Accurate Solution and Gradient Computation for Interface Problems

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Abstract

There are numerous applications of ordinary or partial differential equations of boundary value problems (BVPs) such as the Navier-Stokes equations for bubble simulations or the Stefan problem modeling the interface between ice and water that are known as interface problems. For many interface problems, the free boundary or moving interface depends on the gradient of the solution. It is important to obtain not only the accurate solution but also accurate first order derivatives of the solution. There are several effective numerical methods such as finite difference or finite element methods for numerical ODE/PDEs that can generate accurate solutions but less accurate derivatives. During our research, we explored ways to compute solutions and derivatives to ODE/PDE BVPs accurately at the same time, particularly using a finite difference discretization. We began by writing code to solve two-point boundary value problems in one dimension, then moved our focus to problems with singular sources described by Dirac Delta functions, variable but discontinuous coefficients. We have implemented both Peskin's Immersed Boundary (IB) Method and Li's Immersed Interface Method (IIM). In our research, we have confirmed that IB method is first order accurate while IIM is second order in the L^∞ norm. We further confirmed that the computed derivatives at the interface using one-sided finite differences were only first order accurate in general while the two sided approach using the IIM were second order accurate. The second conclusion is new and significant in this area. Multiple examples were examined that allowed us to confirm these findings. A proof for this result has yet to be found, and is a possibility for future work.

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1 Introduction

The physical phenomena of interactions at an interface are vast in the field of physics, which are described by the use of ordinary differential equations (ODE's) and partial differential equations (PDE's). Some examples of interface problems are water and ice, two masses with different heat conductivity that are in contact, and bubbles in a fluid. In general, interface problems introduce

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discontinuous coefficients and solutions, and they may also introduce point forces. These three factors make the mathematics of solving them more challenging. Accurate numerical methods exist for problems with smooth solutions, but they fail when the interface introduces such irregularities. It is also significantly important to be able to approximate the derivatives of the solutions at an interface, but few methods can do this accurately. The two finite difference methods, which we will discuss in this paper, that approximate the solutions to interface problems include Peskin's Immersed Boundary (IB) method, and the Li's Immersed Interface Method (IIM).

1.1 Derivative at a boundary

Before investigating interface problems, we will examine how to solve for the derivative of a finite difference numerical solution at the boundary using finite difference methods. There are many different formulas that can be applied to suit our needs to find $u'(x)$. The first method we will use utilize is a forward difference at the left boundary

$$u'(x) = \frac{u(x+h) - u(x)}{h},$$

or a backwards difference at the right boundary

$$u'(x) = \frac{u(x) - u(x+h)}{h}.$$

Geometrically, what these formulas compute is the secant line of the point at the interface and the point nearest to it. As the step size goes to zero the secant line becomes more of a tangent line at the boundary which will give us the derivative at a boundary.

The second types of difference formula examined were three point one sided forward and backward differences. These can be derived using the method of undetermined coefficients [3]. At the left boundary the stencil forward stencil is used, so for a problem where the domain is $[a, b]$ then,

$$u'(a) = -\frac{3}{2h}u(a) + \frac{2}{h}u(a+h) - \frac{1}{2h}u(a+2h)$$

and at the right boundary the stencil reads

$$u'(b) = \frac{3}{2h}u(b) - \frac{2}{h}u(b-h) + \frac{1}{2h}u(b-2h).$$

A third approximation scheme we explored was a rearrangement of the ghost point method used for approximating Poisson problems with Neumann boundary conditions with second order accuracy. The formula for the method was given in Zhillin Li's notes for the class MA 584 [3]

The difference formulas above were derived and applied to multiple numerically approximated finite difference solutions of 1-D boundary value problems so that derivatives may be approximated. Through numerical experimentations, we found that for all the cases examined, that the standard boundary value problems using the two point stencil yielded a first order accurate derivative while both the three point one sided and the ghost point methods yielded second order accurate derivatives.

1.2 Second order convergence for u'(x) with a three point finite difference stencil

Proof: For a regular problem we know that the solution will be smooth across the entire domain.

$$u''(x) = f(x), \quad a < x < b, \quad u(a) = u_a, \quad u(b) = u_b$$

Consequently, we know that the local truncation error is

$$\tau_i = \frac{u_{i-1} - 2u_i + u_{i+1}}{h^2} - f(x_i)$$

We assume that the approximate solution is equal to the exact solution plus an error term

$$U_i = u_i + c_i h^2.$$

Solving for u_i and substituting back into the local truncation equation we get

$$\tau_i = \frac{(U_{i-1} - c_{i-1}h^2) - 2(U_i - c_i h^2) + (U_{i+1} - c_{i+1}h^2)}{h^2} - f(x_i).$$

Rearranging this equation yields

$$\tau_i = \frac{U_{i-1} - 2U_i + U_{i+1}}{h^2} - f(x_i) - (c_{i-1} - 2c_i + c_{i+1}).$$

Because of the definition of the finite difference stencil the above equation is simplified to

$$\tau = -Ach^2$$

where A is a tridiagnal coefficient matrix and c is a column vector. Rearranging the equation gives

$$c = -A^{-1}\frac{\tau}{h^2}.$$

We know that the solution is smooth across the domain which allows us to conclude that τ also will be smooth and $O(h^2)$, leaving us with the result that c is smooth and of $O(1)$.

We now look at the approximation for the derivative

$$\frac{U_{i+1} - U_{i-1}}{2h} \approx u'(x).$$

Considering error we get

$$\frac{U_{i+1} - U_{i-1}}{2h} = \frac{u(x_{i+1}) + c_{i+1}h^2 - u(x_{i-1}) - c_{i-1}h^2}{2h}$$

$$= \frac{u_{i+1} - u_{i-1}}{2h} + \frac{c_{i+1} - c_{i-1}}{2h}h^2$$

Using taylor series expansion for the first term, and realizing that c is O(1) and smooth, the result is

$$= u'(x) + O(h^2)$$

This shows that using this method gives $u'(x) \approx O(h^2)$ thus completing the proof. //

1.3 Examples

Example 1.1. *Here is an example Robin boundary condition problem whose solution was computed numerically along with the approximation's derivatives at the boundary.*

$$u''(x) = 2\pi e^{x}\cos(x)$$

$$u(0) + \frac{\partial u}{\partial x}(0) = \pi, \quad u(\pi) = 0 \quad x \in [0, \pi]$$

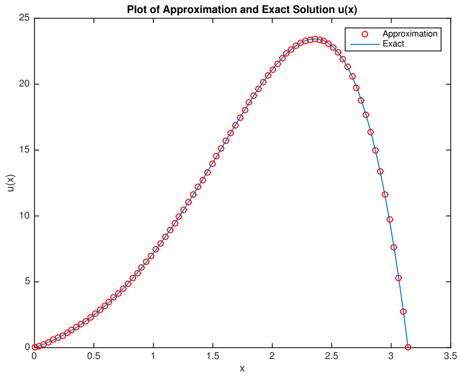

Figure 1: (a): Approximation of solution and exact solution.

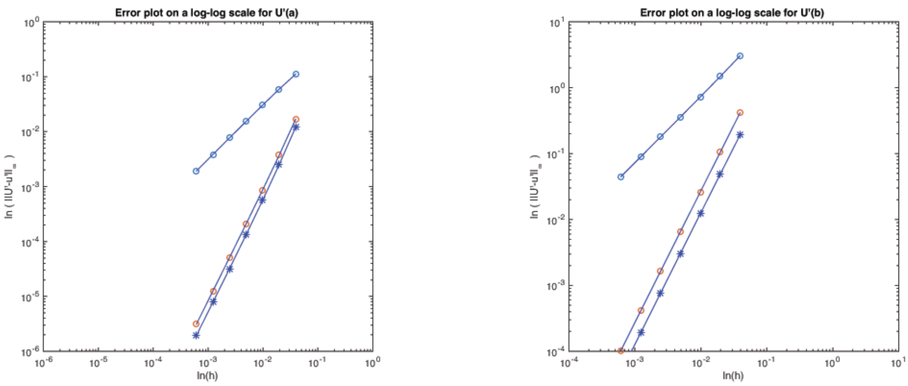

Figure 2: (a): Grid refinement analysis of the derivative of the finite difference solution at the left boundary to the problem presented. Note the the blue circles, red circles, and blue asterisks represent the forward, 3pt. one-sided, and ghost point methods respectively (b): Note the the blue circles, red circles, and blue asterisks represent the backward, 3pt. one-sided, and ghost point methods respectively

2 Interface Problems and Computational Methods for Interface Problems

2.1 Simple Model Example of an Interface Problem

An example of an interface problem is the pulling of a rubber band at a point when it is fixed at both ends. Note that the force that is pulling the rubber band is a point force. Consequently, the parts of the band that are to the left and to the right of the point force have different tension (modeled by a discontinuous β). The following diagram illustrates this problem [5]

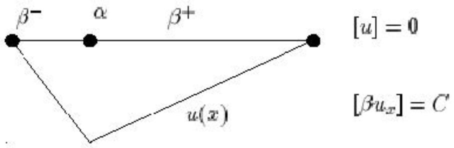

Figure 3: A diagram of the solution. The solution is not smooth at the interface $x = \alpha$ due to the singular delta function source modeling the application of the force

The above problem has the following mathematical formulation as a two point boundary value problem with an interface:

$$(\beta u')' = f + c\delta(x - \alpha), \quad 0 < x < 1, \quad 0 < \alpha < 1 \quad u(0) = u(1) = 0$$

There are two equivalent ways in which this problem can be formulated. The first way is the formulation above over the domain $(0, 1)$ with the explicit use of the Dirac delta function to model the discontinuity of the derivative.

The second way to formulate the problem is by splitting the domain into two subdomains around the singularity and expressing the discontinuity of the problem using the jump conditions which can be found from integrating the problem from $x = \alpha^-$ to $x = \alpha^+$ [5].

$$(\beta u_x)_x = f(x), \quad x \in (0, \alpha) \cup (\alpha, 1)$$

$$[u]_{x=a} = 0 \qquad [\beta u_x]_{x=\alpha} = v$$

Where the notation $[u]$ implies:

$$[u]_{x=\alpha} = \lim_{x \to \alpha^+} u(x) - \lim_{x \to \alpha^-} u(x).$$

Note here that the following assumptions are made in this formulation: $f(x) \in L^2(0, 1), \sigma(x) \in C(0, 1), \beta(x) \in C^1(0, \alpha) \cup (\alpha, 1)$ [5]. Using finite differences, we computed solutions of this interface problem and more general problems using both formulations.

2.2 Review of Finite Difference Methods for Interface Problems and Their Application to the Rubber Band Problem

There are many methods which can be used to approximate solutions to interface problems with the finite difference method. One of the easiest methods to apply is the Peskin's Immersed Boundary method. The main idea of the method is to directly approximate the Dirac Delta function at the interface with a direct discretization of the Dirac Delta function. The main goal of our research however, is to examine the order of accuracy of the Immersed Interface Method's(IIM) approximate solution's derivative using the IIM at the interface of interface problems. So, the primary method we will use to approximate solutions to interface problems will be the IIM. The IIM uses the second formulation of the 1-D interface boundary value problem, and uses the jump conditions to find the finite difference equations and corection terms to be used at points directly before, after, or at the interface.

2.3 Peskin's Method

The first method investigated was Peskin's Immersed Boundary method which implements the first formulation of the problem. Peskin's method seeks to model the interface by using a discretization of the Dirac Delta function. One example of the function is called the hat delta function which is given by [5]

$$\delta_\epsilon(x) = \begin{cases} \frac{\epsilon-|x|}{\epsilon^2}, & \text{if } |x| < \epsilon \\ 0, & \text{if } |x| \geq \epsilon \end{cases}$$

Another way to express the delta function is with the cosine delta function which is given by [5]

$$\delta_\epsilon(x) = \begin{cases} \frac{1}{4\epsilon}(1 + cos(\frac{\pi x}{2\epsilon})), & \text{if } |x| < 2\epsilon \\ 0, & \text{if } |x| \geq 2\epsilon \end{cases}$$

To implement the Peskin's Immersed Boundary method, one uses the standard three point finite difference scheme with the modified right hand side including the discrete Dirac Delta function [5]

$$\frac{U_{j-1} - 2U_j + U_{j+1}}{h^2} = c\delta_h(x_j - \alpha).$$

Note that when δ_h is the hat delta function this gives an exact solution. So, $U_i = u(x_i)$ at all grid points for this model problem in 1-D. On the other hand, the smooth cosine discretization of the delta function originally published by Peskin results in only a first order accurate solution.

2.4 Immersed Interface Method

The Immersed Interface Method is inspired by Peskin's Immersed Boundary Method, but it treats interface problems differently. Peskin's method discretizes the interface while the Immersed Interface boundary method uses jump conditions to work around the delta function. As an example of how the method is derived, consider the rubber band model problem given by [5]

$$\beta u'' = f + c\delta(x - \alpha), \quad 0 < x < 1, 0 < \alpha < 1 \quad u(0) = u(1) = 0.$$

Where β can be thought of as the string tension and is piecewise constant [5].

$$\beta = \begin{cases} \beta^-, & 0 < x < \alpha \\ \beta^+, & \alpha < x < 1 \end{cases}$$

From the problem we know that:

$$[u] = u^+ - u^- = 0$$

And by integrating the ODE from $x = \alpha^-$ to $x = \alpha^+$ we get the following jump condition

$$[\beta u_x] = \beta^+ u^+ - \beta^- u^- = c$$

One can derive the second derivative jump condition from the ODE itself. Rearranging the jump terms, we get the three jump conditions [5]

$$u^+ = u^-, \quad u_x^+ = \frac{\beta^-}{\beta^+}u_x^- + \frac{c}{\beta^+}, \quad u_{xx}^+ = \frac{\beta^- u_{xx}^-}{\beta^+}$$

The above conditions are used to derive a two sided formula at points near the interface. The points directly at or next to the interface are called irregular grid points. However, all other points are called regular grid points therefore the standard central finite difference scheme

$$\frac{U_{i-1} - 2U_i + U_{i+1}}{h^2} = f_i$$

is used to provide a second order accurate approximation of $u(x)$ at $x = x_i$.

The only task now is to derive a finite difference scheme around the irregular grid points, those around the interface. We call the point at or directly left of the interface x_j, and the point directly to the right of the interface x_{j+1}. We begin by using the method of undetermined coefficients to derive a difference stencil for the x_j point [5].

$$\gamma_1 U_{j-1} + \gamma_2 U_j + \gamma_3 U_{j+1} = f_j.$$

To find the scheme at the irregular grid points we want to minimize the local truncation error at the irregular grid points x_j and x_{j+1} by using taylor expansions about $x = \alpha$ .The truncation error is given by [5]

$$T_j = \gamma_1 u_{j-1} + \gamma_2 u_j + \gamma_3 u_{j+1} - f(x_j) - C_j$$

Using the Taylor expansion of each point about $x = \alpha$ we get [5]

$$u(x_{j-1}) = u^- + u_x^-(x_{j-1} - \alpha) + \frac{(x_{j-1} - \alpha)^2}{2} u_{xx}^- + O(h^3)$$

$$u(x_j) = u^- + u_x^-(x_j - \alpha) + \frac{(x_j - \alpha)^2}{2} u_{xx}^- + O(h^3)$$

$$u(x_{j+1}) = u^+ + u_x^+(x_{j+1} - \alpha) + \frac{(x_{j+1} - \alpha)^2}{2} u_{xx}^+ + O(h^3).$$

The Taylor expansion for the point u_{j+1} is expressed in u^+ because it is on the right side of the interface. To use the method of undetermined coefficients to solve for γ_1 , γ_2 , γ_3 and C_j, we must express u_{j+1} in terms of u^-. This is the main idea of the IIM. We express the expansion of the point of the opposite side using terms from the side of the other two points using the interface relations(from jump conditions). To do this we use the jump relationships to get [5]

$$u_{j+1} = u^- + (\frac{\beta^-}{\beta^+} u_x^- + \frac{c}{\beta^+})(x_{j+1} - \alpha) + \frac{\beta^-}{\beta^+} \frac{(x_{j+1} - \alpha)^2}{2} u_{xx}^- + O(h^3)$$

Next we substitute the expanded points into the truncation equation to get [5]

$$T_j = \gamma_1(u^- + u_x^-(x_{j-1} - \alpha) + \frac{(x_{j-1} - \alpha)^2}{2} u_{xx}^- + O(h^3))$$

$$+\gamma_2(u^- + u_x^-(x_j - \alpha) + \frac{(x_j - \alpha)^2}{2} u_{xx}^- + O(h^3))$$

$$+\gamma_3(u^- + (\frac{\beta^-}{\beta^+} u_x^- + \frac{c}{\beta^+})(x_{j+1} - \alpha) + \frac{\beta^-}{\beta^+} \frac{(x_{j+1} - \alpha)^2}{2} u_{xx}^- + O(h^3)) - f_j - C_j$$

When we collect by u^-, $u_x,^-$ u_{xx}^- we are left this linear system of equations for the coefficients when the expression is set equal to the ODE [5]

$$\gamma_1 + \gamma_2 + \gamma_3 = 0$$

$$\gamma_1(x_{j-1} - \alpha) + \gamma_2(x_j - \alpha) + \gamma_3 \frac{\beta^-}{\beta^+}(x_{j+1} - \alpha) = 0$$

$$\gamma_1 \frac{(x_{j-1} - \alpha)^2}{2} + \gamma_2 \frac{(x_j - \alpha)^2}{2} + \gamma_3 \frac{\beta^-}{\beta^+} \frac{(x_{j+1} - \alpha)^2}{2} = \beta^-$$

and the correction term

$$C_j = \gamma_1(\frac{c}{\beta^+}(x_{j+1} - \alpha)).$$

With this, the system of equations can be solved for each γ and the finite difference stencil for the irregular grid point x_j will be found. The same method is then applied to the other irregular grid point x_{j+1}. With stencils for both irregular grid points computed, the approximate solution may be computed at the interface.

2.5 The IIM for General 1-D Elliptic Interface problems

In the previous section we explored the derivation of the Immersed Interface Method when the derivative of a function had a jump but the function itself and its' solution were continuous. In the most general case form of a 1-D elliptic interface problem, the function, its' solution, and the derivative can all jumps. Meaning the coefficients $\beta(x)$ and $\sigma(x)$, as well as $f(x)$ can have a finite jump at $x = \alpha$ while the solution may also have a jump $[u] = w$.

To begin the derivation of these types of problems we must determine the finite difference coefficients at $x = x_j$ which is the solution to the following linear system [5]:

$$\begin{cases} \gamma_{j,1} + \gamma_{j,2} + \left(1 + \dfrac{(x_{j+1}-\alpha)^2}{2\beta}[\sigma]\right)\gamma_{j,3} & = 0 \\ (x_{j-1}-\alpha)\gamma_{j,1} + (x_j-\alpha)\gamma_{j,2} + \Big\{\dfrac{\beta^-}{\beta^+}(x_{j+1}-\alpha) & \\ \qquad\qquad + \left(\dfrac{\beta_x^-}{\beta^+} - \dfrac{\beta^-\beta_x^+}{(\beta^+)^2}\right)\dfrac{(x_{j+1}-\alpha)^2}{2}\Big\}\gamma_{j,3} & = \beta_x^- \\ \dfrac{(x_{j-1}-\alpha)^2}{2}\gamma_{j,1} + \dfrac{(x_j-\alpha)^2}{2}\gamma_{j,2} + \dfrac{(x_{j+1}-\alpha)^2\beta^-}{2\beta^+}\gamma_{j,3} & = \beta^- \end{cases} \tag{1}$$

From the system we get $\gamma_{j,1}, \gamma_{j,2}$, and $\gamma_{j,3}$, now the correction term at $x = x_j$ that accounts for the jumps can be computed as [5]:

$$C_j = \gamma_{j,3}\{w + (x_{j+1}-\alpha)\frac{v}{\beta^+} - \frac{(x_{j+1}-\alpha)^2}{2}\left(\frac{\beta_x^+ v}{(\beta^+)^2} - \sigma^+\frac{w}{\beta^+} - \frac{[f]}{\beta^+}\right)\} \tag{2}$$

The linear system to find the coefficients of finite difference equation at $x = x_{j+1}$ [5] is:

$$\begin{cases} \left(1 - \dfrac{(x_j-\alpha)^2}{2\beta^-}[\sigma]\right)\gamma_{j+1,1} + \gamma_{j+1,2} + \gamma_{j+1,3} & = 0 \\ \Big\{\dfrac{\beta^+}{\beta^-}(x_j-\alpha) + \left(\dfrac{\beta_x^+}{\beta^-} - \dfrac{\beta_x^-\beta^+}{(\beta)^2}\right)\dfrac{(x_j-\alpha)^2}{2}\Big\}\gamma_{j+1,1} & \\ \qquad\qquad + (x_{j+1}-\alpha)\gamma_{j+1,2} + (x_{j+2}-\alpha)\gamma_{j+1,3} & = \beta_x^+ \\ \dfrac{(x_j-\alpha)^2}{2}\dfrac{\beta^+}{\beta^-}\gamma_{j+1,1} + \dfrac{(x_{j+1}-\alpha)^2}{2}\gamma_{j+1,2} + \dfrac{(x_{j+2}-\alpha)^2}{2}\gamma_{j+1,3} & = \beta^+ \end{cases} \tag{3}$$

Finally, the correction term for C_{j+1} [5] is:

$$C_{j+1} = \gamma_{j+1,1}\Big\{-w - (x_j-\alpha)\frac{v}{\beta^-} - \frac{1}{2}(x_j-\alpha)^2\left(-\frac{\beta_x^- v}{(\beta^-)^2} + \sigma^-\frac{w}{\beta^-} + \frac{[f]}{\beta^-}\right)\Big\} \tag{4}$$

Note that it is clearly shown that the linear systems for x_j and x_{j+1} is are the same if we switch the '+' and '-' symbols.

2.6 Using the IIM to Compute Derivatives of IIM Computed Approximations

Approximate solutions from the IIM are guaranteed to be second order accurate. In areas where the derivative and possibly the solution are not smooth, it is well known that standard one sided differences may often yield $O(h)$ accurate derivatives. It is also known that standard two sided difference formulas are incapable of yielding 2nd order accurate derivatives along the interface for derivatives which are not smooth. Considering that many problems will not have smooth solutions nor smooth derivatives it is significant to have a method which can produce 2nd order accurate results for the derivative along an interface. The IIM can be applied to approximate solutions yielded by the IIM to produce second order accurate approximate derivatives at an interface.

2.7 General derivation for $u'(x)$ at the interface

The IIM guarantees that the approximated solutions to the interface are second order. To derive a two sided difference formula for the derivative of the solution at the interface, we must apply the IIM a second time to the solutions originally given. Note that: methods used to derive the derivative were identical to those used to derive the IIM

$$T_j = \gamma_1 u_{j-1} + \gamma_2 u_j + \gamma_3 u_{j+1} - f(x_j) - C_j$$

$$T_j = \gamma_1 (u^- + u_x^-(x_{j-1} - \alpha) + \frac{(x_{j-1} - \alpha)^2}{2} u_{xx}^- + O(h^3))$$

$$+\gamma_2 (u^- + u_x^-(x_j - \alpha) + \frac{(x_j - \alpha)^2}{2} u_{xx}^- + O(h^3))$$

$$+\gamma_3 (u^- + w + (\frac{\beta^-}{\beta^+} u_x^- + \frac{c}{\beta^+})(x_{j+1} - \alpha) + \frac{\beta^-}{\beta^+} \frac{(x_{j+1} - \alpha)^2}{2} u_{xx}^- + O(h^3)) - f_j - C_j$$

Once we have collected by u and its derivatives we set the u' equal to one and the other linear equations to zero to derive a formula for u' at the interface.

$$\gamma_1 + \gamma_2 + \gamma_3 = 0$$

$$\gamma_1 (x_{j-1} - \alpha) + \gamma_2 (x_j - \alpha) + \gamma_3 \frac{\beta^-}{\beta^+} (x_{j+1} - \alpha) = 1$$

$$\gamma_1 \frac{(x_{j-1} - \alpha)^2}{2} + \gamma_2 \frac{(x_j - \alpha)^2}{2} + \gamma_3 \frac{\beta^-}{\beta^+} \frac{(x_{j+1} - \alpha)^2}{2} = 0$$

and the correction term

$$C_j = \gamma_1 (w + \frac{c}{\beta^+}(x_{j+1} - \alpha)).$$

When this system is solved for γ_1, γ_2, and γ_3 we are left with the 2 sided stencil for $u'(x)$ at an interface. This derivation is to give the reader a general overview of how solving for the derivative at an interface can be done using the IIM. This is how our Matlab codes solves for the $u'(x)$. In this derivation we assume $u = U$ when really what we should be considering is $u = U + ch^2$ because we are using IIM approximated solutions. It may seem as though this should not be second order because of this fact, however examples show that the approximation for $u'(x)$ is in fact 2nd order. A formal proof explaining why this is second order is still in progress. Never the less, we have found a way to obtain 2nd order accurate results for the derivative at an interface using a two sided stencil, which is something that is significant and can not be found in standard literature.

2.8 Examples of Second Order Accurate Solutions and Derivatives Using the IIM

Here are some sample computations demonstrating the second order accurate derivative at the interface for the 1-D interface problem presented in "The Immersed Interface Method" by Dr.Li by using a two sided method directly related to the IIM. The 1-D Interface problem where $x \in (0, \alpha) \cup (\alpha, 1)$ is often expressed as:

$$(\beta_x u)_x - \sigma u = f$$

In the examples presented here, all the functions have finite jumps at the interface α. The same β and σ are used throughout, and the proper Dirichlet boundary condition according the the actual solution are always chosen. Note

$$\beta(x) = \begin{cases} 1 + \frac{\cos(x)}{2} & \text{if} \quad x < \alpha \\ 1 + x^2 \quad \text{if} \quad x > \alpha \end{cases}$$

and

$$\sigma(x) = \begin{cases} (1+x)^2 & \text{if} \quad x < \alpha \\ \ln(2+x) & \text{if} \quad x > \alpha \end{cases} .$$

Example 2.1. *Consider the problem where*

$$f(x) = \begin{cases} (120)^2(-(\frac{\cos(x)}{2}+1))\sin(120x) - \frac{120}{2}\sin(x)\cos(120x) - (1+x)^2\cos(120x) & \textit{if} \quad x < \alpha \\ (30)(-30(x^2+1)\cos(30x) - 2x\sin(30x)) - \ln(2+x)\cos(30x) & \textit{if} \quad x > \alpha. \end{cases}$$

The exact solution can be shown to be

$$u(x) = \begin{cases} \sin(120x) & \textit{if} \quad x < \alpha \\ \cos(30x) & \textit{if} \quad x > \alpha \end{cases}$$

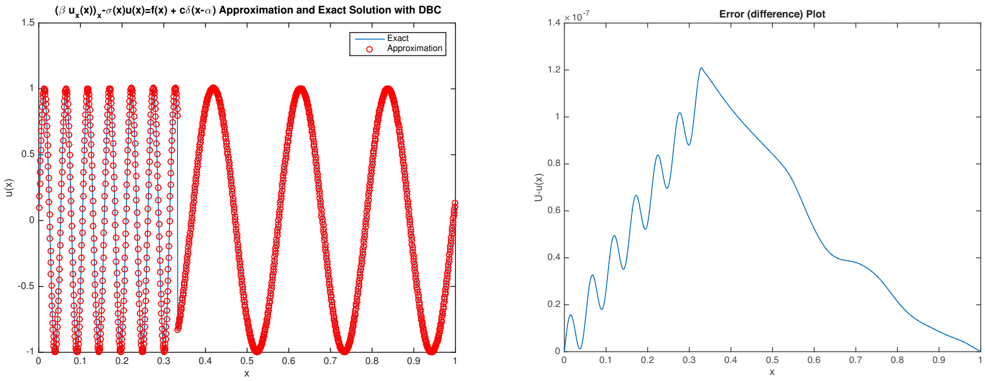

Figure 4: (a): An example of a computed solution with $n = 1280$ grid divisions. Note the actual solution has its discontinuity connected by the plotter. (b): The error difference of the solution and actual solution at the grid points.

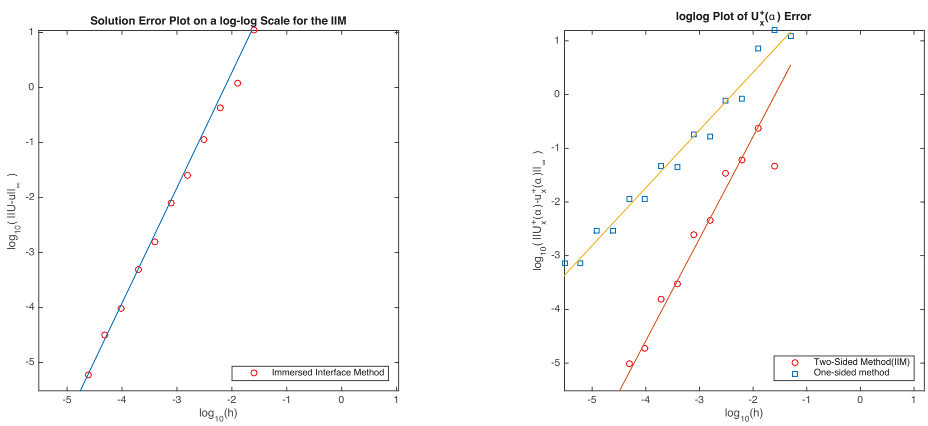

Figure 5: (a): Grid refinement analysis of the approximate solution with 15 refinements starting at $n = 20$. Note that the axis has been adjusted so some points may not be visible. The slope of the regression line fit is 2.1 (b):Grid refinement analysis of the right derivative at the interface with the one-sided and two-sided(IIM) methods. Note that a linear regression fit shows that the slope of the line of best fit is 1.08 and 1.90 for the one-sided and two-sided methods respectively. This shows the IIM two sided method gave an order 2 accurate approximation while standard one-sided methods gave a first order accurate approximation.

Example 2.2. *Consider the problem where*

$$f(x) = \begin{cases} (120)^2(-(\dfrac{\cos(x)}{2}+1))\sin(120x) - \dfrac{120}{2}\sin(x)\cos(120x) - (1+x)^2\sin(120x) & \text{if} \quad x < \alpha \\ \dfrac{x^2+200x-1}{(x+100)^2} - \ln(2+x)\ln(100+x) & \text{if} \quad x > \alpha. \end{cases}$$

The exact solution can be shown to be

$$u(x) = \begin{cases} \sin(120x) & \text{if} \quad x < \alpha \\ \ln(100+x) & \text{if} \quad x > \alpha \end{cases}$$

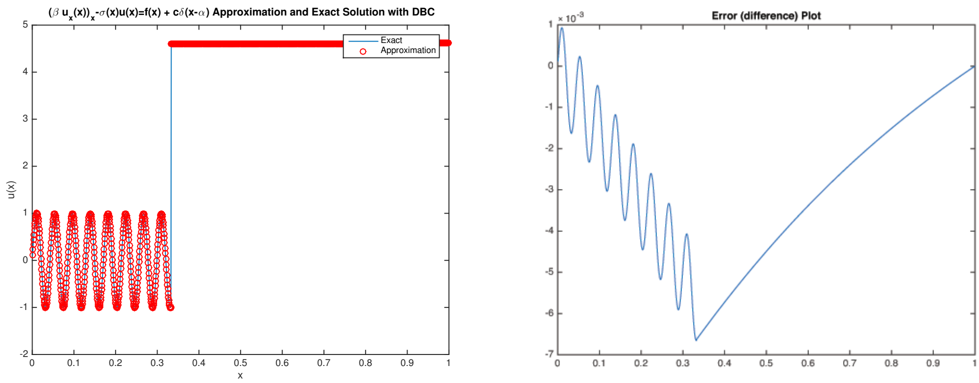

Figure 6: (a): An example of a computed solution with $n = 1280$ grid divisions. Note the actual solution has its discontinuity connected by the plotter. Note that the axis has been adjusted so some points may not be visible. (b): The error difference of the solution and actual solution at the grid points.

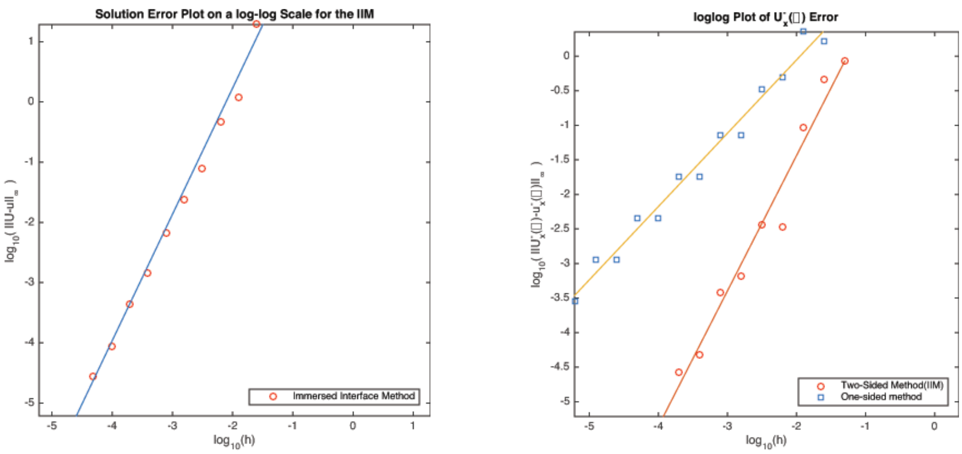

Figure 7: (a): Grid refinement analysis of the approximate solution with 14 refinements starting at $n = 20$. Note that the axis has been adjusted so some points may not be visible. The slope of the regression line fit is 2.1 (b):Grid refinement analysis of the left derivative at the interface with the one-sided and two-sided(IIM) methods. Note that a linear regression fit shows that the slope of the line of best fit is about 1.06 and 1.96 for the one-sided and two-sided methods respectively. This shows the IIM two sided method gave an order 2 accurate approximation while standard one-sided methods gave a first order accurate approximation.

Example 2.3. *Consider the problem where*

$$f(x) = \begin{cases} (15)^2(1+\dfrac{\cos(x)}{2})\sinh(15x) - (15)\dfrac{\sin(x)}{2}\cosh(15x) - (1+x)^2\sinh(15x) & \text{if} \quad x < \alpha \\ (-(x^2+1)\cosh(x) - 2x\sinh(x)) - \ln(2+x)\cosh(x) \quad \text{if} \quad x > \alpha. \end{cases}$$

The exact solution can be shown to be

$$u(x) = \begin{cases} \sinh(15x) & \text{if} \quad x < \alpha \\ \cosh(x) & \text{if} \quad x > \alpha \end{cases}$$

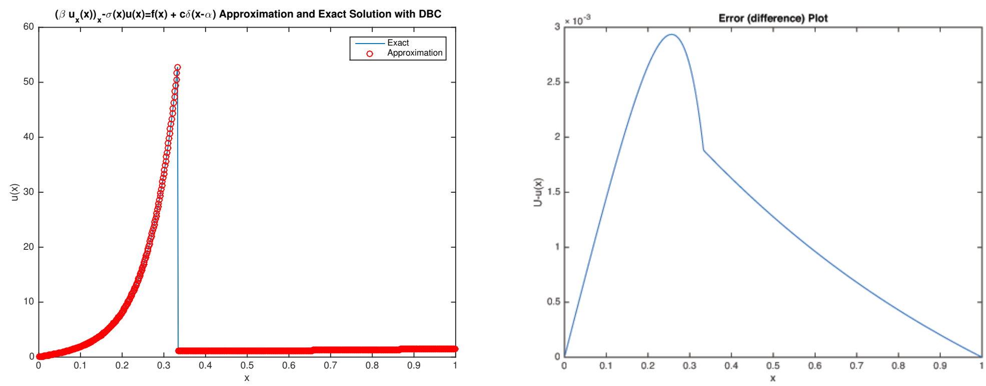

Figure 8: (a): An example of a computed solution with $n = 640$ grid divisions. Note the actual solution has its discontinuity connected by the plotter. (b): The error difference of the solution and actual solution at the grid points.

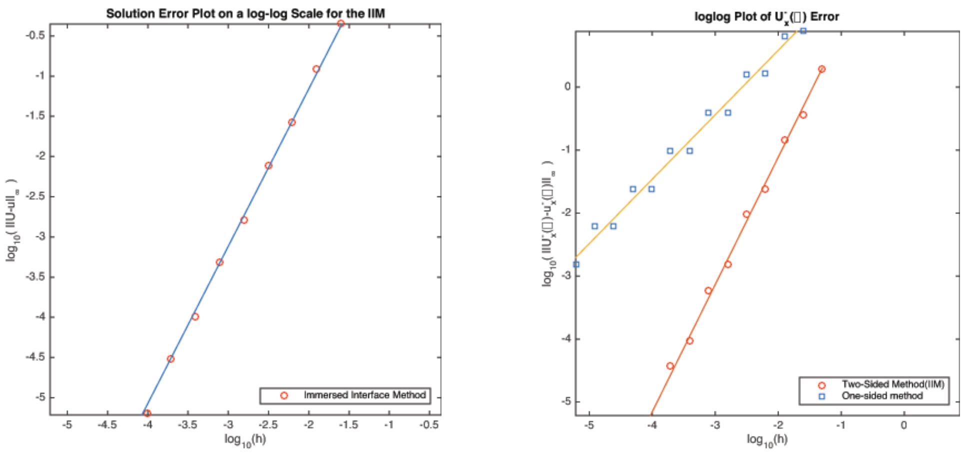

Figure 9: (a): Grid refinement analysis of the approximate solution with 14 refinements starting at $n = 20$.Note that the axis has been adjusted so some points may not be visible. The slope of the regression line fit is 1.96 (b):Grid refinement analysis of the left derivative at the interface with the one-sided and two-sided(IIM) methods. Note that a linear regression fit shows that the slope of the line of best fit is about 1.02 and 2.02 for the one-sided and two-sided methods respectively. This shows the IIM two sided method gave an order 2 accurate approximation while standard one-sided methods gave a first order accurate approximation.

3 Interface Problem in Polar coordinates with Axis-Symmetry

Up to this point the problems we have considered have been 1 dimensional in cartesian coordinates. In cartesian coordinates we have generally explored that the IIM was second order accurate for $u(x)$ and $u'(x)$ so we then chose to investigate how the accuracy of the IIM behaved when working with ODE's in new coordinate systems. In polar coordinates the Poisson equation is [3]

$$\frac{1}{r}\frac{\partial}{\partial r}(r\beta\frac{\partial u}{\partial r}) + \frac{1}{r^2}\frac{\partial^2 u}{\partial \theta^2} = f(r,\theta).$$

However, it is important to note that for our purposes we have chosen to use the axis-symmetric case, and turned the problem into an interface problem. The equation now is

$$\frac{1}{r}\frac{\partial}{\partial r}(r\beta\frac{\partial u}{\partial r}) = f(r)$$

Where $r \in (0,\alpha) \cup (\alpha, 1)$. Note that β, u_r, and u have finite jumps at α. Note that β is piece-wise constant for simplicity.

3.1 Finite Differences in Polar Coordinates

If the origin is not in the domain, $R_1 \leq r \leq R_2$, we can use a uniform grid to discretize the equation:

$$r_i = R_1 + i\Delta r, \qquad i = 0, 1, ..., m, \qquad \Delta r = \frac{R_2 - R_1}{m}$$

The finite difference stencil using the conservative form is [3]

$$\beta^{\pm}\frac{1}{r_i}\frac{r_{i-\frac{1}{2}}U_{i-1} - \left(r_{i-\frac{1}{2}} + r_{i+\frac{1}{2}}\right)U_i + r_{i+\frac{1}{2}}U_{i+1}}{(\Delta r)^2} = f(r_i)$$

3.2 Treating the boundary conditions

When the origin is within the domain of the boundary additional methods are needed to discretize the problem. There are various methods to deal with the pole singularity, but they will often lead to an undesirable structure of the coefficient matrix. One of the ways which will preserve the diagonal dominant coefficient matrix is to use a staggered grid [3]:

$$r_i = (i - \frac{1}{2})\Delta r, \qquad \Delta r = \frac{R_2}{m - \frac{1}{2}}, \qquad i = 1, 2...m.$$

We can use the conservative form of the discretization at $i = 2, \ldots, m-1$ except for $i = 1$ however at $i = 1$ we use the non-conservative form to work around the pole singularity. It can be shown that we get is [3]

$$\frac{-2U_1 + U_2}{(\Delta r)^2} + \frac{1}{r_1}\frac{U_2}{2\Delta r} = f(r_1).$$

With this we have what is needed to solve the interface problem at regular gridpoints. When the point directly at or to the left of the interface (r_j) or the point directly to the right of the interface (r_{j+1}) are of concern, we apply the IIM to solve for the solutions and their derivatives at the irregular points. The IIM changes only slightly in the new coordinate system since the problem is still a 1-D elliptic problem.

3.3 IIM

A polar coordinate problem presented in the form:

$$\frac{1}{r}\frac{\partial}{\partial r}(r\beta\frac{\partial u}{\partial r}) = f(r)$$

can be rewritten in the following format:

$$\frac{1}{r}(r\beta u_r)_r = f$$

We are given the jump conditions $[u] = v$, $[\beta u_r] = c$ which implies,

$$u^+ - u^- = v, \beta^+ u_r^+ - \beta^- u_r^+ = c$$

Multiplying the equation by r yields $(r\beta u_r)_r = rf$ and subsequently expanding the equation gives $\beta u_r + \beta r u_{rr} = rf$. Applying the jump conditions at $r = \alpha$ gives the equation $[\beta u_{rr}] = [f] - \frac{c}{\alpha}$ Rearranging the jump conditions we have

$$u^+ = v + u^-, u_r^+ = \frac{c}{\beta^+} + \frac{\beta^- u_r^-}{\beta^+}, u_{rr}^+ = \frac{[f]}{\beta^+} - \frac{c}{\alpha\beta^+} + \frac{\beta^- u_{rr}^-}{\beta^+}$$

To derive a stencil at the point r_j , we apply the method of undetermined coefficients to the truncation equation

$$T_j = \gamma_{j,1}u_{j-1} + \gamma_{j,2}u_j + \gamma_{j,3}u_{j+1} - rf_j - C_j$$

The Taylor series expansions at $r = j-1, j$, and $j+1$ about α are given below

$$u(r_{j-1}) = u^- + u_r^-(r_{j-1} - \alpha) + u_{rr}^-\frac{(r_{j-1}-\alpha)^2}{2} + O(h^3)$$

$$u(r_j) = u^- + u_r^-(r_j - \alpha) + u_{rr}^-\frac{(r_j-\alpha)^2}{2} + O(h^3)$$

$$u(r_{j+1}) = u^+ + u_r^+(r_{j+1} - \alpha) + u_{rr}^+\frac{(r_{j+1}-\alpha)^2}{2} + O(h^3)$$

Substituting terms on the '+' side in terms of '-'s gives the following for $r = j+1$

$$u(r_{j+1}) = v + u^- + \left(\frac{c}{\beta^+} + \frac{\beta^- u_r^-}{\beta^+}\right)(r_{j+1} - \alpha) + \left(\frac{[f]}{\beta^+} - \frac{c}{\alpha\beta^+} + \frac{\beta^- u_{rr}^-}{\beta^+}\right)\frac{(r_{j+1}-\alpha)^2}{2} + O(h^3)$$

Expanding the terms of the truncation equation gives

$$T_j = \gamma_{j,1}\left(u^- + u_r^-(r_{j-1} - \alpha) + u_{rr}^-\frac{(r_{j-1}-\alpha)^2}{2}\right)$$

$$+\gamma_{j,2}\left(u^- + u_r^-(r_j - \alpha) + u_{rr}^-\frac{(r_j-\alpha)^2}{2}\right)$$

$$+\gamma_{j,3}\left(v + u^- + \left[\frac{c}{\beta^+} + u_r^-\frac{\beta^-}{\beta^+}\right](r_{j+1} - \alpha) + \left[\frac{[f]}{\beta^+} - \frac{c}{\alpha\beta^+} + u_{rr}^-\frac{\beta^-}{\beta^+}\right]\frac{(r_{j+1}-\alpha)^2}{2}\right) - rf_j - C_j$$

Collecting the u^-, u_r^-, and u_{rr}^- terms and setting them equal to the ODE, creates the following system of equations

$$\begin{cases} \gamma_{j,1} + \gamma_{j,2} + \gamma_{j,3} & = 0 \\ (r_{j-1}-\alpha)\gamma_{j,1} + (r_j - \alpha)\gamma_{j,2} + (r_{j+1}-\alpha)\frac{\beta^-}{\beta^+}\gamma_{j,3} & = \beta^- \\ \dfrac{(r_{j-1}-\alpha)^2}{2}\gamma_{j,1} + \dfrac{(r_j-\alpha)^2}{2}\gamma_{j,2} + \dfrac{(r_{j+1}-\alpha)^2\beta^-}{2\beta^+}\gamma_{j,3} & = \alpha\beta^- \end{cases}$$

The correction term

$$C_j = \gamma_{j,3}\left(v + \frac{c}{\beta^+}(r_{j+1}-\alpha) - \left[\frac{c}{\alpha\beta^+} - \frac{[f]}{\beta^+}\right]\frac{(r_{j+1}-\alpha)^2}{2}\right)$$

At $r = j+1$ using the same method , the system of equations are

$$\begin{cases} \gamma_{j+1,1} + \gamma_{j+1,2} + \gamma_{j+1,3} & = 0 \\ \dfrac{\beta^+}{\beta^-}(r_j-\alpha)\gamma_{j+1,1} + (r_{j+1}-\alpha)\gamma_{j+1,2} + (r_{j+2}-\alpha)\gamma_{j+1,3} & = \beta^+ \\ \dfrac{\beta^+(r_j-\alpha)^2}{2\beta^-}\gamma_{j+1,1} + \dfrac{(r_{j+1}-\alpha)^2}{2}\gamma_{j+1,2} + \dfrac{(r_{j+2}-\alpha)^2}{2}\gamma_{j+1,3} & = \alpha\beta^+ \end{cases}$$

The correction term

$$C_{j+1} = \gamma_{j+1,1}\left(-v - \frac{c}{\beta^-}(r_{j+1}-\alpha) + \left[\frac{c}{\alpha\beta^-} - \frac{[f]}{\beta^-}\right]\frac{(r_{j+1}-\alpha)^2}{2}\right)$$

3.4 Examples of Second Order Accurate Solutions and Derivatives Using the IIM in Polar Coordinates with Axis-Symmetry

The axis-symmetric interface problem in polar coordinates where $r \in (0,\alpha) \cup (\alpha,1)$ can be expressed as:

$$\frac{1}{r}(r\beta u_r)_r = f$$

In the examples presented here, β, u_r, u have finite jumps at the interface α. The same β is used throughout, and the proper Dirichlet boundary condition according the the actual solution are always chosen. Note that

$$\beta = \begin{cases} 1 & \text{if} \quad r \le \alpha \\ 100 & \text{if} \quad r > \alpha \end{cases}$$

Example 3.1. *Consider the problem where*

$$f(r) = \begin{cases} \dfrac{-(\sin(r) + r\cos(r))}{r} & \textit{if} \quad r \le \alpha \\ \dfrac{9\cos(9r)}{r} - 81\sin(9r) & \textit{if} \quad r > \alpha. \end{cases}$$

The exact solution can be shown to be

$$u(r) = \begin{cases} \cos(r) & \textit{if} \quad r \le \alpha \\ \sin(2r) & \textit{if} \quad r > \alpha \end{cases}$$

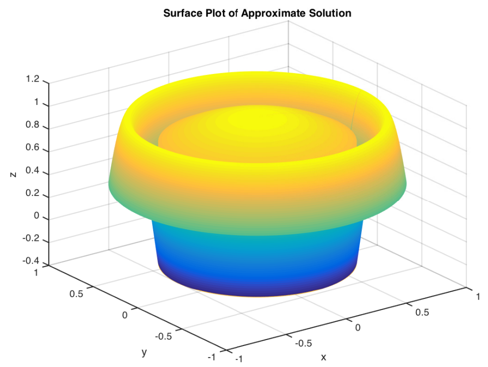

Figure 10: (a): The surface of the approximation .

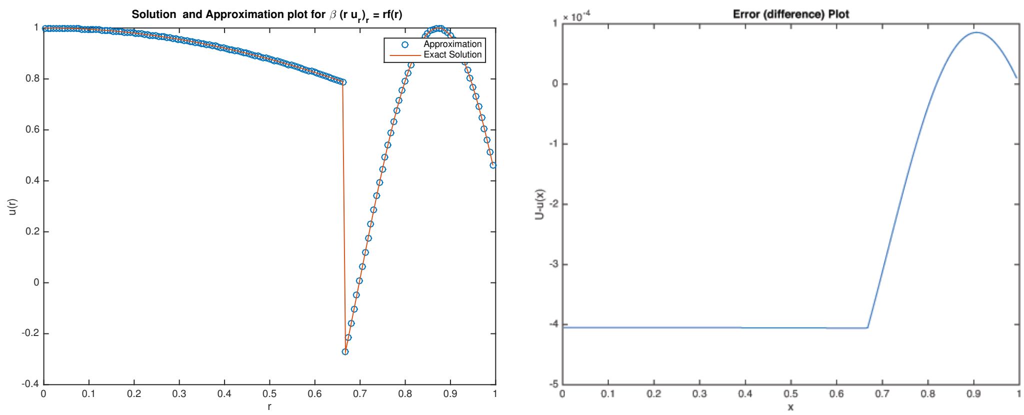

Figure 11: (a): An example of a computed solution with $n = 160$ grid divisions. Note the actual solution has its discontinuity connected by the plotter. Note that the axis has been adjusted so some points may not be visible. (b): The error difference of the solution and actual solution at the grid points.

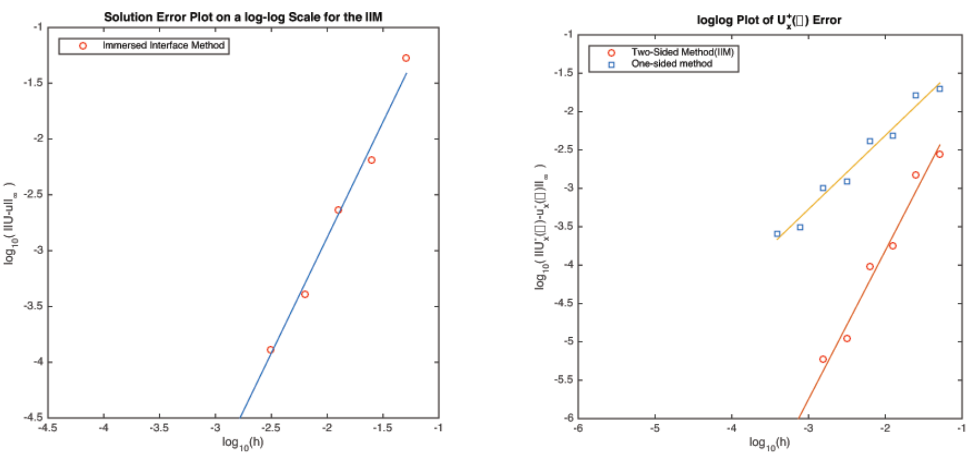

Figure 12: (a): Grid refinement analysis of the approximate solution with 8 refinements starting at $n = 20$. Note that the axis has been adjusted so some points may not be visible. The slope of the regression line fit is 2.07 (b):Grid refinement analysis of the left derivative at the interface with the one-sided and two-sided(IIM) methods. Note that a linear regression fit shows that the slope of the line of best fit is about 0.96 and 1.94 for the one-sided and two-sided methods respectively. This shows the IIM two sided method gave an order 2 accurate approximation while standard one-sided methods gave a first order accurate approximation.

Example 3.2. *Consider the problem where*

$$f(r) = \begin{cases} \dfrac{-2(\sin(2r) + 2r\cos(2r))}{r} & \textit{if} \quad r \leq \alpha \\ \dfrac{-r^2\sin(r) + \sin(r) - r\cos(r)}{r^3} & \textit{if} \quad r > \alpha. \end{cases}$$

The exact solution can be shown to be

$$u(r) = \begin{cases} \cos(2r) & \textit{if} \quad r \leq \alpha \\ \dfrac{\sin(r)}{r} & \textit{if} \quad r > \alpha \end{cases}$$

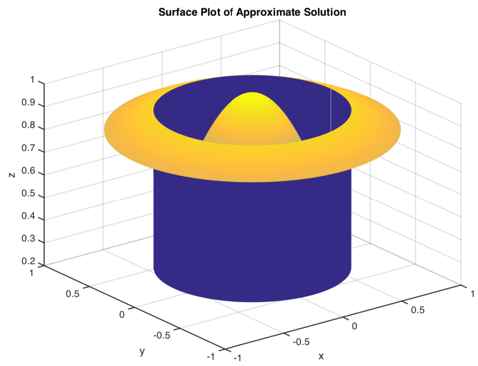

Figure 13: (a): The surface of the approximation .

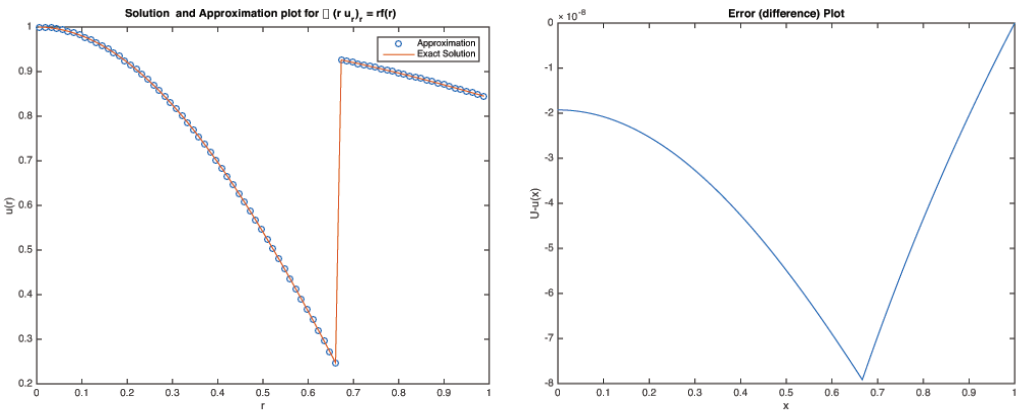

Figure 14: (a): An example of a computed solution with $n = 160$ grid divisions. Note the actual solution has its discontinuity connected by the plotter. Note that the axis has been adjusted so some points may not be visible. (b): The error difference of the solution and actual solution at the grid points.

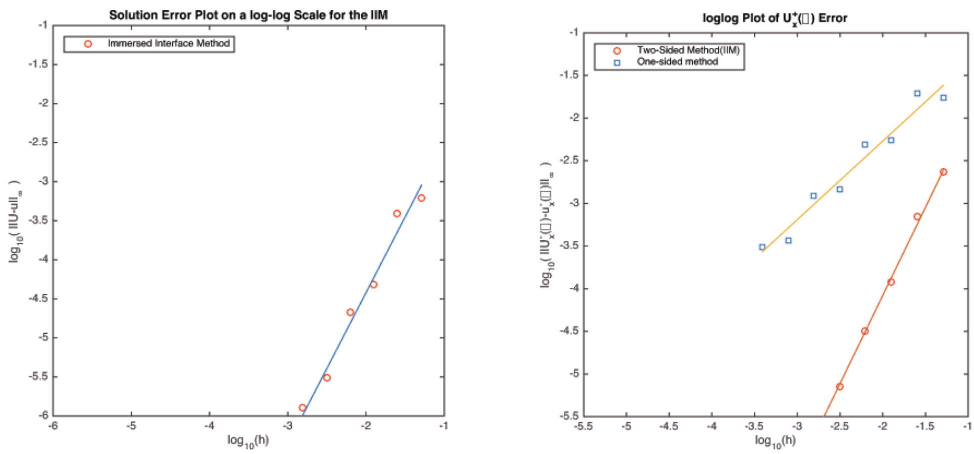

Figure 15: (a): Grid refinement analysis of the approximate solution with 8 refinements starting at $n = 20$. Note that the axis has been adjusted so some points may not be visible. The slope of the regression line fit is 1.99 (b):Grid refinement analysis of the left derivative at the interface with the one-sided and two-sided(IIM) methods. Note that a linear regression fit shows that the slope of the line of best fit is about 0.92 and 2.07 for the one-sided and two-sided methods respectively. This shows the IIM two sided method gave an order 2 accurate approximation while standard one-sided methods gave a first order accurate approximation.

Example 3.3. *Consider the problem where*

$$f(r) = \begin{cases} \dfrac{2}{r(2+r)^2} & \text{if} \quad r \leq \alpha \\ \dfrac{-(\sin(r) + r\cos(r))}{r} & \text{if} \quad r > \alpha. \end{cases}$$

The exact solution can be shown to be

$$u(r) = \begin{cases} \ln(2+r) & \text{if} \quad r \leq \alpha \\ \cos(r) & \text{if} \quad r > \alpha \end{cases}$$

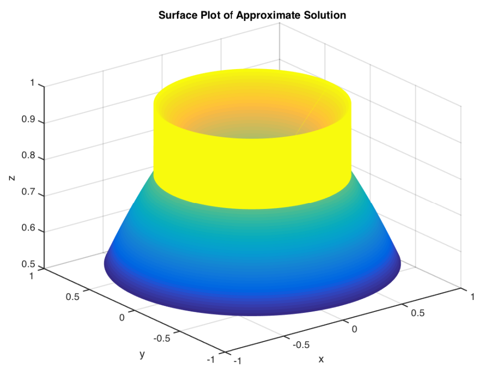

Figure 16: (a): The surface of the approximation .

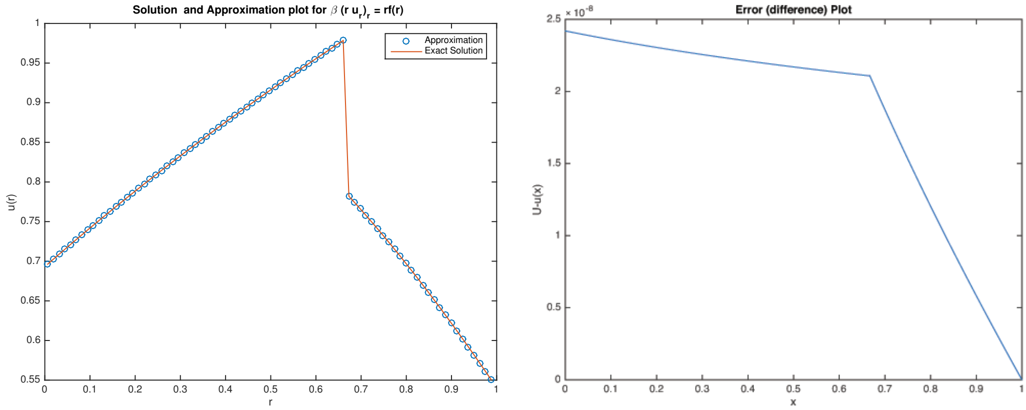

Figure 17: (a): An example of a computed solution with $n = 160$ grid divisions. Note the actual solution has its discontinuity connected by the plotter. Note that the axis has been adjusted so some points may not be visible. (b): The error difference of the solution and actual solution at the grid points.

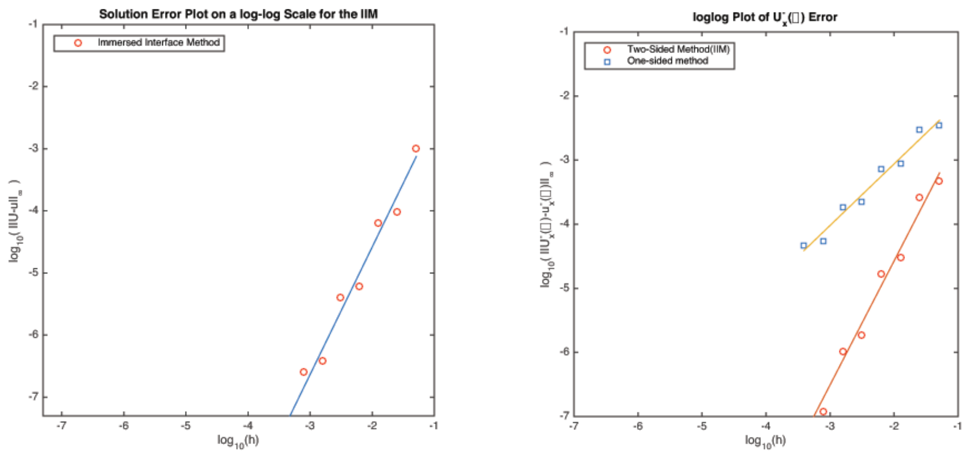

Figure 18: (a): Grid refinement analysis of the approximate solution with 8 refinements starting at $n = 20$. Note that the axis has been adjusted so some points may not be visible. The slope of the regression line fit is 2.05 (b):Grid refinement analysis of the left derivative at the interface with the one-sided and two-sided(IIM) methods. Note that a linear regression fit shows that the slope of the line of best fit is about 0.96 and 1.93 for the one-sided and two-sided methods respectively. This shows the IIM two sided method gave an order 2 accurate approximation while standard one-sided methods gave a first order accurate approximation.

4 Conclusion

In conclusion, our overall goal was to compute accurate solutions and gradients to interface problems. We achieved this goal by using Li's finite difference formulation of the Immersed Interface Method (IIM) to compute the solutions and gradients of various interface problems. We first found that derivatives of finite difference solutions at the boundary of standard boundary value problems using 3 point central differences had smooth error and were second order accurate. We then computed second order accurate finite difference solutions to interface problems using the IIM, and examined the derivative of the finite difference solutions to interface problems. Furthermore, we found that one sided differences did not consistently yield second order accurate gradient approximations at the interface. We then explored a two sided method at the interface using the IIM which lead us to find that approximated solutions and derivatives for the most general case of 1-D interface problems were second order accurate. This was a new finding that could not be found in literature. The IIM also produced second order accurate solutions and derivatives of axis symmetric 2-D polar cases. Our research showed that the Immersed Interface Method was consistently accurate for the approximations of solutions and gradients at the interface for all the types of interface problems we explored. However, a proof has yet to be found, and is a possibility for future work.

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