Harmonic map heat flow

MASTER THESIS

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Preface

What you are reading is my master thesis. I talked to my supervisor Prof. Dr. R. van der Hout about the subject in 2004, but I did not start really until summer 2005. After a few months of wrestling through all the theory it finally became clear to me. The next thing to do was numerically constructing the behaviour predicted in the theory, and after that writing this report.

Most of all I want to thank my supervisor Prof. Dr. R van der Hout for all of his support. We almost met weekly and discussed the progress. I want to thank Dr. J.B. van den Berg for letting me use figures 2.5 and 2.6. I want to thank Peter Bruin for helping me including a flipbook in this thesis of the differential equation I studied. I also want to thank my parents for their support during my study. Finally I want to thank all the other people who supported me during my studies.

Contents

Chapter 1

Introduction & Summary

This report is about the harmonic map heat flow from the disk to the sphere. We consider basically the heat equation for a function $u : D^2 \to S^2$ in a radially symmetric case. Physically it is a simplified model for the behaviour of nematic liquid crystals.

In the radially symmetric case we obtain a nonlinear, inhomogeneous, second order differential equation for the polar angle θ in spherical coordinates. We can easily construct an energy $E(\theta(.,t))$ such that the dynamics is described by the gradient flow of that energy. We restrict ourselves to positive solutions, that is, $\theta \geq 0$.

Under certain conditions a classical solution exists only up to a finite time T. At that time the derivative blows up, the solution θ jumps at $r = 0$ (for example from 0 to π) and the energy jumps too. We remark that such jumps of the solution θ correspond to downward jumps of the energy. So we argue that when the solution θ jumps energy is stored in (or released from) the origin.

Since the dynamics is described by the gradient flow of the energy E, the energy is decreasing in time. Suppose the solution has made a jump at $t = T$ in $r = 0$ from $\theta = 0$ to $\theta = \pi$ (where the energy jumps downward), then we have stored energy in the origin. Since the model describes a physical system we expect that in some cases the energy can be released again. But when that happens the energy decreasing principle is violated locally. This would imply that the solution is not unique.

Next we construct a minimal solution $\hat{\theta}$ for all these solution. The solution is minimal in a sense that $\hat{\theta} \leq \theta$ for all (weak) solutions θ, so it jumps down first. We try to do the construction numerically by implementing a finite element method. The result can be viewed as a flipbook when holding the report backward and then flipping the paper.

The structure of the report is as follows. Chapter 2 describes the theory (we consider a slightly more general problem then the radially symmetric harmonic map heat flow from D^2 to S^2) and chapter 3 describes the numerical construction of the minimal solution

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Chapter 2

Overview of the theory

2.1 The main problem

This report studies the problem:

Problem 2.1.

$$\begin{cases} \theta_t & = & \theta_{rr} + \frac{\theta_r}{r} - \frac{g(\theta)}{r^2} & (r,t) & \in & (0,1) \times (0,\infty) \\ \theta(1,t) & = & \Theta & t & \in & (0,\infty) \\ \theta(r,0) & = & \theta_0(r) & r & \in & (0,1) \end{cases} \tag{2.1}$$

We require that $\Theta \in (0,\infty)$. *For the function g we require:*

1. $g \in C^\infty(\mathbb{R})$,
2. $g(0) = g(A) = 0$ *for some* $A > 0$,
3. $g'(0) > 0$,
4. *there exists an* $A_0 \in (0,A)$ *such that* $(A_0 - \theta)g(\theta) > 0$ *when* $\theta \in [0,A] \backslash \{0, A_0, A\}$.
5. *Define:* $G(\theta) := \int_0^\theta g(s)ds$. *We distinguish between three cases:*
   (a) $G(A) < 0$ *and* $g(\theta) > 0$ *for* $\theta > A$. A^* *is the unique positive zero of G in* $(0,A)$,
   (b) $G(A) = 0$ *and g is A-periodic,*
   (c) $G(A) > 0$ *(in section 2.6 we prove this case in not as interesting as the other ones). Unless stated otherwise we assume we are not in this case.*

The requirements for g (in the case where $G(A) < 0$*) imply roughly that g looks like figure 2.1. For simplicity we will take* $g'(0) = 1$ *instead of* $g'(0) > 0$. *In cases* $G(A) \neq 0$ *we restrict ourselves to the case* $u \leq A$.

2.1.1 Boundary conditions at $r = 0$ & energy considerations

Note that no boundary condition has been specified at $r = 0$. One might recognize $\theta_{rr} + \frac{\theta_r}{r}$ as the Laplacian in 2-dimensional cylindrical coordinates and then argue $\theta_r(r = 0) = 0$ is a good boundary condition (since $r = 0$ is not the the boundary of the disk). This however is not a good idea since we have a singularity at $r = 0$ that will force θ_r to change.

How to resolve this? Let us first find the associated energy for the equation. Multiply the equation by $-r\theta_t$ to obtain

$$-r\theta_t^2 = -\theta_t \frac{\partial}{\partial r}(r\theta_r) + \frac{\theta_t g(\theta)}{r}$$

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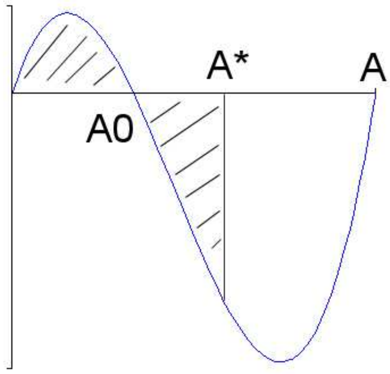
Figure 2.1: Rough sketch of g in the case where $G(A) < 0$.



and try to establish the form $\int -r\theta_t^2 = \frac{d}{dt}\int ... \leq 0$. The latter integral (with the $\frac{d}{dt}$ in front) is called the associated energy and is non-increasing in time. Working this out gives

$$\int_0^1 -r\theta_t^2 dr = \int_0^1 -\theta_t \frac{\partial}{\partial r}(r\theta_r) + \frac{\theta_t g(\theta)}{r} dr = \int_0^1 \theta_r r \frac{\partial \theta_t}{\partial r} + \frac{\theta_t g(\theta)}{r} dr.$$

The boundary term $[-\theta_t \theta_r r]_0^1$ vanishes at $r = 0$ (we require θ_r is finite, this can be achieved certainly for finite time, see theorem 2.9) and at $r = 1$ $\theta_t(1, t) = 0$ (we fix the value of θ at $r = 1$). Continuing the derivation gives

$$\int_0^1 -r\theta_t^2 dr = \int_0^1 \frac{\partial}{\partial t}\left[\frac{\theta_r^2}{2} + \frac{G(\theta)}{r^2}\right] r dr = \frac{d}{dt}\int_0^1 \left[\frac{\theta_r^2}{2} + \frac{G(\theta)}{r^2}\right] r dr.$$

If we define

$$E(t) := \int_0^1 \left[\frac{\theta_r^2}{2} + \frac{G(\theta)}{r^2}\right] r dr, \tag{2.2}$$

then we have the relation

$$\frac{d}{dt}E(t) = \int_0^1 -r\theta_t^2 dr \leq 0. \tag{2.3}$$

We call $E(t)$ the associated energy of the system. Equation 2.3 guarantees that (for classical solutions) the energy $E(t)$ is non-increasing in time. We remark that there exist weak solutions with non-increasing energy. Unless stated otherwise we consider such solutions. Later on we will extend this class to solutions for which we only require

$$E(t) \leq E(0),$$

which is automatically fulfilled for classical solutions.

From now on we suppose we start with finite energy. What does this imply for problem 2.1? We already noticed that we did not specify a boundary condition at $r = 0$. But if we want finite energy at $t = 0$ then we conclude that it is necessary to require

$$\theta(0, 0) \in \{x \in \mathbb{R} : G(x) = 0\}. \tag{2.4}$$

So $\theta(0, 0)$ can have only discrete values, moreover we have $\theta(0, t) = \theta(0, 0)$ as long as θ is continuous. It will turn out that a solution does not have to exist for all time, but only for $t < T$ for some $T > 0$. At

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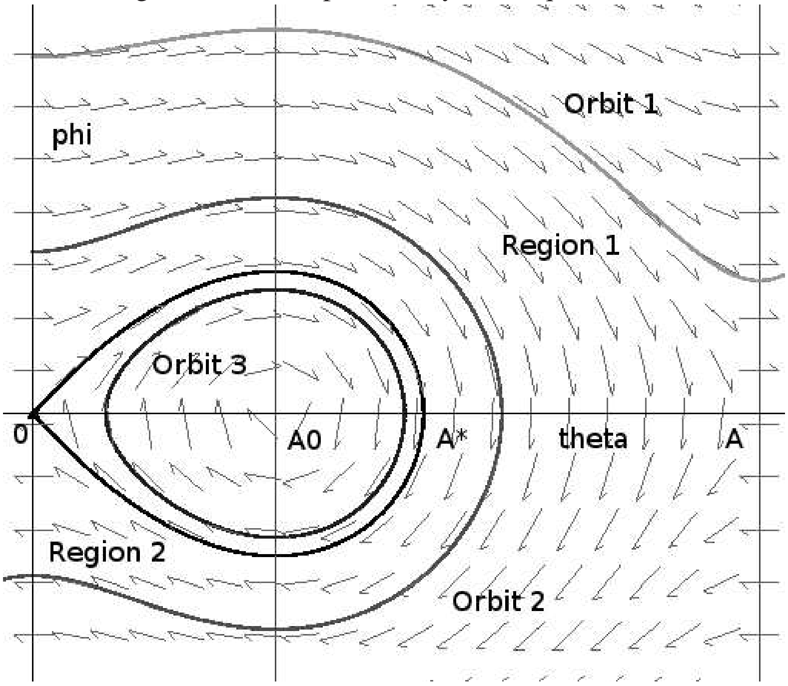
Figure 2.2: Phase plane analysis of equation 2.6.



$t = T$ the solution makes a jump at $r = 0$ from 0 (if $\theta(0,0)$) to A (this is not clear at this point yet). This also coincides with blow-up in the derivative. So we have

$$\begin{aligned} \theta(r = 0, t) &= 0 \quad t < T, \\ \theta(r = 0, t) &= A \quad r \geq T, \\ \limsup_{r \to 0, t \uparrow T} |\theta_r(r, t)| &= \infty. \end{aligned}$$

After the jump the energy will be $-\infty$ (in the case $G(A) < 0$). So in that case the energy is unbounded from below. This might all sound a little vague at the moment, but it will become more clear later on, since this is the lead we will follow.

2.1.2 Stationary solutions

Let's now look for stationary solutions of 2.1. This means we have to solve

$$\theta_{rr} + \frac{\theta_r}{r} - \frac{g(\theta)}{r^2} = 0. \tag{2.5}$$

Make the transformation $r = e^{-y}$, write $\tilde{\theta}(y) = \theta(r)$ and omit the tilde. Put $\phi = \theta_y$ and let $\dot{}$ denote differentiation with respect to y then we get the system

$$\begin{cases} \dot{\theta} = \phi \\ \dot{\phi} = g(\theta) \\ \theta(y = \infty) = \theta(r = 0) \in \{0, A\} \\ \theta(y = 0) = \theta(r = 1) = \Theta \\ 0 \leq \Theta \leq A. \end{cases} \tag{2.6}$$

Look at figure 2.1 to quickly recall the definition of A. Let us look for nullclines. Solving $\dot{\phi} = 0$ gives $\theta \in \{0, A_0, A\}$ and solving $\dot{\theta} = 0$ gives $\phi = 0$. Phase plane analysis gives us the picture of figure 2.2. The following proposition comes from [1], where the proof has been omitted.

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Proposition 2.2. *1. If $\Theta \in \{0, A^*\}$, then 2.5 has a unique classical solution θ with $\theta(0) = 0$.*

2. *If $\Theta \in (0, A^*)$, then 2.5 has two different classical solutions $\theta_1 \leq \theta_2$. The solution θ_1 is increasing. The solution θ_2 is increasing in $(0, \bar{r})$ and decreasing in $(\bar{r}, 1)$ for some $\bar{r} < 1$, moreover $\theta(\bar{r}) = A^*$.*

3. *If $\Theta > A^*$, then 2.5 does not have a solution such that $\theta(0) = 0$*

4. *If $0 \leq \Theta \leq A$, then 2.5 has a unique solution θ^* such that $\theta^*(0) = A$ and $\theta^*(1) = \Theta$. When $\Theta < A$ then θ^* is decreasing.*

Proof. Look at figure 2.2. It is enough to prove the existence of orbits 1, 2 and 3. That means: there are orbits starting on the ϕ-axes which look like 1 and 2 and there is an orbit starting on the θ-axis which looks like 3. We define the following regions:

$$\text{Region 1} \quad := \quad \left\{(\theta, \phi) \in \mathbb{R}^2 : 0 \leq \theta \leq A, \phi \geq 0\right\}, \tag{2.7}$$

$$\text{Region 2} \quad := \quad \left\{(\theta, \phi) \in \mathbb{R}^2 : 0 \leq \theta \leq A, \phi \leq 0\right\}. \tag{2.8}$$

Suppose we start an orbit at (θ_0, ϕ_0), then we have

$$G(\theta(y)) - G(\theta_0) = \int_{\theta(0)}^{\theta(y)} g(s)ds = \int_0^y g(\theta(s))\dot{\theta}(s)ds = \int_0^y \dot{\phi}(s)\phi(s)ds = \frac{1}{2}(\phi(y)^2 - \phi(0)^2). \tag{2.9}$$

Conclusion:

$$G(\theta(y)) - \frac{1}{2}\phi(y)^2 \tag{2.10}$$

is constant along an orbit.

Let's first look at orbits 2 and 3. Note that the orbits are symmetric with respect to the θ-axis, since $\dot{\phi}$ is independent of ϕ and $\dot{\theta}|_{(\theta,\phi)} = -\dot{\theta}|_{(\theta,-\phi)}$. So it is enough to prove the following: suppose we start an orbit at $(\theta_0, 0)$ with $0 \leq \theta_0 < A$, then if $A^* < \theta_0 < A$ we leave region 2 through the ϕ-axis and if $0 \leq \theta_0 < A^*$ we leave region 2 through the θ-axis. Let Y denote the "time" at which we leave region 2 when we start an orbit in $(\theta_0, 0)$, then from 2.10 we get $G(\theta(Y)) - \frac{1}{2}\phi(Y)^2 = G(\theta(0)) - \frac{1}{2}\phi(0)^2 = G(\theta_0)$. If $A^* < \theta_0 < A$ then $G(\theta_0) < 0$, so we must have $\phi(Y) < 0$, that means we leave region 2 through the ϕ-axis. If $0 < \theta_0 < A^*$ then $G(\theta_0) > 0$, so we must have $\theta(Y) > 0$, that means we leave region 2 through the θ-axis.

Let's now look look at orbit 1. We start an orbit in the point $(0, \phi_0)$ ($\phi_0 > 0$) and try to figure out whether it is possible to leave region 1 through the line $\theta = A$. Let Y be the time we leave region 1. From 2.10 we get: $G(\theta(Y)) - \frac{1}{2}\phi(Y)^2 = -\frac{1}{2}\phi(0)^2$. Note: $G(\theta(Y)) \leq 0$ and it is a fixed value. If we choose $\phi(0)$ big enough we must have $\phi(T) > 0$, that means we leave region 1 through the line $\theta = A$. □

From this phase plane analysis we can make a graph of the stationary solutions (see figure 2.3) which satisfy $\theta_0(r = 0) = 0$. Note that we did not draw the zero solution and that the r-axis ranges from 0 to some big value (not necessarily up to $r = 1$). There's another thing we can see from the phase plane analysis: the stationary solutions attain their maxima in r_{A^*}, that is, $\theta_0(r_{A^*}) = A^*$.

Let us finally note some other nice feature of equation 2.5. Suppose that $\theta(r)$ satisfies this equation, that means

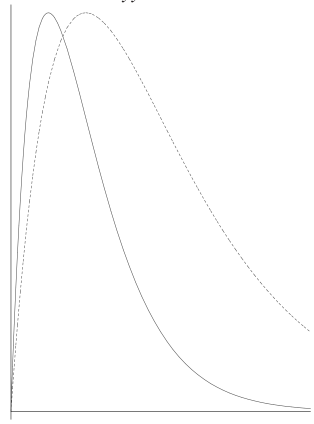
$$\theta_{rr} + \frac{\theta_r}{r} - \frac{g(\theta)}{r^2} = 0.$$

What equation does $\psi(r) := \theta(\alpha r) = \theta(s)$ satisfy (where $s = \alpha r$)? Note that we know

$$\theta_{ss} + \frac{\theta_s}{s} - \frac{g(\theta)}{s^2} = 0,$$

1

Figure 2.3: Stationary solutions of equation $\theta_{yy} = g(\theta(y))$, rescalings are also stationary solutions.



so we get

$$\psi_{rr} + \frac{\psi_r}{r} - \frac{g(\psi)}{r^2} = \alpha^2\theta_{ss} + \alpha\frac{\theta_s}{r} - \frac{g(\theta)}{r^2} = \alpha^2\left(\theta_{ss} + \frac{\theta_s}{\alpha r} - \frac{g(\theta)}{\alpha^2 r^2}\right) = \alpha^2\left(\theta_{ss} + \frac{\theta_s}{s} - \frac{g(\theta)}{s^2}\right) = 0.$$

So $\psi(r)$ satisfies the same equation. Conclusion: *rescalings of stationary solutions are also stationary solutions!*

2.2 Harmonic map heat flow

In the so called 'harmonic map heat flow'-case we take $g(\theta) = \frac{1}{2}\sin(2\theta)$. To be able to refer easily to this case we reformulate problem 2.1:

Problem 2.3.

$$\begin{cases} \theta_t & = \theta_{rr} + \frac{\theta_r}{r} - \frac{\sin 2\theta}{2r^2} & \text{in} \quad (0,1)\times(0,\infty) \\ \theta(1,t) & = \Theta & \text{in} \quad (0,\infty) \\ \theta(r,0) & = \theta_0(r) & \text{in} \quad (0,1) \end{cases} \tag{2.11}$$

2.2.1 Energy

From equation 2.2 we find the energy associated to the equation:

$$E(t) := \int_0^1 \left[\theta_r^2 + \frac{\sin^2\theta}{r^2}\right]\frac{r}{2}dr. \tag{2.12}$$

Note that $E(t) \geq 0$, in combination with 2.3 we obtain for smooth θ

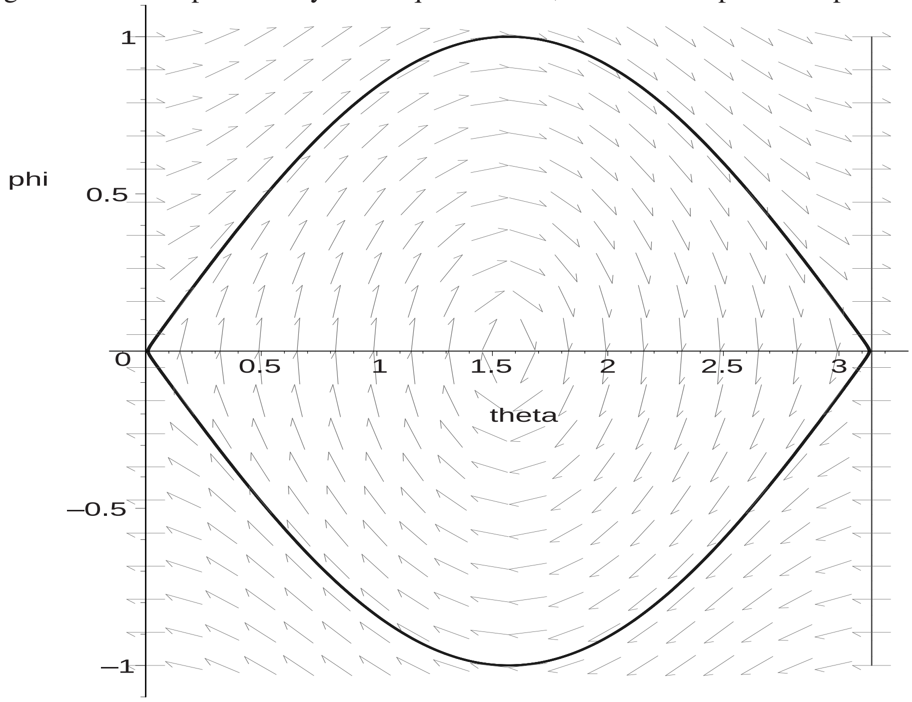
$$0 \leq E(t) \leq E(0).$$

So in this case the energy is bounded from below. That means starting out with finite energy implies that the energy will remain finite for all time. This leads to the following condition:

$$\theta(0,t) \in \pi\mathbb{Z}. \tag{2.13}$$

1

Figure 2.4: Phase plane analysis of equation 2.14, note that the picture is periodic.



2.2.2 Stationary solutions

We look for stationary solutions. We solve the equation

$$\theta_{rr} + \frac{\theta_r}{r} - \frac{\sin 2\theta}{2r^2} = 0.$$

To do this make the transformation $r = e^{-s}$ or $s = -\log r$. We obtain

$$\frac{d^2\theta}{ds^2} = \frac{1}{2}\sin 2\theta.$$

If we multiply this equation by $\frac{d\theta}{ds}$ and integrate with respect to s we obtain

$$\left(\frac{d^2\theta}{ds^2}\right)^2 = \sin^2 2\theta + C'.$$

To determine the C' we do phase plane analysis. We put $\phi = \theta_s$, from formula 2.6 we get

$$\begin{cases} \dot{\theta} = \phi \\ \dot{\phi} = \frac{1}{2}\sin(2\theta) \\ \theta(s = \infty) = \theta(r = 0) \in \pi\mathbb{Z} \\ \theta(s = 0) = \theta(r = 1) = \Theta \\ \Theta \in (0, \infty). \end{cases} \tag{2.14}$$

In figure 2.4 we see the direction field. With techniques similar to the ones used in proposition 2.2 we can prove that the only orbits that go to $k\pi$ as $s \to \infty$ are the heteroclinic orbits that you see in figure 2.4. If we now let $s \to \infty$ then we conclude $\theta \to k\pi$ and $\frac{d\theta}{ds} \to 0$. From this we conclude $C' = 0$. We now end up with

$$\frac{d^2\theta}{ds^2} = \pm \sin 2\theta.$$

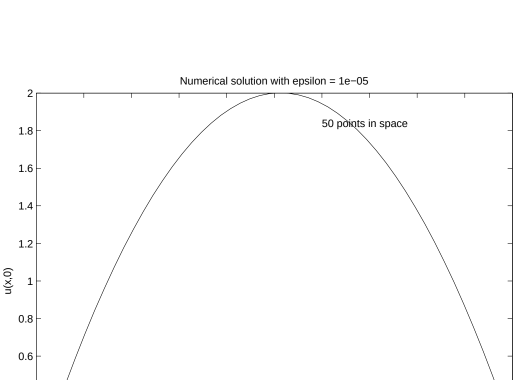

Numerical solution with epsilon = 1e−05
50 points in space
u(x,0)
x
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
1.8
2
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1

Figure 2.5: Different initial profiles, the figure comes from [5].

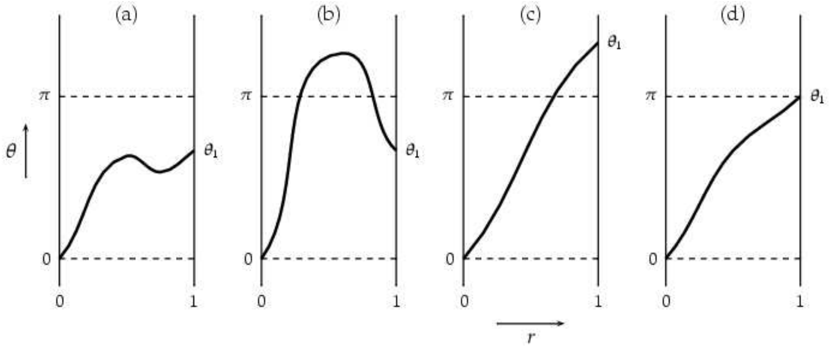
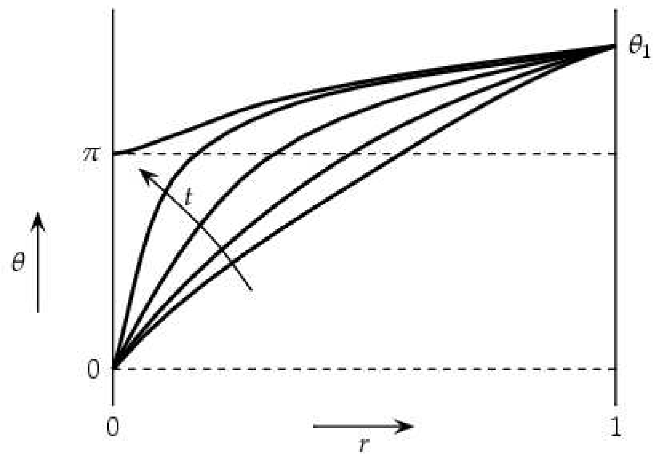


Figure 2.6: Sketch of a jump at the origin, the figure comes from [5].



We immediately see $\theta = k\frac{\pi}{2}$ is a solution to this equation. However the odd multiples $\frac{\pi}{2}$ do not have finite energy, so only $\theta = k\pi$ remains. And that if $\theta \neq k\pi$ then $(m-1)\pi < \theta < m\pi$ because of the the condition $\theta(s = \infty) \in \pi\mathbb{Z}$. This equation can be solved by making the substitution $\psi = \tan\frac{\theta}{2}$. Note that this substitution is bijective since if $\theta \neq k\pi$ (for all $k \in \mathbb{Z}$) then $(m-1)\pi < \theta < m\pi$ (for some $m \in \mathbb{Z}$). From this we find $\sin\theta = \frac{2\psi}{1+\psi^2}$ and $d\theta = \frac{2d\psi}{1+\psi^2}$. An easy computation shows that the general solution (with finite energy) is of the form:

$$\begin{cases} \theta(r) = 2\arctan\alpha r + k\pi \\ k \in \mathbb{Z} \\ \alpha \in \mathbb{R}. \end{cases} \tag{2.15}$$

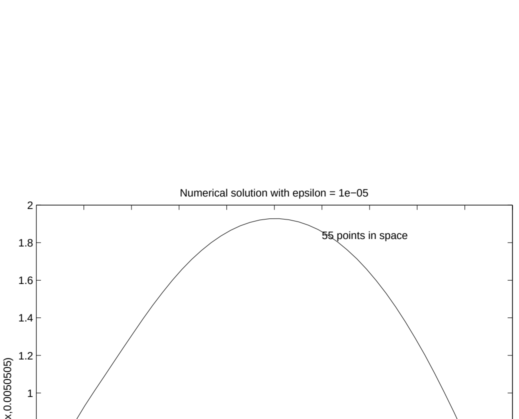
From the derivation it follows that these are all the stationary solutions with finite energy. It is useful to notice that we can rewrite the stationary solutions in the following way:

$$\theta(r) = \arccos\frac{1-\alpha^2 r^2}{1+\alpha^2 r^2}. \tag{2.16}$$

The form of equation 2.16 is used in several references on the subject.

2.2.3 Different initial profiles

The following results are also covered in a similar way in the introduction of [5]. We distinguish between four different cases (see figure 2.5). Suppose we start with an initial profile from figure 2.5(c). Recall that from starting with finite energy we got the condition: $\theta(0,t) \in \pi\mathbb{Z}$ (equation 2.13). There is a no



Numerical solution with epsilon = 1e−05
55 points in space
u(x,0.0050505)
x
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
1.8
2
0.1
0.3
0.5
0.7
0.9

stationary solution which connects 0 and Θ if $\Theta > \pi$. Since we will converge to one of the stationary solutions (for this to happen we must require non-increasing energy, but more on that later) a jump at the origin must occur (figure 2.6).

In the case of figure 2.5(a) $\Theta < \pi$, so a jump does not have to occur. In fact it can be proven that a jump in this case will not occur, but we will come to that later. However if the function has a peak high enough, the case of figure 2.5(b) a jump must occur under certain conditions. This is the topic of [1], which was the main resource for my thesis. When the profile form figure 2.5(d) is chosen infinite time blow-up occurs. In [8] it is shown that: if $\theta_0 \leq \pi$ then the solution exists for all time. Since (as we prove later on) we converge in this case to a stationary solution we will converge to $\theta = \pi$. Conclusion: when we start with the profile of 2.5(d) we have infinite time blow-up.

2.3 Nematic Liquid Crystals

Let us now give some motivation for why problem 2.3 is interesting to study. In fact in the case where we take $g(\theta) = \frac{1}{2}\sin(2\theta)$ the equation is a model for incompressible nematic liquid crystals in an infinity long cylinder. We are not going to do any physics, so we will not discuss what nematic liquid crystals exactly are. But let us notice that liquid crystals for instance are used in LCD-screens (Liquid Crystal Displays), so somehow it's clear that they are important. All we have to know about them is that we can view them as a fluid consisting of molecules which point in some direction (locally). In our case we have an infinitely long cylinder filled with the fluid. The fluid is equipped with a unit vector field (the director field), representing the local molecular directions. We remark that opposite directions should be considered equivalent.

What we are now going to discuss is covered in more detail in [2]. Suppose we have some infinitely long cylinder with radius R and axis along the z-axis. We impose a pressure gradient to make the fluid flow through the cylinder. We make the following assumptions:

1. The velocity of the flow and the molecular directions at the boundary of the cylinder can be prescribed.
2. We assume we have a continuous distribution of directors in the cylinder.
3. Radial symmetry.
4. There is no shear rate. That means if we see the flow in the cylinder as $v = f(r)e_z$, the $f'(r) = 0$. The $f'(r) \neq 0$ case is covered in more detail in [2].
5. Suppose we look at some value of z, then the profile is invariant under shifts in the z-direction.

The following description is also in figure 2.7. Using this z-invariance we conclude that we only have to look at a cross section of the cylinder. Furthermore we define an equivalence relation $\sim$ on S^2 by $x \sim y$ iff $x = -y$. We can view the dynamics as a mapping form $D^2 \times [0, T)$ to $S^2/\sim$. The dynamics are now described by the equation of problem 2.3.

The energy associated to the system is called the Frank Oseen energy. It is some sort of elastic energy due to variations in the director field. The Frank Oseen Energy is given by

$$F(t) = \int_0^1 \frac{K}{2}\left(\theta_r^2 + \frac{\sin^2\theta}{r^2} + \frac{\sin 2\theta}{r}\theta_r\right) r dr, \tag{2.17}$$

where $K \in \mathbb{R}$ is some constant. There is a relation between the Frank Oseen energy and the energy $E(t)$ which we defined in equation 2.12:

$$F(t) = KE(t) + \frac{K}{2}\int_0^1 \left(\frac{\sin 2\theta}{r}\theta_r\right) r dr = KE(t) + \frac{K}{2}\int_{k\pi}^{\Theta} \sin 2\theta d\theta = KE(t) + \frac{K}{2}\sin^2\Theta.$$

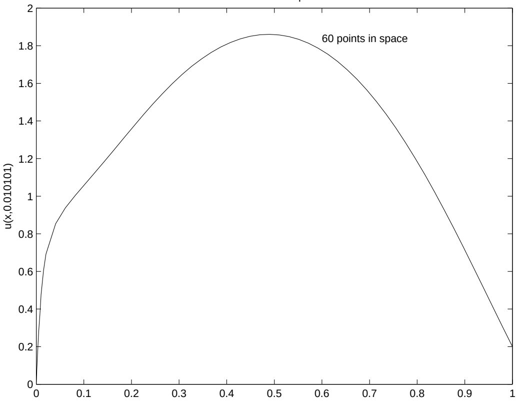
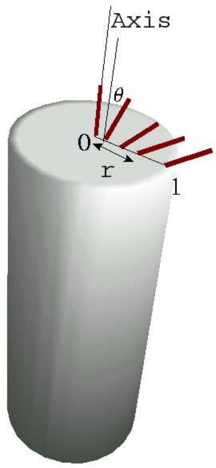

Numerical solution with epsilon = 1e−05
60 points in space
u(x,0.010101)
x
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
1.8
2

Figure 2.7: Physical visualization.



Remark that Θ (and therefore also the last part of the above expression) is constant. Finiteness of the Frank Oseen energy implies (as we already saw before) $\theta(0,t) \in \pi\mathbb{Z}$.

Now suppose we start with some configuration taken from figure 2.5. And suppose that we get blow-up (as in figure 2.6). In view of nematic liquid crystals we can see this as some spring winding up at the origin (the angle of the director at $r = 0$ jumps by π). So we can say that, when $\theta(0,t)$ jumps, energy is stored in the origin.

The expression for the Frank Oseen energy can be used to estimate how much energy is stored. The reasoning is as follows. Look at figure 2.8. The energy in the region $r = 0 \ldots h$ in the limit $h \to 0$ is the energy stored in the origin when solution jumps in $r = 0$ from $\theta = 0$ to $\theta = \pi$. We fix a point of the solution near $r = h$, say at $r = h - \delta$, as indicated in figure 2.8. If we would consider the problem on $r = 0 \ldots h - \delta$ then in time the energy will decrease and the profile will eventually converge to the stationary solution. So we can estimate the energy of the solution on $r = 0 \ldots h - \delta$ from below by calculating the energy of the stationary solution which satisfies the same boundary conditions. We write

$$\begin{aligned}
\theta(r) &= 2\arctan(\alpha r), \\
\theta_r(r) &= \frac{2\alpha}{1+\alpha^2 r^2}.
\end{aligned}$$

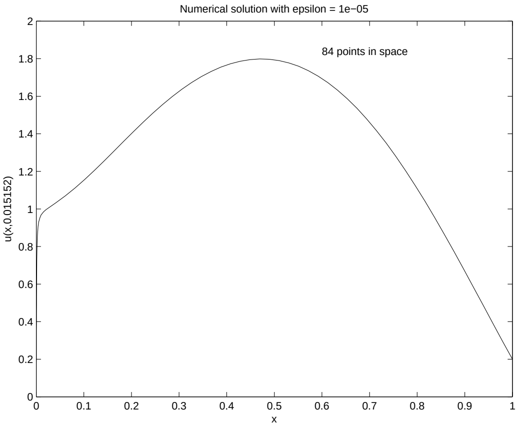
Substitute those expressions in the expression for the energy:

$$\begin{aligned}
\int_0^{h-\delta} \left(\frac{\theta_r^2}{2} + \frac{\sin^2\theta}{2r^2} \right) r dr &= \int_0^{h-\delta} \left(\frac{4\alpha^2}{(1+\alpha^2 r^2)^2} + \frac{4\alpha^2 r^2}{r^2 (1+\alpha^2 r^2)^2} \right) \frac{r}{2} dr = \left. \frac{-2}{1+\alpha^2 r^2} \right|_0^{h-\delta} \\
&= 2 - \frac{2}{1+\alpha^2 (h-\delta)^2} = 2 - \frac{2}{1+\tan^2\frac{\tilde{\theta}}{2}} = \tilde{E}(\tilde{\theta}).
\end{aligned}$$

Sending $h - \delta \to 0$ corresponds to sending $\tilde{\theta} \to \pi$, so we get

$$\lim_{\tilde{\theta}\to\pi} \tilde{E}(\tilde{\theta}) = 2.$$

In some papers the energy is defined slightly different. If one encounters 4π instead of 2 this is due to the integration in polar coordinates, the energy they defined had an extra factor 2π. If one encounters 8π the integration in performed in polar coordinates and the factor $\frac{1}{2}$ is dropped in the energy.


Numerical solution with epsilon = 1e−05
84 points in space
u(x,0.015152)
x
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
1.8
2
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1

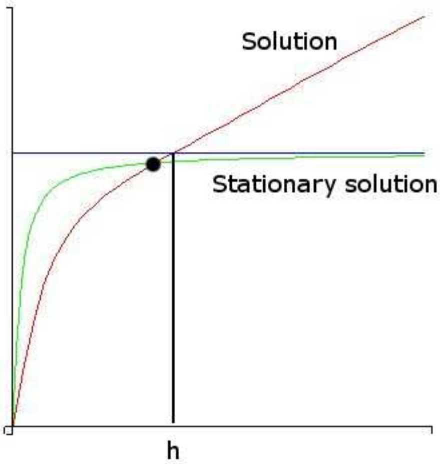


Figure 2.8: One can estimate the energy in the region $r = 0...h$ with the help of the stationary solutions. In the limit $h \to 0$ this is the energy stored in the origin when the solution jumps in $r = 0$ from $\theta = 0$ to $\theta = \pi$.

Physically one expects that in some cases this energy will be released again. Suppose we are in such a case and that the solution jumps at $r = 0$ from $\theta = 0$ to $\theta = \pi$. Problem 2.3 which describes the dynamics in this physical case has infinitely many solutions. But there can only be one physical solution. We supposed that we were in a case where a physically valid solution will eventually release the energy stored in the origin. So after the blow-up (the jump to π) there must be an instance of jumping back. It has been proven in [3] that the jump back time can be controlled. In fact once the solution is below $\theta = \pi$ and has we finite angle with the line $\theta = \pi$ we can force the jumping back. There are multiple choices for the physical solution, since the instance of jumping back does not follow uniquely from the model. What we can do is construct a minimal solution $\hat{\theta}$ in the sense that $\hat{\theta} \leq \theta$ for all solutions θ. The minimal solution will release the energy first (which corresponds in the case we consider to jumping back at $r = 0$ from $\theta = \pi$ to $\theta = 0$). The numerical construction of the minimal solution will be a main goal in this thesis.

2.4 Harmonic maps

What does this all have to do with harmonic maps? Everyone knows the definition of a harmonic function $u : \mathbb{R}^2 \to \mathbb{R}$, we just require $\Delta u = 0$. Can we extend this definition for more general $u : M \to N$ where M and N are Riemannian manifolds? It is well know that the solution of $\Delta u = 0$ minimizes the following integral:

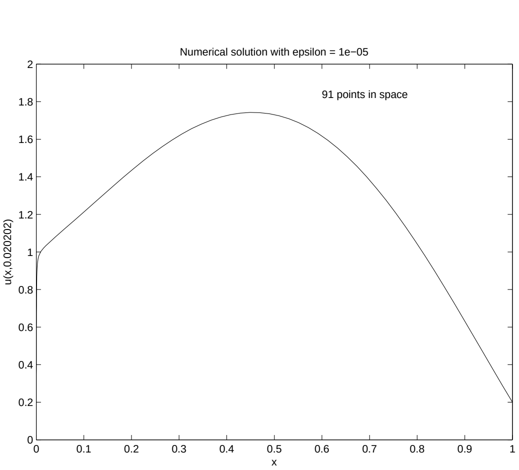
$$\int |\nabla u|^2.$$

We can use this to extend our definition of harmonic.

Definition 2.4. *A differentiable map $u : M \to N$ is called harmonic if it is a stationary point of*

$$E(u) = \int_M |\nabla u|_M^2,$$

where $|\nabla .|_M^2$ denotes differentiation in the context of manifolds. Note that in $\mathbb{R}^n$ $|\nabla u|^2 = \sum_{i,j} \left(\frac{\partial u_i}{\partial x_j}\right)^2$.



Numerical solution with epsilon = 1e−05
91 points in space
u(x,0.020202)
x
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
1.8
2
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1

2.4.1 Harmonic maps from $D^2 \to S^2$

As we saw in the previous section we can describe our nematic liquid crystal problem by a map $u : D^2 \to S^2$. Let's try to answer the following question: what equation does u satisfy if $M = D^2$ and $N = S^2$? This question in also answered in [9]. Consider the disk and the sphere as embedded in $\mathbb{R}^3$:

$$\begin{aligned} D^2 &= \left\{(x_1, x_2, x_3) \in \mathbb{R}^3 : x_1^2 + x_2^2 = 1, x_3 = 0\right\}, \\ S^2 &= \left\{(x_1, x_2, x_3) \in \mathbb{R}^3 : x_1^2 + x_2^2 + x_3^2 = 1\right\}. \end{aligned} \tag{2.18}$$

We write $u = [u_1, u_2, u_3]$. Since $u \in S^2$ we have $u_1^2 + u_2^2 + u_3^2 = 1$. We now have to minimize $\int_{D^2} |\nabla u|^2$ given the constraint $u_1^2 + u_2^2 + u_3^2 = 1$. Suppose u minimizes $E(u)$ and consider some proper perturbation (we will make precise what we mean by that) $u + \epsilon\psi$ of u, then the perturbation must satisfy

$$\frac{d}{d\epsilon} E(u + \epsilon\psi)|_{\epsilon=0} = 0.$$

Working this out gives

$$0 = \frac{d}{d\epsilon} \int_{D^2} \sum_{i,j} \left(\frac{\partial u_i}{\partial x_j} + \epsilon \frac{\partial \psi_i}{\partial x_j}\right)^2 dx \Bigg|_{\epsilon=0} = 2 \int_{D^2} \sum_{i,j} \frac{\partial u_i}{\partial x_j} \frac{\partial \psi_i}{\partial x_j} dx = -2 \int_{D^2} \sum_{i,j} \frac{\partial^2 u_i}{\partial x_j^2} \psi_i dx. \tag{2.19}$$

For the integration by parts we used $\psi|_{\partial D^2} = 0$. This is one requirement for ψ, since we want $u + \epsilon\psi$ to satisfy the same boundary conditions as u. But for ψ to be a good perturbation we must also require that $u + \epsilon\psi$ maps to S^2, that means

$$\sum_i (u_i + \epsilon\psi_i)^2 = 1.$$

Working this out gives

$$\sum_i 2\epsilon u_i \psi_i + \epsilon^2 \psi_i^2 = 0.$$

Since ϵ can be chosen as small as we want, so we can drop the ϵ^2, rewriting this gives

$$< u, \psi >= 0. \tag{2.20}$$

If we see u as a vector from the origin to a point $s \in S^2$, then 2.20 implies that ψ lies in the tangent plane of s in S^2. Rewriting 2.19 gives

$$\int_{D^2} < \psi, \Delta u >= 0. \tag{2.21}$$

If we combine 2.20 with 2.21 we obtain

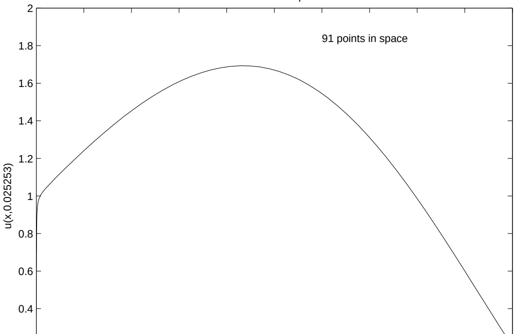
$$\lambda u = \Delta u. \tag{2.22}$$

Since suppose in some point $d \in D^2$ Δu has a component $\hat{\xi}(d)$ perpendicular to u. By continuity we have $\hat{\xi}(d) \neq 0$ in some neighbourhood $N(d) \subset D^2$ of $d \in D^2$. Choose a function $\bar{\psi} : D^2 \to \mathbb{R}$ with support only in the neighbourhood $N(d)$. Now $\bar{\psi}(d)\hat{\xi}(d)$ is a good perturbation, but for this perturbation we have $\int_{D^2} < \bar{\psi}\hat{\xi}, \Delta u > \neq 0$. The next step is to determine λ. Taking the inner product with u and using $< u, u >= 1$ gives

$$\lambda =< u, \Delta u > .$$

Two times differentiating the equation $u_1^2 + u_2^2 + u_3^2 = 1$ with respect to x_i and summing over i gives $< u, \Delta u >= -|\nabla u|^2$. If we substitute this into 2.22, we obtain the differential equation for a harmonic map $u : D^2 \to S^2$:

$$\Delta u + |\nabla u|^2 u = 0.$$



Numerical solution with epsilon = 1e−05
91 points in space
u(x,0.025253)
x
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
1.8
2
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1

2.4.2 The radially symmetric case

Consider the following time dependent problem:

Problem 2.5.

$$\begin{cases} u_t - \Delta u = |\nabla u|^2 u \\ u(x,0) = u_0(x) \\ u(x,t) : D^2 \times [0,T] \to S^2 \\ u(x,t)|_{\partial D^2} = U. \end{cases} \tag{2.23}$$

$[0,T]$ is the maximum time interval on which we can define everything. What we just proved is that stationary solutions of this equation are harmonic maps. Consider $u : D^2 \to S^2$, embed them both in $\mathbb{R}^3$ (as in 2.18) and equip the preimage with cylindrical and the image with spherical coordinates. We use the notation of cylindrical and spherical coordinates as described in the appendix. Suppose u_0 is of the form:

$$u_0 : D^2 \ni r\hat{r}_{D^2}(r,\phi,z=0) \mapsto \hat{r}_{S^2}(1,\phi,\theta(r)) \in S^2,$$

where $\hat{r}$ is a unit vector in the radial direction in respectively cylinder and spherical coordinates. It has been proven in [8] that if we start with a radially symmetric situation then the profile remains radially symmetric in time. So this means that if u_0 is of this form then $u(.,t)$ will also be of the form:

$$u(.,t) : D^2 \ni r\hat{r}_{D^2}(r,\phi,z=0) \mapsto \hat{r}_{S^2}(1,\phi,\theta(r,t)) \in S^2.$$

What equation will $\theta(r,t)$ satisfy? This can be a very long nasty calculation if choosing an inconvenient approach. But with the help of the material in the appendix, the calculation should not be too long. We use A.1 and A.3 to compute $\Delta_{\text{Cylinder}}\hat{r}_{S^2}(1,\phi,\theta(r,t))$ to be

$$\Delta_{\text{Cylinder}}\hat{r}_{S^2}(1,\phi,\theta(r,t)) = \left(\theta_{rr} + \frac{\theta_r}{r} - \frac{\sin\theta\cos\theta}{r^2}\right)\hat{\theta}_{S^2} + \left(-\theta_r^2 - \frac{\sin\theta}{r^2}\right)\hat{r}_{S^2}. \tag{2.24}$$

We use A.2 to calculate:

$$|\nabla u|^2 = \theta_r^2 + \frac{\sin^2\theta}{r^2}. \tag{2.25}$$

Plugging 2.24 and 2.25 in 2.23 gives:

$$\left(\theta_{rr} + \frac{\theta_r}{r} - \frac{\sin\theta\cos\theta}{r^2}\right)\hat{\theta}_{S^2} = 0.$$

Solutions to this equation are just the stationary solutions of problem 2.3! The conclusion of the section reads: *stationary solutions of problem 2.3 correspond to harmonic maps.*

2.4.3 Stationary solutions as backward stereographic projection

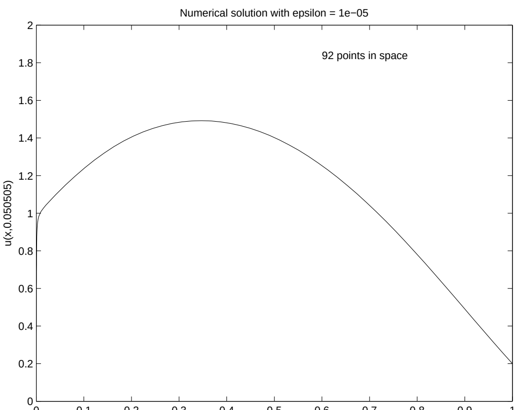
Figure 2.9 shows how we can construct a point on the circle (which can be viewed as a cross section of the sphere S^2) when starting with a point on the line below the circle. One can see in this figure that:

$$\tan\frac{\theta}{2} = \alpha r,$$

this implies:

$$\theta(r) = 2\arctan\alpha r,$$

which are the stationary solutions we also obtained in equation 2.15.


Numerical solution with epsilon = 1e−05
92 points in space
u(x,0.050505)
x
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
0.2
0.4
0.6
0.8
1.2
1.4
1.6
1.8
2

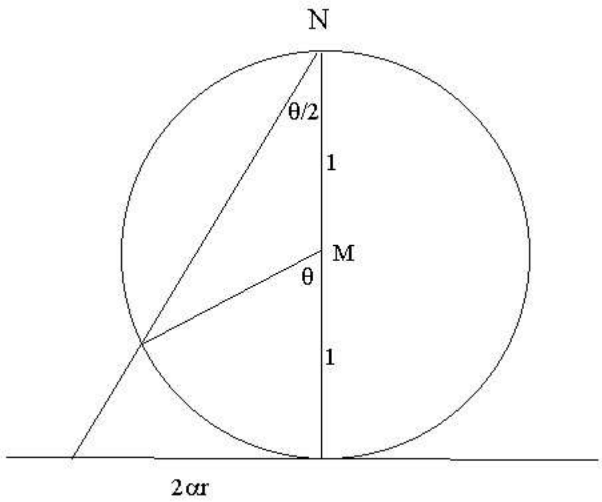


Figure 2.9: Stationary solutions as backward stereographic projection.

2.5 Well known results

This section covers some well know results related to problem 2.1 and 2.3.

2.5.1 Existence of solutions

We start this section with the definition of $H^1(D^2; S^2)$.

Definition 2.6. *Consider D^2 and S^2 as embedded in $\mathbb{R}^3$, then define*

$$H^1(D^2, \mathbb{R}^3) := \left\{u : u, Du \in L^2(D^2; \mathbb{R}^3)\right\}$$

and

$$H^1(D^2, S^2) := \left\{u \in H^1(D^2, \mathbb{R}^3) : u(x) \in S^2 \textit{ for almost every } x \in D^2\right\}$$

Consider problem 2.5. Chang, Ding and Ye proved in [10] that in general a classical solution exists only for finite time. Struwe proved in [7] that if $u_0 \in H^1(D^2; S^2) := \left\{u : u, Du \in L^2(D^2; S^2)\right\}$ then problem 2.5 has a solution satisfying

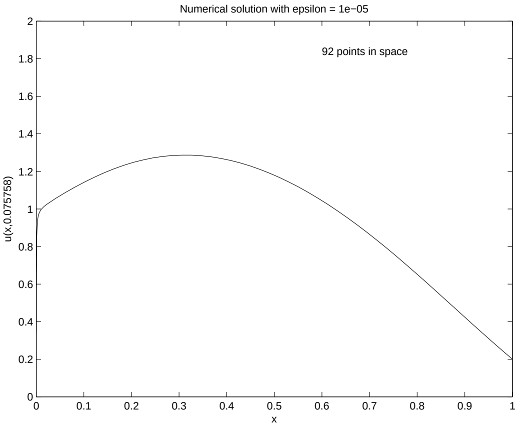
$$\int_{D^2} |\nabla u(t)|^2 \leq \int_{D^2} |\nabla u_0(t)|^2 \quad t > 0. \tag{2.26}$$

Results of Struwe in [14], Chang in [15] and Freire in [6] showed that if we sharpen condition 2.26 to

$$t \mapsto \int_{D^2} |\nabla u(t)|^2 \quad \text{is nonincreasing for } t > 0, \tag{2.27}$$

then there exists a unique solution. The solution that satisfies criterium 2.27 is called the Struwe solution. Remark that a solution that evolves in time without jumping (a classical solution) always satisfies criterium 2.27. Only at jumps can this condition be violated.

Consider problem 2.3. Criterium 2.27 also guarantees that the solution will converge to a stationary solution. To be more precise, we can find a subsequence $u(., t_n)$ that converges a.e. to a stationary solution. We prove this in this paragraph. First we remark the following three facts:



Numerical solution with epsilon = 1e−05
92 points in space
u(x,0.075758)
x
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
1.8
2
0.1
0.3
0.5
0.7
0.9

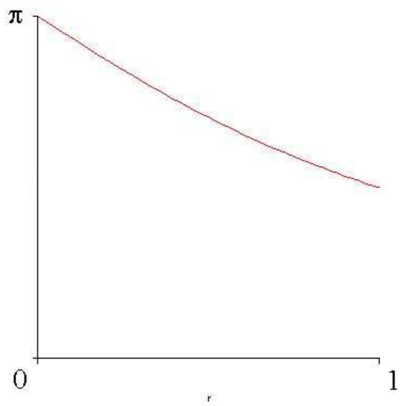


Figure 2.10: A picture of the stationary profile of the Struwe solution, we start with the profile form figure 2.5(b).

1. The criterium implies that the *energy* $E(t)$ *(formula 2.12) tends to a limit* $\bar{E}$ since $E(t)$ is bounded from below by 0.

2. *There exists a* $k \in \mathbb{Z}_{>0}$ *such that* $\theta(., t) \leq k\pi$ *for all* $t \geq 0$, since for smooth θ_0 we have $\theta_0(r) \leq k\pi$ for some $k \in \mathbb{Z}_{>0}$. The result follows from the comparison principle (2.7, which we are about to formulate).

3. From formula 2.3 we conclude $E(t)$ *is stationary iff* $\theta_t = 0$. This means we are in a stationary solution.

Choose a minimizing sequence t_n for the energy, that is $E(t_n) \to \bar{E}$. Consider the corresponding sequence $\theta(., t_n)$. This sequence is uniformly bounded in $H^1(D^2, \mathbb{R})$ since the energy is decreasing and $\theta(r, .) \leq k\pi$ for some $k \in \mathbb{Z}$. From Sobolev embedding theorems we get: $H^1(D^2) \subset\subset L^2(D^2)$. So in fact we have a strongly convergent subsequence $u(., t_{n'}) \to u$ in $L^2(D^2)$. We conclude there is a subsequence $u(., t_{n''})$ that converges to u a.e. General theory of calculus of variations states that (for the energy we defined) the limit u minimizes the energy if the mapping $\theta_r \mapsto |\theta_r|^2$ is convex (see e.g. [23] section 8.2). This condition can easily be checked. The fact that u is a stationary solution follows from point 3.

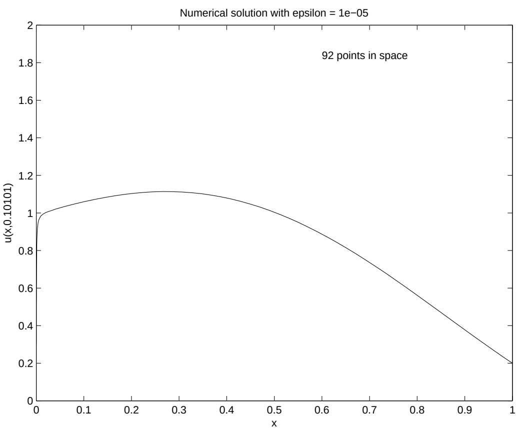
Most of the time we will be dealing with the situation of figure 2.5(b). The Struwe solution converges then to the stationary profile of figure 2.10. Suppose we weaken condition 2.27 to 2.26, Bertsch, Dal Passo and Van der Hout proved in [3] that in this case there are infinitely many solutions. The authors do this by constructing solutions which jumps back from the stationary profile of the Struwe solution (figure 2.10) to the case of figure 2.5(a). Backjumping can be forced once the solution is below $\theta = \pi$ and has a finite angle with the line $\theta = \pi$. In this way infinitely many solutions are obtained. Later it turned out that the same result has been obtained independently by Topping (see [4]). An important tool the authors use is the comparison principle, we will formulate the principle for the more general case where g is still unspecified.

Theorem 2.7. *(The comparison principle) Let* $Q_T := (0, 1) \times (0, T]$ *and* $\Sigma_T := \partial Q_T \setminus \{(r, T) : r \in [0, 1]\}$. *Let* θ *and* ψ *be functions with the following properties:*

1. $\theta, \psi \in C(\bar{Q}_T) \bigcap W^{1,2}_{\text{loc}}(Q_T)$;

2. $\theta(0, 0) = \psi(0, 0) = 0$;

3. ψ *and* θ *have finite energy in the sense of 2.2 for* $t \in [0, T]$;



Numerical solution with epsilon = 1e−05
92 points in space
u(x,0.10101)
x
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
1.8
2
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1

4. $\int\int_{Q_T} r\theta_t\xi \le -\int\int_{Q_T} r\left(\xi_r\theta_r + \frac{g(\theta)}{r^2}\xi\right)$ *and*
$\int\int_{Q_T} r\psi_t\xi \ge -\int\int_{Q_T} r\left(\xi_r\psi_r + \frac{g(\psi)}{r^2}\xi\right)$
for all $0 \le \xi \in H_0^1(Q_T)$ *with compact support in* Q_T.

If $\theta \le \psi$ *on* Σ_T, *then* $\theta \le \psi$ *in* $\bar{Q}_T$.

Proof. The proof is similar to the proof in the appendix of [3], where only the case $g(\theta) = \frac{1}{2}\sin 2\theta$ is done. □

The space $W^{1,2}_{\text{loc}}(\Omega)$ is defined as follows: let $\Omega \subset \mathbb{R}^n$ and $f : \Omega \to \mathbb{C}$, then $f \in W^{1,2}_{\text{loc}}(\Omega)$ iff $f\phi \in H^1(\mathbb{R}^n)$ for all $\phi \in C_c^\infty(\Omega)$. Note that requirement 4 is just a weak formulation of equation 2.1 (with inequality instead of equality signs).

In [3] the authors prove a more general version of this principle. Condition 2 is dropped and finitely many discontinuities in $(0, t_i)$ are allowed under reasonable conditions.

2.5.2 Smoothness of solutions

Let's make a remark about the smoothness of the solution. The techniques in the proof come from [2].

Theorem 2.8. *Let* $\theta(r,t)$ *be a solution of problem 2.3 then:*

$$E(t) := \int_0^1 \left[\theta_r^2 + \frac{\sin^2\theta}{r^2}\right]\frac{r}{2}dr < \infty \implies \theta(r,t) \in C([0,1]) \quad \text{for all } t > 0$$

Proof. Let $\theta(r,t)$ satisfy the requirements of the theorem. If $\theta(r,t)$ is a solution of problem 2.3 then $\theta(r,t) < k\pi$ for some $k \in \mathbb{Z}$. Since $E(t) < \infty$ we have: $\theta_r \in L^2([0,1])$ and there exists a $k \in \mathbb{Z}$ such that $\frac{\theta - k\pi}{r} \in L^2([0,1])$.

Consider $\theta|_{(r,1]}$ (where $0 < r < 1$), then we have both $\theta|_{(r,1]}, \theta_r|_{(r,1]} \in L^2((r,1])$, so $\theta|_{(r,1]} \in H^1((r,1])$. Now we use the fact that: $H^1(I) \subset C(\bar{I})$ (I is an interval in $\mathbb{R}$). So we get $\theta|_{(r,1]} \in C([r,1])$ for every $r \in (0,1)$. This implies $\theta \in C((0,1])$. So also $\theta^2 \in C((0,1])$. Actually it can be made even stronger! From [20] section 4.9 we obtain that θ and then also θ^2 are absolutely continuous on compact subintervals of $(0,1]$.

It is well know that absolute continuity is equivalent to having a derivative in L^1, so we conclude

$$\frac{1}{2}\left(\theta^2\right)' = \theta\theta' \in L^1(0,1).$$

We claim that this implies $\lim_{r\to 0}\theta^2(r)$ exists and is finite. Write

$$|\theta(r)^2| = \left|\theta(0)^2 + 2\int_0^r \theta\theta' ds\right| \le \theta(0)^2 + 2\int_0^r |\theta\theta'| ds < \infty,$$

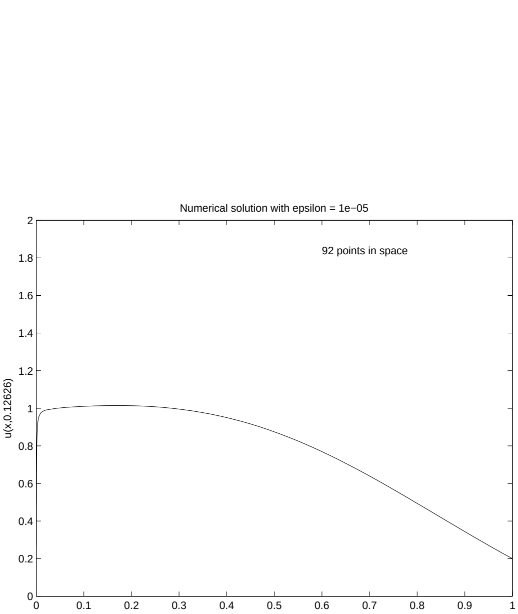
the right hand side is an increasing function of r (so it decreases as $r \downarrow 0$) and bounded from below by 0. This proves the claim.

We already proved $\theta \in C((0,1])$ so we conclude $\lim_{r\to 0}\theta(r)$ also exists and equals $\theta(0)$:

$$\theta(0) = \sqrt{\theta(0)^2} = \sqrt{\lim_{r\to 0}\theta^2(r)}. \tag{2.28}$$

□

Note that we did not really prove continuity of $\theta(r,t)$, but that the equivalence class of θ (in the subspace of L^2 where $E(t)$ is finite) contains a continuous function. Equation 2.28 can seen as a definition of $\theta(0)$ which makes θ continuous. Freire formulates the following theorem in [6]:



Numerical solution with epsilon = 1e−05
92 points in space
u(x,0.12626)
x
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
1.8
2
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1

Theorem 2.9. *For any initial value* $u_0 \in H^1([0,1];\mathbb{R})$ *there exists a number* $T_0 = T_0(u_0) > 0$ *and a unique solution*

$$u \in \bigcap_{T'<T_0} H^1([0,1]\times[0,T'];\mathbb{R}) \cap L^\infty([0,T'];H^1([0,1],\mathbb{R})) \cap L^2([0,T'];H^2([0,1],\mathbb{R}))$$

of problem 2.3 which satisfies criterium 2.27 and $u(.,0) = u_0$*. Moreover,*

1. *u is smooth in* $[0,1]\times(0,T_0]$ *with the exception of finitely many points* (x_i, T_0), $1 \le i \le K$;
2. *the solution can be continued as a weak solution in* $[0,1]\times[0,\infty)$.

Since the energy in bounded from above, the singularities must necessarily occur in the origin.

2.6 Blow-up

2.6.1 Nonuniqueness of solutions for problem 2.3 with criterium 2.26

The material in this section is also discussed in [3]. Consider problem 2.3 with criterium 2.26 and initial data $\theta_0(r)$ that satisfy

$$\begin{array}{l} \theta_0 \in C^\infty([0,1]), \\ \theta_0^{(2m)}(0) = 0, \\ \theta_0\left(\frac{1}{2}\right) \in (\pi, 2\pi), \\ \theta_0(1) \in (0,\pi). \end{array}$$

A solution that satisfies criterium 2.27 is certainly a solution that satisfies criterium 2.26. As long as the solution is classical the solution will satisfy criterium 2.27. The following proposition is proved in [3].

Proposition 2.10. *There exists a function* θ_0 *satisfying requirements 2.29 such that problem 2.3 with criterium 2.27 has a smooth solution* $\tilde{\theta}$ *in* $[0,1]\times[0,\infty)$ *with the exception of the point* $(0,t_1)$*, for some* $t_1 > 0$. θ_0 *is the initial data. Furthermore the solution* $\tilde{\theta}$ *satisfies the properties:*

$$\begin{array}{l} \lim_{r\to 0}\tilde{\theta}(r,t_1) = \pi, \\ \tilde{\theta}(0,t) = \left\{ \begin{array}{lll} 0 & if & 0 \le t < t_1 \\ \pi & if & t > t_1, \end{array} \right. \\ \frac{\partial^{2m}\tilde{\theta}}{\partial r^{2m}} = 0, \\ \textit{the map } t \mapsto E\left(\tilde{\theta}(.,t)\right) \textit{ is decreasing in } [0,\infty). \end{array} \tag{2.29}$$

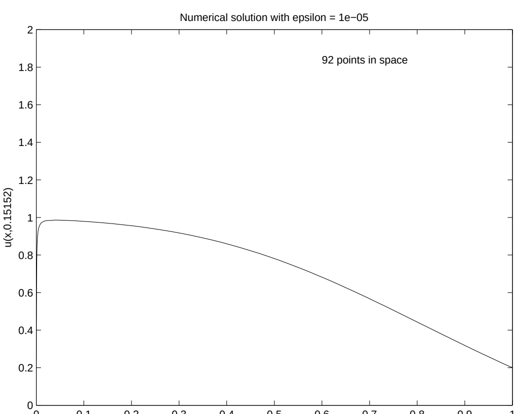
This is exactly what the Struwe solution does. The next step is to force the solution to jump back from $\theta(0,.) = \pi$ to $\theta(0,.) = 0$. But this is certainly going to violate criterium 2.27, since the energy stored in the origin will then be released. For this reason criterium 2.27 is weakened to 2.26 at the instance of the jump. The next main result is;

Proposition 2.11. *Let* θ_0, $\tilde{\theta}$ *and* t_1 *as in proposition 2.10. Then there exists an* $\epsilon > 0$ *and a* $t_2 > t_1$ *such that*

$$\tilde{\theta}(r,t) \le \pi - \epsilon r,$$

for $0 \le r \le 1$ *and* $t \ge t_2$*. Moreover there exist a* $t_3 \ge t_2$ *and a smooth (with the exception of the points* $(0,t_1)$ *and* $(0,t_3)$ *solution* $\bar{\theta}$ *of problem 2.3 such that:*

$$\begin{array}{l} \bar{\theta} = \tilde{\theta} \textit{ in } [0,1]\times[0,t_3], \\ \bar{\theta}(0,t) = 0 \textit{ for } t > t_3, \\ \textit{the map } t \mapsto E(\bar{\theta}(.,t)) \textit{ is decreasing in } (t_3,\infty) \end{array} \tag{2.30}$$


Numerical solution with epsilon = 1e−05
92 points in space
u(x,0.15152)
x
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
1.8
2
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1

Proposition 2.11 in combination with the proof in [3] tells us that we can force the jumping back once $\theta(r,t)$ makes a finite angle with the line $\theta = \pi$.

The basic ingredient for proving proposition 2.10 is

Lemma 2.12. *Let $\delta, \lambda_0, \mu \in \mathbb{R}^+$ and let $\epsilon \in (0,1)$. Let $\lambda(t)$ be the solution of*

$$\lambda' = -\delta\lambda^\epsilon, \quad t > 0 \quad, \lambda(0) = \lambda_0.$$

If $T_\lambda \coloneqq \sup\{t > 0 : \lambda(t) > 0\}$, then the function

$$\Phi(r,t) \coloneqq 2\arctan(\lambda(t)r) + 2\arctan\left(\mu r^{1+\epsilon}\right),$$

with $(r,t) \in [0,1] \times [0,T_\lambda]$, satisfies the following properties:

1. $\Phi \in C^\infty([0,1] \times [0,T_\lambda] \backslash \{(0,T_\lambda)\})$*;*
2. $$\lim_{r\to 0} \Phi(r,t) = \begin{cases} 0 & \text{for } t \in [0,T_\lambda) \\ \pi & \text{for } t = T_\lambda; \end{cases}$$
3. *there exists $\bar{\mu} > 0$ such that for every $\mu > \bar{\mu}$ it is possible t find $\bar{\delta} > 0$, depending only on ϵ and μ, such that for all $\delta \leq \bar{\delta}$*

$$\Phi_{rr} + \frac{1}{r}\Phi_r - \frac{\sin 2\Phi}{2r^2} - \Phi_t \geq 0 \text{ in } (0,1) \times (0,T_\lambda).$$

Proof. The proof can be found in [10]. □

What lemma 2.12 basically tells us is that $\Phi(r,t)$ is a subsolution if that forces θ to jump from 0 to π. Of course we have to make sure that we choose all the parameters in the right way. That is the hard part of the proof. The proof of proposition 2.11 uses a similar function to force θ to develop a finite angle with the line $\theta = \pi$.

2.6.2 A minimal solution

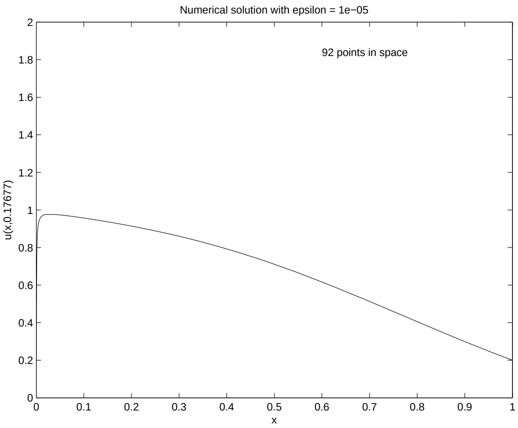
Consider problem 2.3 and recall criteria 2.26 and 2.27. Criterium 2.27 guarantees uniqueness, we converge to a stationary solution (which if we start with the profile form figure 2.5(b) looks like figure 2.10). If we weaken criterium 2.27 to criterium 2.26 then in [3] (this paper was described in section 2.6.1) it is shown that solution is not unique. In [1] the authors construct a minimal solution. In fact the minimal solution is constructed for the more general case of problem 2.1. This section is a preparation for the numerical results in the next chapter where the minimal solution is constructed numerically.

Definition 2.13. *A solution $\theta \geq 0$ to problem 2.1 or 2.3 is called minimal iff each solution $\hat{\theta} \geq 0$ satisfies $\hat{\theta} \geq \theta \geq 0$.*

By definition the minimal solution is unique, but does it exist? The answer is yes and the proof of it is in [1]. Although the proof there is very clear we also include it here since the proof also tells us how to construct the minimal solution.

Theorem 2.14. *Problem 2.1 (and therefore also problem 2.3) admits a minimal solution. For $T > 0$ small enough, it is continuous in $[0,1] \times [0,T]$ and it vanishes at $r = 0$ for $0 \leq t \leq T$.*

Before we can prove this theorem we first need to formulate another problem and prove a lemma.


Numerical solution with epsilon = 1e−05
92 points in space
u(x,0.17677)
x
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
0.2
0.4
0.6
0.8
1.2
1.4
1.6
1.8
2

Problem 2.15. *For $0 < \epsilon < 1$, $\sigma_0 \in C^\infty([\epsilon, 1])$ with $\sigma_0(\epsilon) = 0$, $\sigma_0(1) = \Theta$ and $0 \le \sigma_0 \le A$ we consider the problem:*

$$P_\epsilon \begin{cases} \sigma_t &= \sigma_{rr} + \frac{\sigma_r}{r} - \frac{g(\sigma)}{r^2} \quad \text{in} \quad (\epsilon, 1) \times (0, \infty) \\ \sigma(1,t) &= \Theta \quad \text{in} \quad (0, \infty) \\ \sigma(\epsilon, t) &= 0 \quad \text{in} \quad (0, \infty) \\ \sigma(r, 0) &= \sigma_0(r) \quad \text{in} \quad (\epsilon, 1). \end{cases} \tag{2.31}$$

Lemma 2.16. *Problem 2.15 has a unique solution in $C^\infty((\epsilon, 1] \times [0, \infty))$.*

Proof. We use [22] section 7.3.2 theorem 7.3.3 (iii) to deduce that the problem has a smooth solution for some time $T > 0$. From [22] section 7.3.2 theorem 7.3.4 to deduce that $T = \infty$. The main ingredient of the argument is that the right hand side of equation 2.31 consists of smooth and bounded functions. □

We are now ready to start the proof of theorem 2.14.

Proof of theorem 2.14. The idea is to construct a sequence of problems P_{ϵ_i} of the form of problem 2.15 such that the solution in the limit $\epsilon_i \to 0$ converges in some sense to the solution of problem 2.1. Choose a sequence $\epsilon_i \to 0$ and a corresponding sequence of initial data σ^*_{0i} such that:

1. $\sigma^*_{0i} = \begin{cases} 0 & 0 \le r \le \epsilon_i \\ \ge 0 \ \& \ \le \theta_0(r) & \epsilon_i < r < 1 \\ \Theta & r = 1; \end{cases}$
2. $\sigma^*_{0i} \le \sigma^*_{0j}$ for $i \le j$;
3. $\sigma^*_{0i} \to \theta_0$ uniformly in $[0, 1]$;
4. $\sigma_{0i} := \sigma^*_{0i}|_{[\epsilon_i, 1]} \in C^\infty([\epsilon_i, 1])$.

Let σ_i denote the solution of problem P_{ϵ_i}. From the comparison principle (theorem 2.7) we get $0 \le \sigma_i \le \sigma_j \le A$ for $i \le j$, $0 \le t < \infty$. This implies that the pointwise limit $\hat{\theta} = \lim_{i\to\infty} \sigma_i$ exists. What we now want to prove is that $\hat{\theta}$ solves problem 2.1. If so combining requirement 1 and the comparison principle implies that $\hat{\theta}$ will be the minimal solution. Now several theorems on parabolic equations are applied (the proper references can be found in [1]) and we derive: $\hat{\theta}$ is a continuous classical solution of problem 2.1 in regions bounded away from $r = 0$. We still have to prove that $\hat{\theta}$ is continuous up to $r = 0$ and that it vanishes at $r = 0$ (for small t). To prove this we construct a local barrier function and apply the squeeze theorem. As noted earlier most the constructions made for this equation rely on property that if $\psi_0(r)$ satisfies

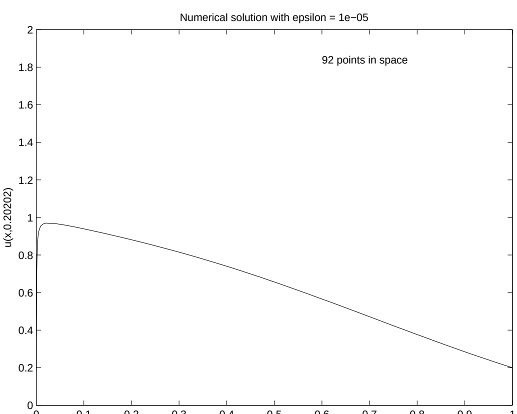
$$\psi_{rr} + \frac{\psi_r}{r} - \frac{g(\psi)}{r^2} = 0, \tag{2.32}$$

then $\psi_0(r/\lambda)$ also satisfies this equation. Let's exploit that fact here. Let ψ_0 be a the unique solution of 2.32 with boundary data $\psi_0(0) = 0$ and $\psi_0(1) = A^*$. We want $\psi_0(r/\lambda)$ to be the local barrier function in the region $[0, \lambda] \times [0, T]$. Choose $\lambda > 0$ and $T > 0$ so small that $\hat{\theta}(\lambda, t) \le A^*$ for $0 \le t \le T$ and $0 \le \theta_0(r) \le \psi_0(r/\lambda)$ for $0 < r < \lambda$. From the comparison principle and the squeeze theorem we obtain:

$$0 \le \lim_{r\to 0} \hat{\theta}(r, t) \le \lim_{r\to 0} \psi_0(r/\lambda) = 0 \quad \text{for} \quad 0 \le t \le T.$$

By comparison we also conclude $\hat{\theta} \ge \sigma_i$, so $\hat{\theta}$ is indeed minimal. □

In the previous section we discussed [3] where the authors describe a construction with which you make a whole bunch of solutions. What does blow-up then mean for a problem with more than one solution? Well fortunately we constructed a minimal solution. With the help of this we can define the blow-up time for problem 2.1:


Numerical solution with epsilon = 1e−05
92 points in space
u(x,0.20202)
x
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
1.8
2

Definition 2.17. *Let θ be the minimal solution of problem 2.1 and define*

$$\bar{T} := \sup\left\{T > 0 : \theta \in C([0,1] \times [0,T))\right\}.$$

If $\bar{T} < \infty$ or if $\bar{T} = \infty$ and $\{\theta(.,t)\}$ does not converge uniformly as $t \to \infty$, then $\bar{T}$ is called the blow-up time of problem 2.1.

The part about the uniform convergence is to capture infinite time blow-up. The following theorem shows that blow-up in the sense of definition 2.17 coincides with blow-up in the derivative at $r = 0$.

Theorem 2.18. *Let θ be the unique solution of problem 2.3 with criterium 2.27 and let $\bar{T} < \infty$. Then the solution blows up at time $\bar{T}$ iff*

$$\left|\limsup_{r \to 0, t \uparrow \bar{T}} \frac{\partial \theta(0,t)}{\partial r}\right| = \infty.$$

Proof. Note that theorem 2.9 guarantees that the solution is unique and smooth (at least for some time before $\bar{T}$). Suppose at time $\bar{T}$ we have $\left|\lim_{t \uparrow \bar{T}} \frac{\partial \theta(0,t)}{\partial r}\right| = \infty$, then $\theta(r,t)$ is not differentiable in $(r = 0, t = T)$. So $\theta(r,t) \notin C([0,1] \times [0,T])$, but $\theta(r,t) \in C([0,1] \times [0,T))$. Conclusion:

$$\bar{T} = \sup\left\{T > 0 : \theta \in C([0,1] \times [0,T))\right\}.$$

For the contrary suppose we have blow-up in the sense of definition 2.17. From the main theorem in [11] we deduce there exists a sequence $\theta(r_n, t_n)$ where $r_n \to 0$ and $t_n \uparrow \bar{T}$ such that $\theta(r_n, t_n) \to \pi$. For this sequence we have

$$\frac{\theta(r_n, t_n) - \theta(0, t_n)}{r_n} = \frac{\theta(r_n, t_n) - 0}{r_n} \to \infty \quad \text{as } n \to \infty.$$

This proves the assertion. □

Consider the more general problem 2.1. And look back to what we required for g. Recall that we defined

$$G(\theta) := \int_0^{\theta} g(s) ds.$$

There are three important cases to consider: $G(A) > 0$, $G(A) = 0$ and $G(A) < 0$.

2.6.3 Case I: $G(A) > 0$

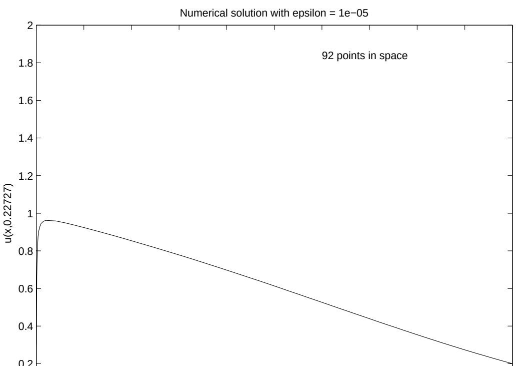
Let's first look at the case $G(A) > 0$. We will prove that we cannot have blow-up in this case. Recall that we defined in 2.2

$$E(t) := \int_0^1 \left[\frac{\theta_r^2}{2} + \frac{G(\theta)}{r^2}\right] r dr.$$

Note that what we require for g (look at figure 2.1) that we have $G(\theta) > 0$ for $\theta \in (0, A]$. From 2.3 we also have the relation

$$\frac{d}{dt} E(t) = \int_0^1 -r\theta_t^2 dr \leq 0.$$

Conclusion: the energy $E(t)$ is bounded by $E(0)$. Can we have blow-up at $r = 0$? From definition 2.17 it is clear that the (minimal) solution should then make some kind of jump (in either finite or infinite time). Well what would want to jump to? Whenever $\theta(0,t)$ becomes non-zero, the $\frac{G(\theta)}{r^2}$ term will explode. The condition $E(t) \leq E(0)$ can than no longer be satisfied, which leads to a contradiction.



Numerical solution with epsilon = 1e−05
92 points in space
u(x,0.22727)
x
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
1.8
2
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1

In this case we can prove there exists a global smooth solution for all time. If we do the phase plane analysis for this equation we can see that for every $\Theta > 0$ there exists a stationary solution $\bar{\theta}$ that satisfies $\bar{\theta}(0) = 0$ and $\bar{\theta}(1) = \theta$. If we start with a smooth initial profile we can always bound the solution by a stationary solution. By comparison this implies the solution remains bounded as long as it exists.

But what is the maximal existence time? We again want to use [22] section 7.3.2 theorem 7.3.3 (iii) and theorem 7.3.4 to deduce there exists a global smooth solution. The main ingredient of the argument is that the right hand side of our differential equation must consists of smooth and bounded functions. This however is not (yet) the case. Define

$$\psi = \frac{\theta}{r},$$

the differential equation for ψ then reads

$$\psi_t = \psi_{rr} + \frac{3}{r}\psi + \frac{r\psi - g(r\psi)}{r^3}. \tag{2.33}$$

We claim that in this equation there is no singularity any more! We claim the first part, $\psi_{rr} + \frac{3}{r}\psi$, in equation 2.33 can be interpreted as the Laplacian in $\mathbb{R}^4$. We can do this if $r = 0$ is not really a boundary of equation 2.33, that is, we have to prove that we can take $\psi_r(0, t) = 0$ as boundary condition and that $\psi(0, t)$ remains bounded. The latter follows immediately, we can always bound the initial profile θ_0 by a stationary solution, so we can also bound the derivative at $r = 0$. We proceed as follows, extend the equation and the solution to $r = -1 \dots 1$ by defining $g(-\theta) = -g(\theta)$ and $\theta(-r) = -\theta(r)$. From this we obtain $\theta''(0, t) = 0$, so $\psi_r = \frac{r\theta_r - \theta}{r^2}\ \theta_{rr}$. This implies

$$\psi_r(0, t) = 0,$$

so this is a good boundary condition. To prove that $\frac{r\psi - g(r\psi)}{r^3}$ has no singularity at $r = 0$ we impose the condition

$$g''(0) = 0.$$

Making a Taylor expansion gives near $r\psi = 0$ gives

$$\frac{r\psi - g(r\psi)}{r^3} \approx \frac{r\psi - g'(0)r\psi - \frac{1}{6}g'''(0)r^3\psi^3}{r^3} = \frac{\psi^3}{6}.$$

Conclusion there is a global smooth solution ψ and thus also a global smooth solution θ.

From the condition $0 \leq E(t) \leq E(0)$ we deduced that the energy will finally go to a limit. By repeating the arguments used in section 2.5.1 we can prove that there is a subsequence $\theta(r, t_n)$ that converges to a stationary solution as $n \to \infty$.

2.6.4 Case II: $G(A) < 0$

By similar reasoning we see no restriction for upward jumps. Remark that condition 2.4 does not imply that the solution θ will jump at $r = 0$ to another zero of G! If we do not jump to another zero of G the energy will become $-\infty$ and will then have no lower bound.

2.6.5 Case III: $G(A) = 0$

In this case we have the condition $0 \leq E(t) \leq E(0)$. From the comparison principle we deduce that the solution remains bounded.

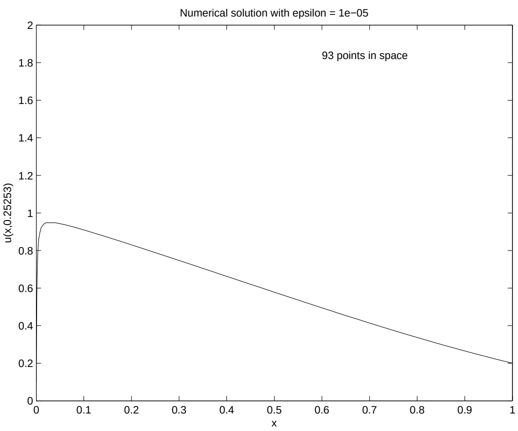
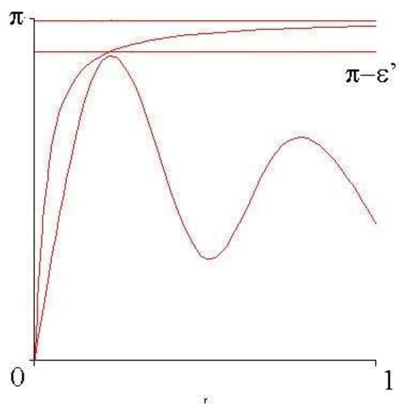

Numerical solution with epsilon = 1e−05
93 points in space
u(x,0.25253)
x
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
1.8
2
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1

Figure 2.11: After a while the solution will have finite angle with the y-axis and will still be smaller than $\pi - \epsilon'$.



2.6.6 General blow-up conditions

As an application of the comparison principle we proof the following:

Proposition 2.19. *Let $\theta(r, t)$ be the unique solution solution of problem 2.3 with criterium 2.27. Assume there exists an $\epsilon' > 0$ such that $\theta_0(r) < \pi - \epsilon'$, then there is no blow-up.*

Proof. From theorem 2.9 we conclude that the solution will immediately develop a finite angle at $r = 0$ with the θ-axis, the solution then looks like figure 2.11. Recall that the stationary solutions (with finite energy) of problem 2.3 are

$$\bar{\theta}(r) = 2 \arctan \alpha r + k\pi.$$

We can adjust this α to transform one of the stationary solutions into a solution completely above the other one (see also figure 2.11. Theorem 2.7 (the comparison principle) now implies $\theta(r, t) \leq \bar{\theta}(r)$ in $[0, T]$ for some $T > 0$. □

We could also have required that $\theta_0(r) < \pi$ together with some continuity for $\theta_0(r)$. In fact the result can even be made stronger! In [8] it is shown that: if $\theta_0 \leq \pi$ then there is no blow-up.

Now consider the more general problem 2.1 where g is still unspecified. We want to find conditions for g to guarantee blow-up. Bertsch, Van der Hout and Villucchi proved in [1] the following theorem:

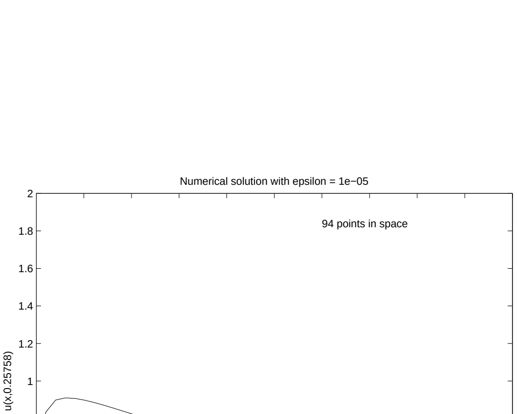
Theorem 2.20. *Consider problem 2.1, assume $G(A) < 0$, let $\bar{T}$ be the blow-up time of the problem. Then we have:*

1. *Suppose that $g'(\theta) < 4$ for all $0 \leq \theta \leq A^*$ and that $\Theta > A^*$. Then $\bar{T} < \infty$.*
2. *If $\bar{T} < \infty$, then $\lim_{r \to 0} \theta(r, t) = A$ for all $t > \bar{T}$.*

In the next section we will go deeper into the techniques used in this paper.

2.7 M. Bertsch, R. van der Hout and E. Villucchi: *Blow-Up Phenomena for a Singular Parabolic Problem*

The purpose of this section is not to rewrite the article but rather to present techniques and ideas used in this paper.



Numerical solution with epsilon = 1e−05
94 points in space
u(x,0.25758)
x

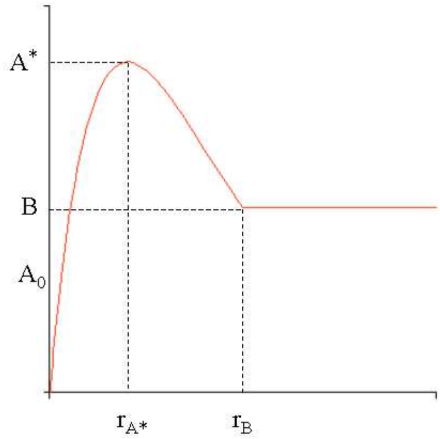


Figure 2.12: A graph of equation 2.35.

2.7.1 A subsolution that blows up in finite time

In this section we try to give insight in the proof of theorem 2.20 part 1. The techniques used are resemble in some sense the techniques presented in section 2.6.1. We try to construct a subsolution that blows up in finite time. Recall the function $\Phi(r,t)$ we used as a subsolution in lemma 2.12. If we look more carefully at this function we see that $\Phi(r,t) = \phi_1(\lambda(t)r) + \phi_2(\mu r^{1+\epsilon})$, where ϕ_1 and ϕ_2 are stationary solutions.

This time we use a slightly different subsolution. Let $\lambda(t)$ satisfy the differential equation:

$$\begin{cases} \lambda' = \beta\lambda^{2-\epsilon} \\ \lambda(0) = \lambda_0. \end{cases} \tag{2.34}$$

This equation has finite time blow-up since we can write

$$f'(t) := \frac{\lambda'}{\lambda^{2-\epsilon}} = -\left(\frac{1}{\lambda^{1-\epsilon}}\right)' \frac{1}{1-\epsilon} = \beta.$$

Solving for $f(t)$ gives

$$f(t) + C = \beta t,$$

where C is a constant dependent on λ_0. Now choose t^* such that $C = \beta t^*$, then at that time we must have $f(t^*) = 0$. That means $\lambda(t) \to \infty$ as $t \to t^*$.

Let ψ_0 be the unique solution of the stationary problem associated to problem 2.1. For $A_0 < B \leq A^*$, let $r_B \geq r_{A^*}$ be the point such that $\psi_0(r_B) = B$. Let's define

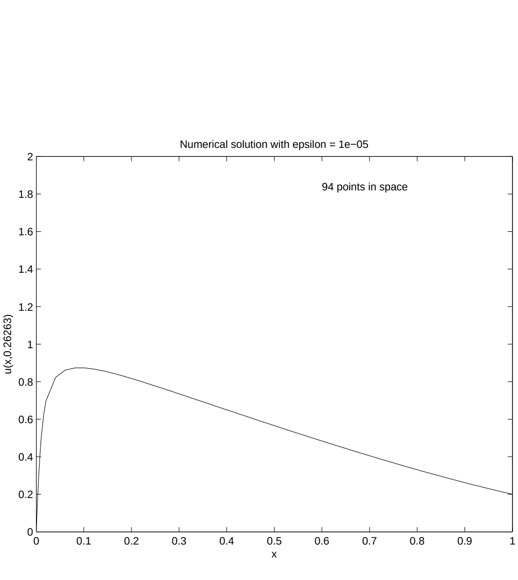
$$\psi_B^* := \begin{cases} \psi_0(r) & r \leq r_B \\ B & \text{otherwise}, \end{cases} \tag{2.35}$$

this means ψ_B^* looks like figure 2.12. Our subsolution will be

$$\phi(r,t) = \psi_B^*(\lambda(t)r) + \psi_0(\alpha r^{1+\epsilon}). \tag{2.36}$$

For $\lambda(t)r$ very big (this will happen in finite time, since $\lambda(t)$ blows up in finite time)

When λ increases, that is t goes to the blow-up time, the shape of the subsolution changes as indicated in figure 2.13. If one tries to prove $\psi(r,t)$ is indeed a subsolution, you have to distinguish between two regions: $\lambda(t)r \leq r_B$ and $\lambda(t)r > r_B$. To prove that $\phi(r,t)$ is a subsolution in the latter region is quite straightforward, it comes down to choosing α small. In the other region it is more difficult, the details are in [1].



Numerical solution with epsilon = 1e−05
94 points in space
u(x,0.26263)
x
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
1.8
2
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1

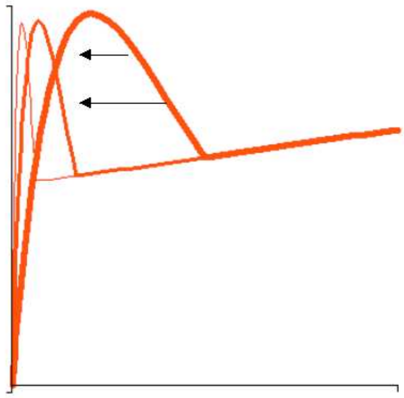


Figure 2.13: A graph of equation 2.36, when λ increases the shape of the subsolution changes as indicated.

2.7.2 The jump is to A

This section is not supposed to repeat all the details discussed in [1], but merely to highlight some key points. We proceed with the proof of theorem 2.20 part 2. We want to prove the jump in $r = 0$ is to A. We want to know what happens just after the blow-up time. Therefore we transform to the similarity variables:

$$\begin{aligned} \eta &= \tfrac{r}{\sqrt{t-T}}, \\ \tau &= \log(t-T) \quad \text{for} \quad t > T, \end{aligned} \tag{2.37}$$

where $T \geq \bar{T}$ ($\bar{T}$ is the blow-up time for problem 2.1). The differential equation for θ transforms into

$$v_\tau = v_{\eta\eta} + \left(\frac{1}{\eta} + \frac{\eta}{2}\right) v_\eta - \frac{g(v)}{\eta^2}, \tag{2.38}$$

where $\theta(r,t) = v(\eta,\tau)$. These similarity variables can be found in a natural way. Set $\eta = \frac{r}{R(t)}$, where $R(t)$ is an unknown function and try to find a solution of the form $\theta(\eta)$. Working this out gives

$$-\frac{\eta}{2}\theta_\eta \frac{2R'}{R} = \frac{1}{R^2}\left(\theta_{\eta\eta} + \frac{1}{\eta}\theta_\eta - \frac{g(\theta)}{\eta^2}\right). \tag{2.39}$$

Requiring that the differential equation only depends on η gives

$$R' = \frac{1}{2R},$$

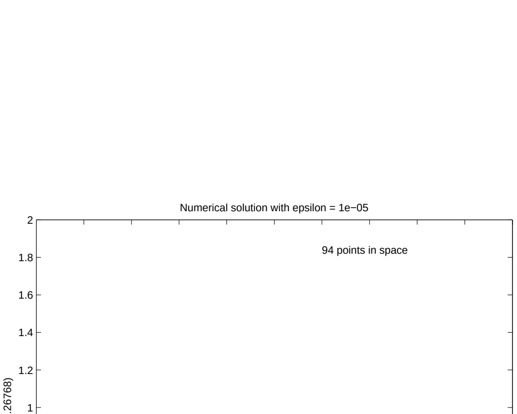
so that $R = \sqrt{t-C}$, where C is a constant. We set $C = T$. Of course, not all solutions are of the form $\theta(\eta)$. In general we need two variables to describe all the solutions. If we compare equations 2.38 and 2.39 we observe that 2.38 is just the time dependent version of the stationary equation 2.39. It can be computed that we can make a time dependent problem of 2.39 if we choose $\tau = \log(t-T)$.

Consider for $\eta_0 > 0$ and $0 < \epsilon < 1$ the stationary problem:

$$Lv := v_{\eta\eta} + \left(\frac{1}{\eta} + \frac{\eta}{2}\right) v_\eta - \frac{g(v)}{\eta^2} = 0, \tag{2.40}$$

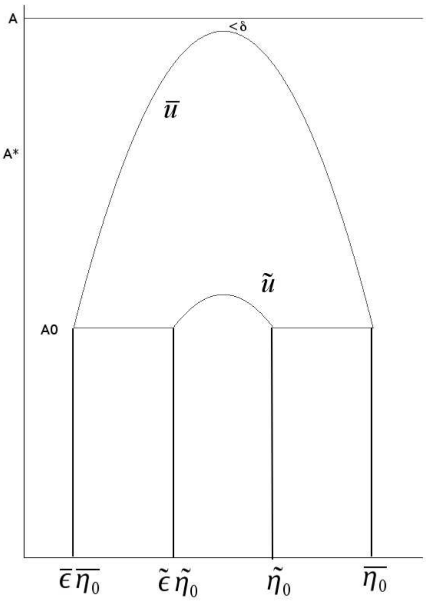
$$v(\epsilon\eta_0) = v(\eta_0) = A_0. \tag{2.41}$$

In [1] it is shown that for any $0 < \epsilon < 1$ this problem has a solution $v > A_0$ if η_0 is sufficiently small. Furthermore by making ϵ and η_0 small(er) we can guarantee that any solution v satisfies $\min\{A - v\} < \delta$.



Numerical solution with epsilon = 1e−05
94 points in space
u(x,0.26768)
x
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
1.8
2
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1

Figure 2.14: A sketch of $\tilde{v}$ and $\bar{v}$.



Another key observation is: there exists an $R > 0$ such that $\theta(r,t) \geq A^*$ for any $r \in (0, R]$, $t \geq \bar{T}$. Accepting these remarks (which are not trivial) we can start the proof.

Let $0 < \delta \ll A - A^*$ and set $T = \bar{T}$ in the similarity variables. We construct a solutions $\bar{v}$ (with $\bar{\epsilon}$ and $\bar{\eta}_0$) of 2.40 such that any solution $\bar{v}$ of 2.40 with $\bar{\epsilon}$ and $\bar{\eta}_0$ satisfies

$$\min\{A - \bar{v}\} < \delta.$$

We also construct a solution $\tilde{v}$ of 2.40 (with $\tilde{\epsilon}$ and $\tilde{\eta}_0$) such that

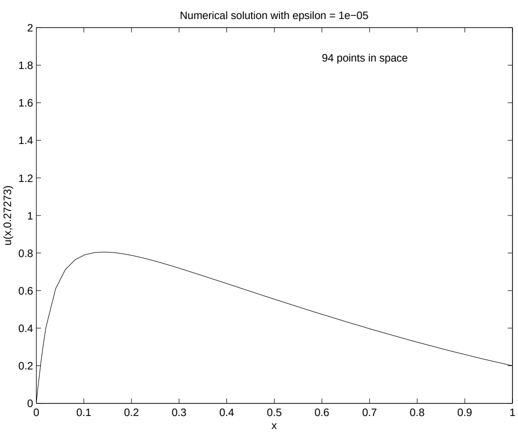
$$\max\{\tilde{v}\} < A^*.$$

From the remarks in the previous paragraph we have that we can choose $\bar{\epsilon}$, $\tilde{\epsilon}$, $\bar{\eta}_0$ and $\tilde{\eta}_0$ such that $\bar{\epsilon}\bar{\eta}_0 < \tilde{\epsilon}\tilde{\eta}_0 < \tilde{\eta}_0 < \bar{\eta}_0$. We extend $\tilde{v}$ by setting $\tilde{v}(\eta) = A_0$ for $\eta \notin (\tilde{\epsilon}\tilde{\eta}_0, \tilde{\eta}_0)$. In figure 2.14 we made a picture of $\bar{u}$ and $\tilde{u}$. Consider the initial value problem

$$\begin{array}{lll} w_\tau = Lw & \text{in} & (\bar{\epsilon}\bar{\eta}_0, \bar{\eta}_0) \times (\tau_0, \infty), \\ w(\bar{\epsilon}\bar{\eta}_0, \tau) = w(\bar{\eta}_0) = A_0 & \text{in} & (\tau_0, \infty), \\ w(\eta, \tau_0) = \tilde{u}(\eta) & \text{in} & (\bar{\epsilon}\bar{\eta}_0, \bar{\eta}_0). \end{array} \tag{2.42}$$

We claim w tends uniformly to a solution of 2.40 as $\tau \to \infty$. It can be shown that we start from a subsolution. So we know the solution will increase in time. Moreover the solution is bounded by $\bar{u}$ so we can define the pointwise limit $\lim_{\tau\to\infty} w(\eta, \tau) =: \phi(\eta)$. Now suppose the convergence is not uniform then we can find a sequence (η_i, τ_i) with $\tau_i \to \infty$ such that $\phi(\eta_i) - w(\eta_i, \tau_i) > \gamma$ for some $\gamma > 0$. By compactness we have a subsequence of the η_i (which we will also call η_i) such that $\eta_i \to \hat{\eta}$). Now choose $\hat{\tau}$ so large that $\phi(\hat{\eta}) - w(\hat{\eta}, T) < \frac{\gamma}{2}$ for $\tau > \hat{\tau}$. By continuity we can find an ϵ neighbourhood $(\hat{\eta} - \epsilon, \hat{\eta} + \epsilon)$ of $\hat{\eta}$ such that $\phi(\eta) - w(\eta, T) < \frac{3\gamma}{4}$ in this neighbourhood. For large τ_i we enter this neighbourhood, we get a contradiction. It can be shown that our limit ϕ is a stationary solution.

So for $\bar{\tau} - \tau_0$ big enough we have $\min\{A - w(., \bar{\tau})\} < \delta$. By making $\bar{\tau}$ and τ_0 both very negative while $\bar{\tau} - \tau_0$ remains constant we can make, if we transform back to the original variables, $t_0 := \bar{T} + e^{\tau_0}$ and $\bar{t} := \bar{T} + e^{\bar{\tau}}$ very close to $\bar{T}$ and also $\eta_0\sqrt{\bar{t} - \bar{T}} < R$. Remark that the latter condition makes w a


Numerical solution with epsilon = 1e−05
94 points in space
u(x,0.27273)
x
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
1.8
2
0.1
0.3
0.5
0.7
0.9

subsolution for θ in the region $[0, R)$, since in this region $w < A^*$ and $\theta > A^*$ initially. If we choose $t > \bar{T}$ sufficiently close to $\bar{T}$ we have by comparison

$$\min_{0<r<1} \{A - \theta(r, t)\} < \delta.$$

We could have done this procedure not only for $\bar{T}$, but for every $T > \bar{T}$. This implies

$$\limsup_{r\to 0} \theta(r, t) = A$$

for $t \geq \bar{T}$.

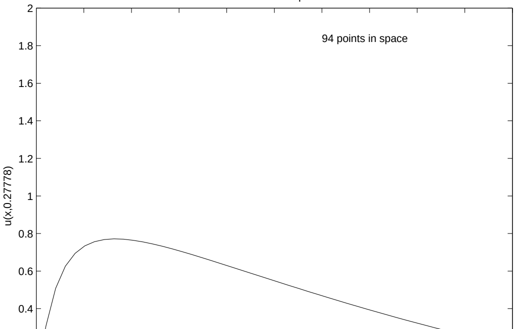
The next thing to do is proving that "lim sup" can be replaced by "lim". We already proved $\min\{A - w(., \bar{\tau})\} < \delta$, so we can choose an $\hat{\eta}$ such that $A - w(\hat{\eta}, \bar{\tau}) < \delta$. Note that we have chosen $\bar{T}$ as the basis for the similarity variables. By transforming back to the original variables we find the corresponding $\hat{r}$ to be $\hat{r} = \hat{\eta} e^{\bar{\tau}/2}$. Now fix $\hat{\eta}$, $\bar{t}$ (defined above) and $\hat{r}$. Define for $r < \hat{r}$ and $T > \bar{T}$

$$r = \hat{\eta} e^{\tilde{\tau}/2}$$

and

$$\tilde{\tau} = \log(\bar{t} - T).$$

So if we change $r < \hat{r}$, then we adjust $\tilde{\tau} < \bar{\tau}$ and T to keep $\hat{\eta}$ and $\bar{t}$ fixed. Applying the same comparison arguments as before we deduce $\theta(r, \bar{t}) > A - \delta$. Thus we have shown that $\lim_{r\to 0} \theta(r, t) = A$ for $t > \bar{T}$.


Numerical solution with epsilon = 1e−05
94 points in space
u(x,0.27778)
x
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
1.8
2
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1

Chapter 3

Numerical results

3.1 Behaviour we want to see

The goal of the numerics is the construction of the minimal solution described by problem 2.15 as $\epsilon \to 0$. We start initially with a situation which looks like figure 3.1(a). In the code we will take we solve the equation for u (instead of σ, which is the unknown function in problem 2.15), with $u(x, 0) = u_0(x)$ as initial condition. Furthermore:

1. $g(\theta) = \frac{1}{2\pi}\sin(2\pi\theta)$, so that we are in the harmonic map heat heat flow case. Note that now everything is rescaled, jumps are now to 1 instead of π.
2. $u_0(x)$ is a parabola through the points $(\epsilon, 0)$, $(\frac{1}{2}, TOP)$ and $(1, \Theta)$, where Θ is the right boundary condition of the problem and $TOP \gg 1$.
3. $\Theta < A_0 = \frac{1}{2}$ (the unique zero of $g(\theta)$, see also figure 2.1).

At $t = 0$ the solution look figure 3.1(a). After some time the solution jumps and will then look like figure 3.1(b). Note that this happens if the initial value of the top is high enough (it follows from the proof of proposition 2.10). Then the profile slowly evolves to the one of figure 3.1(c). Remark that the minimal solution will jump back once the angle with the line $u = 1$ vanishes. Finally the solution will jump back and goes to the stationary solution, figure 3.1(d). The goal of the numerics is constructing this minimal solution and see the predicted behaviour.

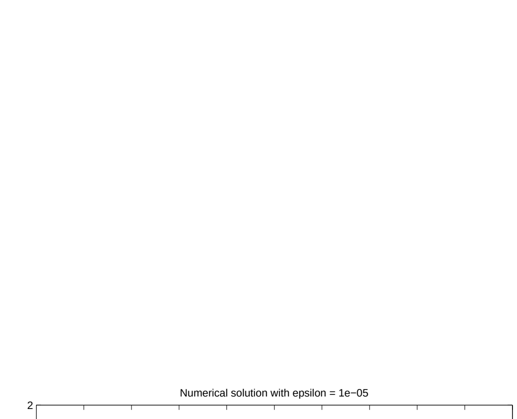
3.2 Numerical methods

There are several methods one can think of to solve parabolic one dimensional PDE's. In general there are two ideas: finite differences and finite elements. The main idea of finite differences is to approximate derivatives by discretization. The main idea of the finite element method is: write down the variational form of the problem and approximate by a finite dimensional function space. Since I liked this variational approach I used the finite element method. The method I used is also called the Galerkin method.

3.2.1 The Galerkin method

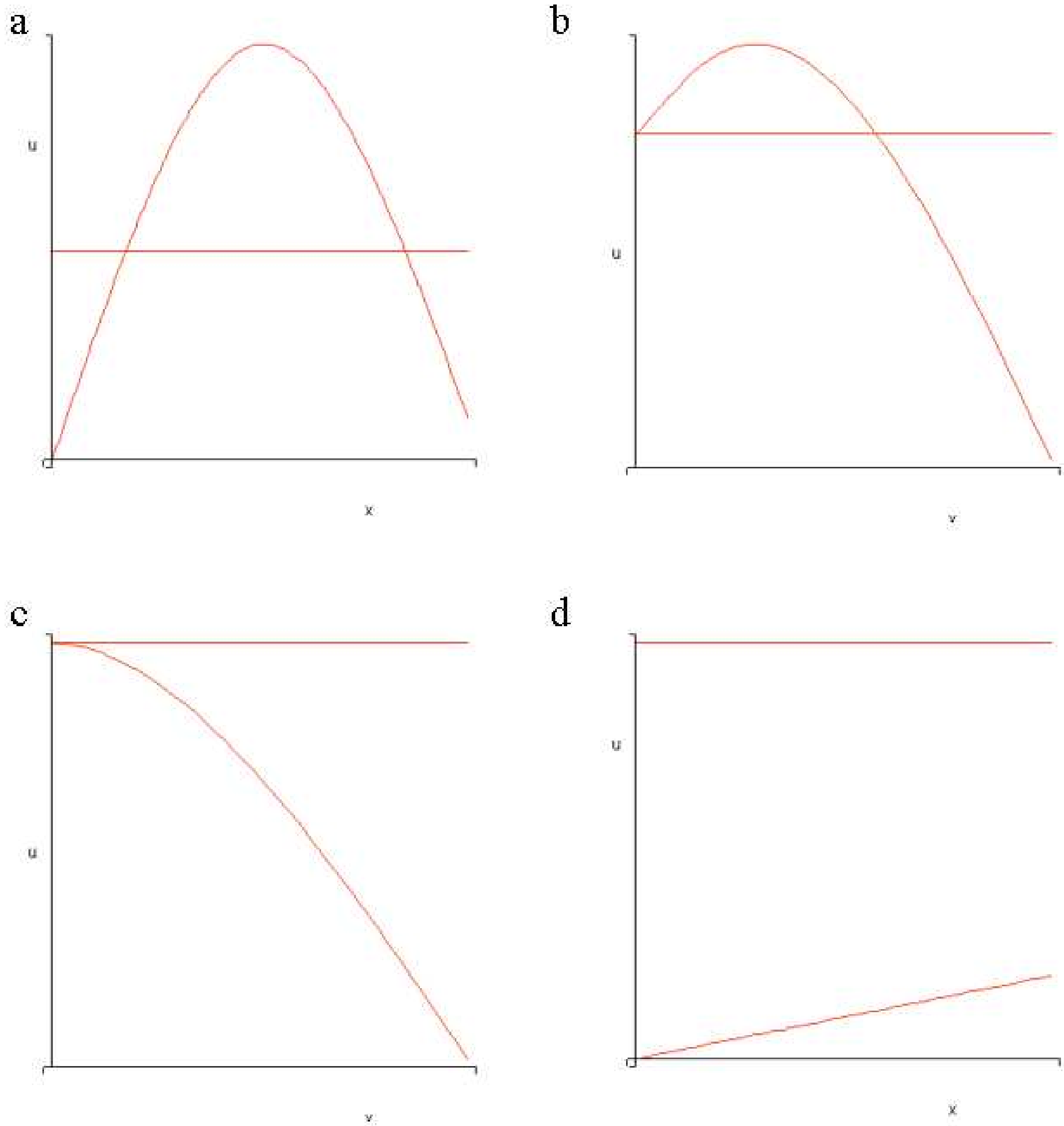
In this section we derive the Galerkin method for our problem. Suppose we start with problem 2.15. Our equation then reads

$$u_t = u_{xx} + \frac{u_x}{x} - \frac{g(u)}{x^2}.$$



Numerical solution with epsilon = 1e−05
94 points in space
u(x,0.28283)
x
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
1.8
2
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1

Figure 3.1: The behaviour of the minimal solution at four snapshots in time. First the initial condition, then the profile after the first and before the second jump, then then profile at the instance of jump back and finally the stationary solution.



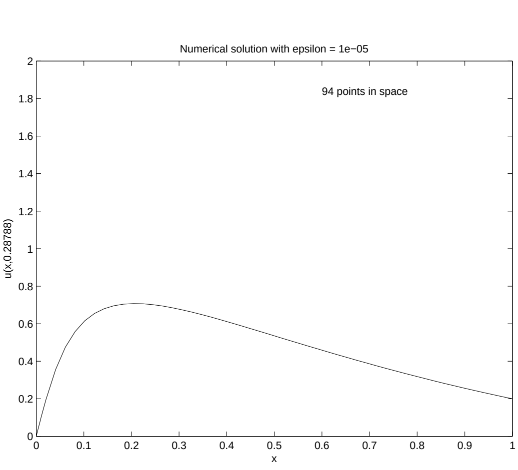
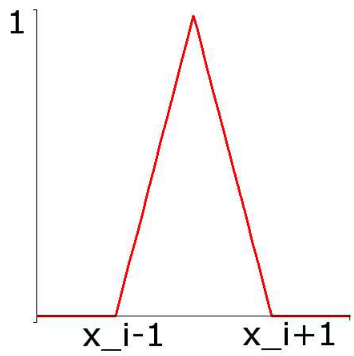

Numerical solution with epsilon = 1e−05
94 points in space
u(x,0.28788)
x
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
1.8
2

Figure 3.2: Graph of the approximating functions $\phi_i(x)$.



We multiply the equation by xv, where $v \in H_0^1(\epsilon, 1)$:

$$xvu_t = v\frac{\partial}{\partial x}(xu_x) - v\frac{g(u)}{x}. \tag{3.1}$$

We are looking for a solution $u - u_0(x) \in H_0^1(\epsilon, 1)$. We are going to approximate this space by a finite dimensional space which we will call S^N. First we make a spatial grid $x_1 = \epsilon, x_2, \ldots, x_N = 1$. And choose functions $\phi_i(x)$ defined by

$$\phi_i(x) = \begin{cases} \frac{x-x_{i-1}}{x_i-x_{i-1}} & \text{for } x_{i-1} \leq x \leq x_i \\ \frac{x-x_{i+1}}{x_i-x_{i+1}} & \text{for } x_i \leq x \leq x_{i+1} \\ 0 & \text{otherwise.} \end{cases} \tag{3.2}$$

This means $\phi_i(x)$ looks like figure 3.2. Note that we start with x_1 (and not x_0) since arrays $x(i)$ in matlab also start with $i = 1$, the notation here then resembles the notation of the numerical code in the appendix. We approximate $H_0^1(\epsilon, 1)$ by

$$S^N = \left\{ \sum_{i=2}^{N-1} c_i\phi_i(x) | c_i \in \mathbb{R} \right\}.$$

But because of the non-zero boundary condition at $r = 1$ we cannot make a good approximation of u in S^N. To resolve this we use the initial condition u_0 of u:

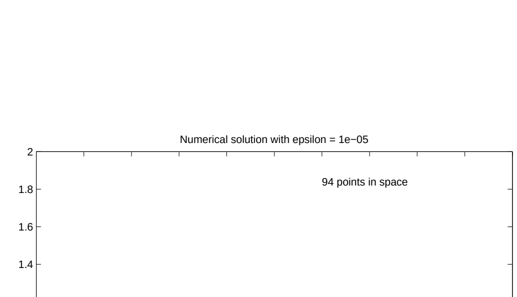
$$u(x,t) \approx U(x,t) := u_0(x) + \sum_{i=2}^{N-1} c_i(t)\phi_i(x).$$

Integration of 3.1 over $[\epsilon, 1]$ and an integration by parts gives

$$\int_\epsilon^1 xvu_t dx = \int_\epsilon^1 \left(-xv_x u_x - v\frac{g(u)}{x}\right) dx. \tag{3.3}$$

For this weak formulation to make sense we need v to be only once piecewise differentiable w.r.t. x, so plugging in the approximation $U(x,t)$ and setting $v = \phi_k(x)$ makes sense. Let $\dot{c}_i := \frac{\partial}{\partial t}c_i$ and $\phi_i' := \frac{\partial}{\partial x}\phi_i$, then we obtain

$$\int_\epsilon^1 \underbrace{x\phi_k \textstyle\sum_i \dot{c}_i\phi_i}_{\text{Part 1}} \, dx = \int_\epsilon^1 \underbrace{-x\phi_k'\left(u_0' + \textstyle\sum_i c_i\phi_i'\right)}_{\text{Part 2}} - \underbrace{\phi_k \frac{g(u_0 + \sum_i c_i\phi_i)}{x}}_{\text{Part 3}} \, dx. \tag{3.4}$$



Numerical solution with epsilon = 1e−05
94 points in space
u(x,0.29293)
x
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
1.8
2
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1

We will now work out part 1, 2 and 3 separately, starting with part 1. Take into account that $\phi_k(x)$ only has support in $[x_{k-1}, x_{k+1}]$ and use Simpson's rule (which states: $\int_a^b f(x)dx \approx \frac{b-a}{6}(f(a)+4f(\frac{a+b}{2})+f(b)))$ to do the integration. Note that Simpson's rule integrates exactly polynomials up to power 3. So also the ϕ_k's are integrated exactly by Simpson's rule if we split up the integral in two parts and apply Simpson's rule on both parts. Furthermore let $x_{k\pm 1/2} := \frac{x_k + x_{k\pm 1}}{2}$. We obtain the following derivation:

$$\begin{aligned}
\int_\epsilon^1 x\phi_k \sum_i \dot{c}_i\phi_i dx &= \int_{x_{k-1}}^{x_k} x\phi_k\left(\dot{c}_k\phi_k + \dot{c}_{k-1}\phi_{k-1}\right)dx + \int_{x_k}^{x_{k+1}} x\phi_k\left(\dot{c}_k\phi_k + \dot{c}_{k+1}\phi_{k+1}\right) \qquad (3.5)\\
&= \dot{c}_k\left(x_k\frac{x_{k+1}-x_{k-1}}{6} + x_{k-1/2}\frac{x_k - x_{k-1}}{6} + x_{k+1/2}\frac{x_{k+1}-x_k}{6}\right)\\
&\quad + \dot{c}_{k-1}\frac{x_k - x_{k-1}}{6}x_{k-1/2} + \dot{c}_{k+1}\frac{x_{k+1}-x_k}{6}x_{k+1/2}.
\end{aligned}$$

We do the same for part 2 of equation 3.4. Note that here we do make an approximation if we use Simpson's rule if $u_0(x)$ is not a polynomial. In the numerics done in this report $u_0(x)$ was always a polynomial of degree 2. We get the derivation:

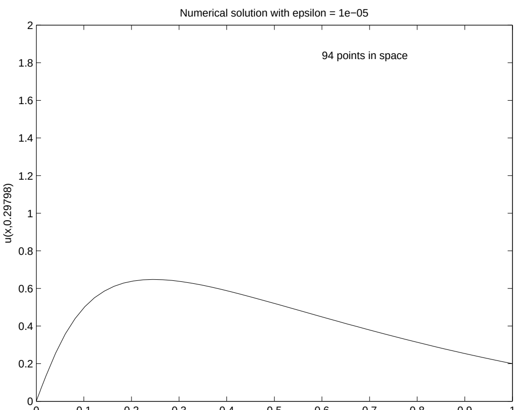
$$\int_\epsilon^1 -x\phi_k'\left(u_0' + \sum_i c_i\phi_i'\right)dx \qquad (3.6)$$

$$\begin{aligned}
&= \int_{x_{k-1}}^{x_k} -\phi_k' x\left(u_0' + \frac{c_{k-1}}{x_{k-1}-x_k} + \frac{c_k}{x_k - x_{k+1}}\right)dx + \int_{x_k}^{x_{k+1}} -\phi_k' x\left(u_0' + \frac{c_k}{x_k - x_{k+1}} + \frac{c_{k+1}}{x_{k+1}-x_k}\right)dx\\
&= \frac{1}{2}(c_{k-1}-c_k)\frac{x_k + x_{k+1}}{x_k - x_{k-1}} + \frac{1}{2}(c_{k+1}-c_k)\frac{x_k + x_{k+1}}{x_{k+1}-x_k}\\
&\quad + \frac{1}{6}\Big[x_{k+1}\left(u_0'(x_{k+1}) + 2u_0'(x_{k+1/2})\right) + x_k\left(2u_0'(x_{k+1/2}) - 2u_0'(x_{k-1/2})\right)\\
&\quad + x_{k-1}\left(-u_0'(x_{k+1}) - 2u_0'(x_{k-1/2})\right)\Big].
\end{aligned}$$

We do the same thing with part 3 and also use the Simpson rule to approximate the integrals:

$$\int_\epsilon^1 \phi_k\frac{g(u_0 + \sum_i c_i\phi_i)}{x}dx \qquad (3.7)$$

$$\begin{aligned}
&\approx \frac{x_{k+1}-x_{k-1}}{6}\frac{g\left(u_0\left(x_k\right) + c_k\right)}{x_k} + 4\frac{x_k - x_{k-1}}{6}\frac{g\left(u_0\left(x_{k-1/2} + \frac{c_k}{2} + \frac{c_{k-1}}{2}\right)\right)}{x_k + x_{k-1}}\\
&\quad + 4\frac{x_{k+1}-x_k}{6}\frac{g\left(u_0\left(x_{k+1/2} + \frac{c_k}{2} + \frac{c_{k+1}}{2}\right)\right)}{x_k + x_{k+1}}.
\end{aligned}$$


Numerical solution with epsilon = 1e−05
94 points in space
u(x,0.29798)
x
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
1.8
2
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1

If we combine 3.5, 3.6 and 3.7 and plug it all into 3.4 we get

$$
\begin{aligned}
&\dot{c}_k\left(x_k\frac{x_{k+1}-x_{k-1}}{6}+x_{k-1/2}\frac{x_k-x_{k-1}}{6}+x_{k+1/2}\frac{x_{k+1}-x_k}{6}\right) \\
&+\dot{c}_{k-1}\frac{x_k-x_{k-1}}{6}x_{k-1/2}+\dot{c}_{k+1}\frac{x_{k+1}-x_k}{6}x_{k+1/2} \\
=\;& \frac{1}{2}(c_{k-1}-c_k)\frac{x_k+x_{k+1}}{x_k-x_{k-1}}+\frac{1}{2}(c_{k+1}-c_k)\frac{x_k+x_{k+1}}{x_{k+1}-x_k} \\
&+\frac{1}{6}\left[x_{k+1}\left(u_0'(x_{k+1})+2u_0'(x_{k+1/2})\right)+x_k\left(2u_0'(x_{k+1/2})-2u_0'(x_{k-1/2})\right)\right. \\
&\left.+x_{k-1}\left(-u_0'(x_{k+1})-2u_0'(x_{k-1/2})\right)\right] \\
&+\frac{x_{k+1}-x_{k-1}}{6}\frac{g\left(u_0\left(x_k\right)+c_k\right)}{x_k}+4\frac{x_k-x_{k-1}}{6}\frac{g\left(u_0\left(x_{k-1/2}+\frac{c_k}{2}+\frac{c_{k-1}}{2}\right)\right)}{x_k+x_{k-1}} \\
&+4\frac{x_{k+1}-x_k}{6}\frac{g\left(u_0\left(x_{k+1/2}+\frac{c_k}{2}+\frac{c_{k+1}}{2}\right)\right)}{x_k+x_{k+1}}.
\end{aligned}
\tag{3.8}
$$

Since we only made a discretization in space we call this method the continuous Galerkin method. At each time step we have to solve system of $N-2$ (where N is the number of grid points in space) nonlinear ordinary differential equations. We use a stiff solver to solve the system. Obviously this introduces a discretization in time as well. We let the ode-solver decide how to to this discretization.

[16], [17] and [18] are good references for this method. [16] are course notes and pretty easy to understand. [17] and [18] are articles from the seventies.

3.2.2 Error Estimates

In [17] and [18] one can find a priori error estimates for the continuous Galerkin method. The error estimates the authors prove are of the form

$$||U-u||_{\dots} \le Ch^{\cdots}\left(||u||_{\dots}+\dots\right).$$

So we know the error goes to zero in the limit $h \to 0$. Note that these estimates assume we solve system 3.8 explicitly. This however is not the case, we use a numerical procedure to solve 3.8.

To estimate the error we use the method suggested in [19]. We estimate the error by using an additional approximation by higher order polynomials. Write

$$u(x,t) \approx U(x,t)+E(x,t)=u_0(x)+\sum_{i=2}^{N-1}c_i(t)\phi_i(x)+\sum_{i=2}^{N}e_i(t)\psi_i(x), \tag{3.9}$$

where $E(x,t)$ is our error estimate and

$$\psi_i(x)=\begin{cases}\frac{4(x-x_i)(x_{i+1}-x)}{(x_{i+1}-x_i)^2} & \text{for } x_i \le x \le x_{i+1} \\ 0 & \text{otherwise.}\end{cases} \tag{3.10}$$

This means that ψ_i looks like figure 3.3. What we have to do is find equations for the $e_i(t)$. We do this by substituting 3.9 and $v=\psi_i$ in equation 3.3. Integrating everything we know exactly and approximating the rest using Simpson's rule gives:

$$
\begin{aligned}
&\frac{4}{15}\left(x_i^2-x_{i-1}^2\right)\dot{e}_i+\frac{1}{15}\left(2x_{i-1}+3x_i\right)\left(x_i-x_{i-1}\right)\dot{c}_i+\frac{1}{15}\left(3x_{i-1}+2x_i\right)\left(x_i-x_{i-1}\right)\dot{c}_{i-1} \\
=\;& -\frac{x_i-x_{i-1}}{6}\left(x_i\psi'(x_i)u_0'(x_i)+x_{i-1}\psi'(x_{i-1})u_0'(x_{i-1})\right)+\frac{2}{3}x_ic_i-\frac{2}{3}x_{i-1}c_{i-1}-\frac{8(x_i+x_{i+1})}{3(x_i-x_{i-1})}e_i \\
&-\frac{x_i-x_{i-1}}{6}4\frac{g(u0(x_{i-1/2})+c_i/2+c_{i-1})/2+e_i)}{x_{i-1/2}}
\end{aligned}
\tag{3.11}
$$

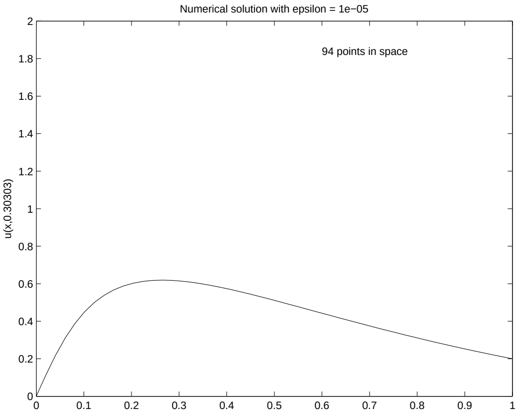
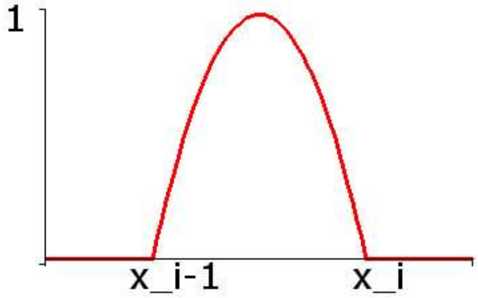

Numerical solution with epsilon = 1e−05
94 points in space
u(x,0.30303)
x
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
1.8
2
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1

Figure 3.3: Graph of the functions $\psi_i(x)$, used to estimate the error.



If we combine equation 3.8 and 3.11 we get a system of differential equations. Initially we take $c_k(0) = e_k(0) = 0$. We solve the full system in matlab at once.

3.2.3 Mesh Refinement

To reduce the error at places where it gets too big we propose the following:

1. Take points $t_1, t_2, \ldots t_M$ in time.
2. Use an ode-solver to compute the solution on time t_{i+1} when the solution is known at t_i.
3. If the estimated local error in the H^1-norm is too big at time t_{i+1}, that means

$$||e_j(t_{i+1})\psi_j||_{H^1} > TOL,$$

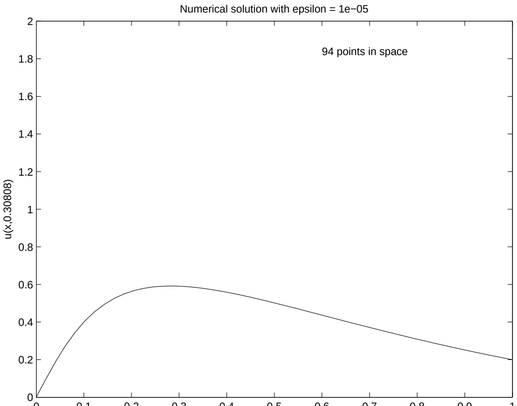
place extra mesh points in space and go back to time t_i.

This is what is called mesh refinement: one refines the mesh on which the solution is computed at places where the error is big. If one thinks the solution (or one of the derivatives) develops a singularity at a fixed point in space then mesh refinement might be best option. Note by increasing the total number of mesh points we increase the computational effort. There are also moving mesh methods. If one thinks the solution will look like a moving front, a moving mesh method suits best to the problem. The mesh then moves along with the problematic part of the solution.

We remark the following. Suppose we add an extra mesh point between x_{i-1} and x_i, then the error is reduced locally by a factor 1/4. This becomes clear from looking at figure 3.4.

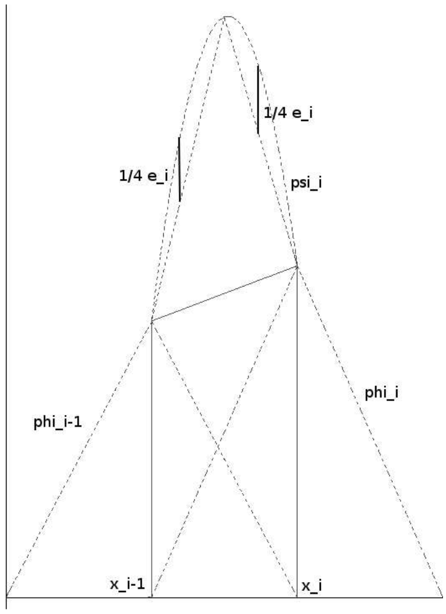
Can we improve on the refinement method? It is obvious that one needs a lot of points when a jump occurs (the solution as function of the space variable is very steep and the derivative changes fast). But after that all these extra points might not be needed any more. So one can improve by not only adding extra points when needed, but also removing superfluous points. For the simulations I did, it will not make any difference. I looked at a case where after all the jumps (that is when expect we can remove points) we go pretty fast to a stationary solution and then the computation stops. So not much is to be gained there. However of course if I would initially start with a too dense mesh (compared to the error I allow) this would unnecessarily increase the computational effort, while a method which also removes mesh points will correct for this.

In [19] the authors implement a similar method. The error is estimated in the same way. Only the way in which extra mesh points are added is different. The authors also show results for their method applied to several problems.



Numerical solution with epsilon = 1e−05
94 points in space
u(x,0.30808)
x
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
1.8
2
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1

Figure 3.4: If an extra mesh point is place between x_{i-1} and x_i the error is reduced locally by a factor $\frac{1}{4}$.



3.2.4 The matlab code

In the appendix a matlab code is included which implements equation 3.8, equation 3.11 and the mesh refinement discussed in the previous section. In the code there are many comments, so it should be readable. The code consists of a main function and some subfunctions which define things like g, $u(x, 0)$, ψ_i, ϕ_i etc. After initializing everything the main loop starts. The ode solver used on line 63 computes the solution of the ode with an absolute tolerance of 10^{-8}. After that we check whether the error is too big locally, if that is the case we place an extra mesh point if we have not reached the maximum number of mesh points and $x_i - x_{i-1} > eps$ (eps is the smallest number in matlab).

3.2.5 Discretization in time

Apart from the continuous Galerkin method there is also the discontinuous Galerkin method where also time is discretized. I did not implement a discretization in time myself, but left that to the ode solver. This paragraph will outline the basic idea's of the method.

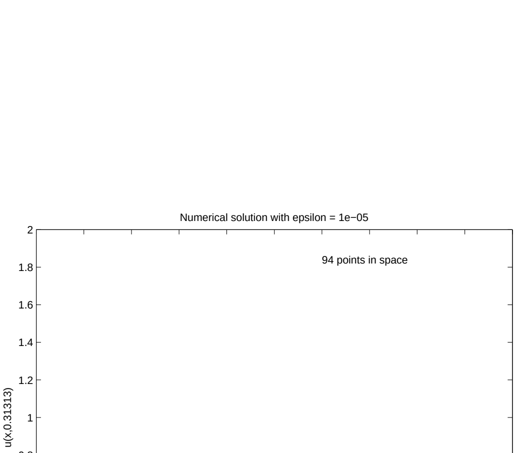
We go back to our weak formulation:

$$\int_{\epsilon}^{1} xvu_t dx = \int_{\epsilon}^{1} -xv_x u_x - v\frac{g(u)}{x} dx.$$

First a discretization in space is performed, we plug in our approximation $U(x, t)$:

$$\int_{\epsilon}^{1} xvU_t dx = \int_{\epsilon}^{1} -xvU - v\frac{g(U)}{x} dx.$$

Now we also discretize in time. Let $t_1 = 0 < t_2 \cdots < t_M = T$, $U_j = U(., t_j)$ and $U_{j,\xi} = \xi U_{j+1} + (1 - \xi)U_j$ for $0 \leq \xi \leq 1$. The ξ is a fixed parameter, for different choices we get different methods. We approximate



Numerical solution with epsilon = 1e−05
94 points in space
u(x,0.31313)
x
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
1.8
2
0.1
0.3
0.5
0.7
0.9

$U_t(x,t_j) \approx \frac{U_{j+1}-U_j}{t_{j+1}-t_j}$. For $j = 1, \ldots, M-1$ we get

$$\int_{\epsilon}^{1} xv\frac{U_{j+1}-U_j}{t_{j+1}-t_j}dx = \int_{\epsilon}^{1} -xvU_{j,\xi} - v\frac{g(U_{j,\xi})}{x}dx.$$

By choosing $v = \phi_k$ again we find a systems of equations for $c_i(t_j)$. If the $c_i(t_{j-1})$ $(i = 2, \ldots, N-1)$ is known we have to solve a system of equations to find the $c_i(t_j)$ $(i = 2, \ldots, N-1)$. If $\xi = \frac{1}{2}$ the method is called the Crank-Nicolson discontinuous Galerkin approximation. If $\xi = 1$ the method is called the backward difference discontinuous Galerkin approximation.

Whether doing the discretization in time yourself is better than leaving it to the ode solver is depends on the problem. If you do the discretization in time yourself you have more control over size of the time steps. You can also decide more precise when you want to add or remove mesh points. An advantage of leaving it to the ode solver is that it makes the method easier to implement (if you already have an implementation for the ode solver).

3.3 Numerical Results

In this section we present the numerical results obtained from the matlab code in the appendix. Recall that the goal of the numerics was the construction of the minimal solution and observing the behaviour that can also be seen in figure 3.1.

3.3.1 Results from the Galerkin method with refinement

The question how small we can make ϵ is related to what error we allow ourselves. Let's first agree on that. We will refine the mesh locally if

$$\|e_i(t)\psi_i\|_{H^1} < 0.01\frac{\text{NSpace}(0)}{\text{NSpace}(t)},$$

where NSpace(t) is the number of mesh points in space we have at time t. However, we will not refine further if $x_i - x_{i-1} > 1000$eps. What follows is a sequence of figures for various times. We took $\epsilon = 10^{-5}$. If ϵ was made smaller the computational effort became the biggest problem The error in the pictures is acceptable.

Note that eventually the solution tends to the stationary solution, as one also sees in the results.

3.3.2 FlexPDE

I also did some simulations with the software package flexpde 5.08. The program implements a finite element method, with error estimation, mesh refinement in space and adaptive time stepping. The pictures looked similar too the pictures I computed.

A great advantage of the program is that you can learn how the program works in a few hours and implement very complicated problems (up to dimension 3) that can take several weeks/months to solve if you need to write your own code. Also the computational time flexpde needed was much and much less than the computation for my matlab code (say several minutes compared to one hour).

However, this software is something like a black box. It is not very clear how the program does the job, what methods are used etc. For example at some point I noticed that it did not make any difference if I made ϵ smaller than approximately 10^{-16}. I took me quite some time to find in the help file that the program worked with a precision of 10^{-16}.

Conclusion: the program can do pretty amazing things, but it is not clear to me whether you can thrust the results.

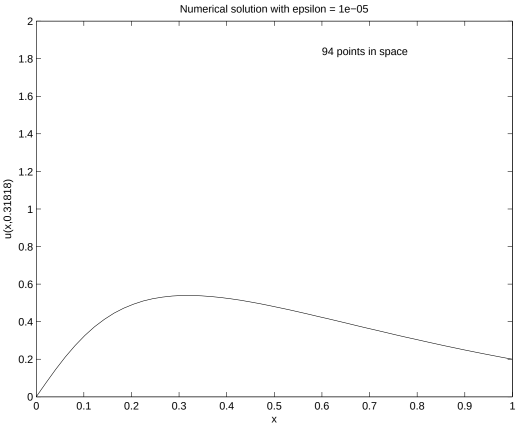
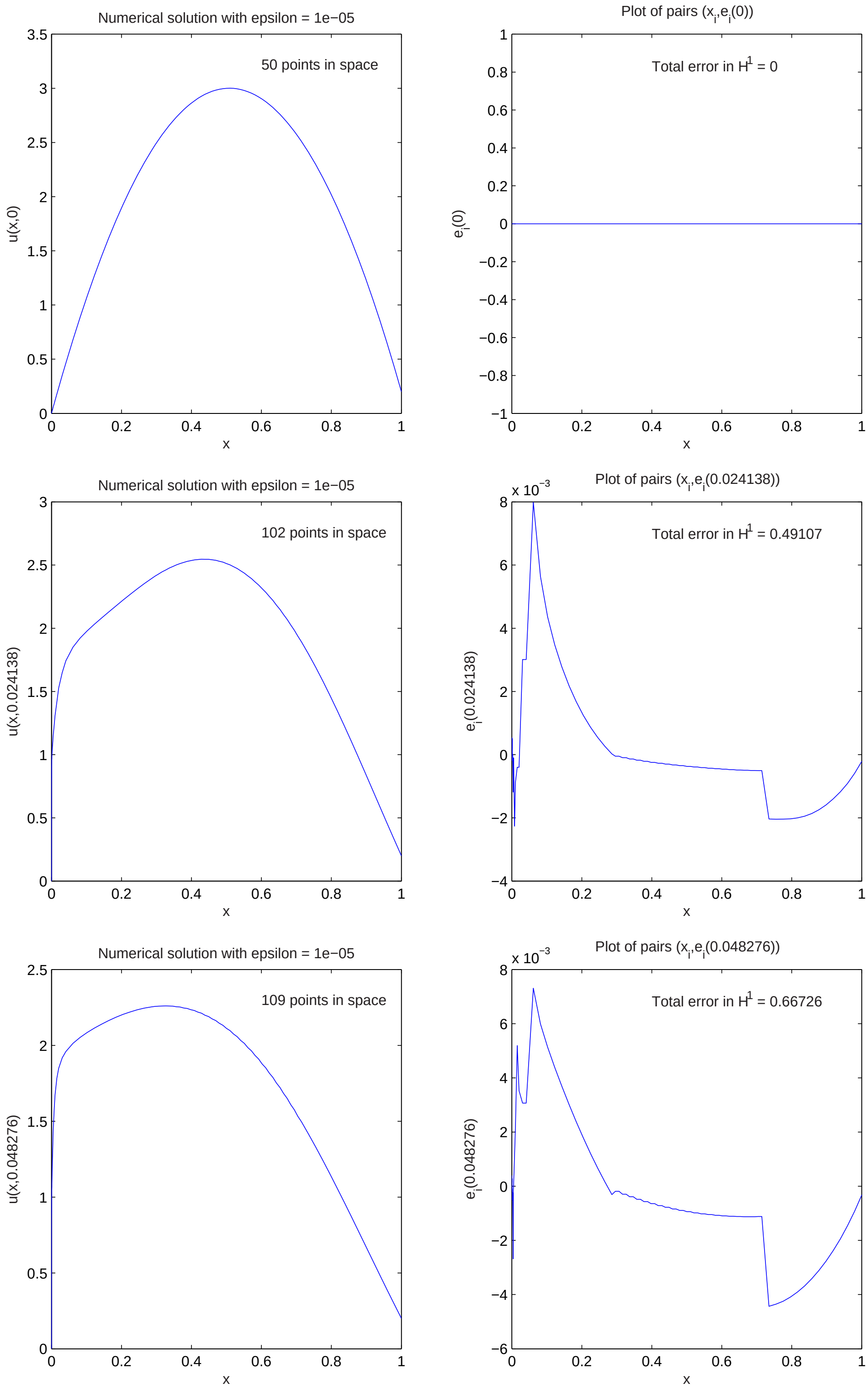

Numerical solution with epsilon = 1e−05
94 points in space
u(x,0.31818)
x
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
1.8
2
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1

Figure 3.5:


Numerical solution with epsilon = 1e−05
50 points in space
u(x,0)
x
Plot of pairs (x_i,e_i(0))
Total error in H^1 = 0
e_i(0)
x
Numerical solution with epsilon = 1e−05
102 points in space
u(x,0.024138)
x
Plot of pairs (x_i,e_i(0.024138))
x 10^−3
Total error in H^1 = 0.49107
e_i(0.024138)
x
Numerical solution with epsilon = 1e−05
109 points in space
u(x,0.048276)
x
Plot of pairs (x_i,e_i(0.048276))
x 10^−3
Total error in H^1 = 0.66726
e_i(0.048276)
x

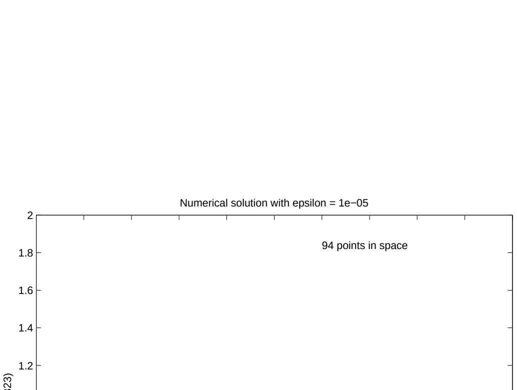
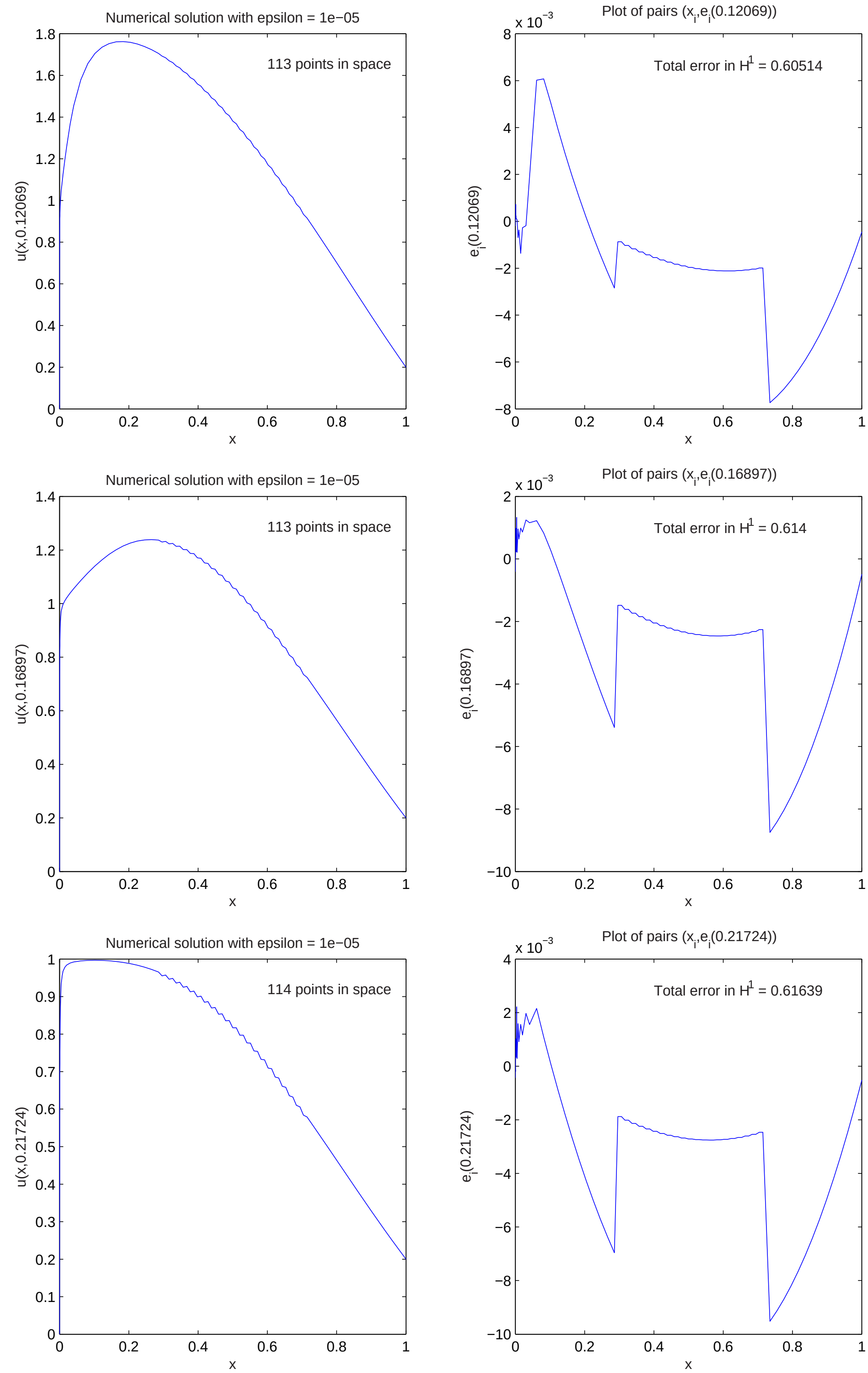

Numerical solution with epsilon = 1e−05
94 points in space
u(x,0.32323)
x
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
1.8
2
0.1
0.3
0.5
0.7
0.9

Figure 3.6:



Numerical solution with epsilon = 1e−05
113 points in space
u(x,0.12069)
x
Plot of pairs $(x_i,e_i(0.12069))$
Total error in H^1 = 0.60514
$e_i(0.12069)$
x 10^{-3}
Numerical solution with epsilon = 1e−05
113 points in space
u(x,0.16897)
Plot of pairs $(x_i,e_i(0.16897))$
Total error in H^1 = 0.614
$e_i(0.16897)$
Numerical solution with epsilon = 1e−05
114 points in space
u(x,0.21724)
Plot of pairs $(x_i,e_i(0.21724))$
Total error in H^1 = 0.61639
$e_i(0.21724)$

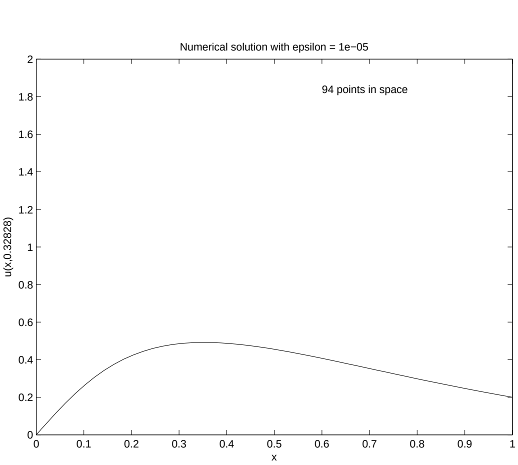
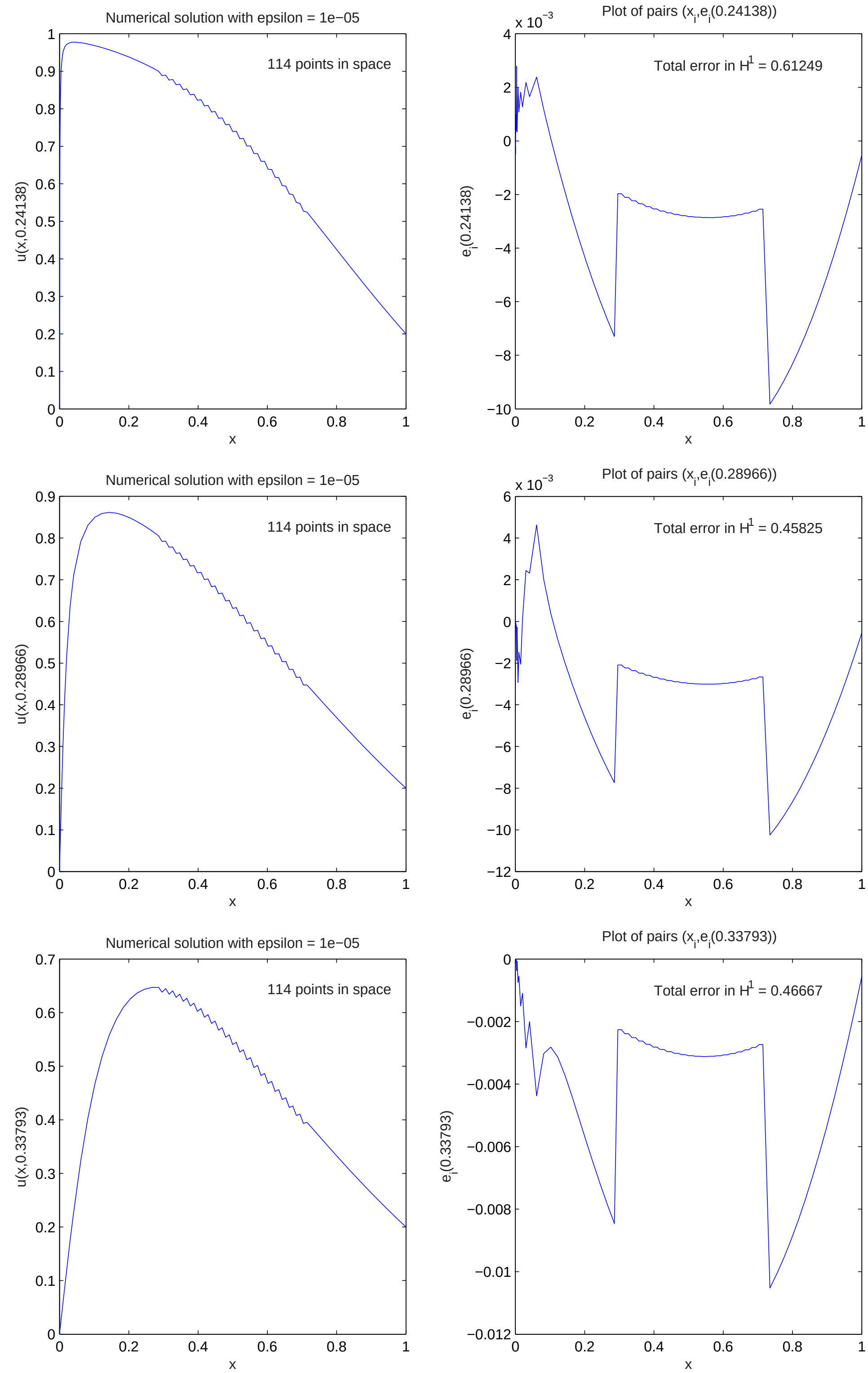
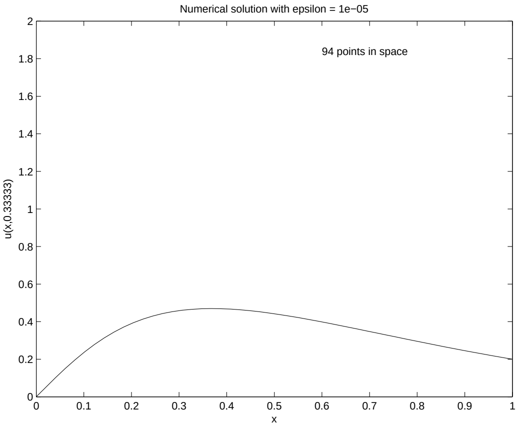

Numerical solution with epsilon = 1e−05
94 points in space
u(x,0.32828)
x
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
1.8
2
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1

Figure 3.7:

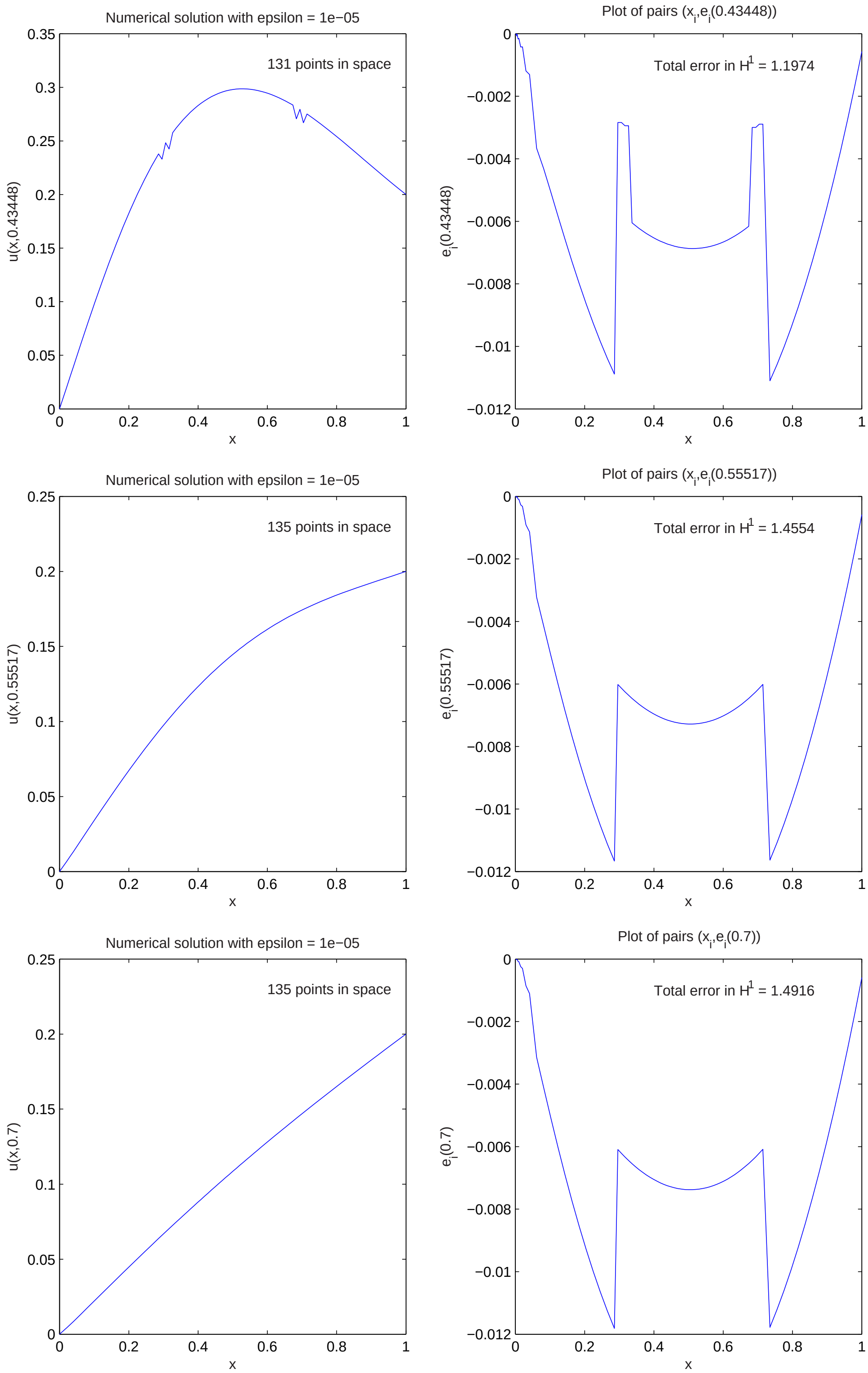


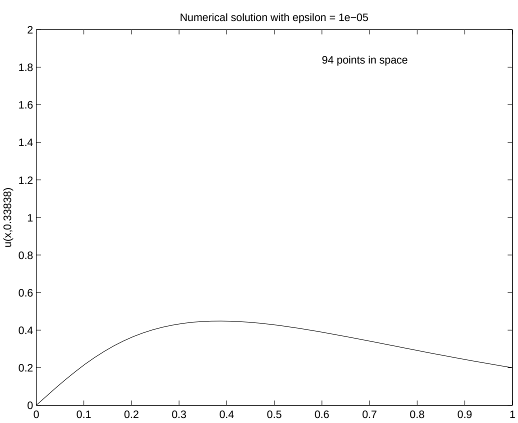
Numerical solution with epsilon = 1e−05
114 points in space
u(x,0.24138)
x
Plot of pairs (x_i,e_i(0.24138))
x 10^-3
Total error in H^1 = 0.61249
e_i(0.24138)
x
Numerical solution with epsilon = 1e−05
114 points in space
u(x,0.28966)
x
Plot of pairs (x_i,e_i(0.28966))
x 10^-3
Total error in H^1 = 0.45825
e_i(0.28966)
x
Numerical solution with epsilon = 1e−05
114 points in space
u(x,0.33793)
x
Plot of pairs (x_i,e_i(0.33793))
Total error in H^1 = 0.46667
e_i(0.33793)
x



Numerical solution with epsilon = 1e−05
94 points in space
u(x,0.33333)
x

Figure 3.8:


Numerical solution with epsilon = 1e−05
131 points in space
u(x,0.43448)
x
Plot of pairs (x_i,e_i(0.43448))
Total error in H^1 = 1.1974
e_i(0.43448)
x
Numerical solution with epsilon = 1e−05
135 points in space
u(x,0.55517)
x
Plot of pairs (x_i,e_i(0.55517))
Total error in H^1 = 1.4554
e_i(0.55517)
x
Numerical solution with epsilon = 1e−05
135 points in space
u(x,0.7)
x
Plot of pairs (x_i,e_i(0.7))
Total error in H^1 = 1.4916
e_i(0.7)
x


Numerical solution with epsilon = 1e−05
94 points in space
u(x,0.33838)
x
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
1.8
2
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1

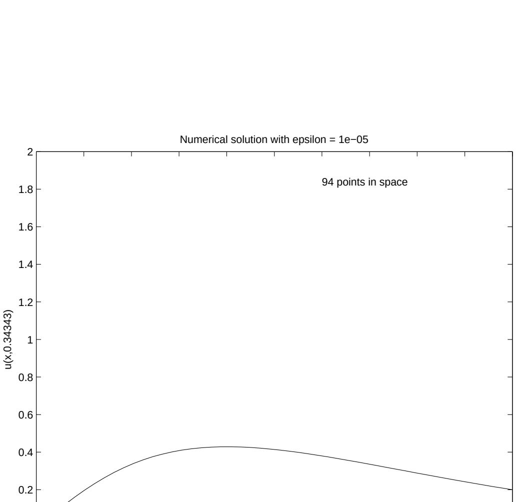
3.3.3 Conclusions

What can we conclude form these results? The smallest ϵ for which we are able to control the error is 0.00001. Of course one can always do better if one allows more mesh points, but then the computational time needed becomes a problem. The computations I did already took several hours. In the numerical results it is not hard to recognize the behaviour of figure 3.1.

3.3.4 Suggestions for further research

I will make some suggestions for directions in which the numerical results can be improved. First of all we solve a nonlinear system of ordinary differential equations at each time step. For a nonlinear equation we cannot expect to get rid of dealing with the nonlinearity, but we should make deal with it in an efficient way. The current situation is that we let the ode solver compute a step forward in time (the solver makes addition smaller steps) and after that we check the error. But if halve way the error too big already we still let the ode solver finish the time step. Part of the work is done for nothing. By doing the discretization in time yourself one might get control over the time stepping and one can make the algorithm more efficient. A second improvement can be the error estimate. If one can find a sharper estimate for the error we might need less mesh points to go to smaller ϵ. One also might improve the refinement method by for instance also removing mesh points. In [19] there are more suggestions for this.

If we are convinced that the results approximate the minimal solution well enough, this might be done by for instance comparing the results for different ϵ, we can try to estimate the blow-up time. An estimate for this time can be interesting for physical situations where the model is applicable.



Numerical solution with epsilon = 1e−05
94 points in space
u(x,0.34343)
x
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
1.8
2
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1

Appendix A

Coordinate systems

A.1 Cylindrical coordinates

In cylindrical coordinates a point $(x, y, z) \in \mathbb{R}^3$ is represented as

$$\begin{bmatrix} r\cos\phi \\ r\sin\phi \\ z \end{bmatrix} = r\hat{r}(r,\phi,z) + z\hat{z}.$$

In these coordinates the direction of unit vectors $\hat{r}$, $\hat{\phi}$ and $\hat{z}$ depends on the coordinates, so we write $\hat{r}(r,\phi,z)$, $\hat{\phi}(r,\phi,z)$ and $\hat{z}(r,\phi,z)$. From [12] we get the following formulas:

$$\begin{aligned} \partial_1\hat{r} &:= \tfrac{\partial\hat{r}}{\partial r} = 0, & \partial_1\hat{\phi} &:= \tfrac{\partial\hat{\phi}}{\partial r} = 0, & \partial_1\hat{z} &:= \tfrac{\partial\hat{z}}{\partial r} = 0, \\ \partial_2\hat{r} &:= \tfrac{\partial\hat{r}}{\partial\phi} = \hat{\phi}, & \partial_2\hat{\phi} &:= \tfrac{\partial\hat{\phi}}{\partial\phi} = -\hat{r}, & \partial_2\hat{z} &:= \tfrac{\partial\hat{z}}{\partial\phi} = 0, \\ \partial_3\hat{r} &:= \tfrac{\partial\hat{r}}{\partial z} = 0, & \partial_3\hat{\phi} &:= \tfrac{\partial\hat{\phi}}{\partial z} = 0, & \partial_3\hat{z} &:= \tfrac{\partial\hat{z}}{\partial z} = 0. \end{aligned} \tag{A.1}$$

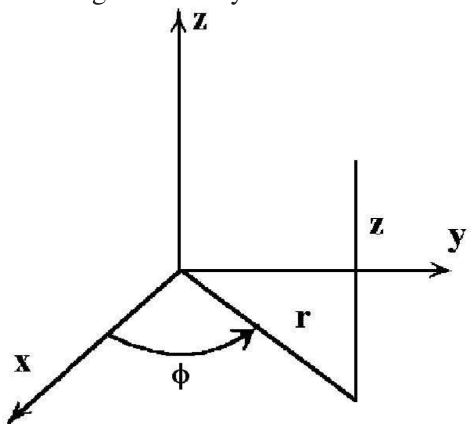
The gradient in cylindrical coordinates is given by

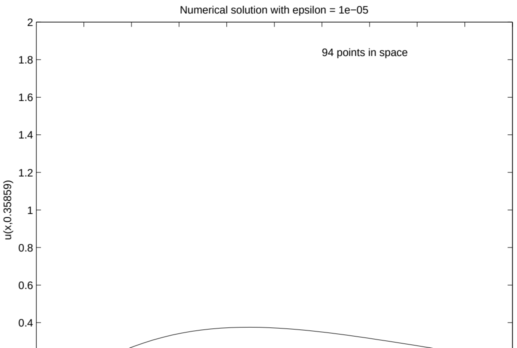
$$\nabla_C = \hat{r}\frac{\partial}{\partial r} + \hat{\phi}\frac{1}{r}\frac{\partial}{\partial\phi} + \hat{z}\frac{\partial}{\partial z}. \tag{A.2}$$

The Laplacian is given by

$$\Delta_C = \frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial\phi^2} + \frac{\partial^2}{\partial z^2}. \tag{A.3}$$

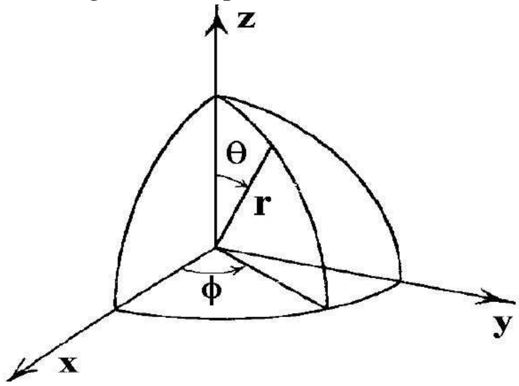
Figure A.1: Cylinder Coordinates.





Numerical solution with epsilon = 1e−05
94 points in space
u(x,0.35859)
x
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
1.8
2
0.1
0.3
0.5
0.7
0.9

Figure A.2: Spherical Coordinates.



A.2 Spherical coordinates

In spherical coordinates a point $(x, y, z) \in \mathbb{R}^3$ is represented as

$$\begin{bmatrix} r\cos\phi\sin\theta \\ r\sin\phi\sin\theta \\ \cos\theta \end{bmatrix} = r\hat{r}(r, \phi, \theta).$$

In these coordinates the direction of unit vectors $\hat{r}$, $\hat{\phi}$ and $\hat{\theta}$ depends on the coordinates, so we write $\hat{r}(r, \phi, \theta)$, $\hat{\phi}(r, \phi, \theta)$ and $\hat{\theta}(r, \phi, \theta)$. From [13] we get the following formulas:

$$\begin{aligned} &\partial_1\hat{r} := \tfrac{\partial\hat{r}}{\partial r} = 0, && \partial_1\hat{\phi} := \tfrac{\partial\hat{\phi}}{\partial r} = 0, && \partial_1\hat{\theta} := \tfrac{\partial\hat{\theta}}{\partial r} = 0, \\ &\partial_2\hat{r} := \tfrac{\partial\hat{r}}{\partial\phi} = \sin\theta\hat{\phi}, && \partial_2\hat{\phi} := \tfrac{\partial\hat{\phi}}{\partial\phi} = -cos\theta\hat{\theta} - \sin\theta\hat{r}, && \partial_2\hat{\theta} := \tfrac{\partial\hat{\theta}}{\partial\phi} = \cos\theta\hat{\phi}, \\ &\partial_3\hat{r} := \tfrac{\partial\hat{r}}{\partial\theta} = \hat{\theta}, && \partial_3\hat{\phi} := \tfrac{\partial\hat{\phi}}{\partial\theta} = 0, && \partial_3\hat{z} := \tfrac{\partial\hat{z}}{\partial\theta} = -\hat{r}. \end{aligned} \tag{A.4}$$

The gradient in spherical coordinates is given by:

$$\nabla_S = \hat{r}\frac{\partial}{\partial r} + \hat{\phi}\frac{1}{r\sin\theta}\frac{\partial}{\partial\phi} + \hat{\theta}\frac{1}{r}\frac{\partial}{\partial\theta}. \tag{A.5}$$

The Laplacian is given by

$$\Delta_S = \frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2} + \frac{\cos\theta}{r^2\sin\theta}\frac{\partial}{\partial\theta} + \frac{1}{r^2}\frac{\partial^2}{\partial\theta^2}. \tag{A.6}$$

Appendix B

The Matlab code

```
function [sol,xmesh,tmesh, err,epsilon,Nspace]= ...
            singpar5(NspaceInitial,MaxNspace,Ntime,FinalTime,ErrorTol, ...
                             LeftBoundary,RightBoundary,Epsilon,HeightTop)

%Parameters corresponding to the boundary values
global left; %the value at x =epsilon
left = LeftBoundary;
global right; %the value at x=1
right = RightBoundary;
global InitTop; %the value of the top of the initial value
InitTop = HeightTop;
global epsilon; %x = epsilon....1, we let epsilon->0
epsilon = Epsilon;

%Parameters corresponding to the accuracy
NumberMeshPointsSpace=NspaceInitial;
NumberMeshPointsTime =Ntime;
EndTime=FinalTime;
%x1=linspace(epsilon,epsilon+0.1,NumberMeshPointsSpace/2);
%x2=linspace(epsilon+0.1,1,NumberMeshPointsSpace/2+1);
global x;
%x=[x1 x2(2:end)];
x=linspace(epsilon,1,NumberMeshPointsSpace);
%we let time range form 0 to EndTime and take ... mesh points in between
global t; t = linspace(0,EndTime,NumberMeshPointsTime);
%to store the coefficients in Sum c_i(t) phi_i(x)
global C; C=zeros(NumberMeshPointsSpace,NumberMeshPointsTime);
%to store the coefficents in Sum e_i(t) psi_i(x)
global E; E=zeros(NumberMeshPointsSpace,NumberMeshPointsTime);
%Store in which time step we are currently working
global CurrentTimeStep; CurrentTimeStep=1;
%how many grid points in space do we have at timestep ....
%used to see afterwards when the extra points were added
Nspace = zeros(Ntime);

%We write the solution as: u0 + Sum c_i(t) phi_i(x)
%where phi_i(x) are piecewise linear functions between x_i-1 and x_i+1
%(in x_i it is 1)
%everywhere else.
%we let i range from 2 to NumberMeshPointsSpace-1
%The ODE-solver solves ODE's of the form M(y,t)y'=f(t,y)
```

```
%The function Mass specifies the mass matrix M
%The function odefun specifies f

%After this we estimate the error in the interval x_i x_i by writing
%the solutioin as u0 + Sum c_i(t) phi_i(x) +Sum e_j(t) psi_j(x)
%The psi_i are parabolas between x_j-1 and x_j
%we let j range from 2 to NumberMeshPointsSpace
%Again an ODE solver solves the e_j

%initialize
%C is aready 0
progressbar;
Nspace(1)=NumberMeshPointsSpace;
%a boolean
RejectTimeStep=0;

%start the main loop
while(CurrentTimeStep<NumberMeshPointsTime)
  %update the progress bar
  progressbar(CurrentTimeStep/NumberMeshPointsTime);
  %compute the new solution bases on CurrentTimeStep
  sol = ode15s(@odefun, [0 EndTime/NumberMeshPointsTime], ...
          [C(:,CurrentTimeStep)' E(:,CurrentTimeStep)']', ...
          odeset('Mass',@Mass,'AbsTol',10^(-8) ));
  %Go one time step further and store the calculated solution and error
  CurrentTimeStep=CurrentTimeStep+1;
  Nspace(CurrentTimeStep)=NumberMeshPointsSpace;
  C(:,CurrentTimeStep)=sol.y(1:NumberMeshPointsSpace,end);
  E(:,CurrentTimeStep)=sol.y(NumberMeshPointsSpace+1:end,end);
  %check if the error gets too big
  i=2;
  while( (NumberMeshPointsSpace<=MaxNspace) && (i<=size(x,2)) )
    progressbar( (CurrentTimeStep-1)/NumberMeshPointsTime ...
                  + i/size(x,2)/NumberMeshPointsTime );
    if( (x(i)-x(i-1)>1000*eps)  &&    OneNorm(i,CurrentTimeStep) > ...
          ErrorTol*Nspace(1)/Nspace(CurrentTimeStep))
      %add mesh point between x(i-1) and x(i)
      %adjust Error, C, x etc.
      x=[x(1:i-1) (x(i)+x(i-1))/2 x(i) x(i+1:end)];
      C=[C(1:i-1,:)                    %the first i-1 rows
          (C(i,:)+C(i-1,:))./2+E(i,:)        %a new row
          C(i:end,:)];                %the i^th till last row
      E=[E(1:i-1,:)
          E(i,:)./4
          E(i,:)./4
          E(i+1:end,:)];
      NumberMeshPointsSpace=NumberMeshPointsSpace+1;
      RejectTimeStep=1;
    end%if
    i=i+1;
  end%while
  i=i+1;
  if(RejectTimeStep==1)
    CurrentTimeStep=CurrentTimeStep-1;
    RejectTimeStep=0;
```

```
  end%if
end%while
progressbar(1)

xmesh=x;
tmesh=t;
err=zeros(NumberMeshPointsSpace,NumberMeshPointsTime);
for i=2:NumberMeshPointsSpace
  for j=2:NumberMeshPointsTime
      err(i,j,1)=OneNorm(i,j);
  end
end
err(:,:,2)=E;
sol=C;
%now add the initial condition to sol
for i=1:NumberMeshPointsSpace
    sol(i,:)=sol(i,:)+u0(x(i));
end

%-----------------------------------------------------------------
%functions related to the ODE-solver for U

function M = Mass(t,y)
global x;
dim = size(x,2);
M=zeros(2*dim);
for i=2:dim-1
    M(i,i) =   (x(i)^2-x(i-1)^2)/12 + (x(i+1)-x(i-1))*x(i)/6 ...
             + (x(i+1)^2-x(i)^2)/12;
    M(i,i-1)=(x(i)^2-x(i-1)^2)/12;
    M(i,i+1)=(x(i+1)^2-x(i)^2)/12;
end
M(1,1)=1;
M(dim,dim)=1;
for i=2:dim
    M(dim+i,dim+i)  = 4/15*(x(i)^2-x(i-1)^2);
    M(dim+i,i-1)    = 1/15*(2*x(i)+3*x(i-1))*(x(i)-x(i-1));
    M(dim+i,i)      = 1/15*(3*x(i)+2*x(i-1))*(x(i)-x(i-1));
end
M(dim+1,dim+1)=1;

function f=odefun(t,c)
global x;
dim=size(x,2);
f=zeros(2*dim,1);
for k=2:dim-1
    f(k,1)=1/2*(c(k-1)-c(k))*(x(k)+x(k-1))/(x(k)-x(k-1)) ...
           +1/2*(c(k+1)-c(k))*(x(k+1)+x(k))/(x(k+1)-x(k)) ...
           +1/6*( x(k+1)*(Du0Dx(x(k+1))+2*Du0Dx((x(k+1)+x(k))/2))...
               +x(k)*(2*Du0Dx((x(k+1)+x(k))/2)-2*Du0Dx((x(k)+x(k-1))/2))...
               +x(k-1)*(-1*Du0Dx(x(k-1))-2*Du0Dx((x(k)+x(k-1))/2)) )...
           -(x(k+1)-x(k-1))/6*  g( u0( x(k) )+c(k) ) / x(k) ...
           -(x(k   )-x(k-1))/6*4 ...
            *g( u0( (x(k)+x(k-1))/2 )+c(k)/2+c(k-1)/2 ) / (x(k)+x(k-1)) ...
           -(x(k+1)-x(k   ))/6*4 ...
```

```
                *g( u0( (x(k)+x(k+1))/2 )+c(k)/2+c(k+1)/2 ) / (x(k)+x(k+1));
end%for
for k=2:dim
    f(dim+k,1)=-(x(k)-x(k-1))/6*(DPsiDx(k,x(k-1))*x(k-1)*Du0Dx(x(k-1))+ ...
                 DPsiDx(k,x(k))*x(k)*Du0Dx(x(k))) ...
               +2/3*x(k)*c(k)+2/3*x(k-1)*c(k-1) -8/3*(x(k-1)+x(k))/ ...
                 (x(k)-x(k-1))*c(k+dim) ...
               -(x(k)-x(k-1))/6*4*2/(x(k)+x(k-1))*g(u0((x(k)+x(k-1))/2)+ ...
               c(k)/2+c(k-1)/2 +c(dim+k)  );
end%for

%-----------------------------------------------------------------
%some addition functions

%the solution is approximated by
%Sum C(i,t) Phi(i,x) +u0(x)
%Phi(i,x) has a peak above x(i)
function z=Phi(k,y)
global x;
dim=size(x,2);
if(k<=1 || k>=dim),             z=0;
elseif(x(k-1)>=y && y<=x(k)), z=(y-x(k-1))/(x(k)-x(k-1));
elseif(y>=x(k) && y<=x(k+1)), z=(y-x(k+1))/(x(k)-x(k+1));
else,                           z=0;
end

%and its derivative
function z=DPhiDx(k,y)
global x;
global epsilon
dim=size(x,2);
if(k<2 || k>dim-1),             z=0;
elseif(y<x(k-1) || y>x(k+1)), z=0;
elseif(y<x(k)),                 z=1/(x(k)-x(k-1));
else,                           z=1/(x(k)-x(k+1));
end

%the error is approximated by
%Sum E(i,t) Psi(i,x)
function z=Psi(k,y)
global x;
dim=size(x,2);
if(k<=1 || k>=dim+1),           z=0;
elseif(x(k-1)>=y && x(k)<=y), z=4*(y-x(k-1))*(x(k)-y)/(x(k)-x(k-1))^2
else,                           z=0;
end

%and it's derivative
function z=DPsiDx (k,y)
global x;
dim=size(x,2);
if(k<=1 || k>=dim+1),           z=0;
elseif(x(k-1)>=y && x(k)<=y), z=4*((x(k-1)-y)+(x(k)-y))/(x(k)-x(k-1))^2
else,                           z=0;
end
```

```
%the solution
%the TStep does not have to be specified
function z = U(y,tau,TStep)
global C;
global t;
z=0;
if(nargin==3)
  for k=1:size(C,1), z=z+C(k,TStep)*Phi(k,y); end
  z=z+u0(y);
else
  TStep=TimeStep(tau);%Now tau lies between t(TStep-1) and t(TStep)
  %interpolate between the two timesteps
  z=((tau-t(TStep-1))*U(y,t,TStep-1)+(t(TStep)-tau)*U(y,t,TStep))/ ...
    (t(TStep)-t(TStep-1))
end

%the initial condition
function z=u0(y)
%we take a parabola as initial function
%we computed A,B,C such that it fits the boundary conditons
%and u0(1/2) = InitTop
global left;
global right;
global InitTop;
global epsilon;
A=-2*(-right+2*right*epsilon+2*InitTop-2*InitTop*epsilon)/ ...
     (1-3*epsilon+2*epsilon^2);
B=epsilon;
C=1/2*(2*right*epsilon-4*InitTop*epsilon-right+4*InitTop)/ ...
    (-right+2*right*epsilon+2*InitTop-2*InitTop*epsilon);
z = A*(y-B)*(y-C);

%and it's exact derivative
function z=Du0Dx(y)
%we take a parabola as initial function
%we computed A,B,C such that it fits the boundary conditons
%and u0(1/2) = InitTop
global left;
global right;
global InitTop;
global epsilon;
A=-2*(-right+2*right*epsilon+2*InitTop-2*InitTop*epsilon)/ ...
     (1-3*epsilon+2*epsilon^2);
B=epsilon;
C=1/2*(2*right*epsilon-4*InitTop*epsilon-right+4*InitTop)/ ...
    (-right+2*right*epsilon+2*InitTop-2*InitTop*epsilon);
z = 2*A*y+A*(-C-B);

%computes the OneNorm of the error over the interval [x_k-1, x_k]
function y=OneNorm(k,TStep)
global x;
global E;
y=E(k,TStep)^2*(8/15*x(k)-8/15*x(k-1))+E(k,TStep)^2*16/3*1/(x(k)-x(k-1));
```

```
function x = g(y)
x=gzero(y);

%the function g with pos integral
function x = gpos(y)
x=3/2*y*(y-2/3)*(y-1);

%the function g with negative integral
function x = gneg(y)
x=3*y*(y-1/3)*(y-1);

%the function g in the harmonic map case
%the integral is now 0
function x = gzero(y)
x=1/2/pi*sin(2*pi*y);
```

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