The Finite Difference Methods for Multi-Phase Free Boundary Problems

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Doctoral Thesis
Stockholm, Sweden 2011

TRITA-MAT-09-MA-04
ISSN 1401-2278
ISRN KTH/MAT/DA 11/02-SE
ISBN 978-91-7178-928-0

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Akademisk avhandling som med tillstånd av Kungl Tekniska högskolan framlägges till offentlig granskning för avläggande av teknologie doktorsexamen i matematik torsdagen den 12 maj 2011 kl 13.00 i sal F3, Kungl Tekniska högskolan, Lindstedtsvägen 26, Stockholm.

Tryck: Universitetsservice US AB

Abstract

This thesis consist of an introduction and four research papers concerning numerical analysis for a certain class of free boundary problems.

Paper I is devoted to the numerical analysis of the so-called two-phase membrane problem. Projected Gauss-Seidel method is constructed. We prove general convergence of the algorithm as well as obtain the error estimate for the finite difference scheme.

In Paper II we have improved known results on the error estimates for a Classical Obstacle (One-Phase) Problem with a finite difference scheme.

Paper III deals with the parabolic version of the two-phase obstacle-like problem. We introduce a certain variational form, which allows us to define a notion of viscosity solution. The uniqueness of viscosity solution is proved, and numerical nonlinear Gauss-Seidel method is constructed.

In the last paper, we study a numerical approximation for a class of stationary states for reaction-diffusion system with m densities having disjoint support. The proof of convergence of the numerical method is given in some particular cases. We also apply our numerical simulations for the spatial segregation limit of diffusive Lotka-Volterra models in presence of high competition and inhomogeneous Dirichlet boundary conditions.

Sammanfattning

Denna avhandling består av en introduktion och fyra vetenskapliga artiklar inom numerisk analys för en viss klass av frirandsproblem.

Den första artikeln är en numerisk analys av det så kallade tvåfasproblemet. Vi konstruerar en ickelinjär Gauss-Seidelmetod, visar generell konvergens av lösningsalgoritmen och ger en feluppskattning för finita differensschemat.

I den andra artikeln förbättrar vi kända resultat för feluppskattningar för det klassiska enfas hinderproblemet med hjälp av ett finita differens-schema.

Den tredje artikeln behandlar en parabolisk version av tvåfas hinderproblemet. En speciell variationsformulering introduceras vilket möjliggör att definiera viskositetslösningar. Vi visar att problemet har en unik viskositetslösning och konstruerar en Gauss-Seidel lösningsmetod för problemet.

I sista artikeln studerar vi ett stationar problem (genom numeriska metoder) for en reaction-diffusion system, med m olika tathet, med distinkta stodd. Vi visar konvergens hos algoritmen visas i specifika fall, och tillampar metoden i problemet med Lotka-Volterra modellen.

Acknowledgments

I wish to express my sincere gratitude to my supervisor Henrik Shahgholian, who gave me a chance to do my PhD in Sweden, and guided during the work on the thesis. I'm also grateful to him for support and many valuable advices (not only in Mathematics). I also thank Björn Gustafsson who acted as my second supervisor.

My special thanks goes to Charles M. Elliott, with whom I had very fruitful discussions during my visit to The University of Warwick, UK. The visit was supported by the Knut and Alice Wallenberg Foundation.

I am grateful to my coauthors Michael Poghosyan, Rafayel Barkhudaryan and Farid Bozorgnia, they all played essential parts in the research behind this thesis.

I owe my deepest gratitude to Norair Arakelyan who was my advisor during my undergraduate studies at Yerevan State University. This thesis I dedicate on the occasion of his 75th anniversary.

I thank my colleagues at KTH and especially my friends Erik Lindgren, Anders Edquist, Teitur Arnarson and Farid Bozorgnia for a nice time I've spent in Sweden.

Finally, I thank my family and all my friends in Armenia for their constant support and encouragement.

Avetik Arakelyan
Stockholm, April 2011

Contents

Chapter 1

Introduction

1.1 Free Boundary Problems

Many problems in physics, industry, finance, biology, and other areas can be described by partial differential equations that exhibit apriori unknown sets, such as interfaces, moving boundaries, shocks, etc. The study of such sets, also known as free boundaries, often occupies a central position in such problems. In this section we give a brief introduction to the free boundary problems (FBPs). We start with the Classical Obstacle Problem which has been widely studied starting form $60'$s. In the second subsection we discuss the so-called Two-Phase Obstacle-Like Problems that are arising in the different branches of physics.

The Classical Obstacle Problem

An obstacle problem arises when an elastic string is held fixed at two ends, A and B, and passes over a smooth object which protrudes between the two ends (see Figure 1.1). We do not know a priori the region of contact between the string and the obstacle, only that either the string is in contact with the obstacle, in which case its position is known, or it must satisfy an equation of motion, which, in this case, says that it must be straight. Beyond this, the string must satisfy two constraints. The first simply says that the string must lie above or on the obstacle, combined with the equation of motion, the curvature of the string must be negative or zero. Another interpretation of this is that the obstacle can never exert a negative force on the string: it can push but not pull. The second constraint on the string is that its slope must be continuous. This is obvious except at points where the string first loses contact with the obstacle, and there it is justified by a local force balance: a lateral force is needed to create a kink in the string, and there is none.

Under these constraints, the solution to the obstacle problem can be shown to be unique. The string and its slope are continuous, but in general the curvature of the string, and hence its second derivative, has discontinuities. Mathematically the problem can be described as a minimization of the certain energy functional over the set of admissible "deformations".

Suppose we are given a certain function $\psi \in C^2(D)$, known as the *obstacle*, satisfying the compatibility condition $\psi \leq g$ on ∂D in the sense that $(\psi - g)^+ \in W_0^{1,2}(D)$. Consider then the problem of minimizing the (Dirichlet) functional

$$J(u) = \int_D \frac{1}{2}|\nabla u|^2 dx,$$

over the constrained set

$$K_{g,\psi} = \{u \in W^{1,2}(D) : u - g \in W_0^{1,2}(D), u \geq \psi \text{ a.e. in } D\}.$$

Since J is continuous and strictly convex on a convex subset $K_{g,\psi}$ of the Hilbert space $W^{1,2}(D)$, it has a unique minimizer on $K_{g,\psi}$.

As before, we may think of the graph of u as a membrane (string) attached to a fixed wire, which is now forced to stay above the graph of ψ. As mentioned above the membrane (string) can actually touch the obstacle, i.e. the set

$$\Lambda = \{u = \psi\},$$

known as the *coincidence set*, may be nonempty. We also denote

$$\Omega = D \backslash \Lambda.$$

The boundary

$$\Gamma = \partial\Lambda \cap D = \partial\Omega \cap D$$

is called the *free boundary*, as it is apriori unknown.

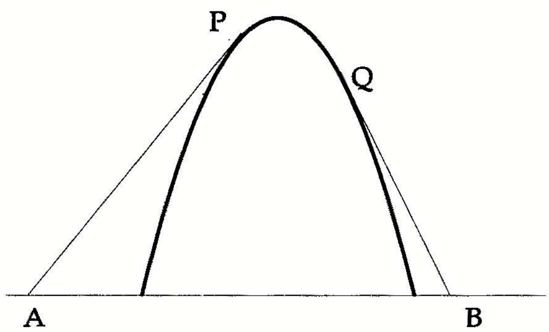

Figure 1.1: The classical obstacle problem: the string is held fixed at A and B. Here P and Q are the free boundary points.

The Two-Phase Obstacle-Like Problems

Given a bounded domain $\Omega \subset \mathbb{R}^n$, and $g \in W^{1,2}(\Omega)$. Assume $\lambda^{\pm}$ are nonnegative bounded measurable functions in Ω. We consider the following minimization problem:

$$\int_{\Omega} \left[\frac{1}{2}|\nabla u|^2 + \lambda^+ \max(u, 0) + \lambda^- \max(-u, 0) \right] dx, \tag{1.1}$$

over the set

$$K_g = \{u \in W^{1,2}(\Omega) : u - g \in W_0^{1,2}(\Omega)\}.$$

The Euler-Lagrange equation for (1.1) reads

$$\begin{cases} \Delta u = \lambda^+ \cdot \chi_{\{u>0\}} - \lambda^- \cdot \chi_{\{u<0\}} & x \in \Omega, \\ u = g & x \in \partial\Omega. \end{cases} \tag{1.2}$$

The two phases for this problem are $\{u > 0\}$ and $\{u < 0\}$, and the free boundary consist of two parts - $\partial\{u > 0\} \cap \Omega$, and $\partial\{u > 0\} \cap \Omega$.

One of the physical interpretation of this problem is the consideration of a thin membrane (film) which is fixed on the boundary of a given domain, and some part of the boundary data of this film is below the surface of a thick liquid (heavier than the film itself). Now the weight of the film produces a force downwards (call it λ^+) on that part of the film which is above the liquid surface. On the other side the part in the liquid is pushed upwards by a force λ^-, since the liquid is heavier than the film. The equilibrium state of the film is given by a minimization of the above mentioned functional.

One of the difficulties one confronts in this problem is that the interface $\{u = 0\}$ consists in general of two parts - one where the gradient of u is nonzero and one, where the gradient of u vanishes. Close to points of the latter part we expect the gradient of u to have linear growth. However, because of the decomposition into two different types of growth, it is not possible to derive a growth estimate by classical techniques. The case $\lambda^- = 0$ and $g \geq 0$ the problem is equivalent to the classical obstacle problem with zero obstacle, see above.

A good reference for this problem is Shahgholian-Uraltseva-Weiss [SUW07].

The parabolic version of the two-phase obstacle-like problem has the following form

$$\Delta u - u_t = \lambda^+ \cdot \chi_{\{u>0\}} - \lambda^- \cdot \chi_{\{u<0\}}, \text{ in } (0, T) \times \Omega, \tag{1.3}$$

where

$$\lambda^{\pm} \in C^{0,1}(\Omega),\ 0 < T < \infty, \text{ and } \Omega \subset \mathbb{R}^n \text{ is a given bounded domain.} \tag{1.4}$$

The problem arises as limiting case in the model of temperature control through the interior described in [DL76, Section 2.3.2].

1.2 Viscosity Solutions

The theory of viscosity solutions has gained much ground since its (formal) introduction in the celebrated paper [CL83] by Crandall and Lions. It provides a notion of solutions to problems for which neither classical nor weak (in the Sobolev sense) solutions are known to exist. Typical examples of such problems are found among non-linear PDEs and free boundary problems. In short, a function can be a viscosity solution as long as it is continuous, no requirements are made regarding existence of derivatives.

Consider a general fully non-linear PDE

$$F(D^2u(x,t), Du(x,t), u_t(x,t), u(x,t), x, t) = 0 \quad \text{in } \Omega, \tag{1.5}$$

and the set of paraboloids $P = \{\varphi : \ \varphi(x,t) = at + x^T Bx + cx + d\}$.

Definition 1.1. *u is a viscosity solution to (1.5) if it is continuous and satisfies for any $\varphi \in P$ and all $(x_0, t_0) \in \Omega$:*

a) If $u - \varphi$ has a local maximum at (x_0, t_0) then

$$F(D^2\varphi(x_0,t_0), D\varphi(x_0,t_0), \varphi_t(x_0,t_0), \varphi(x_0,t_0), x_0, t_0) \geq 0.$$

b) If $u - \varphi$ has a local minimum at (x_0, t_0) then

$$F(D^2\varphi(x_0,t_0), D\varphi(x_0,t_0), \varphi_t(x_0,t_0), \varphi(x_0,t_0), x_0, t_0) \leq 0.$$

1.3 Barles-Souganidis Theorem

In this section we present a very fundamental theorem related to the convergence of difference schemes. The result has been obtained by G.Barles and P.Souganidis in 1991 (see [BS91]) and since then many applications in numerical analysis of *monotone* difference schemes, has been made.

The equations we are considering are of the form

$$F(D^2u, Du, u_t, u, t, x) = 0 \quad \text{in } [0,T] \times \overline{\Omega}. \tag{1.6}$$

Here Ω is an open subset of $\mathbb{R}^n$, and $\overline{\Omega}$ is its closure. The functions

$$F : \mathbb{S}^n \times \mathbb{R}^n \times \mathbb{R} \times [0,T] \times \overline{\Omega} \to \mathbb{R} \ \text{ and } \ u : [0,T] \times \overline{\Omega} \to \mathbb{R},$$

are bounded (possibly discontiuous), and finally, Du and D^2u stand for the gradient vector and second derivative (Hessian) matrix of u. We say that (1.6) is *elliptic* if for all $x \in \mathbb{R}^n, t > 0, p_t \in \mathbb{R}, p_x \in \mathbb{R}^n$, and $\quad M, N \in \mathbb{S}^n$

$$F(M, p_x, p_t, u, t, x) \leq F(N, p_x, p_t, u, t, x) \quad \text{if} \quad M \geq N.$$

Before stating the theorem we need to define some notions related to the finite difference schemes.

A numerical scheme is an equation of the following form

$$S(h, t, x, u_h(t, x), [u_h]_{t,x}) = 0, \tag{1.7}$$

where u_h stands for the approximation of u and $[u_h]_{t,x}$ represents the value of u_h at other points than (t, x). Here for simplicity we take $\Delta x = \Delta t = h$.

The theory requires the following assumptions:

Monotonicity: If $u \leq v$,

$$S(h, t, x, r, u) \geq S(h, t, x, r, v).$$

Consistency: For every smooth function $\phi(t, x)$,

$$S(h, t, x, \phi(t, x), [\phi(t, x)]_{t,x}) \to F(D^2\phi, D\phi, \phi_t, \phi, t, x),$$

as $\Delta x \to 0$ and $\Delta t \to 0$.

Stability: For every $h > 0$, the scheme has a solution u_h which is uniformly bounded independently of h.

The theorem reads as follows:

Theorem 1.2. ***(Barles-Souganidis)*** *Under the above assumptions, if the scheme* (1.7) *satisfy the* consistency, monotonicity *and* stability *property, then its solution* u_h *converges locally uniformly to the unique viscosity solution of* (1.6).

1.4 Numerical Methods

The three scientific papers presented in this thesis have involved some numerical calculation for graphical illustrations of the presented methods. It is, however, well known that numerical methods tend to perform poorly close to free boundaries. This is in fact one motivation to study free boundary problems analytically. In this chapter we outline the procedure of computing numerical solutions and also mention a few known issues when treating free boundary problems numerically. Our main reference for numerical methods in this class of problems is [WHD95].

The Finite Difference Methods for PDEs

We use *finite difference schemes* to solve free boundary problems. They have the advantage (over *finite element methods*) that they are easy to implement on rectangular domains, which are of interest in our papers. To concretize, we usually consider a space-time domain of points $(x, t) \in [a, b] \times [0, T]$. Discretize the domains with the steps Δx and Δt so that $b = a + (N + 1)\Delta x$ and $T = (M + 1)\Delta t$ and denote $u_n^m = u(a+n\cdot\Delta x, m\cdot\Delta t)$. PDEs can be solved by replacing the involved partial derivatives by their discrete approximations, e.g. $\partial u/\partial t \approx (u_n^{m+1} - u_n^m)/\Delta t$ in the point $(a + m\Delta x, n\Delta t)$. The replacement results in $M \cdot N$ linear equations from which u_n^m can be solved.

We use predominantly the *Implicit* discretization schemes for which $\partial u/\partial t$ is discretized as in the example above and the second spacial derivative is discretized by

$$\frac{\partial^2 u}{\partial x^2} \approx \frac{1}{\Delta x^2}\left(u_{n+1}^{m+1} - 2u_n^{m+1} + u_{n-1}^{m+1}\right),$$

and for the Crank-Nickolson approximation we take

$$\frac{\partial^2 u}{\partial x^2} \approx \frac{1}{2\Delta x^2}\left(u_{n+1}^{m+1} - 2u_n^{m+1} + u_{n-1}^{m+1} + u_{n+1}^{m} - 2u_n^{m} + u_{n-1}^{m}\right).$$

This discretization schemes have the advantage over the *explicit* scheme of being stable also when $\Delta t/\Delta x^2 > 1/2$.

Implicit Schemes for Free Boundary Problems

When applying *explicit* schemes to heat-type PDEs all information for calculating the current time step is given by the previous time step. In other words $u_n^{m+1} = F(u_i^m)$ where $0 \le i \le N+1$ for some function F. *Implicit* schemes, such as the Crank-Nicholson, interconnect all current time steps, $u_n^{m+1} = F(u_i^{m+1})$ for $i \ne n$, hence all values for the current time step must be calculated simultaneously.

This complicates the application of implicit schemes to free boundary problems. For the explicit scheme the free boundary problem can be solved by calculating the PDE solution from the explicit scheme and then applying the obstacle condition., The same procedure does not work for implicit schemes. After applying the obstacle condition the solution would no longer satisfy the PDE.

To overcome this issue we apply the following method, known as the *Gauss-Seidel method*. For each time step we follow an iterative procedure which is initiated with the values from the previous time step. We then borrow the molecule from the scheme we chose, so for Crank-Nicholson, at the $(k+1)$'th step of the iteration we obtain

$$u_n^{m+1,k+1} = F(u_{n-1}^m, u_n^m, u_{n+1}^m, u_{n-1}^{m+1,k+1}, u_{n+1}^{m+1,k}). \tag{1.8}$$

The Gauss-Seidel method converges for increasing k (see [Str89]). It can however be further improved as described in the next section.

Successive Over-Relaxation

The analysis in [Str89] suggests that the rate of convergence of the Gauss-Seidel method can be considerably improved by introducing an *over-relaxation* parameter. The method suggests adding a multiple of the difference $(u^{k+1} - u^k)$ to u^{k+1}. We choose an over-relaxation parameter $\omega \in (1,2)$ and get the following modification of (1.8):

$$u_n^{m+1,k+1} = u_n^{m+1,k} + \omega \left(F(u_{n-1}^m, u_n^m, u_{n+1}^m, u_{n-1}^{m+1,k+1}, u_{n+1}^{m+1,k}) - u_n^{m+1,k} \right). \quad (1.9)$$

The value of the parameter ω is continuously updated for each time step, with the aim of finding the value which minimizes the number of iterations. The method goes by the name of *successive over-relaxation* (SOR). Introducing the obstacle condition does not affect the convergence of the method. In this case it is called the *projected SOR method*.

Chapter 2

Overview of Papers

2.1 Overview of Paper I

In the following paper we discussed the finite difference approximation of the following minimization problem:

$$\int_{\Omega} \left[\frac{1}{2} |\nabla u|^2 + \lambda^+ \max(u, 0) + \lambda^- \max(-u, 0) \right] dx, \tag{2.1}$$

over the set of admissible "deformations" $u \in H^1(\Omega)$ with given boundary data g, where $\Omega \subset \mathbb{R}^n$ is a bounded domain. The Euler-Lagrange equation for (2.1) is

$$\begin{cases} \Delta u = \lambda^+ \cdot \chi_{\{u>0\}} - \lambda^- \cdot \chi_{\{u<0\}}, & x \in \Omega, \\ u = g, & x \in \partial\Omega. \end{cases} \tag{2.2}$$

Here $\lambda^+, \lambda^- > 0$, g are given Lipschitz functions. The two phases for this problem are $\{u > 0\}$ and $\{u < 0\}$, and the free boundary consist of two parts - $\partial\{u > 0\} \cap \Omega$, and $\partial\{u > 0\} \cap \Omega$.

The optimal $C^{1,1}_{loc}$ regularity for the solution to (2.2) has been proved by Ural'tseva [Ura01] and Shahgholian [Sha03]. The regularity for the free boundary has been studied by Shahgholian, Ural'tseva and Weiss [SW06], [SUW07].

Discretized Solution

We consider the following nonlinear problem

$$\begin{cases} \min(-\Delta u + \lambda^+, \max(-\Delta u - \lambda^-, u)) = 0, \\ u = g. \end{cases} \tag{2.3}$$

The next Proposition shows the connection between the problems (2.3) and (2.2).

Proposition 2.1. *If u is the solution (in the weak sense) to (2.2), then it is a viscosity solution to (2.3). Moreover, u satisfies (2.3) a.e.*

Let $N \in \mathbb{N}$ be a positive integer $h = 1/N$ and define the partition points

$$x_i = ih,\ y_j = jh,\ i, j = 0, 1, ..., N.$$

A point of the form (x_i, y_j) is called a grid point and we are interested in computing approximate solution values at the grid points. We use the notation v_{ij} for an approximation to $v_{ij} = v(x_i, y_j)$ computed from a finite difference scheme. Write $\lambda^+_{ij} = \lambda^+(x_i, y_j)$, $\lambda^-_{ij} = \lambda^-(x_i, y_j)$. Denote

$$N_h = \{(i, j), s.t. 0 \leq i, j \leq N\},$$

$$N_h^o = \{(i, j), s.t. 1 \leq i, j \leq N - 1\},$$

and

$$\partial N_h = N_h \setminus N_h^o.$$

For any node $(i, j) \in N_h^o$, we consider 5-point stencil for the Laplace operator

$$L_h u_{i,j} = -\frac{u_{i-1,j} + u_{i+1,j} - 4u_{i,j} + u_{i,j-1} + u_{i,j+1}}{h^2}.$$

Then we apply the finite difference method to (2.3) and obtain the following nonlinear system:

$$\begin{cases} \min(L_h u_{i,j} + \lambda^+_{ij},\ \max(L_h u_{i,j} - \lambda^-_{ij}, u_{i,j})) = 0, & (i, j) \in N_h^o, \\ u_{i,j} = g_{i,j} & (i, j) \in \partial N_h. \end{cases} \tag{2.4}$$

The main result in this section is the following lemma:

Lemma 2.2. *There exists a unique solution to the nonlinear system (2.4).*

Error Estimate and Numerical Algorithm

For the unique solution to (2.4), we obtain the following error estimate:

Theorem 2.3. *(Error estimate) Let $\lambda^+(x), \lambda^-(x) \in C^3(\Omega)$ and u and u_h are the solutions of (2.2) and (2.4), respectively. Then there exist a constant $K > 0$, independent of h, such that*

$$|u(x) - u_h(x)| \leq K \cdot h^{2/7}, \quad x \in \Omega.$$

In particular, $u_h \to u$ as $h \to 0$.

We use an idea from Krylov [Kry97, Kry00]. The approach follows the following steps: First, we consider a regularized problem for which the solution is smooth. Next, we derive error estimates between the solutions of the regularized problem and the original problem - this is done for both continuous solutions and the finite difference solutions. We then estimate the error between the continuous and the finite difference solutions for the regularized problems. Finally, combining all the estimates, we obtain the convergence rate.

Concerning the numerical algorithm of the problem we refer to the well-known Projected Gauss-Seidel Method. Our method reads as follows:

Given initial approximation

$$u^0 = (u_1^0, u_2^0, ..., u_n^0) = (a, 0, ..., 0, b),$$

we set

$$u_1^k = a; \quad u_n^k = b \quad \forall k.$$

For every $k = 1, 2, ...$ and $2 \leq i \leq n-1$ we denote

$$z_i^1 = \frac{1}{2}\left(u_{i-1}^k + u_{i+1}^{k-1} - h^2 \cdot \lambda_i^+\right),$$

$$z_i^2 = \frac{1}{2}\left(u_{i-1}^k + u_{i+1}^{k-1} + h^2 \cdot \lambda_i^-\right).$$

Here h is a discretized mesh size.

Then we proceed as follows:

$$\begin{aligned} &\text{if } \ z_i^1 \geq 0, && \text{then} \quad \tilde{u}_i^k = z_i^1; \\ &\text{if } \ z_i^2 \leq 0, && \text{then} \quad \tilde{u}_i^k = z_i^2; \\ &\text{if } \ z_i^1 < 0 < z_i^2, && \text{then} \quad \tilde{u}_i^k = 0. \end{aligned} \tag{2.5}$$

The sequence $\tilde{u}^k = \left(\tilde{u}_1^k, \tilde{u}_2^k, ..., \tilde{u}_{N-1}^k\right)$ constructed in this way we will call the sequence obtained by PGS method. For the method we obtain the following convergence result:

Theorem 2.4. *(Convergence of Algorithm) Constructed Projected Gauss-Seidel method converges towards to the unique solution of* (2.4)*.*

Remark 2.5. We emphasize that for finite element discretization the constructed nonlinear Gauss-Seidel method will work as well, moreover the prove of convergence of the algorithm can be repeated by taking into account certain differences between the Finite Difference and Finite Element Methods.

2.2 Overview of Paper II

In the following paper we revisited the One-phase (Obstacle) Problem:

$$\begin{cases} -\Delta u(x) \geq \lambda(x), & x \in \Omega, \\ -\Delta u(x) = 0, & x \in \{u(x) > \psi(x)\}, \\ w(x) \geq \psi(x), & x \in \Omega, \\ w(x) = g(x), & x \in \partial\Omega. \end{cases} \tag{2.6}$$

Here the inequality and equation for Laplacian of u should be understood in the *weak sense*, but using the optimal $C^{1,1}(\Omega)$ regularity result for One-Phase Obstacle Problems over sufficiently smooth obstacles (cf. [Fre72], [Caf98]), we can assure that they hold *a.e.*. The aim of this paper is for optimal regular solution of (2.6), to prove that the sequence u_h converges towards u as $h \to 0$, and to obtain approximation error estimate in terms of h.

Here we use the technique that was used in [HLJ09] to prove the convergence of Finite Difference Scheme for One-Phase Obstacle problem.

Preliminaries

Let $\Omega \subset \mathbb{R}^n$ be bounded open set, $\lambda \in L^2(\Omega)$ and $\psi \in H^2(\Omega)$.

It is well-known fact, that the classical (One-Phase) Obstacle problem, i.e. the problem of minimization of the functional

$$\mathcal{E}(u) = \frac{1}{2}\int_\Omega |\nabla u(x)|^2 dx + \int_\Omega \lambda(x) u(x) dx,$$

over the set $\mathbb{K}_\psi$ can be transformed to the minimization of the functional

$$\mathcal{J}(u) = \frac{1}{2}\int_\Omega |\nabla u(x)|^2 dx + \int_\Omega f(x) u(x) dx, \tag{2.7}$$

over the set

$$\mathbb{K} = \{v \in H^1(\Omega) : v - \psi \in H^1_0,\ v(x) \geq 0 \text{ in } \Omega\}, \tag{2.8}$$

where $f(x) = \lambda(x) - \Delta\psi(x)$, and the later can be formulated as

$$\min\{-\Delta u(x) + f(x), u(x)\} = 0.$$

If we denote

$$\mathcal{F}(v) = \min\{-\Delta v(x) + f(x), v(x)\},$$

then the classical Obstacle problem (2.7)-(2.8) can be written as

$$\begin{cases} \mathcal{F}(u) = 0 & in \quad \Omega, \\ u = g & on \quad \partial\Omega. \end{cases} \tag{2.9}$$

Let $\Delta_h u$ be the Finite Difference Scheme approximation operator for Laplace operator.

We denote

$$\mathcal{F}_h(v) = \min\{-\Delta_h v(x) + f(x), v(x)\},$$

and by u_h we denote the solution of the following problem:

$$\begin{cases} \mathcal{F}_h(u_h) = 0 & in \quad \Omega, \\ u_h = g & on \quad \partial\Omega. \end{cases} \tag{2.10}$$

Error estimate

The Finite Difference Scheme were extensively used for numerical solutions to One-Phase Obstacle problems of elliptic and parabolic type. The method is easily implementable and the rate of approximation is good enough in practice, so there is theoretical and practical interest for investigation and mathematical justification of convergence. Strangely enough, there were no convergence and error estimate results up to 2006, when Xiao-liang and Lian (see [CX06]) proved the quadratic convergence of the FDS for the two-dimensional Classical Obstacle Problem under the condition, that the solution belongs to $C^4(\Omega)$. This is not surprising result, since for $u \in C^4(\Omega)$, by the Taylor expansion, the local estimate

$$\Delta u(x) - \Delta_h u(x) = O(h^2)$$

is true (Δ_h is the FDS approximation to Laplacian). But it is known (see [Caf98]), that in general, even for infinite differentiable obstacle ψ, the solution u of the Obstacle Problem belongs only to $C^{1,1}(\Omega)$.

Our main result reads

Theorem 2.6. *Let f and g be as above and u and u_h are the solutions of* (2.9) *and* (2.10)*, respectively. Then there exists a constant $C_0 > 0$, independent of h, such that*

$$|u(x) - u_h(x)| \leq C_0 \cdot h^{4/11}, \quad x \in \Omega.$$

In particular, $u_h \to u$ as $h \to 0$.

2.3 Overview of Paper III

In this paper we study the finite difference approximation for two-phase parabolic obstacle-like problem,

$$\Delta u - u_t = \lambda_+ \cdot \chi_{\{u>0\}} - \lambda_- \cdot \chi_{\{u<0\}}, \quad (t, x) \in (0, T) \times \Omega, \tag{2.11}$$

where $0 < T < \infty, \lambda_+, \lambda_- > 0$ are Lipschitz continuous functions, and $\Omega \subset \mathbb{R}^n$ is a bounded domain. Denote $\Omega_T = (0, T) \times \Omega$.

Variational form

The idea of constructing the numerical scheme is to define a variational form that will provide us the same solution (in viscosity sense) as the solution to (2.11). In the paper we consider the following variational equation:

$$G[D^2u, u, u_t] = \min(u_t - \Delta u + \lambda^+, \max(u_t - \Delta u - \lambda^-, u)) = 0, \tag{2.12}$$

where λ^+ and λ^- are as in (2.11).

We prove the following lemma:

Lemma 2.7. *If u is the solution (in the weak sense) to* (2.11)*, then it is a viscosity solution to* (2.12)*.*

Similarly for the two-phase membrane problem discussed in the paper I, we considered the following variational form:

$$F[D^2u, u] = \min(-\Delta u + \lambda^+, \max(-\Delta u - \lambda^-, u)) = 0. \tag{2.13}$$

We define for parabolic two-phase obstacle-like variational equation a notion of viscosity solution and prove the following uniqueness result

Theorem 2.8. *(Uniqueness of viscosity solution) There exists at most one viscosity solution of* (2.12)*.*

Note that the same result holds true for the elliptic two-phase membrane problem as well.

Convergence of schemes

Elliptic case

Consider the nonlinear, degenerate elliptic partial differential equation with Dirichlet boundary conditions,

$$\begin{cases} F[u](x) = 0 & \text{in } \Omega, \\ u(x) = g(x) & \text{on } \partial\Omega. \end{cases} \tag{2.14}$$

Definition 2.9. *The equation F is degenerate elliptic if*

$$F(x, r, p, X) \le F(x, s, p, Y) \quad \textit{whenever } r \le s \quad \textit{and } Y \le X,$$

where $Y \le X$ means that $Y - X$ is a nonnegative definite symmetric matrix.

In our case for the two-phase membrane problem we have,

$$F[u](x) = \min(-\Delta u + \lambda^+, \max(-\Delta u - \lambda^-, u)). \tag{2.15}$$

Hence

$$F(x, r, p, X) = \min(-\text{trace}(X) + \lambda^+, \max(-\text{trace}(X) - \lambda^-, r)).$$

Lemma 2.10. *The two phase-membrane problem* (2.15) *is degenerate elliptic.*

Proof. In order to prove degenerate ellipticity one has to check the definition stated above. Since we have that

$$-\mathrm{trace}(X) \leq -\mathrm{trace}(Y), \quad \textit{whenever} \quad Y \leq X,$$

and

$$\max(-\mathrm{trace}(X) - \lambda^-, r)) \leq \max(-\mathrm{trace}(X) - \lambda^-, s)), \quad \textit{whenever} \quad r \leq s.$$

Therefore

$$\begin{aligned} F(x,r,p,X) &= \min(-\mathrm{trace}(X) + \lambda^+, \max(-\mathrm{trace}(X) - \lambda^-, r)) \\ &\leq \min(-\mathrm{trace}(X) + \lambda^+, \max(-\mathrm{trace}(X) - \lambda^-, s)) \\ &= F(x,s,p,Y). \end{aligned}$$

This completes the proof of the lemma. □

We define the approximation scheme for the elliptic two-phase membrane problem as follows:

$$F^i[u] \equiv F^{h,i}[u_i, u_i - u_j] = \min\left(L_h u_i + \lambda_i^+, \max\left(L_h u_i - \lambda_i^-, u_i\right)\right), \tag{2.16}$$

where

$$L_h u_i = \sum_{j=1}^{N(i)} \frac{1}{h^2}(u_i - u_j), \quad i = 1, ..., N. \tag{2.17}$$

For this scheme we show that it is a degenerate elliptic scheme (see[Obe06]), which in turn implies the *monotonicity* and *stability* for the scheme (2.16). Then by applying the Barles-Souganidis theorem we prove the following theorem:

Theorem 2.11. *(Convergence) The finite difference scheme given by* (2.16) *converges uniformly on compacts subsets of* Ω *to the unique viscosity solution of the two phase-membrane variational equation* (2.13).

Parabolic case

We follow the notations of [BDR95]. A numerical scheme can be written as

$$S(m, \tilde{u}) \equiv S(\Delta t, \Delta x, m, j, u_j^m, \tilde{u}) = 0,$$

for $1 \leq j \leq N$ and $1 \leq m \leq M$, where N and M are respectively the number of grid points in space and in time. Here $\tilde{u}$ denotes the vector $(u_k^l)_{k,l}$ in $\mathbb{R}^{NM}$. Finally Δt and Δx denote the time and the space mesh size respectively. For parabolic case we consider the following *explicit scheme*:

$$S(m+1, \tilde{u}) = \min(\tilde{S}(\tilde{u}) + \Delta t {\lambda^+}_j^m; \max(\tilde{S}(\tilde{u}) - \Delta t {\lambda^-}_j^m, \Delta t u_j^{m+1})), \tag{2.18}$$

where

$$\tilde{S}(\tilde{u}) = u_j^{m+1} - u_j^m + \frac{\Delta t}{(\Delta x)^2} L u_j^m, \text{ and } L u_i^m = \sum_{j=1}^{N(i)} (u_i^m - u_j^m), \quad i = 1, \ldots, N.$$

We prove the following lemma

Lemma 2.12. *The scheme* (2.18) *is* monotone *and* stable *provided the following non-linear CFL condition holds*

$$\frac{\Delta t}{(\Delta x)^2} \leq \frac{1}{K}, \tag{2.19}$$

where $K = \max_{1 \leq i \leq N} N(i)$.

Finally again applying the Barles-Souganidis theorem we obtain the following convergence result for parabolic two-phase obstacle-like problem:

Theorem 2.13. *(Convergence for parabolic case) The solution* $\tilde{u}$ *of* (2.18) *converges as* $\Delta t, \Delta x \to 0$ *uniformly on compacts subsets of* Ω_T *to the unique viscosity solution of the two-phase parabolic obstacle-like variation equation* (2.12) .

Numerical Method

For constructing a numerical method we refer to nonlinear Gauss-Seidel method. Suppose u^m is a shorthand of $(u_j^m)_j$. We proceed as follows:

- **First Step**.

$$u^{m+\frac{1}{2}} = \min\left(u^m - \frac{\Delta t}{(\Delta x)^2} L u^m + \Delta t \lambda^-, 0\right),$$

- **Second Step**.

$$u^{m+1} = \max\left(u^m - \frac{\Delta t}{(\Delta x)^2} L u^m - \Delta t \lambda^+, u^{m+\frac{1}{2}}\right).$$

At the end of the paper the numerical simulations are presented.

2.4 Overview of Paper IV

In this paper, we study a numerical approximation for a class of stationary states for reaction-diffusion system with m densities having disjoint support, which are governed by a minimization problem. We consider the following two problems called Problem (A) and Problem (B).

Problem (A)

$$\text{Minimize } E(u_1, \cdots, u_m) = \int_\Omega \sum_{i=1}^{m} \left(\frac{1}{2}|\nabla u_i|^2 + f_i u_i \right) dx, \tag{2.20}$$

over the set

$$S = \{(u_1, \dots, u_m) \in (H^1(\Omega))^m : u_i \geq 0, u_i \cdot u_j = 0, u_i = \phi_i \quad \text{on} \quad \partial\Omega\}.$$

Here $\phi_i \in H^{\frac{1}{2}}(\partial\Omega)$ with property $\phi_i \cdot \phi_j = 0$, $\phi_i \geq 0$ on the boundary $\partial\Omega$. Also we assume that f_i is uniformly continuous and $f_i(x) \geq 0$.

First of all we discuss the existence and uniqueness of minimizer (2.20). The existence follows from the general theory of calculus of variations for coercive and convex functionals (see [Str90]). For the uniqueness we prove the following proposition:

Proposition 2.14. *The minimizer of* (2.20) *is unique.*

We use quantitative properties of the solution and free boundaries to derive our scheme. Suppose there is a grid on the domain Ω; then our method can be formulated as follows:

- **Initialization:** For $l = 1, \cdots, m$, set

$$u_l^0(x_i, y_j) = \begin{cases} 0 & (x_i, y_j) \in \Omega^\circ, \\ \phi_l(x_i, y_j) & (x_i, y_j) \in \partial\Omega. \end{cases}$$

- **Step $k+1$, $k \geq 0$:** For $l = 1, \cdots, m$, we iterate for all interior points

$$u_l^{(k+1)}(x_i, y_j) = \max\left(\frac{-f_l h^2}{4} + \overline{u}_l^{(k)}(x_i, y_j) - \sum_{p \neq l} \overline{u}_p^{(k)}(x_i, y_j), \, 0 \right). \tag{2.21}$$

For the scheme discussed above we prove the following lemma:

Lemma 2.15. *The iterative method* (2.21) *satisfies*

$$u_l^{(k)}(x_i, y_j) \cdot u_q^{(k)}(x_i, y_j) = 0,$$

for all $k \in \mathbb{N}$ *and* $q, l \in \{1, 2, \dots, m\}$, *where* $q \neq l$.

Convergence of the scheme in particular case is shown.

Problem (B)

Known results

The second problem appears in the study of population ecology. In this case high competitive interactions between different species occurs. As the rate of interaction of two different species goes to infinity, then the competition-diffusion systems shows a limiting configuration with segregated state. We refer the reader to [CTV05, CDH07, CDH$^+$04, DD94] and in particular to [DHMP99] for models involving Dirichlet boundary data. A complete analysis of the stationary case has been studied in [CTV05]. Also numerical simulation for the spatial segregation limit of two diffusive Lotka-Volterra models in presence of strong competition and inhomogeneous Dirichlet boundary conditions is provided in [SZ08].

Let d_i, λ be positive numbers. Consider the following system of m differential equations

$$\begin{cases} -d_i \Delta u_i = \lambda u_i(1-u_i) - \frac{1}{\varepsilon} u_i \sum_{j\neq i} u_j^2 & \text{in } \Omega, \\ u_i(x,y) = \phi_i(x,y) & \text{on } \partial\Omega, \end{cases} \tag{2.22}$$

for $i = 1, \cdots, m$, where again $\phi_i \in H^{\frac{1}{2}}(\partial\Omega)$ with property $\phi_i \cdot \phi_j = 0$, $\phi_i \geq 0$ on the boundary $\partial\Omega$. Our aim is to present numerical approximation for this system as $\varepsilon \to 0$. This system can be viewed as steady state of the following system in the case that boundary values are time independent.

$$\begin{cases} \frac{d}{dt} u_i - d_i \Delta u_i = \lambda u_i(1-u_i) - \frac{1}{\varepsilon} u_i \sum_{j\neq i} u_j^2 & \text{in } \Omega \times (0,\infty), \\ u_i(x,y,t) = \phi_i(x,y,t) & \text{on } \partial\Omega \times (0,\infty), \\ u_i(x,y,0) = u_{i,0}(x,y) & \text{in } \Omega, \end{cases} \tag{2.23}$$

for $i = 1, \cdots, m$.

Numerical approximation of Problem (B)

We present a numerical scheme for elliptic system in Problem (B) as $\varepsilon \to 0$.

For m components we obtain the following iterative method: For all $l = 1, \ldots, m$,

$$u_l^{(k+1)}(x_i, y_j) = \max\left(\frac{2\overline{w_l}^{(k)}(x_i, y_j)}{d_l - \alpha + \sqrt{(d_l-\alpha)^2 + 4\alpha \overline{w_l}^{(k)}(x_i, y_j)}}, 0 \right), \tag{2.24}$$

where

$$\overline{w_l}^{(k)}(x_i, y_j) = d_l \overline{u_l}^{(k)}(x_i, y_j) - \sum_{p\neq l} d_p \overline{u_p}^{(k)}(x_i, y_j),$$

here $\alpha = \lambda h^2/4$.

Again by using the same approach as in Lemma 2.15, one can prove the same result for this method as well.

Lemma 2.16. *If* $\min_l d_l > \alpha$, *then the iterative method* (2.24) *satisfies*

$$u_l^{(k)}(x_i, y_j) \cdot u_q^{(k)}(x_i, y_j) = 0,$$

for all $k \in \mathbb{N}$ *and* $q, l \in \{1, 2, \dots, m\}$, *where* $q \neq l$.

The main idea of deriving the numerical scheme is consider two components case and generalize it for m components. For two components we proceed as follows:

We have

$$d_2 \Delta v - d_1 \Delta u = \lambda u(1-u)\chi_{\{u>0\}} - \lambda v(1-v)\chi_{\{v>0\}}.$$

This equation is solved numerically by employing second order, centered, finite differences on the given grid i.e,

$$-\frac{d_1}{h^2}[4\overline{u}(x_i, y_j) - 4u(x_i, y_j)] + \frac{d_2}{h^2}[4\overline{v}(x_i, y_j) - 4v(x_i, y_j)] = \tag{2.25}$$

$$\lambda u(x_i, y_j)(1 - u(x_i, y_j))\chi_{\{u(x_i,y_j)>0\}} - \lambda v(x_i, y_j)(1 - v(x_i, y_j))\chi_{\{v(x_i,y_j)>0\}}.$$

It is easy to see that the equation (2.25) is a quadratic equation with respect to $u(x_i, y_j)$ and $v(x_i, y_j)$. If $u(x_i, y_j) > 0$ then we set $v(x_i, y_j) = 0$ and vice versa. Let $4\alpha = \lambda h^2$ then from (2.25) we get the following iterative formulas

$$u^{(k+1)}(x_i, y_j) = \max\left(\frac{2(d_1\overline{u}^{(k)}(x_i, y_j) - d_2\overline{v}^{(k)}(x_i, y_j))}{d_1 - \alpha + \sqrt{(d_1 - \alpha)^2 + 4\alpha(d_1\overline{u}^{(k)}(x_i, y_j) - d_2\overline{v}^{(k)}(x_i, y_j))}}, 0\right)$$

and

$$v^{(k+1)}(x_i, y_j) = \max\left(\frac{2(d_2\overline{v}^{(k)}(x_i, y_j) - d_1\overline{u}^{(k)}(x_i, y_j))}{d_2 - \alpha + \sqrt{(d_2 - \alpha)^2 + 4\alpha(d_2\overline{v}^{(k)}(x_i, y_j) - d_1\overline{u}^{(k)}(x_i, y_j))}}, 0\right).$$

In the last section of the paper numerical examples are presented.

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