = -K_L \mathrm{D}u_L \tag{2.3}$$
$$\boldsymbol{\phi}_S = -K_S \mathrm{D}u_S \tag{2.4}$$

where K_i is the is the material's conductivity for liquid with $i = L$ and solid $i = S$, and we assume $u \in C^1$. By energy conservation it is natural to assume that the total heat absorbed in equation (2.2) is equal to

$$\begin{aligned} Q = \int_{t_0}^{t_1} \int_A [\boldsymbol{\phi}_L \cdot \hat{x} + \boldsymbol{\phi}_S \cdot (-\hat{x})] \,\mathrm{dA}\, \mathrm{d}\tau = \\ \int_{t_0}^{t_1} \int_A [-K_L \mathrm{D}u_L(s(\tau),\tau) \cdot \hat{x} - K_S \mathrm{D}u_S(s(\tau),\tau) \cdot (-\hat{x})] \,\mathrm{dA}\, \mathrm{d}\tau, \end{aligned} \tag{2.5}$$

where $\hat{x}$ is the unit vector in the $x-$direction. Integrating expression (2.5) over the spatial coordinates gives

$$Q = \mathrm{A} \int_{t_0}^{t_1} [-K_L \frac{\partial u_L}{\partial x}(s(\tau),\tau) + K_S \frac{\partial u_S}{\partial x}(s(\tau),\tau)] \,\mathrm{d}\tau \tag{2.6}$$

we assume this to be equal to expression (2.2). Equating equation (2.2) and (2.6), we get

$$(s(t_1) - s(t_0))\,\rho l = \int_{t_0}^{t_1} \left[-K_L \frac{\partial u_L}{\partial x}(s(\tau),\tau) + K_S \frac{\partial u_S}{\partial x}(s(\tau),\tau)\right] \mathrm{d}\tau \tag{2.7}$$

divide by $(t_1 - t_0)$ and take the limit $t_1 \longrightarrow t_0$ ends up with:

$$l\rho \lim_{t_1 \to t_0} \frac{s(t_1) - s(t_0)}{t_1 - t_0} = \lim_{t_1 \to t_0} \frac{1}{t_1 - t_0} \int_{t_0}^{t_1} \left[-K_L \frac{\partial u_L}{\partial x}(s(\tau),\tau) + K_S \frac{\partial u_S}{\partial x}(s(\tau),\tau)\right] \mathrm{d}\tau. \tag{2.8}$$

Theorem 2.1.1 (The Intermediate Value Theorem)**.** *Let $f : [a,b] \to \mathbb{R}$ and $f \in C$, then f attains all values between the endpoints $f(a)$ and $f(b)$.*

Proof. Is given by for instance [10] □

Theorem 2.1.2 (The Extreme value theorem)**.** *A continuous function f on a bounded and closed interval $[a,b]$, attains both a maximum and a minimum value at least once.*

Proof. Is given by for instance [10] □

Theorem 2.1.3 (The Mean-Value Theorem for integrals)**.** *If $f : [a,b] \to \mathbb{R}$ and $f \in C$ on $[a,b]$, then there exists a number $c \in [a,b]$ such that*

$$\int_a^b f(x)\, dx = (b-a) f(c). \tag{2.9}$$

Proof. It follows from Theorem 2.1.2 that a continuous function $f(x)$ has a minimum value m and a maximum value M on a interval $[a, b]$. From the monotonicity of integrals and $m \leq f(x) \leq M$, it follows that

$$mI = \int_a^b m \, \mathrm{d}x \leq \int_a^b f(x) \, \mathrm{d}x \leq \int_a^b M \, \mathrm{d}x = MI \tag{2.10}$$

where

$$I \equiv \int_a^b \mathrm{d}x = b - a \tag{2.11}$$

using equation (2.11) and dividing by I (assuming $I > 0$) in equation (2.10) gives

$$m \leq \frac{1}{b-a} \int_a^b f(x) \, \mathrm{d}x \leq M. \tag{2.12}$$

From the extreme value theorem we know that both m and M is attained at least once by the integral. Therefore the Intermediate value theorem says that the function f attains all values in $[m, M]$, more specific it exists a $c \in [a, b]$ such that

$$f(c) = \frac{1}{b-a} \int_a^b f(x) \, \mathrm{d}x. \tag{2.13}$$

□

We can with help of Theorem 2.1.3 write equation (2.8) as

$$l\rho s'(t_1) = \lim_{t_1 \to t_0} \frac{1}{t_1 - t_0} \times (t_1 - t_0) f(c) \tag{2.14}$$

where we introduced a new function (for simplicity)

$$f(c) \equiv -K_L u_x(s(c), c) + K_S u_x(s(c), c) \tag{2.15}$$

and $c \in [t_0, t_1]$. But as $t_0 \to t_1$ and f is continuous ($u \in C^1$), then

$$l\rho s'(t_1) = f(t_1). \tag{2.16}$$

However since the same procedure could be done at any time t instead of t_1, we could instead write

$$l\rho s'(t) = f(t) \tag{2.17}$$

and hence with our expression for f we reach

$$l\rho \frac{ds}{dt} = K_S u_x(s(t), t) - K_L u_x(s(t), t) \tag{2.18}$$

which is called the *Stefan condition* and is a boundary condition on the free boundary [2].

2.2 The melting problem in one dimension

The one-dimensional one phase problem could be represented as a semi-infinite solid, for instance a thin block of ice occupying $0 \leq x < \infty$ at the solidification temperature $u = 0$. An assumption needed is that we ignore any volume change in the solidification. At the fixed boundary of the thin block of ice $x = 0$ there could be many different type of "flux functions" $f(t)$. For instance we could have a constant temperature which is above the solidification temperature i.e $u_0 > 0$, or a function depending on time. We assume that the temperature in the solid phase is being constant. Thus the problem is to find the temperature distribution in the liquid phase and the location of the free boundary $s(t)$. Even if there will be two phases present, the problem is called a one-phase problem since it is only the liquid phase which is unknown.

The liquid region,	$0 \leq x < s(t)$
$\frac{\partial u}{\partial t} = \frac{K_L}{C_L \rho} \frac{\partial^2 u}{\partial x^2} = \alpha_L \frac{\partial^2 u}{\partial x^2}$,	The heat equation $0 < x < s(t), t > 0$,
$u(0,t) = f(t)$,	Boundary condition, t>0,
$u(x,0) = 0$,	Initial condition.
The free boundary,	$x = s(t)$
$l\rho \frac{\mathrm{ds}}{\mathrm{dt}} = -K_L \frac{\partial u}{\partial x}$,	Stefan condition,
$s(0) = 0$,	Initial position of the melting interface,
$u(s(t),t) = 0$,	The Dirichlet condition at the interface,
	i.e freezing temperature
Phase 2 − The solid region,	$s(t) < x < \infty$,
$u(x,t) = 0$,	For all t, $x \geq s(t)$.

(2.19)

The boundary condition at $x = 0$ could be anything, but in this thesis we will follow [9] and consider the following cases:

$$\begin{aligned} &(i) \qquad f(t) = 1, \\ &(ii) \quad f(t) = e^t - 1. \end{aligned} \tag{2.20}$$

Actually both of our problems could be solved exactly according to [9].

2.2.1 Rescaling the problem into a dimensionless form

The goal here is to rescale the problem into a more convenient form, and since we have a mathematical approach we only need to make sure that the new expressions satisfy the necessary equations. Consider the following change of variables

$$\begin{cases} u \to av, \\ t \to \gamma\tau \end{cases} \tag{2.21}$$

where γ and a are constants. Put

$$a = \gamma^2 = \alpha \tag{2.22}$$

where $\alpha \neq 0$. With help of (2.21) and (2.22) we can show that the system of equations in (2.19) could be transformed into

$$v_\tau = v_{xx}, \tag{2.23}$$
$$\beta \frac{\mathrm{d}}{\mathrm{d}\tau} s(\gamma\tau) = -v_x(s(\gamma\tau), \gamma\tau) \tag{2.24}$$
$$v(x, 0) = 0 \tag{2.25}$$
$$v(0, \gamma\tau) = f(\gamma\tau)\gamma \tag{2.26}$$

where β is $\frac{l\rho}{K_L}$. Replace the functions by

$$\begin{aligned} &s(\gamma\tau) \to \sigma(\tau) \\ &f(\gamma\tau) \to F(\tau)/\gamma \\ &v(x, \gamma\tau) \to \lambda(x, \tau) \end{aligned} \tag{2.27}$$

and now

$$\begin{aligned} &\lambda_\tau(x, \tau) = \lambda_{xx}(x, \tau) \\ &\beta \frac{\mathrm{d}}{\mathrm{d}\tau} \sigma(\tau) = -\lambda_x(\sigma(\tau), \tau) \end{aligned} \tag{2.28}$$

however, in this thesis we make a mathematical approach, so we change the letters

$$\begin{aligned} &\sigma \to s \\ &\tau \to t \\ &\lambda \to u \\ &F \to f. \end{aligned} \tag{2.29}$$

And we get the rescaled problem as

$$\begin{aligned} &u_t = u_{xx} \\ &u(0, t) = f(t) \\ &u(x, 0) = 0 \\ &\beta \frac{\mathrm{d}s}{\mathrm{d}t} = -u_x(s(t), t). \end{aligned} \tag{2.30}$$

2.2.2 Similarity solution

Here will we consider the Stefan problem defined in system (2.19) with condition (i) at the boundary $x = 0$ and derive an explicit expression for the solution,

$$u_t = \alpha_L u_{xx}, \quad 0 < x < s(t), t > 0 \tag{2.31}$$
$$u(s(t), t) = 0, \quad t \geq 0 \tag{2.32}$$
$$l\rho \frac{\mathrm{d}s}{\mathrm{d}t} = -K_L u_x(s(t), t), \quad t > 0 \tag{2.33}$$
$$s(0) = 0 \tag{2.34}$$
$$u(0, t) = u_0 > 0, \ t > 0. \tag{2.35}$$

If we first consider the ordinary rescaled heat equation $u_t - u_{xx} = 0$ a solution on the bounded domain $0 < x < s(t)$ is found by a change of variables with dilatation scaling. By similar argument we try to introduce the similarity variable

$$\xi = \frac{x}{\sqrt{t}} \tag{2.36}$$

and thus seeks a solution of the form

$$u(x, t) = F(\xi(x, t)) \tag{2.37}$$

where $F(\xi)$ is an unknown function yet to be found. Substituting equation (2.37) in the heat equation (2.31) gives

$$\frac{\partial u}{\partial t}(x, t) = \frac{\mathrm{d}F}{\mathrm{d}\xi}\frac{\partial \xi}{\partial t} = \frac{-x}{2t\sqrt{t}}\frac{\mathrm{d}F}{\mathrm{d}\xi} \tag{2.38}$$
$$\frac{\partial u}{\partial x}(x, t) = \frac{\mathrm{d}F}{\mathrm{d}\xi}\frac{\partial \xi}{\partial x} = \frac{1}{\sqrt{t}}\frac{\mathrm{d}F}{\mathrm{d}\xi} \tag{2.39}$$
$$\alpha_L \frac{\partial^2 u}{\partial x^2}(x, t) = \alpha_L \frac{1}{\sqrt{t}}\frac{\mathrm{d}}{\mathrm{d}\xi}\left(\frac{\mathrm{d}F}{\mathrm{d}\xi}\right)\frac{\partial \xi}{\partial x} = \alpha_L \frac{1}{t}\frac{\mathrm{d}^2 F}{\mathrm{d}\xi^2}. \tag{2.40}$$

Equation (2.38) and (2.40) gives the second order linear homogeneous differential equation

$$\frac{\mathrm{d}^2 F}{\mathrm{d}\xi^2} + \frac{\xi}{2\alpha_L}\frac{\mathrm{d}F}{\mathrm{d}\xi} = 0 \tag{2.41}$$

which can be solved with an integrating factor

$$M(\xi) = e^{\int_{s_0}^{\xi} \frac{s}{2\alpha_L}\,\mathrm{d}s} = C_1 e^{\frac{\xi^2}{4\alpha_L}} \tag{2.42}$$

where C_1 is an integration constant. $M(x)$ in equation (2.42) is multiplied with equation (2.41) and by identifying the product rule we have

$$\frac{\mathrm{d}^2 F}{\mathrm{d}\xi^2}M(\xi) + \frac{\xi}{2\alpha_L}M(\xi)\frac{\mathrm{d}F}{\mathrm{d}\xi} = \frac{\mathrm{d}}{\mathrm{d}\xi}\left(M(\xi)\frac{\mathrm{d}F}{\mathrm{d}\xi}\right) = 0 \tag{2.43}$$

and by integrating equation (2.43) we get

$$M(\xi)\frac{\mathrm{d}F}{\mathrm{d}\xi} = C_2 \tag{2.44}$$

where C_2 is an integration constant. From the fundamental theorem of calculus the solution of equation (2.44) is

$$F(\xi) = C\int_0^{\xi} e^{-\frac{s^2}{4\alpha_L}}\,\mathrm{d}s + D \tag{2.45}$$

where D is an integration constant. By using the substitution $y = \frac{s}{\sqrt{2\alpha_L}}$, equation (2.45) could be written in terms of the error function (defined in 'List of notations')

$$F(\xi) = A\,\mathrm{erf}\left(\frac{\xi}{2\sqrt{\alpha_L}}\right) + D \tag{2.46}$$

and thus the solution to equation (2.31) is

$$u(x,t) = F(\frac{x}{\sqrt{t}}) = A\mathrm{erf}\left(\frac{x}{2\sqrt{t\alpha_L}}\right) + D. \tag{2.47}$$

From the boundary condition at $x = 0$ and $x = s(t)$ we get

$$D = u_0 \tag{2.48}$$

and

$$A = \frac{0 - u_0}{\mathrm{erf}(\lambda)} \tag{2.49}$$

where

$$\lambda \equiv \frac{s(t)}{2\sqrt{t\alpha_L}} \tag{2.50}$$

since A in equation (2.49) is a constant, it follows that λ must also be constant, thus

$$s(t) = 2\lambda\sqrt{\alpha_L t} \tag{2.51}$$

and with the constants A and D, the solution is:

$$u(x,t) = u_0 - \frac{u_0}{\mathrm{erf}(\lambda)}\mathrm{erf}\left(\frac{x}{2\sqrt{\alpha_L t}}\right). \tag{2.52}$$

About the parameter λ
The Stefan condition at the free boundary $x = s(t)$ is

$$l\rho\frac{\mathrm{d}s}{\mathrm{d}t} = -K_L u_x(s(t),t) \tag{2.53}$$

and the time derivative of $s(t)$ is

$$\frac{\mathrm{d}s(t)}{\mathrm{d}t} = \frac{\mathrm{d}}{\mathrm{d}t}\left(2\lambda\sqrt{\alpha_L t}\right) = \lambda\frac{\sqrt{\alpha_L}}{\sqrt{t}} \tag{2.54}$$

and for the other derivative in the Stefan condition we need to first take the spatial derivative of the solution u given by equation (2.52)

$$u_x(x,t) = -\frac{u_0}{\operatorname{erf}(\lambda)} \frac{2}{\sqrt{\pi}} \frac{\mathrm{d}}{\mathrm{d}x} \int_0^{\frac{x}{2\sqrt{\alpha_L t}}} e^{-y^2}\, \mathrm{d}y = -\frac{u_0}{\operatorname{erf}(\lambda)} \frac{1}{\sqrt{\pi}} \frac{e^{-\frac{x^2}{4\alpha_L t}}}{\sqrt{\alpha_L t}} \tag{2.55}$$

and at $x = s(t)$

$$u_x(s(t),t) = -\frac{u_0}{\operatorname{erf}(\lambda)} \frac{e^{-\lambda^2}}{\sqrt{\alpha_L t}\sqrt{\pi}}. \tag{2.56}$$

By putting in equation (2.56) and (2.54) in the Stefan condition (2.53) and solving for λ, we get the following transcendental equation

$$\lambda e^{\lambda^2} \operatorname{erf}(\lambda) = \frac{K_L}{\rho l \alpha_L} \frac{u_0}{\sqrt{\pi}} = \frac{C_L(u_0)}{\sqrt{\pi} l} \equiv \frac{St_L}{\sqrt{\pi}} \tag{2.57}$$

where St_L is the *Stefan number* [1].

Summing up the solution of $u(x,t)$ and $s(t)$, and the condition for λ, gives

$$\begin{cases} u(x,t) & = u_0 - \frac{u_0}{\operatorname{erf}(\lambda)} \operatorname{erf}\left(\frac{x}{2\sqrt{\alpha_L t}}\right) \\ s(t) & = 2\lambda\sqrt{\alpha_L t} \\ \lambda e^{\lambda^2} \operatorname{erf}(\lambda) & = \frac{St_L}{\sqrt{\pi}}. \end{cases} \tag{2.58}$$

2.2.3 Nonlinearity

If we look at the problem before the free boundary $s(t)$ we have only the heat equation, which is a linear equation. Now we want to analyse the problem how it behaves at the free boundary $x = s(t)$. As shown in section 2.1 with energy conservation, the boundary condition at the free boundary is

$$-K_L \frac{\partial u}{\partial x}(s(t), t) = l\rho \frac{\mathrm{d}s}{\mathrm{d}t}. \tag{2.59}$$

The value at the free boundary is

$$u(s(t), t) = 0 \tag{2.60}$$

for any t, where $s(t) \propto \sqrt{t}$, which can be seen in Figure 2.

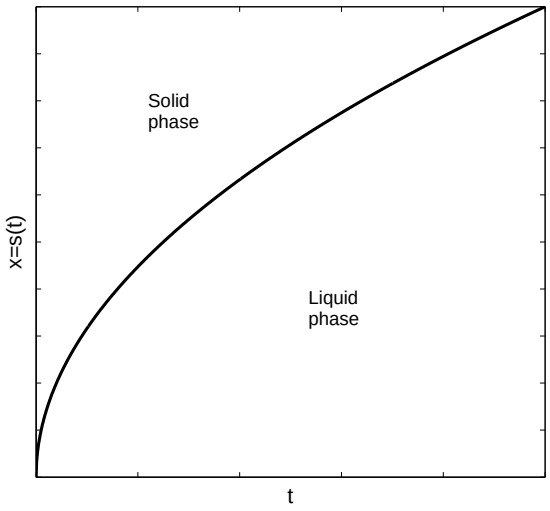

Figure 2: *The free boundary $s(t)$ against time t*

.

The curve of the free boundary in the (x, t)-plane could be described with

$$\mathbf{r}(t) = (x(t), t) = (s(t), t). \tag{2.61}$$

The rate of change of the temperature u is then the directional derivative of u along $\mathbf{v} = \frac{\mathrm{d}\mathbf{r}}{\mathrm{d}t}$.

$$\mathbf{v} \cdot \mathrm{D}u = \frac{\partial u}{\partial x}\frac{\mathrm{d}s}{\mathrm{d}t} + \frac{\partial u}{\partial t} = 0 \tag{2.62}$$

and thus

$$\frac{\partial u}{\partial x} = -\frac{\frac{\partial u}{\partial t}}{\frac{\mathrm{d}s}{\mathrm{d}t}}. \tag{2.63}$$

By multiplying equation (2.59) with equation (2.63) gives

$$-K_L \left(\frac{\partial u}{\partial x}(s(t), t) \right)^2 = -l\rho \frac{\partial u}{\partial t}(s(t), t) = -\frac{lK}{C} \frac{\partial^2 u}{\partial x^2}(s(t), t) \tag{2.64}$$

which implies that the Stefan problem is a *nonlinear problem*.

2.3 The maximum principle

In our domain of interest, the solution is given by the heat equation, which we give a discussion about here.

A very common and important tool in the study of partial differential equations is the maximum principle. The maximum principle is nothing more than a generalization of the single variable calculus fact that the maximum of a function f is achieved at one of the endpoints a and b of the interval $[a, b]$ where $f'' > 0$. Hence we could say more generally that functions which satisfy a differential inequality in any domain Ω posses a maximum principle, since their maximum is achieved on the boundary $\partial\Omega$. The maximum principle help us obtain information about the solution of a differential equation even without any explicit information of the solution itself. For example, the maximum principle is an important tool when an approximative solution is searched for. The following theory could be found in [11].

Definition 2.3.1 (The parabolic boundary)**.** Since the heat equation is often prescribed with its temperature initially and at the endpoints. The most natural approach is to consider the region

$$E_T = \{(x, t) : 0 < x < l(t), 0 < t \leq T\} \tag{2.65}$$

in the (x, t)-plane. We suppose that the temperature is known on the remaining sides of E_T:

$$S_1 : \{x = 0, 0 \leq t \leq T\}, \qquad S_2 : \{0 \leq x \leq l(t), t = 0\},$$
$$S_3 : \{x = l(t), 0 \leq t \leq T\}.$$

Lemma 2.3.2. *Assume the function $u(x, t) \in C^2_{(1)}$ and satisfies the differential inequality*

$$L[u] \equiv \frac{\partial^2 u}{\partial x^2} - \frac{\partial u}{\partial t} > 0 \tag{2.66}$$

in E_T. Then u cannot attain its maximum value at the interior of the closure $\overline{E_T}$ of E_T.

Proof. Assume that u obtain its maximum value at an interior point $P = (x_0, t_0)$ of $\overline{E}$. As the point P is a critical point, the derivative u_t is 0 and since it is a maximum $u_{xx}(x_0, t_0) \leq 0$. However this contradicts $L[u] > 0$ and thus cannot u have a maximum at an interior point. □

Theorem 2.3.3 (The weak maximum principle)**.** *Suppose the function $u(x, t)$ satisfies the differential inequality*

$$L[u] \equiv \frac{\partial^2 u}{\partial x^2} - \frac{\partial u}{\partial t} \geq 0 \tag{2.67}$$

in the rectangular region E_T given by (2.65)*. Then the maximum value of u on the closure $\overline{E_T}$ must occur on one of the remaining boundaries S_1, S_2 or S_3.*

Proof. Let M be the largest value of u that occur on S_1, S_2 and S_3 and assume that there is a point in the interior $P = (x_0, t_0)$ where $u(x_0, t_0) = M_1 > M$.

Define the help function

$$w(x) = \frac{M_1 - M}{2l^2}(x - x_0)^2, \tag{2.68}$$

from w and u we define the function

$$v(x,t) \equiv u(x,t) + w(x). \tag{2.69}$$

On the boundaries S_1, S_2 and S_3 we have $u \leq M$ and $0 < x < l$ and thus

$$v(x,t) \leq M + \frac{M_1 - M}{2} < M_1. \tag{2.70}$$

At the interior point (x_0, t_0) we have

$$v(x_0, t_0) = u(x_0, t_0) + 0 = M_1 \tag{2.71}$$

and in E_T we have

$$L[v] \equiv L[u] + L[w] = L[u] + \frac{M_1 - M}{l^2} > 0. \tag{2.72}$$

From the conditions (2.70) and (2.71) we can conclude that the maximum $v(x_0, t_0)$ must be attained either on the interior of E or along

$$S_4 : \{0 < x < l <,\ t = T\}$$

From lemma 2.3.2 we know that the inequality (2.72) gives us no possibility for an interior maximum. If we instead would have a maximum on S_4, we get $\frac{\partial^2 v}{\partial x^2} \leq 0$ which implies that $\frac{\partial v}{\partial t}\big|_{t=T} < 0$. Hence must v have a larger value at an earlier time $t < T$ and from this contradiction we can see that our assumption $u(x_0, t_0) > M$ is wrong. □

Remark. Notice that Theorem 2.3.3 is only the weak maximum principle and the theorem permits the maximum to occur on the interior points as well, in addition to the boundary [11].

Theorem 2.3.4 (The strong maximum principle)**.** *Suppose that there is a* (x_0, t_0) *in* E_T *such that* $u(x_0, t_0) = max_{\overline{E_T}} u$*. Then is* $u(x,t) \equiv u(x_0, t_0)$ *for all* $(x,t) \in E_T$*.*

Proof. The proof could be found in [11] □

2.4 Existence and uniqueness

To be "allowed" to use any kind of numerical analysis in this thesis it is essential to show that this problem is well-posed. A *well-posed* problem for a partial differential equation is required to satisfy following criteria, e.g. [4]:

1. A solution to the problem exists
2. The solution is unique

   and

3. The solution depends continuously on the given data

To give any conclusions about the solution to a partial differential equation, we require the existence of a unique solution. If we would not have one unique solution any prediction made, would depend on which of the solutions we have chosen to be the "right" one. The last requirement is important in the problems from physical applications, since it is preferable if our solution would not change much when the initial conditions are perturbed.
We therefore need to present and give a proof of the existence and uniqueness of the Stefan Problem defined in (2.19). In this thesis we present a special case of the theorem stated in the book by Friedman [5, p.216], due to less general boundary conditions in (2.19).

Theorem 2.4.1 ([5], Theorem 1, page 216)**.** *For boundary condition* $u(0,t) = f(t)$ *(which is continuously differentiable) and* $u(x,0) =$*constant there exists a unique solution* $\{u(x,t), s(t)\}$ *of the system in* (2.19) *for all* $t < \infty$*.*

Proof. The proof is beyond the scope of this thesis and could be found in the book by Avner Friedman [5, p.222]. □

When we now know that there truly exist one unique solution to (2.19) we can show the following theorem:

Theorem 2.4.2 ([5], Theorem 1, page 217)**.** *If* u *and* $s(t)$ *gives a solution to* (2.19) *for all* $t < \sigma$*, where* σ *is a finite number, then* $x = s(t)$ *is a monotone non-decreasing function.*

Proof. From the weak Maximum Principle given by Theorem 2.3.3 we know that $u(x,t) \geq 0$ for $0 < x < s(t)$. Since the temperature u is 0 at the boundary $x = s(t)$, the rate of change in temperature with respect to x at the free boundary $x = s(t)$ is lesser or equal to 0. Thus we get from the Stefan condition that $\frac{\mathrm{d}s}{\mathrm{d}t} \geq 0$, i.e, the free boundary $s(t)$ is *monotone non-decreasing.* □

3 Numerical analysis

The theory of partial differential equation is of fundamental importance for numerical analysis. At the undergraduate level the main goal in partial differential equations is to find solutions that could be expressed explicitly in terms of elementary functions. There exist several methods of finding those solutions to various problem, but to most problems an explicit solution could not be found. When this occurs, numerical methods are useful to give some further information about the problem and the solutions. In differential equations the contributions from analysis often lies in to find conditions to ensure uniqueness and existence of the solution, not construct the explicit solution. Both the case of the existence of an unique solution and the reverse case are interesting to study in their own way. When searched for existence and uniqueness in analysis, the problems are posed on an infinite dimensional space. This is a contrast to numerical analysis, where the problems are discrete and posed on a finite dimensional space. In addition to the existence and uniqueness which are needed to be found valid for different discretizations, error estimates are also required to be found for the approximations.

There does not exist any general numerical algorithm to every PDE you may encounter, but in reality there are a lot of different types of numerical schemes depending on what problem you need to approximate. To approximate the solution of a partial differential equation with numerical methods, the procedures can be largely decomposed into two types. In the first procedure the solution is searched for at a finite number of nodes in the domain of definition. The other procedure is about expanding the solution as a sum of basis functions defined on the domain of definition and find the coefficients for this expansion. In this thesis we are only going to look at the first procedure, namely a finite difference method.

3.1 Finite difference method

The main idea of the finite difference method is to use approximation of the appearing derivatives in a PDE by sums and differences of function values. The function values are defined on a discrete set of points (nodes), which often are uniformly spaced. In this thesis the 1 dimensional heat equation is considered. Two methods will be used, the Forward Euler scheme and Crank-Nicholson scheme.

3.1.1 Forward Euler scheme

Forward Euler is a numerical method for approximating solutions to differential equations. This method is explicit since we can express the solution at time step $n+1$ in terms of the values of former step n. To demonstrate this method let us start out with a simple example:

$$\begin{aligned} u_t &= u_{xx} && (x,t) \in (0,1) \times (0,\infty), \\ u(x,0) &= v(x) && \text{in } (0,1), \\ u(0,t) &= u(1,t) = 0, && \text{for } t > 0. \end{aligned} \tag{3.1}$$

The first step of this procedure is to make space and time discrete. Put

$$\begin{aligned} x \to x_j &= x_0 + jh \quad j = 0,1,2...M, \\ t \to\ t^n &= t_0 + nk \quad n = 0,1,2... \end{aligned}$$

where $x_0 = t_0 = 0$, M the number of nodes, k the size of the time step and h is spatial step given by

$$h = \frac{1}{M}. \tag{3.2}$$

We denote the numerical solution U_j^n of u as

$$U_j^n \approx u(jh, nk). \tag{3.3}$$

which is the approximative solution of u at time step n and spatial step j. For the spatial derivatives, introduce the forward and backward difference quotients with respect to space and time as

$$\begin{aligned} \partial_x U_j^n &= \tfrac{U_{j+1}^n - U_j^n}{h}, \quad & \partial_x U_j^n &= \tfrac{U_{j+1}^n - U_j^n}{h} \\ \overline{\partial}_x U_j^n &= \tfrac{U_j^n - U_{j-1}^n}{h} \quad & \overline{\partial}_x U_j^n &= \tfrac{U_j^n - U_{j-1}^n}{h}\ . \end{aligned} \tag{3.4}$$

The Forward Euler example stated in equation (3.1) is written as

$$\begin{cases} \partial_t U_j^n = \partial_x \overline{\partial}_x U_j^n & \text{for } j = 1,...,M.1, n \geq 0 \\ U_0^n = U_M^n = 0, & \text{for } n > 0, \\ U_j^0 = V_j = v(x_j), & \text{for } j = 0,...,M. \end{cases} \tag{3.5}$$

By introducing the mesh ratio $\lambda = \frac{k}{h^2}$ and solving for U_j^{n+1} in equation (3.5), we get

$$U_j^{n+1} = \lambda(U_{j-1}^n + U_{j+1}^n) + (1 - 2\lambda)U_j^n \tag{3.6}$$

$$U_0^{n+1} = U_M^{n+1} = 0 \tag{3.7}$$

$$U_j^0 = v(x_j) \tag{3.8}$$

and equation (3.6) in matrix form

$$\bar{U}^{n+1} = A\bar{U}^n \tag{3.9}$$

where $\bar{U}^n$ denotes the $(M-1)-$vector related to U^n and A is a symmetric tridiagonal coefficient matrix given by:

$$A = \begin{bmatrix} 1-2\lambda & \lambda & 0 & \dots & 0 \\ \lambda & 1-2\lambda & \lambda & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \lambda & 1-2\lambda & \lambda \\ 0 & \dots & 0 & \lambda & 1-2\lambda \end{bmatrix}. \tag{3.10}$$

This method is however only first order accurate in time, and second order in space as can seen in the Theorem 3.1.2 below. This means that the error in time will dominate unless the time step k is much smaller than the spatial step h. The Forward Euler scheme is stable when the mesh ratio $\lambda \leq \frac{1}{2}$,[8, thm 9.5].

Theorem 3.1.2. *Let U^n and u be the solutions of (3.5) and (3.1), with $\lambda = \frac{k}{h^2} \leq \frac{1}{2}$ and u being fourth order continuous differentiable, then*

$$\|U^n - u^n\|_{\infty,h} \leq Ct^n h^2 \max_{t \leq t^n} |u(x,t)|_{C^4}, \quad \text{for } t \geq 0,$$

Proof. See [8, thm 9.5]. □

Theorem 3.1.2 gives us an error estimate for the numerical approximation, and for this numerical scheme we have a quite restrictive stability condition between time step k and spatial step h. With this method it is not possible to have the same order of magnitude in k and h and still maintain stability.

To give an example of what happens to the numerical simulation with a $\lambda \geq 1/2$, we plot the maximum norm against t^n with the forward Euler scheme shown in Figure 3.

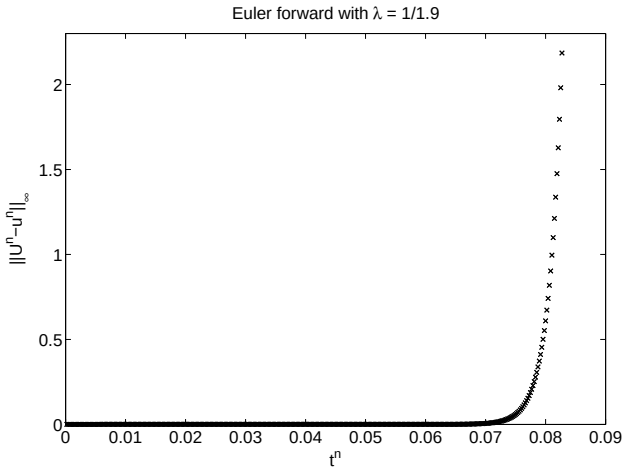

Figure 3: *Plot of the maximum norm of the error against time for the forward Euler scheme with $\lambda > 1/2$.*

3.1.3 Crank-Nicholson scheme

Another finite difference scheme is the Crank-Nicholson method which is an implicit method, which uses a symmetry around a middle point, $(x_j, t_{n+1/2})$, where

$$t_{n+1/2} = \frac{t^{n+1} + t^n}{k}. \tag{3.11}$$

Due to the implicit scheme an algebraic system must thus be solved for each time step. The example given in equation (3.1) with the Crank-Nicholson method is then defined as

$$\begin{cases} \overline{\partial}_t U_j^{n+1} = \frac{1}{2}\partial_x \overline{\partial}_x (U_j^n + U_j^{n+1}) & \text{for } j = 1, ..., M-1, n \geq 0 \\ U_0^{n+1} = U_M^{n+1} = 0, & \text{for } n > 0, \\ U_j^0 = V_j = v(x_j), & \text{for } j = 0, ..., M. \end{cases} \tag{3.12}$$

Rewriting the first equation in (3.12) as

$$(I - \frac{1}{2}k\partial_x\overline{\partial}_x)U_j^{n+1} = (I + \frac{1}{2}k\partial_x\overline{\partial}_x)U_j^n \tag{3.13}$$

where I is the $(M-1)$-Identity matrix, and then using the defined difference quotients and collecting similar terms, we get

$$(1+\lambda)U_j^{n+1} - \frac{1}{2}\lambda(U_{j-1}^{n+1} + U_{j+1}^{n+1}) = (1-\lambda)U_j^n + \frac{1}{2}\lambda(U_{j-1}^n + U_{j+1}^n). \tag{3.14}$$

The matrix form is

$$B\bar{U}^{n+1} = A\bar{U}^n \tag{3.15}$$

where both A and B are tridiagonal matrices given by

$$B = \begin{bmatrix} 1+\lambda & -\frac{1}{2}\lambda & 0 & \dots & 0 \\ -\frac{1}{2}\lambda & 1+\lambda & -\frac{1}{2}\lambda & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & -\frac{1}{2}\lambda & 1+\lambda & -\frac{1}{2}\lambda \\ 0 & \dots & 0 & -\frac{1}{2}\lambda & 1+\lambda \end{bmatrix}$$

and

$$A = \begin{bmatrix} 1-\lambda & \frac{1}{2}\lambda & 0 & \dots & 0 \\ \frac{1}{2}\lambda & 1-\lambda & \frac{1}{2}\lambda & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \frac{1}{2}\lambda & 1-\lambda & \frac{1}{2}\lambda \\ 0 & \dots & 0 & \frac{1}{2}\lambda & 1-\lambda \end{bmatrix}.$$

Solving equation (3.15) we get the solution at time $(n+1)$

$$U^{n+1} = B^{-1}AU^n. \tag{3.16}$$

Previously we had the forward Euler method with only a first order of accuracy in time, which together with the stability criteria limited our numerical analysis. We can see in the Theorem 3.1.4 that the Crank-Nicholson method is second order accurate in time. This method give us no time step restriction.

Theorem 3.1.4. *Let U^n and u be the solutions of* (3.12) *and* (3.1)*, with u being sixth order continuous differentiable, then*

$$\|U^n - u^n\|_{2,h} \leq Ct^n(h^2 + k^2)\max_{t \leq t^n}|u(x,t)|_{C^6}, \quad \textit{for } t \geq 0,$$

Proof. The proof of this Theorem could be found in [8]. □

3.2 Analysis when t → 0

The problem (2.19) gets a degeneracy as $t \to 0$, since the thickness of the melt region is initially zero according to equation (2.34). To solve this problem, we do a change of variable as in the paper by S.L. Mitchell and M. Vynnycky [9]. Another goal here is to attain an initial condition for the new variables. It is a good idea to work in the transformed coordinates suggested by the analytical solution given by (2.47), and we therefore set

$$\xi = \tfrac{x}{s(t)}, \quad u = h(t)F(\xi, t), \tag{3.17}$$

where $h(t)$ is chosen to ensure that we get a well-posed problem as $t \to 0$. The space derivative, in the new coordinates are

$$\frac{\partial u}{\partial x} = h(t)\frac{\partial}{\partial \xi}\Big(F(\xi,t)\Big)\frac{\partial \xi}{\partial x} = \frac{h(t)}{s(t)}\frac{\partial F}{\partial \xi}, \tag{3.18}$$

and

$$\frac{\partial^2 u}{\partial x^2} = \frac{\partial}{\partial \xi}\Big(\frac{h(t)}{s(t)}\frac{\partial F}{\partial \xi}\Big)\frac{\partial \xi}{\partial x} = \frac{h}{s(t)^2}\frac{\partial^2 F}{\partial \xi^2}, \tag{3.19}$$

moreover, the time derivative u_t takes the form

$$\frac{\partial u}{\partial t} = \frac{\mathrm{d}h(t)}{\mathrm{d}t}F + h(t)\left(\frac{\partial F}{\partial t} + \frac{\partial F}{\partial \xi}\frac{\partial \xi}{\partial t}\right) = \frac{\mathrm{d}h}{\mathrm{d}t}F + h\left(\frac{\partial F}{\partial t} - \frac{\xi}{s}\frac{\mathrm{d}s}{\mathrm{d}t}\frac{\partial F}{\partial \xi}\right). \tag{3.20}$$

By equating u_t and u_{xx} and multiplying s^2 on both sides we end up with

$$h\frac{\partial^2 F}{\partial \xi^2} = s\left[s\frac{\mathrm{d}h}{\mathrm{d}t}F + sh\frac{\partial F}{\partial t} - \xi\frac{\mathrm{d}s}{\mathrm{d}t}\frac{\partial F}{\partial \xi}\right]. \tag{3.21}$$

3.2.1 Constant boundary condition

Let $\beta = \frac{l\rho}{K}$, and for the boundary conditions (i) in (2.20) we have

$$h\frac{\partial^2 F}{\partial \xi^2} = s\left[s\frac{\mathrm{d}h}{\mathrm{d}t}F + sh\frac{\partial F}{\partial t} - \xi\frac{\mathrm{d}s}{\mathrm{d}t}\frac{\partial F}{\partial \xi}\right] \tag{3.22}$$

subject to

$$F = 0, \qquad \text{at } \xi = 1, \tag{3.23}$$

$$F = \frac{1}{h(t)}, \qquad \text{at } \xi = 0, \tag{3.24}$$

$$\beta s(t)\frac{\mathrm{d}s}{\mathrm{d}t} = -h\frac{\partial F}{\partial \xi}, \quad \text{at } \xi = 1. \tag{3.25}$$

We need to pick a function $h(t)$ such that F is independent of t as $t \to 0$. Since the numerator in equation (3.24) is constant, we can choose any constant value

to be $h(t)$, to attain the necessary boundary condition, as in system (2.19). A simple and good choice is therefore $h(t) = 1$. By using equation (2.51) with $\alpha = 1$, we get $s(t) = 2\lambda\sqrt{t}$. Equation (3.21) will thus reduce to

$$\frac{\partial^2 F}{\partial \xi^2} = -2\lambda^2 \xi \frac{\partial F}{\partial \xi}, \tag{3.26}$$

with the boundary conditions

$$F(1) = 0 \quad F(0) = 1 \quad 2\lambda^2 \beta = -\frac{\partial F}{\partial \xi}\bigg|_{\xi=1}. \tag{3.27}$$

The equation (3.26) could be solved in a similar way as the previous differential equation found in equation (2.41) and thus is the solution

$$F(\xi) = 1 - \frac{\operatorname{erf}(\lambda \xi)}{\operatorname{erf}(\lambda)}, \tag{3.28}$$

this solution is valid in $t \to 0$. Where the constant λ satisfies (2.57).

3.2.2 Time-dependent boundary condition

The case (ii) in (2.20) is a time-dependent condition and we need to make sure that $F(0,t)$ is independent of time in the limit $t \to 0$. The boundary condition is

$$F = \frac{e^(t)-1}{h(t)} \quad \text{at } \xi = 0 \tag{3.29}$$

and to choose $h(t)$, we look at the Taylor expansion of $e^t - 1$ around $t = 0$

$$f(t) \sim t + \frac{t^2}{2} + \frac{t^3}{6} + O(t^4). \tag{3.30}$$

Hence in the limit as $t \to 0$ an appropriate choice would be $h(t) = t$. The Stefan condition will thus take the form

$$s(t)\frac{\mathrm{d}s}{\mathrm{d}t} = O(t) \tag{3.31}$$

and by integrating both sides with initial condition $s(0) = 0$, we get an expression for the free boundary

$$s(t) = \gamma t, \tag{3.32}$$

where γ is a proportionality constant, which according to Theorem 2.4.2 must be positive. System (3.22) with $h(t) = 1$ will in the limit $t \to 0$ be

$$\frac{\partial^2 F}{\partial \xi^2} = 0 \tag{3.33}$$

subject to

$$F(1) = 0 \quad F(0) = 1 \quad \gamma^2\beta = -\frac{\partial F}{\partial \xi}\bigg|_{\xi=1} \tag{3.34}$$

and the solution is

$$F(\xi) = 1 - \xi. \tag{3.35}$$

From the Stefan condition we get

$$\gamma = \pm\frac{1}{\sqrt{\beta}}, \tag{3.36}$$

where the positive solution is chosen, as proven in Theorem 2.4.2.

3.3 Numerical method for solving the Stefan problem

As seen previously the Crank-Nicholson method is a sufficient stable method for the heat equation. We will therefore use the Crank-Nicolson scheme to approximate the solution of the Stefan problem under the assumption that the discretization of ξ and t is uniform.

3.3.1 Constant boundary condition

For the first case in equation (3.24) at $\xi = 0$, we have $h(t) = 1$ and to simplify the algebra, we put $z \equiv s^2$. The system in equation (3.22) will therefore take the appearance:

$$\begin{cases} \frac{\partial^2 F}{\partial \xi^2} = z\frac{\partial F}{\partial t} - \frac{\xi}{2}\frac{\mathrm{d}z}{\mathrm{d}t}\frac{\partial F}{\partial t}, & \\ F = 0, & \text{at } \xi = 1, \\ \frac{\beta}{2}\frac{\mathrm{d}z}{\mathrm{d}t} = -\frac{\partial F}{\partial \xi}, & \text{at } \xi = 1, \\ F = 1, & \text{at } \xi = 0, \end{cases} \tag{3.37}$$

with the condition $z(0) = 0$. We apply a discretization using the same method as in section (3.1.3) to acquire the Crank-Nicolson scheme. The scheme uses a central difference at time $t^{n+1/2}$ and a second-order central difference for the spatial derivative at position ξ_j. By applying the Crank-Nicolson method as in section (3.1.3), we will end up with

$$\frac{1}{2}\left(\frac{F_{j+1}^{n+1} - 2F_j^{n+1} + F_{j-1}^{n+1}}{h^2}\right) + \left(\frac{F_{j+1}^{n} - 2F_j^{n} + F_{j-1}^{n}}{h^2}\right) = z^{n+1/2}\left[\frac{F_j^{n+1} - F_j^n}{k}\right] - \frac{\xi_j}{2}\frac{z^{n+1} - z^n}{k}\left[\frac{1}{2}\left(\frac{F_{j+1}^{n+1} - F_{j-1}^{n+1}}{2h}\right) + \frac{1}{2}\left(\frac{F_{j+1}^{n} - F_{j-1}^{n}}{2h}\right)\right]. \tag{3.38}$$

The system (3.38) is according to (3.12) valid for $j = 1, 2, ..., M-1$ and $n = 0, 1, 2, ...$. The boundary conditions become

$$\begin{cases} \frac{\beta}{2}\left(\frac{z^{n+1} - z^n}{k}\right) & = -\frac{1}{2}\left(\frac{F_{M+1}^{n+1} - F_{M-1}^{n+1}}{2h}\right) - \frac{1}{2}\left(\frac{F_{M+1}^{n} - F_{M-1}^{n}}{2h}\right) \\ F_0^{n+1} = 1 & \\ F_M^{n+1} = 0. & \end{cases} \tag{3.39}$$

To be able to approximate this numerically we need to write (3.38) in matrix form, and take into account that $F = 1$ at $\xi = 0$. Using the same notation and regrouping system (3.38) we have

$$\tilde{L} = \frac{1}{2h^2}\left(F_{j+1}^{n+1} - 2F_j^{n+1} + F_{j-1}^{n+1}\right) - \frac{z^{n+1/2}}{k}F_j^{n+1} + \frac{z'}{8h}\xi_j\left(F_{j+1}^{n+1} - F_{j-1}^{n+1}\right) \tag{3.40}$$

and

$$\tilde{R} = -\frac{1}{2h^2}\Big(F_{j+1}^n - 2F_j^n + F_{j-1}^n\Big) - \frac{z^{n+1/2}}{k}F_j^n - \frac{z'}{8k}\xi_j\Big(F_{j+1}^n - F_{j-1}^n\Big), \quad (3.41)$$

where

$$z' = \tfrac{z^{n+1}-z^n}{k} \qquad z^{n+1/2} = \tfrac{z^{n+1}+z^n}{2} \quad (3.42)$$

and $\tilde{L}$ and $\tilde{R}$ denote the side at time $(n+1)$ and (n). To take care of the boundary condition $F_0^{n+1} = 1$ we evaluate equation (3.40) (equation (3.41) is done in a similar way) at $j = 1$:

$$\tilde{L}_{j=1} = \frac{1}{2h^2}\Big(F_2^{n+1} - 2F_1^{n+1} + \underset{=1}{F_0^{n+1}}\Big) - \frac{z^{n+1/2}}{k}F_1^n + \frac{z'}{8k}\xi_1\Big(F_2^{n+1} - \underset{=1}{F_0^{n+1}}\Big). \quad (3.43)$$

Sort out the two constant vectors(due the boundary condition) we could put them together into one constant vector

$$C \equiv \begin{bmatrix} \frac{1}{2h^2} - \frac{z'}{8h}\xi_1 \\ 0 \\ \vdots \\ 0 \end{bmatrix}. \quad (3.44)$$

Furthermore the coefficient matrix of the first parenthesis in equation (3.40) is

$$A = \frac{1}{2h^2}\begin{bmatrix} -2 & 1 & 0 & \dots & 0 \\ 1 & -2 & 1 & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & 1 & -2 & 1 \\ 0 & \dots & 0 & 1 & -2 \end{bmatrix} \quad (3.45)$$

and the second coefficient matrix in equation (3.40) is

$$B = \frac{1}{8h}\begin{bmatrix} 0 & \xi_1 & 0 & \dots & \dots & 0 \\ -\xi_2 & 0 & \xi_2 & \ddots & \dots & \vdots \\ 0 & -\xi_3 & 0 & \xi_3 & \dots & 0 \\ 0 & \ddots & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & -\xi_{M-2} & 0 & \xi_{M-2} \\ 0 & \dots & \dots & 0 & -\xi_{M-1} & 0 \end{bmatrix}. \quad (3.46)$$

Then the system (3.38) could be written in matrix form as

$$\Big(A - \frac{z^{n+1/2}}{k} I + z'B\Big) F^{n+1} = \Big(- \frac{z^{n+1/2}}{k} I - z'B - A\Big) F^n - 2C, \qquad (3.47)$$

where I is the $(M-1)-$Identity matrix, and
Denote the two tridiagonal matrix in equation (3.47) as L and R (as in left and right) and then equation (3.47) could be written as

$$LF^{n+1} = RF^n - 2C \qquad (3.48)$$

where

$$L = \Big(A - \tfrac{z^{n+1/2}}{k} I + z'B\Big), \quad R = \Big(- \tfrac{z^{n+1/2}}{k} I - z'B - A\Big). \qquad (3.49)$$

and

$$C = \begin{bmatrix} \frac{1}{2h^2} - \frac{z'}{8h}\xi_1 \\ 0 \\ \vdots \\ 0 \end{bmatrix}. \qquad (3.50)$$

The approximated Stefan condition in equation (3.39) include the extrapolated values F^{n+1}_{M+1} and F^n_{M+1}. To approximate this problem we evaluate equation (3.38) at $j = M$ and thus we can eliminate the extrapolated values by some algebra. This will lead us to the following polynomial equation of second order for z^{n+1}

$$\begin{aligned} \frac{\beta\xi_M}{2k}(z^{n+1})^2 + \Big[- \frac{\beta\xi_M}{k} z^n + \frac{2\beta r}{v} + F^{n+1}_M - F^n_M \Big] z^{n+1} + \frac{\beta\xi_M}{2k}(z^n)^2 \\ - \frac{2\beta r}{v} z^n + (2r + z^n) F^n_M - 2r(F^{n+1}_{M-1} + F^n_{M-1}) = 0. \end{aligned} \qquad (3.51)$$

Flow chart The constant boundary condition

1. Start by introducing all the constants, "Allocate" memory for the vectors, and give the initial conditions their values.

2. From equation (2.57) we can use the Newton-Raphson method (found in the appendix) to approximate the physical constant λ related to the given value of β.

3. Start iterating a time loop for the whole problem. Because equation (3.38) involves z at time level $(n+1)$, we need to iterate the value until a given tolerance is reached.

4. We use the starting guess for the free boundary to be the previous value $z(n)$ and with help of (3.51) we can update z^{n+1} until the tolerance is reached.

5. Convert back the values for the temperature and the free boundary. Save values at each time step for the exact solutions for both the free boundary and the temperature, for later usage.

6. Plot both the numerical and the exact values for both the temperature and the free boundary against time. Plot the error in the numerical temperature and the numerical free boundary against time.

3.3.2 Time-dependent boundary condition

For the second case in equation (3.24), $h(t) = t$

$$\begin{cases} t\frac{\partial^2 F}{\partial \xi^2} = s\Big[sF + st\frac{\partial F}{\partial t} - \xi t\frac{\mathrm{d}s}{\mathrm{d}t}\frac{\partial F}{\partial \xi}\Big], & \\ F = 0, & \text{at } \xi = 1, \\ \beta s\frac{\mathrm{d}s}{\mathrm{d}t} = -t\frac{\partial F}{\partial \xi}, & \text{at } \xi = 1, \\ F = \frac{e^t - 1}{t}, & \text{at } \xi = 0. \end{cases} \tag{3.52}$$

By applying the Crank-Nicolson method as in section (3.1.3), we will end up with

$$t^{n+\frac{1}{2}}\left[\frac{1}{2}\left(\frac{F_{j+1}^{n+1} - 2F_j^{n+1} + F_{j-1}^{n+1}}{h^2}\right) + \frac{1}{2}\left(\frac{F_{j+1}^{n} - 2F_j^{n} + F_{j-1}^{n}}{h^2}\right)\right] = \\ \left(s^{n+\frac{1}{2}}\right)^2\frac{1}{2}\left(F_j^{n+1} + F_j^n\right) + t^{n+\frac{1}{2}}\left(s^{n+\frac{1}{2}}\right)^2\frac{F_j^{n+1} - F_j^n}{k} - \\ \xi_j t^{n+\frac{1}{2}}s^{n+\frac{1}{2}}s'\left[\frac{1}{2}\left(F_{j+1}^{n+1} - F_{j-1}^{n+1}\right) + \frac{1}{2}\left(F_{j+1}^{n} - F_{j-1}^{n}\right)\right], \tag{3.53}$$

where

$$t^{n+\frac{1}{2}} = \tfrac{t^{n+1}+t^n}{2} \quad s^{n+\frac{1}{2}} = \tfrac{s^{n+1}+s^n}{2} \quad s' = \tfrac{s^{n+1}-s^n}{k}. \tag{3.54}$$

The system (3.53) is according to (3.12) valid for $j = 1, 2, ..., M-1$ and $n = 0, 1, 2, \ldots$. The boundary conditions become

$$\begin{cases} \beta s^{n+\frac{1}{2}}s' = -\frac{1}{2}t^{n+\frac{1}{2}}\left(\frac{F_{M+1}^{n+1} - F_{M-1}^{n+1}}{2h}\right) - \frac{1}{2}t^{n+\frac{1}{2}}\left(\frac{F_{M+1}^{n} - F_{M-1}^{n}}{2h}\right) & (3.55) \\ \frac{1}{2}\left(F_0^{n+1} + F_0^n\right) = \frac{1}{2}\left(\frac{e^{t^{n+1}}-1}{t^{n+1}} + \frac{e^{t^n}-1}{t^n}\right) & (3.56) \\ F_M^{n+1} = 0. & (3.57) \end{cases}$$

The system (3.53) involves s at the next time level, so an iteration is needed. We use the value at level n as starting guess for s^{n+1}. To update the value of s^{n+1} we use the Stefan condition in (3.55). However does equation (3.55) involve the two extrapolated values F_{M+1}^n and F_{M+1}^{n+1}. To remove those values, we evaluate equation (3.53) at $j = M$ and this leads to a quartic expression in terms of s^{n+1} :

$$2r(t^{n+1}+t^n)(F_{M-1}^{n+1}+F_{M-1}^n) - \frac{4\beta}{v}\Big[r + \frac{\xi_M}{4h}\big((s^{n+1})^2 - (s^n)^2\big)\Big]\Big((s^{n+1})^2 - (s^n)^2\Big) = 0. \tag{3.58}$$

To be able to approximate this numerically we need to write (3.53) in matrix form, and take into account that $\frac{1}{2}\Big(F_0^{n+1}+F_0^n\Big)=\frac{1}{2}\left(\frac{e^{t^{n+1}}-1}{t^{n+1}}+\frac{e^{t^n}-1}{t^n}\right)$ at $\xi=0$. Denote the left hand side of equation (3.53) as LH and evaluate at $j=1$

$$\mathrm{LH}_{j=1}:=\frac{t^{n+\frac{1}{2}}}{2h^2}\left[F_2^{n+1}-2F_1^{n+1}+F_0^{n+1}+F_2^n-F_1^n+F_0^n\right], \tag{3.59}$$

and the right hand side of (3.53) at $j=1$

$$\mathrm{RH}_{j=1}:=\big(s^{n+\frac{1}{2}}\big)^2F_1^{n+\frac{1}{2}}+t^{n+\frac{1}{2}}\big(s^{n+\frac{1}{2}}\big)^2\frac{F_1^{n+1}-F_1^n}{k}-\frac{\xi_1 t^{n+\frac{1}{2}}s^{n+\frac{1}{2}}s'}{4h}\left[F_2^{n+1}-F_0^{n+1}+F_2^n-F_0^n\right] \tag{3.60}$$

and then by replacing $\frac{1}{2}\Big(F_0^{n+1}+F_0^n\Big)$ with $\frac{1}{2}\left(\frac{e^{t^{n+1}}-1}{t^{n+1}}+\frac{e^{t^n}-1}{t^n}\right)$ in both $RH_{j=1}$ and $LH_{j=1}$, and collect the terms in a time-dependent vector as

$$D(t)=\begin{bmatrix}\Big(\frac{t^{n+\frac{1}{2}}}{2h^2}-\frac{\xi_1 t^{n+\frac{1}{2}}s^{n+\frac{1}{2}}\frac{s^{n+1}-s^n}{k}}{4h}\Big)\left(\frac{e^{t^{n+1}}-1}{t^{n+1}}+\frac{e^{t^n}-1}{t^n}\right)\\0\\\vdots\\0\end{bmatrix}. \tag{3.61}$$

Regrouping equation (3.53) we get

$$LF^{n+1}=RF^n+D(t) \tag{3.62}$$

with

$$\begin{cases}L:=t^{n+\frac{1}{2}}A-\big(s^{n+\frac{1}{2}}\big)^2\big(\frac{1}{2}+\frac{t^{n+\frac{1}{2}}}{k}\big)I+t^{n+\frac{1}{2}}s^{n+\frac{1}{2}}s'B\\R:=-t^{n+\frac{1}{2}}A+\big(s^{n+\frac{1}{2}}\big)^2\big(\frac{1}{2}-\frac{t^{n+\frac{1}{2}}}{k}\big)I-t^{n+\frac{1}{2}}s^{n+\frac{1}{2}}s'B\end{cases} \tag{3.63}$$

where I is the $(M-1)-$Identity matrix, and the two other coefficient matrix are

$$A=\frac{1}{2h^2}\begin{bmatrix}-2&1&0&\dots&0\\1&-2&1&\ddots&\vdots\\0&\ddots&\ddots&\ddots&0\\\vdots&\ddots&1&-2&1\\0&\dots&0&1&-2\end{bmatrix} \tag{3.64}$$

and

$$B = \frac{1}{4h} \begin{bmatrix} 0 & \xi_1 & 0 & \dots & \dots & 0 \\ -\xi_2 & 0 & \xi_2 & \ddots & \dots & \vdots \\ 0 & -\xi_3 & 0 & \xi_3 & \dots & 0 \\ 0 & \ddots & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & -\xi_{M-2} & 0 & \xi_{M-2} \\ 0 & \dots & \dots & 0 & -\xi_{M-1} & 0 \end{bmatrix}. \tag{3.65}$$

Flow chart The time-dependent boundary condition

1. Start by introducing all the constants, "Allocate" memory for the vectors, and give the initial conditions their values.

2. Start iterating a time loop for the whole problem, and because equation (3.53) involves s at time level $(n+1)$, we need to iterate the value until a given tolerance is reached for every time step.

3. Take care of the case with $0/0$ separately at $n = 1$, where the values in the limit $t \to 0$ is analysed previously in section (3.2.2).

4. Due boundary condition at $\xi = 0$ we get a time constant vector D for every time step.

5. Introduce the right and left coefficient matrix for the expression $LF^{n+1} = RF^n + D$ and solve for F^{n+1}.

6. Solve the quartic equation with Newton-Raphson method (found in appendix) with initial guess of $s^{n+1} = s^n$.

7. When a sufficient good value of s^{n+1} is found we add the boundary conditions at $\xi = 0$ and $\xi = 1$. Avoid the $0/0$ case at $n = 1$.

8. Convert back the values for the temperature and the free boundary. Save values at each time step for the exact solutions for both the free boundary and the temperature, for later usage.

9. Plot both the numerical and the exact values for both the temperature and the free boundary against time. Plot the error in the numerical temperature and the numerical free boundary against time.

3.4 Error analysis

In this section we would like to discuss the methods used around the numerical analysis to measure the error.
To investigate the error in the numerical analysis, we use the discrete l_2-norm denoted by $l_{2,h}$ [8, p.133] for the temperature.
The error in the l_2-norm at time t^n is given by

$$E^n := \|U^n - u^n\|_{2,h} = \left(h \sum_{j=0}^{M} (U(x_j, t^n) - U_j^n) \right)^{1/2}, \tag{3.66}$$

where $U(x_j, t^n)$ is the exact solution at (x_j, t^n) and U_j^n is the numerical solution.
The error for the free boundary at time t^n is given by

$$\left| s(t^n) - s^n \right|. \tag{3.67}$$

System (3.38) and (3.53) involves z^{n+1} and s^{n+1}. To be able to get those value we do an iteration on z^{n+1} respectively s^{n+1} for a given tolerance ε using the same value at level n as a starting guess. We get the new update from the Stefan condition (3.39), and keep on updating until the tolerance is reached. If we denote z_m^{n+1} and s_m^{n+1} as the $m : th$ iterated value of z^{n+1} and s^{n+1}, we can write a convergence criterion as

$$\left| z_{m+1}^{n+1} - z_m^{n+1} \right| < \varepsilon \quad \left| s_{m+1}^{n+1} - s_m^{n+1} \right| < \varepsilon.$$

4 Discussion

In this thesis we have introduced the one-dimensional Stefan problem defined on a semi-infinite interval with two different type of boundary conditions. The important Stefan condition for the free boundary was derived under the condition of equal densities for the two phases. That is not realistic, and even for water the small difference will give a volume change in the transition. Due to the change in volume, another term will occur in the heat equation and also change the appearance for the Stefan condition. By taking consideration of this small but realistic feature, the whole problem of ours will get more complex.

Another simplification in this thesis was the start temperature of the solid phase. If the (for our case) solid phase had another temperature then the melting point, a heat flux will flow back into the liquid phase. And thus attain another term for the Stefan condition (seen in equation (2.1)). Furthermore we will need to solve two different heat equations, separately describing the temperature in each phase.

The numerical simulations was made with the Crank-Nicholson method, which have a second order accuracy in both time and space. This method uses an implicit discretization about $(n + \frac{1}{2})$, instead of a more straightforward explicit one. The numerical implementation is harder, but as shown previously, the explicit scheme imposes both lesser accuracy and a restriction of our time step.

4.1 Future studies

It does clearly exist a lot of opportunities to continue with similar problems that I have been working on this semester. In this thesis only one time-dependent boundary condition was analysed and it does exist some other more realistic and exciting conditions, for instance; oscillating functions which could be describing the variation of temperature over a day. Even further it could be possible to expand the model, find an adequate real life problem. It would be very interesting to simulate nature itself.

Furthermore, this was a one-phase problem so we could extend our interest for a problem with the temperature changing over time in both of the phases, two-phase problem. So the temperature would change in both the liquid phase and the solid phase. For any problem we have discussed in this thesis, we have skipped the density difference between the phases, which causes the liquid phase to attain another velocity vector due to volume changes in the phase transition.

For the confident and brave person, the option to go up a dimension does always exist. Look at some weak solutions and maybe discover something exciting. But as far as that I have understood, the level of complexity do increase substantially as we go up in dimensions.

5 List of notations

$x = s(t)$	The position of the free boundary.
C	The specific heat capacity.
ρ	The density of the specific material.
K	Thermal conductivity.
α	Thermal diffusivity.
l	Latent heat.
Open set	A set which does not contain any of its boundary points.
$\mathbb{R}^n$	The n-dimensional real Euclidian space, where $\mathbb{R} = \mathbb{R}^1$.
Du	Gradient vector := $(u_{x1}, u_{x2}, ..., u_{xn})$.
Div $\mathbf{u}$	The divergence of a vector valued function := $\sum_{i=1}^{n} \frac{\partial F_i}{\partial x_i}$.
∂V	The boundary of V.
$\overline{V}$	The closure is defined as $\partial V \cup V$.
C	A function defined on a set is said to be of class C (or C^0) if it is continuous. Thus, C is the class of all continuous functions.
C^K	A function defined on a set is of class C^K if the first K derivatives exists and are continuous.
Smooth	or C^∞. A function is said to be smooth if it has derivatives of all orders.
Test volume	An open and connected subset of $\mathbb{R}^n$ whose boundary is "smooth" enough, but in this essay we demand only C^1 boundary.
$C^2_{(1)}$	A function u is of class $C^2_{(1)}$ when its time derivative u_t is continuous and its spatial derivatives u_x and u_{xx} are continuous.
L	A linear operator acting on functions.
erf(x)	The error function, which is defined as erf(x) = $\frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2}\, \mathrm{d}t$.
$O(h^k)$	Truncation error - An approximation is of order k with respect to h, which mean that the error is proportional to h^k.
$\|x\|$	Norm, a measure of length or size of a vector in a vector space.
$\|x\|_\infty$	Maximum norm, the largest value of the vector x.
$\|x\|_2$	l_2-norm, is defined as $\left(\sum_{i=1}^{n} \|x_i\|^2 \right)^{1/2}$.

F Appendix

To visualize the approximate solutions for our problem given in (2.19), we present the plots here. We follow the paper by Mitchell and Vynnycky [9] and put

$$
\begin{aligned}
&M = 10 \\
&k = h = 1/M \\
&\beta = \{0.2, 2\} \quad \text{For boundary condition } (i) \\
&\beta = 1 \qquad\quad \text{For boundary condition } (ii),
\end{aligned}
$$

where $\beta = \frac{l\rho}{K_L}$ and the boundary conditions both are given in the system (2.19).

Plots for the constant boundary condition with $\beta = 2$

Using the method described in section 3.3.1 we present below the approximate solutions for the temperature u and the free boundary $s(t)$, shown in Figure 4 and Figure 5. The error in $s(t)$ and u which is defined in section 3.4, are also given below, in Figure 7 and Figure 6.

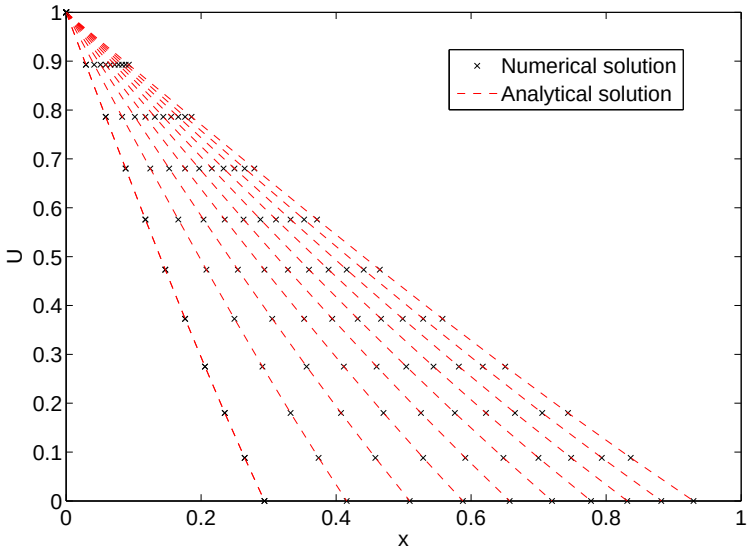

Figure 4: *Plot of the temperature against the position for both the numerical and the analytical solution.* $\beta = 2$.

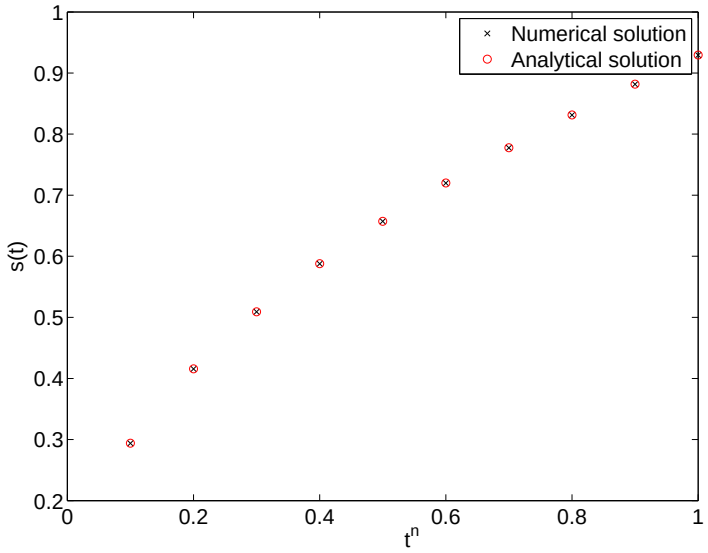

Figure 5: *Plot of the free boundary against the time for both the numerical and the analytical solution.* $\beta = 2$.

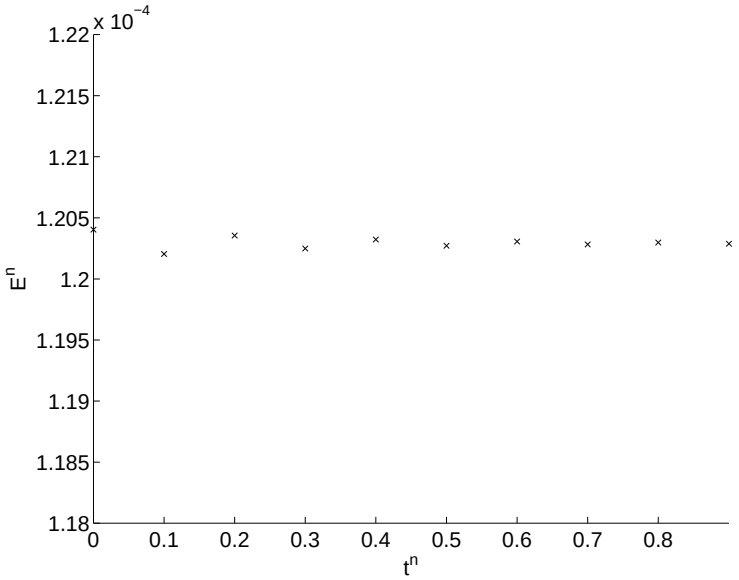

Figure 6: *Plot of* l_2-*error for the temperature against time, with* $\beta = 2$.

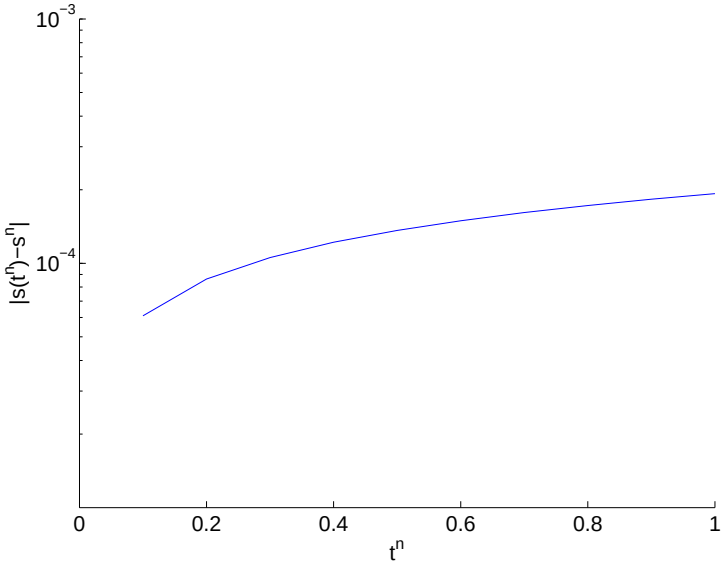

Figure 7: *Plot of the error in the free boundary* $s(t)$ *for* $\beta = 2$.

Plots for the constant boundary condition with $\beta = 0.2$

Using the method described by section 3.3.1 we present below the approximate solutions for the temperature u and the free boundary $s(t)$, shown in Figure 8 and Figure 9. The error in $s(t)$ and u which is defined in section 3.4, are also given below, in Figure 10 and Figure 11.

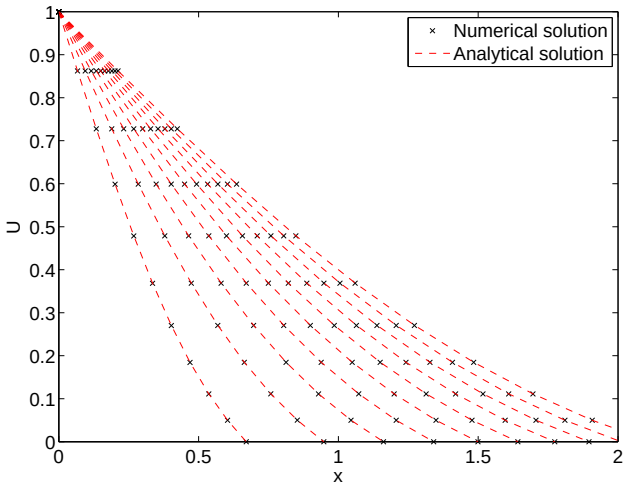

Figure 8: *Plot of the temperature against the position for both the numerical and the analytical solution.* $\beta = 0.2$.

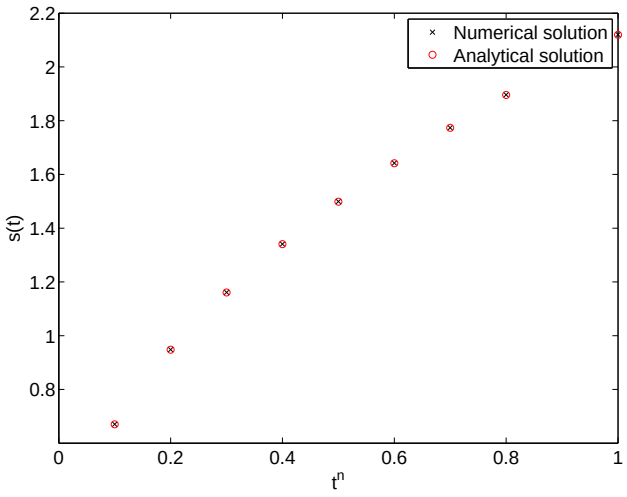

Figure 9: *Plot of the free boundary against the time for both the numerical and the analytical solution.* $\beta = 0.2$.

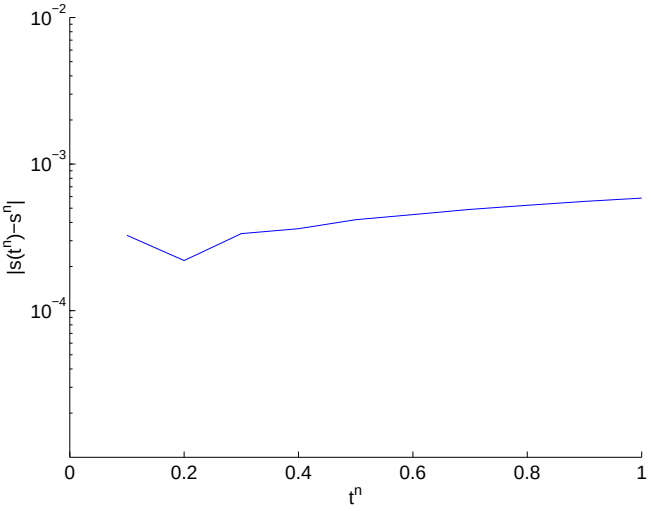

Figure 10: *Plot of the error in the free boundary* $s(t)$ *for* $\beta = 0.2$.

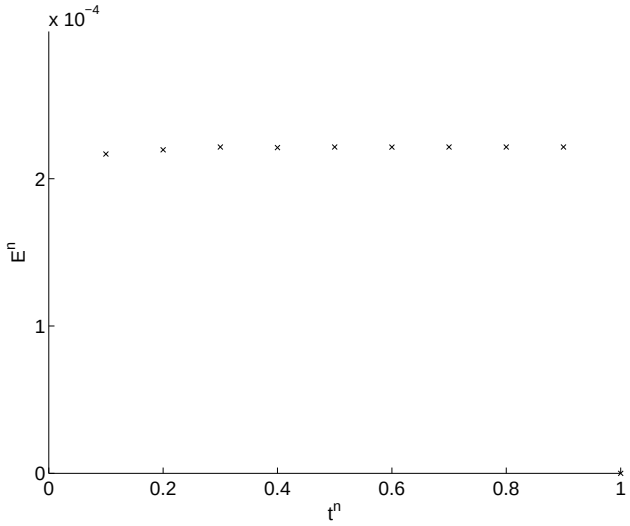

Figure 11: *Plot of* l_2-*error for the temperature with* $\beta = 0.2$.

Plots for the time-dependent boundary condition with $\beta = 1$

Using the method described by section 3.3.2 we present below the approximate solutions for the temperature u and the free boundary $s(t)$, given in Figure 12 and Figure 13. The error in $s(t)$ and u which is defined in section 3.4, are also given below, in Figure 14 and Figure 15.

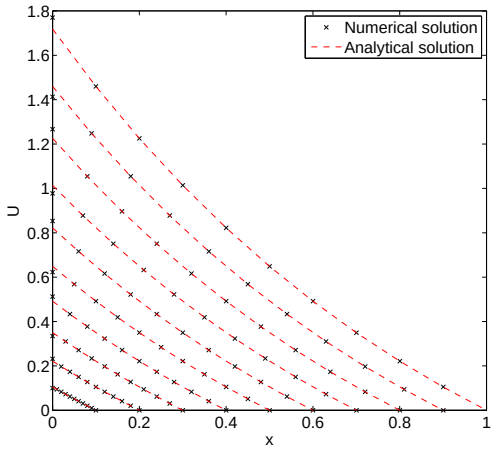

Figure 12: *Plot of the temperature against the position for both the numerical and the analytical solution.*

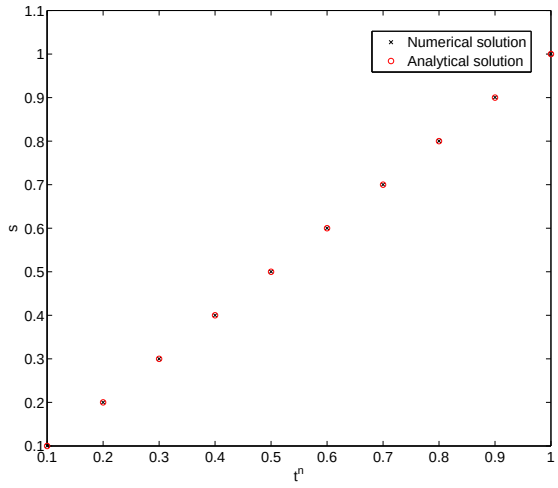

Figure 13: *Plot of the free boundary against the time for both the numerical and the analytical solution.*

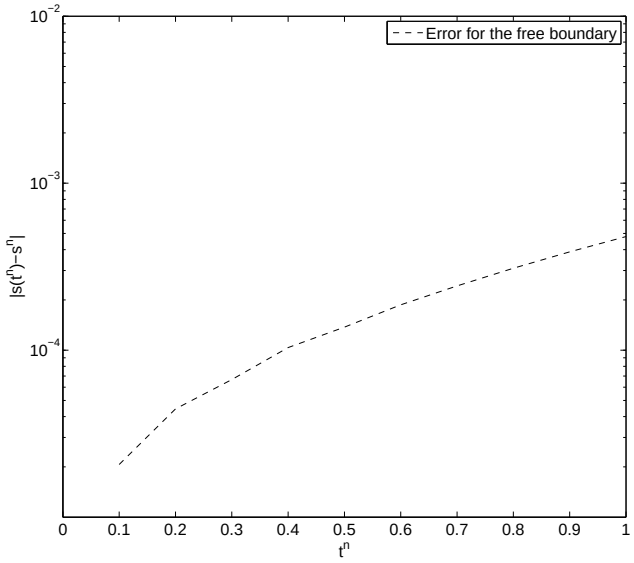

Figure 14: *Error in the free boundary s(t) against time.*

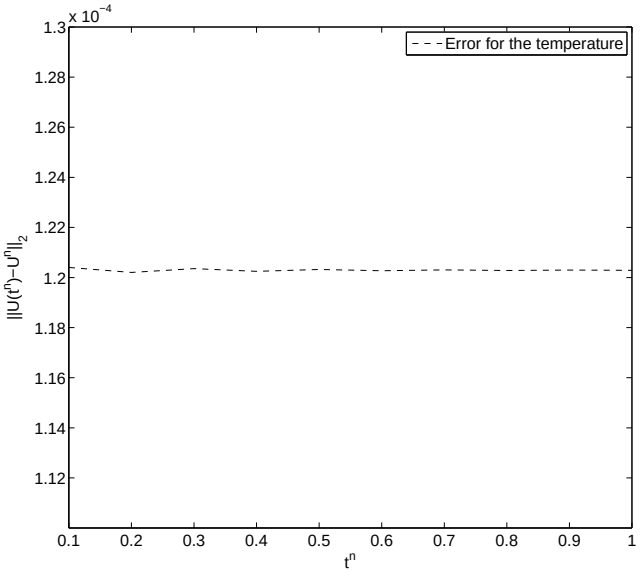

Figure 15: *Error in the temperature U against time* t^n.

G Appendix

The Stefan Problem - Constant boundary condition

```
clear all
close all
%---------------CONSTANTS-----------------%

%Number of nodes
M=10;
%Spatial step size h
h=1/M;
%time step size k
k=h;

%The reciprocal stefan number, found in the stefan condition
beta=0.2;
%To simplify, denote
r=k/h^2;
v=k/h;

%Physical constant, decided by the stefan condition
lambda = newton(beta);

%Number of time steps
NT =M;

%"Allocate" memory
Error_s=zeros(M,1);
Error_F=zeros(M+1,1);
F=zeros(M+1,1); F_analytical=zeros(M+1,1); F_old=zeros(M-1,1);
F_new=F_old;
z=zeros(2,1);
z_error=1e-12;
%The constant vector, taking care of the boundary condition F_0=1
C=zeros(size(F_old));
Error_U=zeros(NT,1);
%The node values for \xi
xi_pos=(0:M)*h;
%Time vector for all timesteps
t=(0:NT)*k;


%Coefficient Matrix
e=ones(M-1,1);
A=1/(2*h^2)*spdiags([e -2*e e],-1:1,M-1,M-1);

xi_above=xi_pos(1:M-1)';
xi_below=xi_pos(3:M+1)';
B=spdiags([-xi_below xi_above],[-1 1],M-1,M-1);
B=1/(8*h)*B;

I=speye(M-1);


%---------initial conditions-------------
F=1-erf(lambda*xi_pos)/erf(lambda);
F_old=F(2:M)';
%----------------------------------------

%Constant coefficient for equation regarding Zn+1
a=beta*xi_pos(M+1)/(2*k);



%iteration for z^(n+1) and the initial guess z(2)=z(1), i.e z^(n
    +1)=z^n
for n=1:NT
    z_error=1e-12;
    while z_error> 1e-13

    %z(n+1/2) and (dz/dt)^n
    z_half= (z(2)+z(1))/2;
    z_prim=(z(2)-z(1))/k;

    %The coefficient matrix for the modifed heat equation: L and
        R,
    %L*Un+1=H*Un
    C(1)=-xi_pos(2)*1/(8*h)*z_prim+1/(2*h^2);
    L=(A-z_half/k*I+z_prim*B);
    R=-(z_half/k*I+A+z_prim*B);

    %Solve for U^(n+1) with our guess

    F_new=L\(R*F_old-2*C);


    %Some coefficients for the quadratic equation giving z^(n+1)
    b=-beta*xi_pos(M+1)/k*z(1)+2*beta*r/v;
    c=beta*xi_pos(M+1)/(2*k)*(z(1))^2-2*beta*r/v*z(1)-2*r*(F_new(
        M-1)+F_old(M-1));


    %roots for the quadratic equation regarding zn+1
    z1=(-b+sqrt(b^2-4*a*c))/(2*a);
    z2=(-b-sqrt(b^2-4*a*c))/(2*a);

    %check if we get complex roots
```

```
if b^2<4*a*c
     disp('Complex roots for z(n+1)')
     break;
end

%Saves the old value of z(n+1)
 zold=z(2);

%z should be positive, for natural reasons, uppdate for z(n
      +1)
if z1>z2
     z(2)=z1;
else
     z(2)=z2;
end
     z_error=abs(z(2)-zold);
end

%Add the boundary conditions
F(2:M)=F_new;
F(1)=1;
F(end)=0;


%----convert back the values of the free boundary at t^(n+1)
      -----%

s_num=sqrt(z(2));
%The exact function for the free boundary
s_exact=2*lambda*sqrt(t(n+1));
%The error for s at timestep t^(n+1)
Error_s(n)=abs(s_num-s_exact);


%Convert back to the temperature U=h(t)F where h(t)=1
U_num=1*F;
%The exact temperature at t^(n+1)
U_exact=1-erf(xi_pos*s_num/(2*sqrt(t(n+1))))/erf(lambda);


%Error for the temperature at timestep t^n
Error_U(n)=sqrt((h*sum((U_exact-U_num).^2)));

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
 %------------THE PLOTS------------%
 figure(1)
 plot(xi_pos*s_num,U_num,'kx',s_num*xi_pos,U_exact,'r--')
     if n==1
       legend('Numerical solution','Analytical solution')
     end

     if n==NT
              xlabel('x')
              ylabel('U')

         end
     hold on

     figure(2)
     plot(t(n+1),s_num,'kx',t(n+1),s_exact,'ro')
          if n==1
           legend('Numerical solution','Analytical solution')
          end

          if n==NT
              xlabel('t^n')
              ylabel('s')
          end
     hold on

    %plot(t(n+1),s,'kx',t(n+1),s_exact,'ro')
   % hold on



  % figure(2)
    %subplot(2,1,2)
  %   plot(xi_pos*s,U,'kx',xi_pos*s,U_exact,'r--')
  % hold on
    %legend('Black is numerical')
  % axis([0 1 0 1])
 %   xlabel('x')
 %   ylabel('U')
     F_old=F_new;
     z=[z(2) z(2)];
     pause(0.1)
end
hold off

%The Error in the temperature against time
figure(4)
plot(t(2:end),Error_U,'k--')
legend('Error for the temperature')
xlabel('t^n')
ylabel('||U(t^n)-U^n||_2')


figure(3)
plot(t(2:end),Error_s,'kx')
legend('Error for the free boundary')
xlabel('t^n')
ylabel('|s(t^n)-s^n|')
```

The Stefan Problem - Time-dependent boundary condition

```
clear all
close all
%--------------CONSTANTS----------------%

%Number of nodes
M=10;
%Spatial step size h
h=1/M;
%time step size k
k=h;

%The reciprocal stefan number, found in the stefan condition
beta=1;
%To simplify, denote
r=k/h^2;
v=k/h;

%Physical constant, decided by the stefan condition
lambda = 1/sqrt(beta);


%Number of time steps
NT =M;

%"Allocate" memory
%Error_s=zeros(M,1);
Error_U=zeros(M+1,1);
F=zeros(M+1,1); F_analytical=zeros(M+1,1); F_old=zeros(M-1,1);
F_new=F_old;
s=zeros(2,1);
s_error=1e-12;
D=zeros(size(F_old));
%The node values for \xi
xi_pos=(0:M)*h;
%Time vector for all timesteps
t=(0:NT)*k;

%Coefficient Matrix
e=ones(M-1,1);
A=1/(2*h^2)*spdiags([e -2*e e],-1:1,M-1,M-1);

xi_above=xi_pos(1:M-1)';
xi_below=xi_pos(3:M+1)';
B=spdiags([-xi_below xi_above],[-1 1],M-1,M-1);
B=1/(4*h)*B;
I=speye(M-1);

%---------initial conditions------------
F=1-xi_pos;
F_old=F(2:M)';
%---------------------------------------
```

```
for n=1:NT
    s_error=1e-12;
    itt=0;
    %iteration for s^(n+1) and the initial guess s(2)=s(1)
    while s_error> 1e-13

    %s at time positon n+1/2
    s_half=(s(2)+s(1))/2;
    %The forward time difference quotient for s
    s_prim=(s(2)-s(1))/k;
    %t at n+1/2
    t_half=(t(n+1)+t(n))/2;



    %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
    %Fixing the time constant D(t)
    %-------------------------------------------------------------------%

    c2=xi_pos(2)*t_half*s_prim*s_half/(4*h);
    c1=t_half/(2*h^2);

    %Avoid the 0/0-case, since t(1)=0
    if n==1

        Y=(exp(t(n+1))-1)/(t(n+1))+1;

    else

    Y=(exp(t(n+1))-1)/(t(n+1))+(exp(t(n))-1)/(t(n));

    end

    D(1)=(c2-c1)*Y;
   %-------------------------------------------------------------------%



    %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
    %The coefficient matrix for F^{n+1} and F^n; LF^{n+1} = RF^{n
        }
    %-------------------------------------------------------------------%

    L=t_half*A-((s_half)^2/2+t_half*(s_half)^2/k)*I+t_half*s_half
        *s_prim*B;
```

```
R=-t_half*A+((s_half)^2/2-t_half*(s_half)^2/k)*I-t_half*
      s_half*s_prim*B;

%-------------------------------------------------------------%

%Solve for the new value at level n+1
F_new=L\(R*F_old+D);

%The quartic equation in terms of s^{n+1}, where x:=s^{n+1}
fun =@(x) 2*r*(t(n+1)+t(n))*(F_new(M-1)+F_old(M-1))-4*beta/v
      *(r+xi_pos(M+1)/(4*h)*(x^2-(s(1))^2))*(x^2-(s(1))^2);
%Saves the old value of s(n+1) before the update
s_old=s(2);
%Newton-raphson method with starting guess of s^n
s(2)=newton3(fun,s(1));

%Saves the error in the free boundary at the m:th iteration
      for s^{n+1}
s_error=abs(s(2)-s_old);

end

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%Adding boundary conditions
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
F(2:M)=F_new;
  %Avoiding the 0/0 at n=1
if n==1
 F(1)=1;
else
 F(1)= (exp(t(n+1))-1)/(t(n+1))+(exp(t(n))-1)/(t(n))-
       Fendpoint;
end
F(end)=0;

%
     %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

%----convert back all the values at t^(n+1)-----%
%
     %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

U_num=F*t(n+1);
s_num=s(2);
%The exact function for the free boundary and the temperature
s_exact=1/sqrt(beta)*t(n+1);

%The error for s at timestep t^(n+1)
Error_s(n+1)=abs(s_num-s_exact);
%The exact temperature at time level t^(n+1)
U_exact=exp(t(n+1)-s_exact*xi_pos)-1;

%Error for the temperature at timestep t^(n+1)
Error_U(n+1)=sqrt((h*sum((U_exact-U_num).^2)));

    %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
    %------------THE PLOTS-------------%
    figure(1)
    plot(xi_pos*s_num,U_num,'kx',s_num*xi_pos,U_exact,'r--')
       if n==1
         legend('Numerical solution','Analytical solution')
       end

       if n==NT
           xlabel('x')
           ylabel('U')

       end
    hold on

    figure(2)
    plot(t(n+1),s_num,'kx',t(n+1),s_exact,'ro')
        if n==1
         legend('Numerical solution','Analytical solution')
        end

        if n==NT
           xlabel('t^n')
           ylabel('s')
       end
    hold on
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

    %
         %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

    %-------- Overwrite the old values for the next time loop
         -------
    %
         %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

    F_old=F_new;
    Fendpoint=F(1);
    s=[s(2) s(2)];

end

%The Error in the free boundary against time
figure(3)
plot(t,Error_s,'k--')
legend('Error for the free boundary')
xlabel('t^n')
ylabel('|s(t^n)-s^n|')

%The Error in the temperature against time
figure(4)
```

```
plot(t,Error_U,'k--')
legend('Error for the temperature')
xlabel('t^n')
ylabel('||U(t^n)-U^n||_2')
```

The Newton Raphson method - constant boundary condition

```
function [ xold] = newton(beta)

f = @(x) sqrt(pi)*beta*x*exp(x^2)*erf(x)-1;
fprim = @(x) sqrt(pi)*beta*(exp(x^2)*erf(x)+2*x^2*exp(x^2)*erf(x)
     +2*x/sqrt(pi));

xold=10;
while 1
    xnew = xold-f(xold)/fprim(xold);
    temp=xold;
     xold=xnew;
    if abs(temp-xold)<0.0001
       break;
    end
end


end
```

The Newton Raphson method - time-dependent condition

```
function [ xold] = newton3(f,xold)

%f = @(x) sqrt(pi)*beta*x*exp(x^2)*erf(x)-1;
%fprim = @(x) sqrt(pi)*beta*(exp(x^2)*erf(x)+2*x^2*exp(x^2)*erf(x
    )+2*x/sqrt(pi));

    function[fprim]=fprim(xold,h)
        fprim=(f(xold+h)-f(xold))/h;
    end

it=0;
%xold=10;
while 1
    xnew = xold-f(xold)/fprim(xold,0.000001);
        temp=xold;
        it=it+1;
         xold=xnew;
        if abs(temp-xold)<0.0001
            break;
        end
end


end
```

Bibliography

[1] V. Alexiades and A.D. Solomon. *Mathematical Modeling of Melting and Freezing Processes*. Hemisphere Publishing Corporation, Washington, 1993.

[2] D. Andreucci. Lecture notes on the Stefan problem. 2002.

[3] J. Crank. *Free and Moving Boundary Problems*. Hemisphere Publishing Corporation, Washington, 1993.

[4] L.C. Evans. *Partial Differential Equations*. American Mathematical Society, Providence, Rhose Island, 2010.

[5] A. Friedman. *Partial Differential Equations of Parabolic Type*. Prentice-Hall, Inc, Englewood Cliffs, N.J., 1964.

[6] S.C. Gupta. *The Classical Stefan Problem - Basic Concepts, Modelling and Analysis*. Elsevier Science B.V, Amsterdam, 2003.

[7] G. Lamé and B.P. Clapeyron. Mémoire sur la solidification par refroidissement d'un globe liquide. *Ann. Chem. Phys 47, pp. 250-256*, 1831.

[8] S. Larsson and V. Thomée. *Partial Differential Equations with Numerical Methods*. Springer, Berlin, 2005.

[9] S.L. Mitchell and M. Vynnycky. Finite-difference methods with increased accuracy and correct initialization for one-dimensional Stefan problems. *Applied Mathematics and Computation 215 1609-1621*, 2009.

[10] F. Morgan. *Real Analysis and Applications*. American Mathematical Society, Providence, Rhode Island, 2005.

[11] M.H. Protter and H.F. Weinberger. *Maximum Principles in Differential Equations*. Prentice-Hall, Inc, London, 1967.

[12] L.I. Rubenstein. *The Stefan Problem*. American Mathematical Society, Providence, Rhode Island, 1971.

[13] D.V. Schroeder. *An Introduction to Thermal Physics*. Addison Wesley Longman, Boston, Massachusetts, 2000.

[14] J. Stefan. Über die Theorie der Eisbildung, insbesondere über die Eisbildung im Polarmeere. *Ann. Physik Chemie 42, pp. 269–286*, 1891.

[15] C. Vuik. Some historical notes about the Stefan problem. *Nieuw Archief voor Wiskunde*, 4e serie 11 (2): 157–167, 1993.