AN ACCURACY INVESTIGATION OF THE IMMERSED INTERFACE METHOD

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Abstract. *A accuracy examination of the Immersed Interface Method is performed. The method is applied to the calculation of the second derivative of the sine function over an uniform grid. This is conducted through the employment of a fourth-order, compact finite differences scheme, subjected to the introduction of Jump Discontinuities at points that do not coincide with grid ones. This justifies the requirement of a correction method to be applied. One of the IIM's inner steps is briefly discussed and the solution generated throught its use is then compared to the exact one. Finally, some qualitative remarks regarding this method's grid refinement requirements are presented.*

Keywords: *Immersed Interface Method, Immersed Boundary Method, Compact Schemes*

1. INTRODUCTION

This article is intended to provide outlines and to spot one limitation of the Immersed Interface Method, as proposed by [2] and [1].

This method has been designed to provide for high-order (4rd order and above) flow simulations around bodies of complex shape over structured, Cartesian grids. It's suited for problems such as the evolution of Tollmien-Schlichting waves, and all sorts of problems which require high near-wall accuray in order to be represented accordingly. One of its key advantages is the possibility of working with fixed, stationary grids, even if the immersed geometry moves within the domain. This may lead to a significant reduction of the overall computational cost.

During the latest year this method has been extensevely analysed by the authors and, though its mathematical formulation does cope with the necessity of order maintenance, one of its inner steps seem to have harsh restrictions regarding grid refinement. This is investigated through its employment to accomplish a simple calculation, that of the second derivative of a sine funtion over an uniform grid. The reason behind the selection of the sine function falls beyond the existence of an analytical solution to be compared with the numerical one. It lies on the fact that the sine function has an infinite number of derivatives. This is of particular importance not only in order to compare the final solutions, but also in order to perform individual tests throughout the IIM's substeps. This will become clearer later on.

2. NUMERICAL METHODOLOGY - THE IMMERSED INTERFACE METHOD

The numerical discretization is performed here through the use of a fourth-order accurate Compact Scheme, in conjuction with the Immersed Interface Method, IIM. The IIM builds upon the fact that implicit methods such as Compact Schemes loose validity when Jump Discontinuities are introduced at points that do not lie on grid ones. The picture below depicts that:

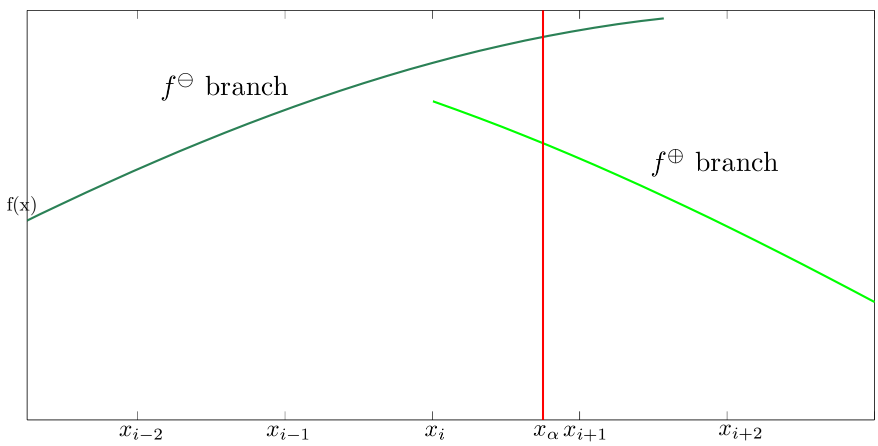

Figure 1. Jump Discontinuity Introduced at the point x_α

Where x_α represents the point at which the Jump Discontinuity is introduced.

The method is depicted here taking as an example the following approximation of a function's first derivative through the use of a Compact Scheme (second and higher order derivatives follow the same guidelines). Assuming that it consists of a set of equations of the form:

$$L_{1,i-1}f'(x(i-1)) + L_{1,i}f'(x(i)) + L_{i+1}f'(x(i+1)) = R_{1,i-1}f(x(i-1)) + R_{1,i}f(x(i)) + R_{1,i+1}f(x(i+1)) \quad (1)$$

Where the coefficients $L_{n,i+m}$ e $R_{n,i+m}$ represent Padé Schemes coefficients, with n refering to the n-th order derivative (0 refers to the function value itself), and the letters L and R indicating left and right coefficients, respectively.

These equations are based upon Taylor Series expansions over different grid points. As those expansions presume function continuity, it becomes clear that the presence of Jump Discontinuities requires some kind of correction to be employed in order to maintain their validity.

Two situations might take place according to where the Jumps are placed, relatively to the interface.

Assuming a scheme centered at the point i, the point at which the function needs to be corrected can be either $i+1$ or $i-1$. These situations are respectively represented as $f^n, n = 0, 1, 2, 3, \ldots$ superscripts $^\ominus$ and $^\oplus$. The negative sign refers to the branch of function downstream the immersed interface, whereas the positive sign refers to the upstream branch.

2.1 Jump Correction for the Downstream Branch Based Scheme

Further simplifying the following terms:

$$f^{\ominus,\oplus}(x(i+1)) = f_{i+1}^{\ominus,\oplus} \quad (2)$$

$$f^{'\ominus,\oplus}(x(i+1)) = f_{i+1}^{'\ominus,\oplus} \quad (3)$$

The equation 1 becomes:

$$L_{1,i-1}f_{i-1}^{'\ominus} + L_{1,i}f_i^{'\ominus} + L_{1,i+1}f_{i+1}^{'\ominus} = R_{1,i-1}f_{i-1}^{\ominus} + R_{1,i}f_i^{\ominus} + R_{1,i+1}f_{i+1}^{\ominus} \quad (4)$$

In this case, the Jump is introduced in the region $x(i) < x_\alpha < x(i+1)$. This is imposed when boundary and interior conditions are applied to satisfy the presence of a physical object within the domain. With that particular introduction, the scheme, that was entirely based on downstream values, now computes two downstream (at points $i-1$ and i) and one upstream value (at the $i+1$-th grid point). With that in mind, and withouth any correction applied, the equation becomes:

$$L_{1,i-1}f_{i-1}^{'\ominus} + L_{1,i}f_i^{'\ominus} + L_{1,i+1}f_{i+1}^{'\oplus} = R_{1,i-1}f_{i-1}^{\ominus} + R_{1,i}f_i^{\ominus} + R_{1,i+1}f_{i+1}^{\oplus} \quad (5)$$

At this stage there's the need to introduce the Jump Correction Term, which intends to be a workaround to that problem. Following the definition provided by [2], this term shall, hereinafter, be represented as $J^n_{\alpha,i+m}$. Its meaning shall be elucidated below.

The next challenge is to find expressions for those corrections. Expanding $f(x(i+1))$ through Taylor Series both to the left and to the right side of the interface, and naming these expansions as $f_{i+1}^{\ominus}$ and $f_{i+1}^{\oplus}$, one has:

$$f_{i+1}^{\oplus} = f_\alpha^{\oplus} + f_\alpha^{1\oplus}dx_\alpha^+ + \frac{f_\alpha^{2\oplus}(dx_\alpha^+)^2}{2!} + \ldots + \frac{f_\alpha^{n\oplus}(dx_\alpha^+)^n}{n!} \quad (6)$$

$$f_{i+1}^{\ominus} = f_\alpha^{\ominus} + f_\alpha^{1\ominus}dx_\alpha^+ + \frac{f_\alpha^{2\ominus}(dx_\alpha^+)^2}{2!} + \ldots + \frac{f_\alpha^{n\ominus}(dx_\alpha^+)^n}{n!} \quad (7)$$

With:

$$dx_\alpha^+ = x(i+1) - x_\alpha \quad (8)$$

$$f_\alpha^{n\oplus,\ominus} = \lim_{x \to x_\alpha{}^{+,-}} f^n(x) \quad (9)$$

If one relates $f_{i+1}^{\oplus}$ to $f_{i+1}^{\ominus}$ then it's possible to equal this expression to a term called $J^{0\ominus}_{\alpha,i+m}$, which ultimately results in:

$$J^{0\ominus}_{\alpha,i+1} = f_{i+1}^{\oplus} - f_{i+1}^{\ominus} \quad (10)$$

This becomes, upon manipulation:

$$J^{0\ominus}_{\alpha,i+1} = [f_\alpha^0] + [f_\alpha^1]dx_\alpha^+ + [f_\alpha^2]\frac{(dx_\alpha^+)^2}{2!} + \ldots + [f_\alpha^n]\frac{(dx_\alpha^+)^n}{n!} \quad (11)$$

With:

$$[f_\alpha^n] = \lim_{x\to x_\alpha^+} f^n(x) - \lim_{x\to x_\alpha^-} f^n(x)$$

After this procedure, it becomes obvious why the term $J^{0\ominus}_{\alpha,i+1}$ is called Jump Correction Term, and one could proceed similarly to obtain an expression for $J^{1\ominus}_{\alpha,i+m}$:

$$J^{1\ominus}_{\alpha,i+1} = [f_\alpha^1] + [f_\alpha^2]dx_\alpha^+ + [f_\alpha^3]\frac{(dx_\alpha^+)^2}{2!} + \ldots + [f_\alpha^n]\frac{(dx_\alpha^+)^{n-1}}{n-1!} \tag{12}$$

These manipulations lead to the corrected equation of the form:

$$L_{1,i-1}f_{i-1}^{'\ominus} + L_{1,i}f_i^{'\ominus} + L_{1,i+1}f_{i+1}^{'\oplus} = R_{1,i-1}f_{i-1}^{\ominus} + R_{1,i}f_i^{\ominus} + R_{1,i+1}f_{i+1}^{\oplus} - (R_{1,i+1}J^{0\ominus}_{\alpha,i+1} + L_{1,i+1}J^{1\ominus}_{\alpha,i+1}) \tag{13}$$

2.2 Jump Correction for the Upstream Branch Based Scheme

The development for this case follows the same guidelines as those from the previous section. Considering an approximation to the first derivative:

$$L_{1,i-1}f_{i-1}^{'\oplus} + L_{1,i}f_i^{'\oplus} + L_{1,i+1}f_{i+1}^{'\oplus} = R_{1,i-1}f_{i-1}^{\oplus} + R_{1,i}f_i^{\oplus} + R_{1,i+1}f_{i+1}^{\oplus} \tag{14}$$

That becomes:

$$L_{1,i-1}f_{i-1}^{'\ominus} + L_{1,i}f_i^{'\oplus} + L_{1,i+1}f_{i+1}^{'\oplus} = R_{1,i-1}f_{i-1}^{\ominus} + R_{1,i}f_i^{\oplus} + R_{1,i+1}f_{i+1}^{\oplus} \tag{15}$$

Using the following Taylos Series expansions around x_α:

$$f_{i-1}^{\oplus} = f_\alpha^{\oplus} - f_\alpha^{1\oplus}dx_\alpha^- + \frac{f_\alpha^{2\oplus}(dx_\alpha^-)^2}{2!} + \ldots + [-1^{(n)}]\frac{f_\alpha^{n\oplus}(dx_\alpha^-)^{(n)}}{(n)!} \tag{16}$$

$$f_{i-1}^{\ominus} = f_\alpha^{\ominus} - f_\alpha^{1\ominus}dx_\alpha^- + \frac{f_\alpha^{2\ominus}(dx_\alpha^-)^2}{2!} + \ldots + [-1^{(n)}]\frac{f_\alpha^{n\ominus}(dx_\alpha^-)^{(n)}}{(n)!} \tag{17}$$

$$f_{i-1}^{1\oplus} = f_\alpha^{1\oplus} - f_\alpha^{2\oplus}dx_\alpha^- + \frac{f_\alpha^{3\oplus}(dx_\alpha^-)^2}{2!} + \ldots + [-1^{(n-1)}]\frac{f_\alpha^{n\oplus}(dx_\alpha^-)^{(n-1)}}{(n-1)!} \tag{18}$$

$$f_{i-1}^{1\ominus} = f_\alpha^{1\ominus} - f_\alpha^{2\ominus}dx_\alpha^- + \frac{f_\alpha^{3\ominus}(dx_\alpha^-)^2}{2!} + \ldots + [-1^{(n-1)}]\frac{f_\alpha^{n\ominus}(dx_\alpha^-)^{(n-1)}}{(n-1)!} \tag{19}$$

Where:

$$dx_\alpha^- = x_\alpha - x(i-1) \tag{20}$$

$$f_\alpha^{n\oplus,\ominus} = \lim_{x\to x_\alpha{}^{+,-}} f^n(x) \tag{21}$$

And the following definitions:

$$J^{0\oplus}_{\alpha,i-1} = f_{i-1}^{\ominus} - f_{i-1}^{\oplus} \tag{22}$$

$$J^{1\oplus}_{\alpha,i-1} = f_{i-1}^{\prime\ominus} - f_{i-1}^{\prime\oplus} \tag{23}$$

The Jump Correction Terms are then written as:

$$J^{0\oplus}_{\alpha,i-1} = -[f_\alpha^0] + [f_\alpha^1]dx_\alpha^- - [f_\alpha^2]\frac{(dx_\alpha^-)^2}{2!} + \ldots + [-1^{(n+1)}][f_\alpha^n]\frac{(dx_\alpha^-)^n}{n!} \tag{24}$$

$$J^{1\oplus}_{\alpha,i-1} = -[f_\alpha^1] + [f_\alpha^2]dx_\alpha^- - [f_\alpha^3]\frac{(dx_\alpha^-)^2}{2!} + \ldots + [-1^{(n)}][f_\alpha^n]\frac{(dx_\alpha^-)^{(n-1)}}{(n-1)!} \tag{25}$$

Where:

$$[f_\alpha^n] = \lim_{x\to x_\alpha^+} f^n(x) - \lim_{x\to x_\alpha^-} f^n(x)$$

Finally, the corrected first derivative equation:

$$L_{1,i-1}f_{i-1}^{'\ominus} + L_{1,i}f_i^{'\oplus} + L_{1,i+1}f_{i+1}^{'\oplus} = R_{1,i-1}f_{i-1}^{\ominus} + R_{1,i}f_i^{\oplus} + R_{1,i+1}f_{i+1}^{\oplus} - (R_{1,i-1}J^{0\oplus}_{\alpha,i-1} + L_{1,i-1}J^{1\oplus}_{\alpha,i-1}) \tag{26}$$

Nevertheless, it's yet to be shown how to obtain approximations to those Jump Terms. The only values know at each iteration of the method are function values themselves. So the only option available is to combine them in such a way that all derivatives at the immersed interface can be estimated accordingly. For the case depicted at this subsection, the desired system can be represented by:

$$\begin{array}{rcccccccc} f(x_\alpha) &=& c_{\alpha,1}f(x_\alpha) &+& c_{i+1,1}f(x_{i+1}) &+& c_{i+2,1}f(x_{i+2}) &+ \ldots +& c_{i+n,1}f(x_{i+n}) \\ f^1(x_\alpha) &=& c_{\alpha,2}f(x_\alpha) &+& c_{i+1,2}f(x_{i+1}) &+& c_{i+2,2}f(x_{i+2}) &+ \ldots +& c_{i+n,2}f(x_{i+n}) \\ \vdots &=& \vdots &+& \vdots &+& \vdots &+ \vdots +& \vdots \\ f^n(x_\alpha) &=& c_{\alpha,n}f(x_\alpha) &+& c_{i+1,n}f(x_{i+1}) &+& c_{i+2,n}f(x_{i+2}) &+ \ldots +& c_{i+n,n}f(x_{i+n}) \end{array} \tag{27}$$

With $f^n(x_\alpha) = f^n_\alpha$ and $f(x_{i+n}) = f^0_{i+n}$, its matrix representation is:

$$\begin{pmatrix} f^0_\alpha \\ f'_\alpha \\ \vdots \\ f^{n-1}_\alpha \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & \ldots & 0 \\ c_{\alpha,2} & c_{i+1,2} & c_{i+2,2} & \cdots & c_{i+n,2} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ c_{\alpha,n} & c_{i+1,n} & c_{i+2,n} & \cdots & c_{i+n,n} \end{pmatrix} \times \begin{pmatrix} f^0_\alpha \\ f^0_{i+1} \\ \vdots \\ f^0_{i+n} \end{pmatrix} \tag{28}$$

The Weierstrass's theorem states that if a function $f(x)$ is continuous over a finite interval $a \leq x \leq b$ then it can be approximated as closely as we please by a power polynomial, provided this polynomial's order is sufficiently large. So, one may want to represent the function values in successive points close to the immersed interface through Taylor Series expansions (according to [2], the fist neighbor point shall be neglected):

$$\begin{pmatrix} f^0_\alpha \\ f^0_{i+1} \\ \vdots \\ f^0_{i+n} \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & \ldots & 0 \\ 1 & (dx^+_\alpha + d_x) & \frac{(dx^+_\alpha + d_x)^2}{2!} & \ldots & \frac{(dx^+_\alpha + d_x)^n}{n!} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & (dx^+_\alpha + nd_x) & \frac{(dx^+_\alpha + nd_x)^2}{2!} & \ldots & \frac{(dx^+_\alpha + nd_x)^n}{n!} \end{pmatrix} \times \begin{pmatrix} f^0_\alpha \\ f'_\alpha \\ \vdots \\ f^{n-1}_\alpha \end{pmatrix} \tag{29}$$

Using:

$$[C] = C_{n,n} = \begin{pmatrix} 1 & 0 & 0 & \ldots & 0 \\ c_{\alpha,2} & c_{i+1,2} & c_{i+2,2} & \cdots & c_{i+n,2} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ c_{\alpha,n} & c_{i+1,n} & c_{i+2,n} & \cdots & c_{i+n,n} \end{pmatrix} \tag{30}$$

And:

$$[D] = D_{n,n} = \begin{pmatrix} 1 & 0 & 0 & \ldots & 0 \\ 1 & (dx^+_\alpha + d_x) & \frac{(dx^+_\alpha + d_x)^2}{2!} & \ldots & \frac{(dx^+_\alpha + d_x)^n}{n!} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & (dx^+_\alpha + nd_x) & \frac{(dx^+_\alpha + nd_x)^2}{2!} & \ldots & \frac{(dx^+_\alpha + nd_x)^n}{n!} \end{pmatrix} \tag{31}$$

We can change between systems:

$$(f) = [D](f^n_\alpha) \tag{32}$$

$$[D]^{-1}(f) = [D]^{-1}[D](f^n_\alpha) \tag{33}$$

Upon close inspection, we conclude that [D] is always invertible. Finally:

$$[C] = [D]^{-1} \tag{34}$$

A brief discussion regarding the order maintenance of these expansions is found in [2]. As for the fourth-order Compact Scheme used:

$$\begin{pmatrix} 1 & 11 & 0 & \dots & \dots & \dots \\ 1 & 10 & 1 & \dots & \dots & \dots \\ 0 & 1 & 10 & 1 & \dots & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \dots & \dots & 1 & 10 & 1 & 0 \\ \dots & \dots & \dots & 1 & 10 & 1 \\ \dots & \dots & \dots & 0 & 11 & 1 \end{pmatrix} \text{ and } \begin{pmatrix} 39a & -81a & 45a & -3a & \dots & \dots \\ 1b & -2b & 1b & 0 & \dots & \dots \\ 0 & 1b & -2b & 1b & \dots & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \dots & \dots & 1b & -2b & 1b & 0 \\ \dots & \dots & 0 & 1b & -2b & 1b \\ \dots & \dots & -3a & 45a & -81a & 39a \end{pmatrix}$$

With:

$$a = 1/3dx^2 \tag{35}$$

$$b = 12/dx^2 \tag{36}$$

2.3 Grid Refinement Test Guidelines

A Selection of five different grids have been used:

Grid	Number of Points
1	21
2	41
3	81
4	161
5	321

The errors are based on two norms, and their definitions follow [3]:

$$L_1 = \left[\sum_{n=1}^{j} |f_{ex}(n) - f_{calc}(n)| \right] /j \tag{37}$$

$$L_\infty = max|f_{ex}(n) - f_{calc}(n)| \quad ; \quad n = 1, 2, \dots, j \tag{38}$$

Where the index n represents the number of grid points.

3. RESULTS AND REMARKS

Here are presented some results of the application of the method to the calculation of the second derivative of $f(x) = sin(x)$.

The selected $sine$ profile is shown below. The domain has a lenght $L = 10$ and the Jump Discontinuities are placed at $x_{\alpha_1} = 1.97875$ and $x_{\alpha_2} = 8.02125$:

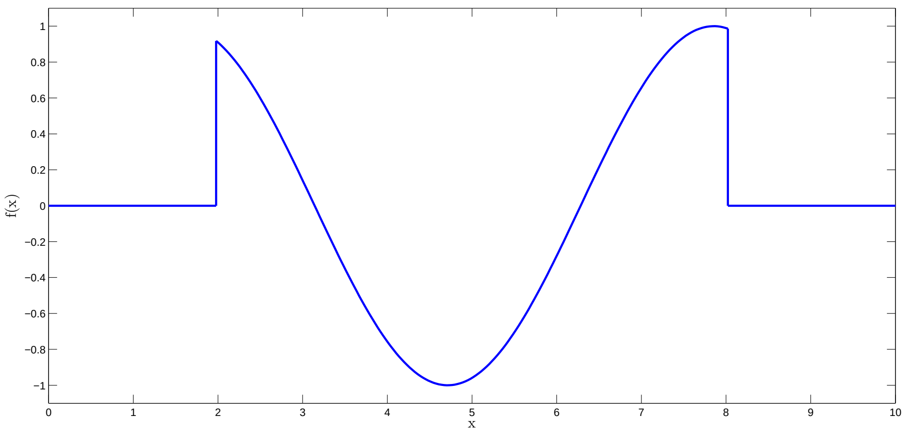

Figure 2. Jump Discontinuity Introduced at the points x_{α_1} and x_{α_2}

Below there are plots from two numerical solutions, from grids number 1 and number 5, plus the exact solution. Numerical solutions are represented by dots, whereas the analytical one is represented by a red line.

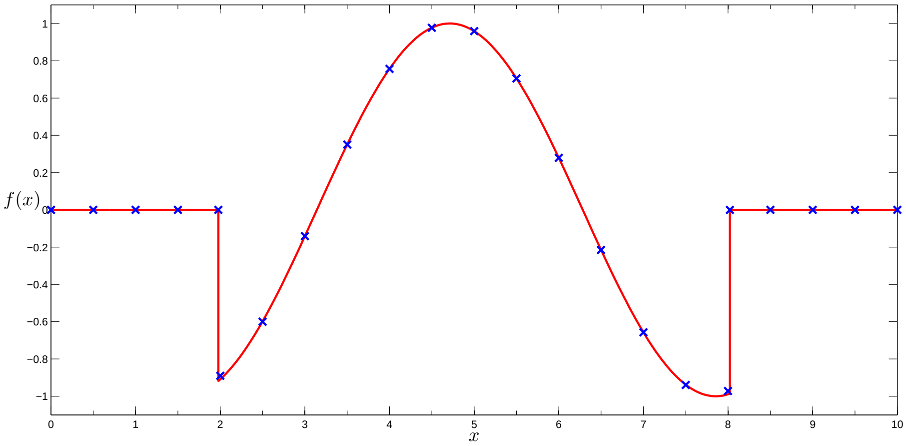

Figure 3. $sine$ Numerical Solution vs Analytical Solution - GRID 1

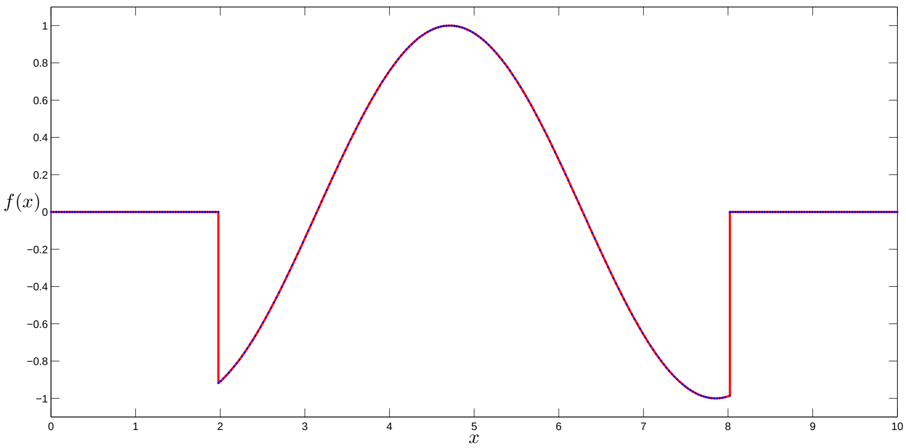

Figure 4. $sine$ Numerical Solution vs Analytical Solution - GRID 5

The following graph contains plots regarding the grid refinement test.

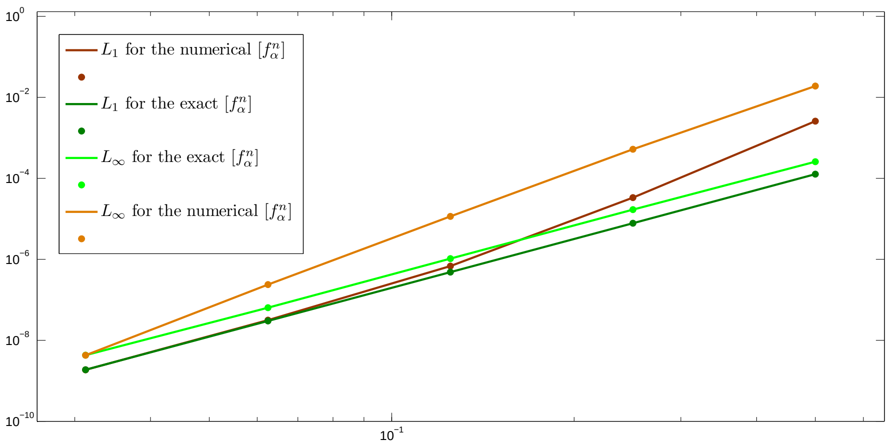

Figure 5. Grid Refinement Test

The numerical solution with Jump Terms based upon analytical values depict 4th-order behaviour both for L_∞ and L_1. That's in consonance with the method's formulation.

In their turn, the two lines related to the entirely numerical solution reflect a degradation of the solution as the grid becomes less refined. This behaviour rises the question of how effective is the approximation of those derivatives at points x_{α_n} by the linear combination of the function values.

This approximation always requires the same amount of neighbor points to be carried over, but one can imediately point out that their positions along the coordinate axis change as the grid becomes more refined. Additionally, what can be seen is that this collection of points become more (or less) collapsed as we change from one grid to the next, and thus the curve that is actually being computed by this process also changes from one run of the code to the next.

What has been shown is that this effect seems to have direct influence over the order maintenance of this method, which could ultimately render it unfitted for its original proposition, which involves mantaining the order of the Compact Scheme used.

The issue could lie on a bad implementation for the inversion process of the [D] matrix, from section 2. That doesn't seem to be the case, though. If [C] is [D]'s inverse matrix, their product should yield the Identity Matrix, and that's precisely what happens throughout all 5 runs from the entirely numerical solution.

With that in mind, one of the preliminary conclusions regarding the subject of this paper is that this linearization process is a critical limitation of the Immersed Interface Method as it has been presented.

Further results and studies are still being performed, and the aim now is to provide a quantitative appreciation of this issue, rather than a qualitative one.

4. ACKNOWLEDGEMENTS

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5. REFERENCES

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