TWO-DIMENSIONAL STEFAN PROBLEM USING LEVEL SET METHOD

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To my beloved mother and father, my siblings and my friends

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ABSTRACT

Cancer cell invasion across the surrounding tissues is driven by finger-like protrusions known as invadopodia. Plasma membrane of a cancer cell has the elastic characteristic that gives the idea to employ the knowledge of Stefan problem to solve the problem in cancer cell invasion. For this purpose, plasma membrane is treated as a free boundary interface. In fact, Stefan problem is a well-known free boundary problem that requires the solution of moving interface(s) as time proceeds along with the change in the temperature distribution. Hence, this study investigated two-dimensional free boundary Stefan problem that focused on the solidification process. A mathematical model of solidification is first introduced by Chen $et\,al.$ (1997) considering the jump of the temperature distribution from the liquid to the solid regions. The velocity concerning the movement of the interface is calculated by taking the first derivative of the temperature with respect to space. The model is solved numerically by using finite-difference of level set method [13]. Two algorithms of the level set method are presented in modelling and discretization parts, to handle the topology changes of Stefan problem, systematically. Results of the interface movement and temperature distribution are presented graphically and discussed in order to visualize the solidification process.

ABSTRAK

Serangan sel kanser terhadap keseluruhan tisu adalah didorong oleh bonjolan-bonjolan berbentuk jejari yang dikenali sebagai invadopodia. Sifat kekenyalan yang dimiliki oleh membran plasma sel kanser telah memberi idea untuk mengaplikasikan konsep masalah Stefan dalam menyelesaikan masalah serangan sel kanser ini. Untuk tujuan ini, membran plasma dianggap sebagai antara muka sempadan bebas. Secara faktanya, masalah Stefan terkenal dengan masalah sempadan bebas yang memerlukan penyelesaian dalam pergerakan antara muka mengikut perubahan masa dan juga taburan suhu. Maka, pembelajaran ini adalah untuk mengkaji sempadan bebas masalah Stefan dalam dua dimensi yang fokus kepada proses penyejukbekuan. Model matematik tentang penyejukbekuan telah diperkenalkan oleh Chen $et\ al.$ (1997) dengan mempertimbangkan lompatan suhu dari kawasan cecair kepada kawasan pepejal. Halaju mengenai pergerakan antara muka dikira dengan mengambil terbitan pertama suhu terhadap ruang. Model ini diselesaikan secara berangka menggunakan beza terhingga bagi kaedah set aras [13]. Dua algoritma bagi kaedah set aras dikemukakan dalam bahagian permodelan dan bahagian pendiskretan, untuk mengawal perubahan topologi masalah Stefan secara sistematik. Keputusan-keputusan berkaitan pergerakan antara muka dan tebaran suhu dikemukakan secara grafik dan dibincangkan untuk menggambarkan proses penyejukbekuan.

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LIST OF ABBREVIATIONS

BC	-	Boundary condition
BVP	-	Boundary value problem
CFL	-	Courant-Friedreichs-Lewy
ECM	-	Extracellular matrix
ENO	-	Essentially non oscillatory
HJ	-	Hamilton-Jacobi
LU	-	Lower upper
PDE	-	Partial differential equation
TVD	-	Total variation diminishing

LIST OF SYMBOLS

a	-	Velocity field
c_s	-	Volumetric heat capacity in solid
c_l	-	Volumetric heat capacity in liquid
D	-	Domain for two phase Stefan problem
d	-	Distance from the front
F	-	Speed function
$f(\mathbf{x})$	-	Continuous function
$g(\mathbf{x})$	-	Melting temperature function
k_s	-	Thermal diffusivity in solid
k_l	-	Thermal diffusivity in liquid
L_h	-	Latent heat of solidification
L	-	Length of domain D
$N, \mathbf{n}$	-	Outward normal vector at the front
T	-	Tangential vector
T_m	-	Melting temperature of material
t	-	Time taken
$U(\mathbf{x}, t)$	-	Temperature of the material
U_l	-	Temperature in liquid region
U_m	-	Positive constant
U_s	-	Temperature in solid region
V	-	Normal velocity

V_n, F	-	Speed at the front
V_t	-	Tangential velocity
S	-	Sign function
$\mathbf{x}$	-	Nodes in x and y axis
$\mathbf{x}_I$	-	Nodes in x and y axis at the boundary
x_c	-	Closest point on the interface to $\mathbf{x}$

Greek symbol

$\Gamma(t)$	-	Boundary between two phases
$<$	-	Less than
$\geq$	-	Greater than or equal to
$>$	-	Greater than
$\in$	-	An element of
κ	-	Curvature at front
$\leq$	-	Less than or equal to
∇	-	Gradient operator
$\neq$	-	Not equal to
$\notin$	-	Not element of
Ω	-	Domain occupied individual cancer cell
Ω^l	-	Material in liquid region
Ω^s	-	Material in solid region
ω_c^t	-	Intracellular
ω_n^t	-	Extracellular
$\psi(\mathbf{x}, t)y$	-	Level set function
∂	-	Partial derivative
θ	-	angle between $\mathbf{x}$ axis and $\mathbf{n}$
θ_0	-	angle symmetry axis upon which the crystal growth
ε_c	-	Surface tension coefficient
ε_V	-	molecular kinetic coefficient

Constant

A	-	Constant
k_A	-	Constant
$\overline{\varepsilon_c}$	-	Constant
$\overline{\varepsilon_V}$	-	Constant

CHAPTER 1

INTRODUCTION

1.1 Introduction

Cancer is a critical societal and scientific problem. Researchers from various fields spend many years to understand the behaviour of the cancer cells in order to find the cure. Normally, humans cells grow and divide to form new cells as the body needs them. Cells grow old or become damage and they die, and new cells take their place. But, cancer will develop when this orderly process breaks down.

Saitou $et\,al.$ [1] said that cancer cells at an early stage of invasion possess the ability to invade the surrounding tissue. This ability leads to metastasis where cells from primary tumour move to the distant sites in the body to form secondary tumour. Metastasis is a major cause of death in cancer patients, and thus preventing this secondary spread of the tumour leads to an increase of the survival rate. Accordingly, Saitou $et\,al.$ [1] carried out a mathematical model of invadopodia formation observed as sub-cellular structures of invasive tumor cells.

Invadopodia are invasive cancer cells with a special sub-cellular membrane structure which carries a pivotal process in cancer invasion. They are membrane protrusions that localized enzyme required for extracellular matrix (ECM) degradation. Besides, invadopodia are composed of a variety of proteins such as actin and actin regulatory protein, adhesion molecules, membrane remodelling and signalling proteins. Figure 1.1 shows the movement of a cancer cell that is driven by invadopodia which engenders migratory pathways through the ECM. But, Saitou's model however has a problem where the region of actin, $n > 0$ becomes disconnected as time progresses.

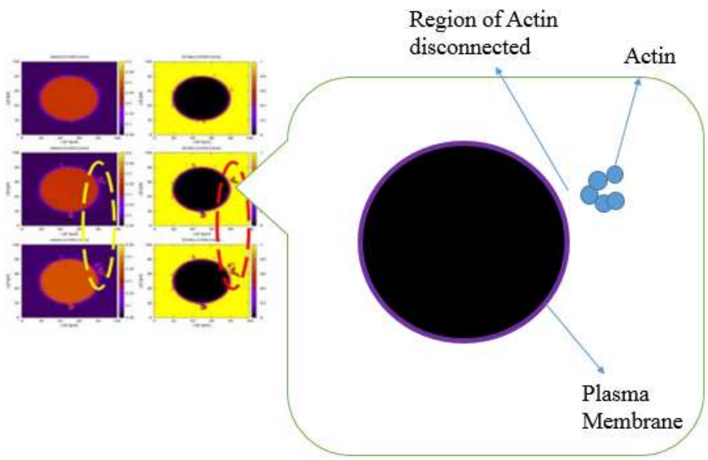

Figure 1.1 Actin disconnected from the membrane as time progresses [2].

Admon [2] investigated a one-dimensional signal transduction with integrated penalty of cancer cell model to overcome the problem in Saitou $et\,al.$ [1] which is shown in Figure 1.2 where domain Ω occupied by an individual cancer cell. ω_c^t and ω_n^t represent intracellular and extracellular respectively. Admon's model was able to make the region of actin from Figure 1.1 continuous as time advances. He proposed to treat the plasma membrane as a free boundary interface to overcome the region of actin disconnection problem. Since the formation involves a free boundary problem, a two dimensional simulation is needed to get a clear picture of formation of invadopodia. Figure 1.3 shows the proposed two-dimensional signal transduction with integrated penalty of cancer cell model.

This proposed model is similar to Chen's model [3] as shown in Figure 1.4. Chen's model is about the process of solidification involving two phases which are liquid and solid phases in free boundary problem. Thus, this study is focusing on modelling a two-dimensional solidification problem and simulating it by using a level

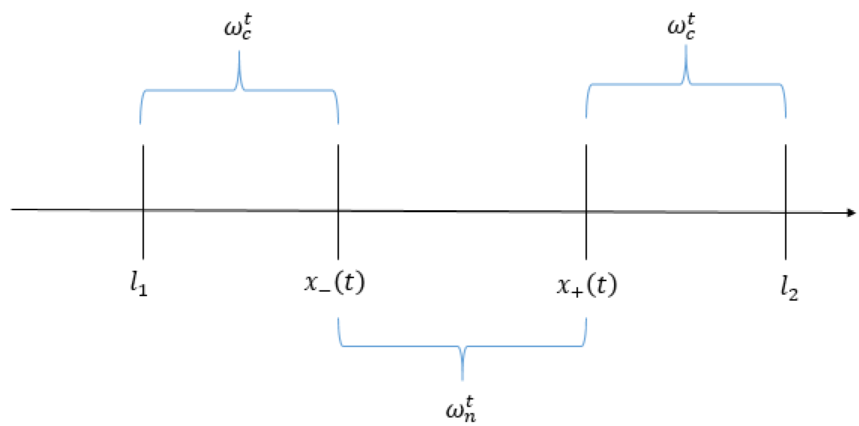

Figure 1.2 Domain of one-dimensional cancer cell model [2].

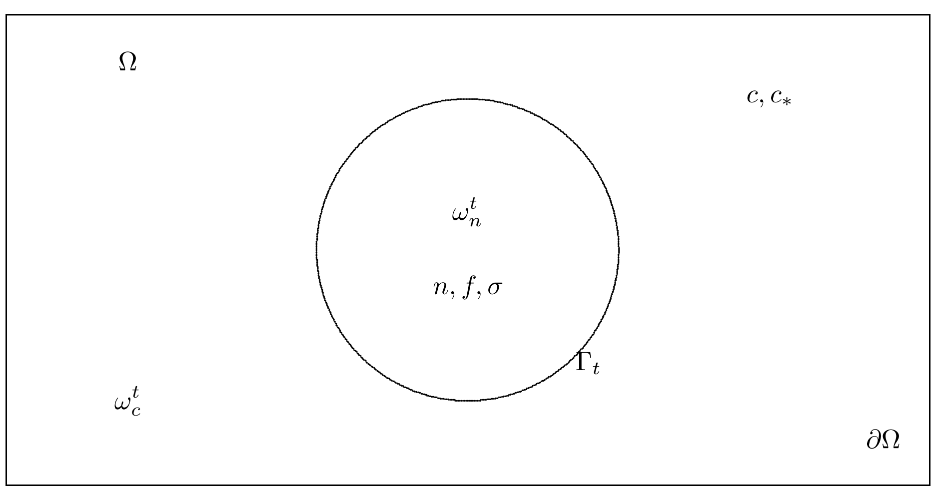

Figure 1.3 Domain of two-dimensional cancer cell model [2].

set method.

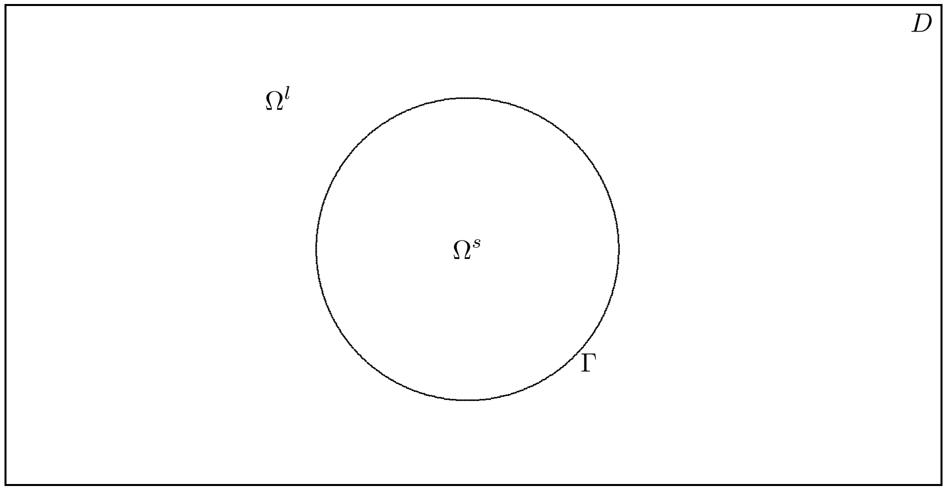

Figure 1.4 Domain D for the model of dendritic solidification in $2-D$ case [3].

1.2 Research Background

1.2.1 Stefan Problem

Stefan problem is a well-known boundary value problem concerning melting or solidification process that requires the solution of a moving interface as time progresses along with the change in the temperature distribution. Oftentimes, the goal of studying and developing algorithm for solving Stefan problems is to adapt and apply various methods such as the finite element method, front tracking method and level set method to the problem of modelling unstable or dendritics solidification [3]. The model of unstable solidification in the supercooled condition concern with an anistropic curvature and velocity dependent boundary condition. It is said to be unstable when the topology changes and complicated interface shapes are formed.

Various models of Stefan problems have been proposed. These problems involve n-dimensions but most researchers focus on the research up to three dimensions only. As for one dimension, most researchers frequently consider liquid phase only as found in Murphy [4], Brattkus and Meiron [5], Dunbar $et\,al.$ [6], and Sethian and Straint [7].

There are researchers who investigated two dimensional Stefan problems in which they considered solid and liquid phases. Gammon and Howarth [8] solved the two dimensional Stefan problem of solidification in a half-space where the heat flux at the wall is a slightly varying function of position along the wall. Other examples for two dimensional problems can be seen in Sussman $et\,al.$ [9], Juric and Tryggvason [10], Wang and Sekerka [11] and Chen $et\,al.$ [3].

1.2.2 Numerical Methods for Stefan Problem

Numerous numerical approaches to solve Stefan problems have been conducted by many researchers. Brattkus and Meiron [5] used boundary integral method to solve an integral equation on the moving boundary. But, this method works well only in one dimension. Schmidt [12] used finite elements methods to solve Stefan problems in three dimension. He shows that finite element method is most suitable method compared with other numerical approaches. Juric and Tryggvason [10] employed front-tracking methods, a common way of solving moving boundary problem by using immersed boundary method for transferring information from the moving boundary to the fixed temperature. They successfully modelled various physical features of dendritics solidification. However, a special care has to be taken when a topological change occurs such as when merging happens at the front.

Employing phase-field method is also one of the ways to simulate Stefan problems. The model of Stefan problem is used to track the boundary implicitly by partial differential equation (PDE) for the temperature field and its boundary conditions on the moving boundary by two coupled PDEs involving the temperature field and a new field. The new field is the phase field that keep the track. Wang and Sekerka [11] used phase field model of solidification in two dimensions in the context of dendritic growth. However, they failed to eliminate the interface tracking which is the advantage of using phase-field model.

Level set method is a well suited method for solidification problem which is essentially a problem involving moving boundary. In this method, instead of tracking the boundary or front using Lagrange approach, one can instead capture the front on a fixed grid by using Eulerian approach. Sethian and Straint [7] simulated dendritic growth by combining boundary integral formulation of the equation of motion coupled with a level set method for advancing the propagating interface. It ables to follow the evolution of extremely intricate shape, exhibiting complex behaviour such as lingering, tip splitting, and side branching as well as profound topological changes. But their technique is slightly complicated and computationally expensive for solving the solidification problem.

Hence in this study, the level set method is used in which the moving front is always represented by the zero level set of smooth, continuous function. Finite difference method is used to compute the normal velocity at the interface. The numerical results obtained from the computation using Matlab software are validated with results by Mitchell [13].

1.3 Problem Statement

By realizing the fact that cancer is a critical societal and scientific problem, the importance of the study of a cancer cell movement that is driven by invadopodia which causes migratory pathways through the ECM in two dimensional model is acknowledged. In this research, plasma membrane is treated as a free boundary similar to Stefan problem. The main interest of this particular study is due to these few problem statements:

i. How to construct a mathematical model of a cancer cell growth based on the Stefan problem associated with solidification of a crystal growth?

ii. How to discretize the model using level set approach?

iii. Are the numerical results obtained from the computation using Matlab fitted well with those results from Mitchell [13]?

1.4 Objectives of the Study

The objectives of this study are:

i. To construct the mathematical modeling of Stefan problem associated with solidification of water.
ii. To employ the level set method for solving two phase Stefan problem in two dimensional case.
iii. To discretize the algorithm of level set method by using finite difference method.
iv. To assemble the results for interface movements and temperature distributions for the solidification process.

1.5 Scope of the Study

This study concerns on the modelling of the solidification process of water surrounding the ice on two-dimension. Neumann boundary condition is considered on the square domain, D. The model is then simulated by using a level set method where values of the interface function ψ are taken as negative (ice), zero (on the boundary of ice-water) and positive (water) constants.

1.6 Significance of the Study

The outcome from this study is to visualize the behaviour of the moving front that arises from the unstable solidification of pure substance. This study also helps in better understanding on the cases related with moving boundaries such as alloy solidification [14] and dendritic growth [3]. Also, by considering the moving boundary concepts, we are able to understand the behaviour of a cancer cell invasion that is driven by invadopodia which engenders migratory pathways through the ECM in two dimensional model in which we treat the plasma membrane as a free boundary [2].

1.7 Research Methodology

The research starts from studying on unstable solidification process (Stefan problem) in two dimension. Then, the mathematical modelling of the solidification process in two dimensional Stefan problem is constructed. The level set method is employed for solving Stefan problem. Next, the model is discretized by using finite difference method. Finally, numerical simulation is computed by using Maltab software.

1.8 Thesis Outline

There are six chapters in this research project. This chapter which is Chapter 1 is the introduction chapter that includes the research background, statement of the problem, research objectives, significance of the study and scope of the study. Chapter 2 presents the literature review of this study. Various works by different researchers regarding Stefan problems and solidification are presented. Some numerical methods used to simulate solidification process are also discussed in

Chapter 2.

Mathematical formulation is stated in Chapter 3. The chapter is started with the governing equation followed by algorithm of the solution. Four steps for simulating the model are given in this chapter. In Chapter 4, discretization by using finite difference method is shown. Essentially-non oscillatory (ENO) method and upwind method are also considered in this chapter. The result and discussion for this research are given in Chapter 5. In Chapter 6, the conclusion of the research is presented and recommendation for future work is delivered.

REFERENCES

1. Saitou, T., Rouzimaimaiti, M., Koshikawa, N., Seiki, M., Ichikawa, K. and Suzuki, T. 2012. Mathematical Modeling of Invadopodia Formation. *Journal of Theoretical Biology*. 298, 138-146.

2. Mohd Ariff Bin Admon. 2015. *Mathematical Modeling and Simulation in an Individual Cancer Cell Associated with Invadopodia Formation.* PHD Thesis, Osaka University, Japan.

3. Chen, S., Merriman, B., Osher, S. and Smereka, P. 1997. A Simple Level Set Method for Solving Stefan Problems. *Journal of Computational Physics*. 135(1), 8-29.

4. Murphy, K. 1989. Parameter Estimation in the Multidimensional Stefan Problem. *Decision and Control, 1989. Proceedings of the 28th IEEE Conference on IEEE*. 608-612.

5. Brattkus, K. and Meiron, D. 1992. Numerical Simulations of Unsteady Crystal Growth. *SIAM Journal on Applied Mathematics*. 52(5), 1303-1320.

6. Dunbar, W. B., Petit, N., Rouchon, P. and Martin, P. 2003. Boundary Control of a Nonlinear Stefan Problem. *Decision and Control, 2003. Proceedings. 42nd IEEE Conference on IEEE*. 1309-1314.

7. Sethian, J. A. and Straint, J. 1992. Crystal Growth and Dendritic Solidification. *Journal of Computational Physics*. 77(2), 231-253.

8. Gammon, J. and Howarth, J. 1995. The Two-Dimensional Stefan Problem with Slightly Varying Heat Flux. *International communications in Heat and Mass Transfer*. 22(5), 629-638.

9. Sussman, M., Smereka, P. and Osher, S. 1994. A Level Set Approach for Computing Solutions to Incompressible Two-Phase Flow. *Journal of Computational Physics*. 114(1), 146-159.

10. Juric, D. and Tryggvason, G. 1996. A Front-Tracking Method for Dendritic Solidification. *Journal of Computational Physics*. 123(1), 127-148.

11. Wang, S. L. and Sekerka, R. F. 1996. Algorithms for Phase Field Computation of the Dendritic Operating State at Large Supercoolings. *Journal of Computational Physics*. 127(1), 110-117.

12. Schmidt, A. 1996. Computation of Three Dimensional Dendrites with Finite Elements. *Journal of Computational Physics*. 125(2), 293-312.

13. Mitchell, I. M. 2008. The Flexible, Extensible and Efficient Toolbox of Level Set Methods. *Journal of Scientific Computing*. 35(2-3), 300-329.

14. Tan, L. and Zabaras, N. 2006. A Level Set Simulation of Dendritic Solidification with Combined Features of Front-Tracking and Fixed-Domain Methods. *Journal of Computational Physics*. 211(1), 36-63.

15. Rubinshtein, L. 1971. *The Stefan Problem.* American Mathematical Soc.

16. Barry, S. I. and Caunce, J. 2008. Exact and numerical solutions to a Stefan problem with two moving boundaries. *Applied Mathematical Modelling*. 32(1), 83-98.

17. Geng Tian. 2005. *Level Set Methods and Sloshing Problems.* Master Thesis, Saint Marys University, Halifax.

18. Voller, VR. and Falcini, F. 2013. Two exact solutions of a Stefan problem with varying diffusivity. *International Journal of Heat and Mass Transfer*. 58(1), 80-85.

19. Matano, H 1983. Asymptotic behavior of the free boundaries arising in one phase Stefan problems in multi-dimensional spaces. *North-Holland Mathematics Studies*. 81, 133-151.

20. Lun, L., Yeckel, A. and Derby, J. J. 2010. A Schur Complement Formulation for Solving Free-Boundary, Stefan Problems of Phase Change. *Journal of Computational Physics*. 229(20), 7942-7955.

21. Flemings, M. C. 1974. Solidification Processing. *Metallurgical Transactions*. 5(10), 2121-2134.

22. Barrett, J. W., Garcke, H. and Nurnberg, R. 2010. On Stable Parametric Finite Element Methods for the Stefan Problem and the MullinsSekerka Problem with Applications to Dendritic Growth. *Journal of Computational Physics*. 229(18), 6270-6299.

23. Wang, G. X. and Matthys, E. 1992. Numerical Modelling of Phase Change and Heat Transfer during Rapid Solidification Processes: Use of Control Volume Integrals with Element Subdivision. *International Journal of Heat and Mass Transfer*. 35(1), 141-153.

24. Shingu, P. H. and Ozaki, R. 1975. Solidification Rate in Rapid Conduction Cooling. *Metallurgical Transactions A*. 6(1), 33-37.

25. Osher, S. and Fedkiw, R. 1992. *Level Set Methods and Dynamic Implicit Surfaces.* Verlag New York Inc.:Springer Science and Business Media.

26. Shaikh, J., Sharma, A. and Bhardwaj, R,. 2016. On Sharp-Interface Level-Set Method for Heat and/or Mass Transfer Induced Stefan Problem. *International Journal of Heat and Mass Transfer*. 96, 458-473.

27. Shu, C-W. and Osher, S. 1988. Efficient Implementation of Essentially Non-Oscillatory Shock-Capturing Schemes. *Journal of Computational Physics*. 77(2), 439-471.

28. Russo, G. and Smereka, P. 2000. A Remark on Computing Distance Functions. *Journal of Computational Physics*. 163(1), 51-67.

29. Fedkiw, R, P., Aslam, T., Merriman, B. and Osher, S. 1999. A Non-Oscillatory Eulerian Approach to Interfaces in Multimaterial Flows (The Ghost Fluid Method). *Journal of Computational Physics*. 152(2), 457-492.

30. Rouy, E. and Tourin, A. 1992. A Viscosity Solutions Approach to Shape-From-Shading. *SIAM Journal on Numerical Analysis*. 29(3), 867-884.