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CODE VERIFICATION TEST IN HIGH-ORDER CALCULATIONS AROUND JUMP SINGULARITIES

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Abstract. *In this paper, a verification test using the method of manufactured solution (MMS) was applied in a derivative calculation code of functions with jump singularities. Calculations around jump singularities can be a good methodology to simulate a three-dimentional flow that contains an immersed surface. It has been intitled of the immersed interface method (IIM). This is an alternative to the established immersed boundary method (IBM) and presents the folowing advantages: to guarantee the order of accuracy implemented in the code; it doesn't use interpolation between Eulerian and Lagrangian meshes; it allows the use of rectangular mesh to simulation complex geometries and it doesn't work with delta funcion or forcing terms in the equation to simulate an immersed surface in the flow. The calculation is performed in a simple manner using one-sided finite difference to correct the method in the points near the jumps. High order of accuracy can be reached using this methodology. In this paper, it is presented a mesh refinement test and an error analysis, recording the order of accuracy implemented in the code. First of all, but didn't show in this paper, the derivative calculation of a function with a jump singularities was performed using compact finite difference schemes at* 6^{th} *order of accuracy. After, a domain assuring a region limited by jump singularities was also adopted and results were discussed. The results showed that, in both cases, it is possible to guarantee the order of accuracy in all domain, inclusive in the critical region of the domain around that limited by jumps.*

Keywords: *immersed interface method, method of manufactured solution, high-order compact finite difference schemes*

1. INTRODUCTION

The study about problems of initial/boundary-value on domains, with complex geometric boundaries, instigates the numerical analysis in the attempt to quantify the accuracy of the obtained numerical solution. Therefore, several results are presented by literature by immersed boundary methods (IBM). One of the most difficulty here is to develop an efficient method to guarantee the accuraccy yet implemented to the calculations around the immersed boundary in the domain. In fact, this region involves for modelling using functions with discontinuities, and a large scale of methods don't work very well, because they attempt there assuming the hypothesis of regular functions. In this sense, the need for regular points to represent the Taylor expansion was negligible. However, more recent studies have considered this hypothesis. The goal those studies were to correct the Taylor expansion at the neighbhoard of the singularities, called of immersed interface method (IIM) (LeVeque and Li, 1994). Linnick and Fasel (2005) present results to the IIM at high accuracy using high-order compact finite difference schemes.

The IIM using high order in the calculations should give reliability that the intended accuracy can be reached. Therefore, verification tests can be applied. It evaluates the implementation of equations, boundary conditions and discretization scheme as a whole, in order to ensure the absence of programming errors. There are many ways to execute a code verification, such as, comparisons between the numerical solution and an analytical solution, comparisons code to code and the method of manufactured solutions (MMS) (Silva *et al.*, 2010). The basic idea of the MMS is to introduce a source term in the equations, creating a non-realistic problem, but with an analytical solution. This analytical (manufactured) solution can be used for comparisons with numerical results and a mesh refinement test can be performed to obtain the order of accuracy of the calculations.

The proposal this work was to perform a verification test in a code that uses the methodology by IIM, using the method of manufactured solutions. A derivative calculation routine for one-dimensional analytical function $f(x)$ was modified to the current application (Silva *et al.*, 2010). This genuine routine utilizes compact finite difference methods at 6^{th} order of accuracy to the interior points and 5^{th} order of accuracy to the boundary points in the domain. It was modified to calculate the derivative of $f(x)$ in a domain with discontinuities, but maintaining the formal order of accuracy. Two situations were studied. In fact, one situation involved to suppose a function $f(x)$ analytic in a domain, except only one jump discontinuity, while in other situations, the domain presented one region limited by two jump discontinuities where in this region nothing calculations were performed. The first situation was based on the literature found in (Wiegmann and Bube, 2000). There, it is possible to elaborate one correction of the finite difference methods used to the derivative calculation of points near the jump by one-sided finite difference schemes. In that paper, finite difference schemes at second order of accuracy were tested. The second situation was developed by Linnick and Fasel (2005) for several applications. There, the methodology was to apply the theory presented in (Wiegmann and Bube, 2000), however, it was adapted to simulate the derivative calculations of a function in a domain with one region limited by two jump discontinuities. f and $f^{'}$ were assumed to be null in the region limited by two jump singularities and the derivative calculations were performed only outside this region.

The paper is composed as follows. Section 2presents details of methodology assumed to perform the correction of the finite difference schemes to the points near the singularities. Section 3presents the results of the verification test in the modified code by adjusting the calculations near the singularities, as mentioned in Section 2. Section 4presents some remarks and future proposals. The results showed that the routine was able to perform the derivative calculations without loss of accuracy in the critical regions, where jumps are present.

2. Methodology

Case with only one jump

We are supposing a function $f(x)$, analytic everywhere in the domain $D = \{x|x_{i-1} \leq x \leq x_{i+1}\}$, except at the point $x = x_a$, as represented by Figure 1.

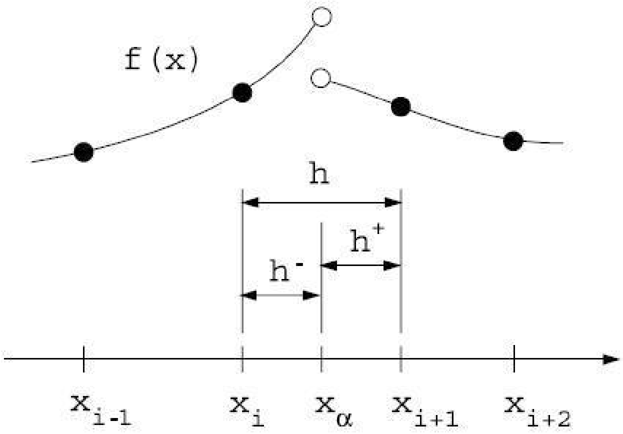

Figure 1. Function with discontinuity at $x = x_a$. Available from Linnick and Fasel (2005).

The goal this work is to write a Taylor series at point x_i to evaluate $f(x)$ at point x_{i+1} except at the point x_a where it has a jump discontinuity in the function value itself and/or higher derivatives. If $x_i < x_a$, the standard Taylor series cannot proceed through x_a to correctly predict $f(x_{i+1})$ unless a correction term J_a is added:

$$f(x_{i+1}) = f(x_i) + f^{'}(x_i)h + \frac{f^{''}(x_i)h^2}{2!} + \cdots + J_a \tag{1}$$

where J_a is

$$J_a = [f]_a + [f^{'}]_a h^+ + \frac{[f^{''}]_a (h^+)^2}{2!} + \cdots, \tag{2}$$

$h = x_{i+1} - x_i$ and $h^+ = x_{i+1} - x_a$. The term $[f]_a$ represents the jump in the value of f at $x = x_a$, that is

$$[f]_a = \lim_{x \leftarrow x_a^+} f(x) - \lim_{x \leftarrow x_a^-} f(x), \tag{3}$$

so that $[f]_a$ represents the jump in the function value at $x = x_a$, $[f^{'}]_a$ the jump in the value of the first derivative of the function, and so on. Eq. (1) is termed the corrected Taylor series. The corrected Taylor series will be used to correct finite-difference schemes that have been obtained using the standard Taylor series, as follow. This section, the first derivative of a function $f(x)$ at point x_i is computed using an explicit finite difference with jump correction:

$$f_i^{'} = R_{i-1} f_{i-1} + R_i f_i + R_{i+1} f_{i+1} - R_{i+1} J_{a0} \tag{4}$$

and truncated jump correction term

$$J_{a0} = [f^{(0)}]_a + [f^{(1)}]_a h^+ + \frac{[f^{(2)}]_a (h^+)^2}{2!} + \frac{[f^{(3)}]_a (h^+)^3}{3!} \cdots, \tag{5}$$

The expressions (4) and (5) together form an expression of second order of accuracy for $f_i^{'}$ in the presence of a jump singularity at the point $x = x_a$. The terms $[f^{(n)}]_a$ in eq.(5) are computed by:

$$[f^{(n)}]_a = f^{(n)}_{F.D.+} - f^{(n)}_{F.D.-}, \tag{6}$$

where

$$f^{(n)}_{F.D.+} = c_{n_a+}f_a^+ + c_{n_{i+2}+}f_{i+2} + c_{n_{i+3}+}f_{i+3} + c_{n_{i+4}+}f_{i+4}, \tag{7}$$

and

$$f^{(n)}_{F.D.-} = c_{n_a-}f_a^- + c_{n_{i-1}+}f_{i-1} + c_{n_{i-2}+}f_{i-2} + c_{n_{i-3}+}f_{i-3}. \tag{8}$$

The coefficients c_{n_i} are used to determine a numerical approximation to the nth derivative of f by a linear combination of the f_i. The + and - superscripts on f_a indicate, respectively, right and left limits at x_a. Note that the points x_i and x_{i+1} have intentionally not been used and that because of this, many problems, numerical stability in particular, have been avoided. Each expressions (7) and (8) form n-order linear systems, in the variable c_{n_i}, which can be solved by a linear system solver. So, the number n depends on chosen term quantitative in the expression (2).

Case with one region limited by two jumps

Figure 2.illustrates the situation where one region limited by two jumps is adopted. Therefore, the finite difference method with jump correction was applied in two jump singularities, x_α and x_β. In this case, it is assumed $f^{(n)}_{F.D.+} = 0$ in the expression (6) to the corrections near x_α and $f^{(n)}_{F.D.-} = 0$ in the expression (6) to the corrections near x_β. Details these calculations can be found in Linnick and Fasel (2005).

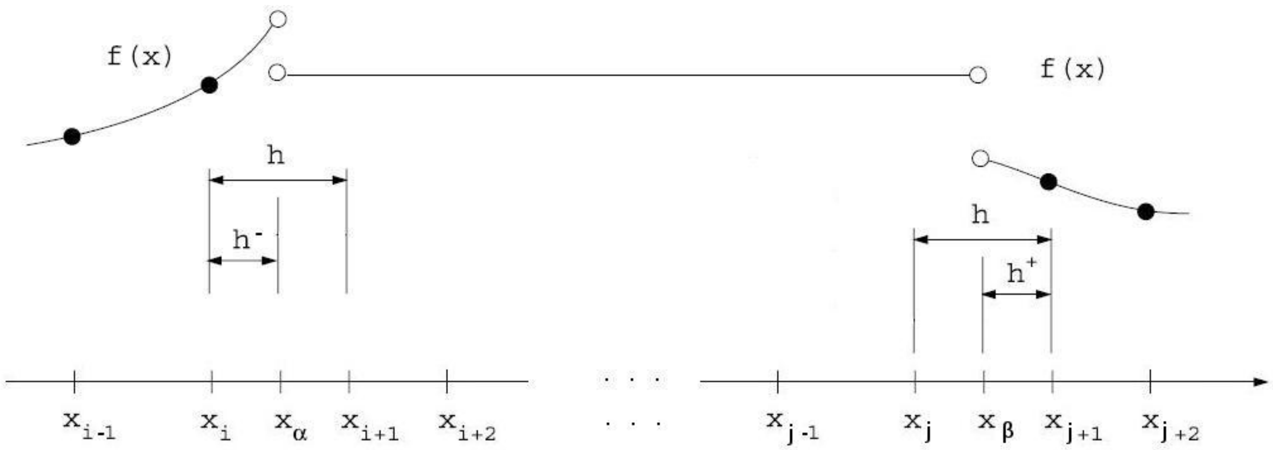

Figure 2. Function with a region limited by two discontinuities at x_α and x_β.

3. RESULTS

The derivative calculations of a function in a domain with region of discontinuity was performed. The chosen domain was $[0, 2\pi]$, where the sine function was defined along of $[0, x_\alpha]$ and cossine function was defined along of $[x_\beta, 2\pi]$. The x_α and x_β values represent the limits of discontinuity region of the chosen domain. In the test, $x_\alpha = 3.3$ and $x_\beta = 4.3$ were used. The calculation was performed only to the points inside of domain, but out of the limited region by x_α and x_β. The null value was assumed inside of discontinuity region. Trigonometrical functions are good choices to evaluate the discretization error in a mesh refinement test because the dominant term of Taylor series doesn't became null, except to some points. This allows studying the order of accuracy of the methods without doubts. More details about the better characteristics should a well-manufactured solution can be found in (Roache, 1998). Figure 3presents comparisons between analytical and numerical solutions to the derivative calculations in the mesh with 49 points. It is possible to see a very good approximation to the numerical results.

The numerical error, given by magnitude of difference between analytical and numerical solution (absolute error), was analized in a refinement mesh test using 10 mesh levels in local and global analysis. This choice can be useful to evaluate the convergence and it reaching the asymptotic range (Roache, 1998). Both maximum and mean errors were applied to global error analysis. The wavenumber α was set 1 and the length of the domain was set 2π, for all the cases. The number

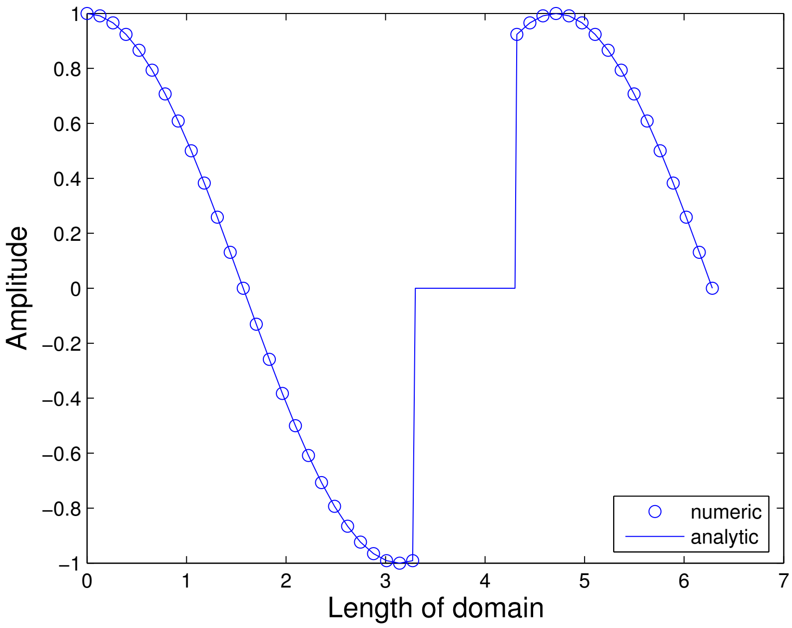

Figure 3. comparisons between analytical and numerical solutions in the mesh with 49 points.

Table 1. Number of points used in the mesh refinement test.

n	7	15	49	97	193	385	769	1537	3073

of points in each mesh (n) was doubled from one to other and the spacing was $dx = \frac{2\pi}{n-1}$. Table 1 presents the chosen number of points in the simulations.

For this application the derivative calculations of the function with jump singularities involved a correction to the points near of x_α and x_β using 6^{th} order one-sided finite difference schemes. In fact, the calculations at the points $i-2; i-1; i; i+1$ and $i+2$ near x_α and x_β, as illustrated by Fig 2. were corrected using the expression (5). So, the correction terms $[f^{(n)}]_\alpha\,[f^{(n)}]_\beta)$ composing the expressions 6 were discretized satisfying 6^{th} order of accuracy to the $[f^{(1)}]_\alpha\,([f^{(1)}]_\beta)$, and successively to other terms: 5^{th} order of accuracy to $[f^{(2)}]_\alpha\,([f^{(2)}]_\beta)$; 4^{th} order of accuracy to $[f^{(3)}]_\alpha\,([f^{(3)}]_\beta), \cdots, 1^{th}$ order of accuracy to $[f^{(6)}]_\alpha\,([f^{(6)}]_\beta)$.

Figure 3presents the mesh refinement test to the 7 correction terms on the mesh levels by table 1. Similar results were reached to $[f^{(n)}]_\beta$ and the calculations were omitted.

When the first meshes were utilized, there was a transient and the results had experimented one adjust. This fact is normal when doesn't have the minimum resolution for this calculation. However, after the third level mesh, the convergence had in agreement with the theory and the results reached the asymptotic range.

Figure 5 presents the global error analysis using maximum and mean norms for the derivative calculations by implemented schemes. Similar to Fig. 3.there was a transient. The results experimented one adjust when fewer refinement meshes were utilized. However, it was possible to reach an asymptotic convergence at 6^{th} order of accuracy to the mean error and 5^{th} order of accuracy to the maximum error. The different results in the different norms is usual in this study. The maximum error captures the points where the most magnitude error occurs. In this scheme, compact finite difference scheme at 5^{th} order of accuracy was utilized to the first and last points of the domain. The results showed that the boundary error calculation was dominant and it remained isolated. Therefore, it didn't affected the calculation at interior points of the domain. On the other hand, the mean error analysis indicated 6^{th} order of accuracy, because the interior points in the domain used compact finite difference scheme at 6^{th} order of accuracy. More details this explanation also be found in Silva *et al.* (2010).

Figure 6 presents the local error analysis in the points 0, π and 2π respectively. The results showed that, after the less refinement meshes, the convergence was 6^{th} order of accuracy to the points $x = 0$ and $x = \pi$ and 5^{th} order of accuracy to the point $x = 2\pi$. Such explained above, 5^{th} order of accuracy to the calculation at the boundary and 6^{th} at the interior of domain is the expected by scheme. However, in contrary to the theory, the results showed 6^{th} order of accuracy to the boundary $x = 0$. This is done due of the nature of chosen function, that was sine function at $x = 0$ and cossine function at $x = 2\pi$. In fact, the discretization error by Taylor series truncation, to the derivative calculation in the boundary depended of $f^{(VI)}(x)dx^5$. For the current function, at $x = 0$ $f^{(VI)}(0) = sin(0) = 0$ and the dominant term of discretization error is

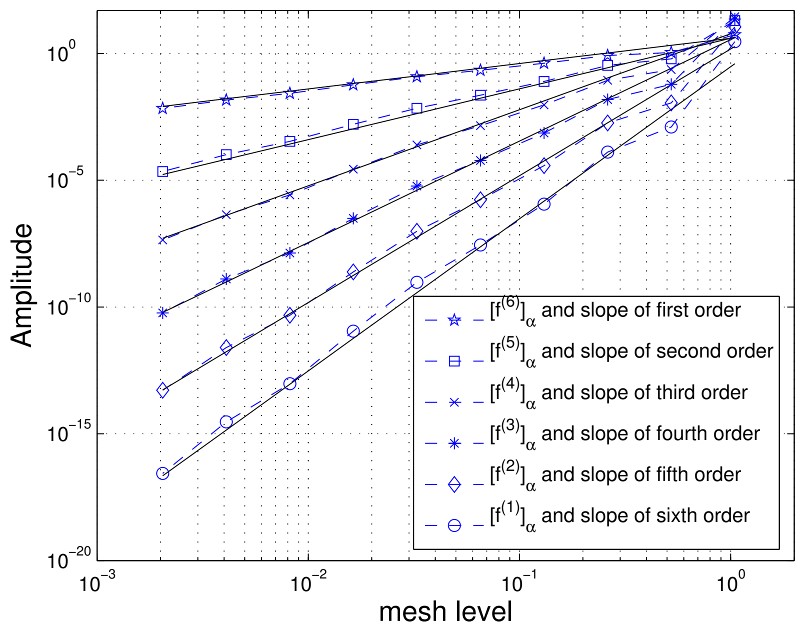

Figure 4. Mesh refinement test to the 7 correction terms used in the expression 5.

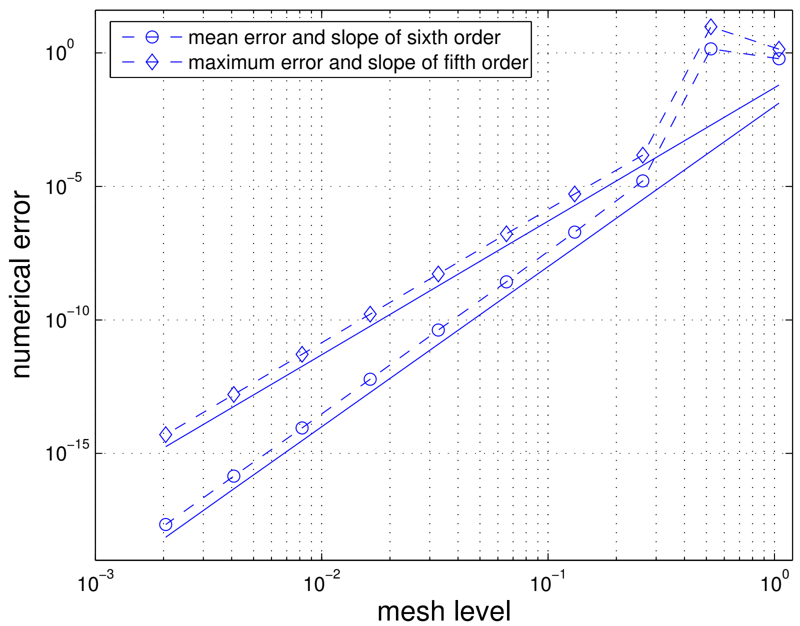

Figure 5. Global error analysis.

dominated by next term $f^{(VII)}(0)dx^6 = cos(0)dx^6 \neq 0$, reaching 6^{th} order of accuracy. On the other hand, this situation doesn't occurs to the last point of domain, $x = 2\pi$, because the dominant term of the discretization error at $x = 2\pi$ depends of $f^{(VI)}(0)dx^5 = cos(0)dx^5 \neq 0$. This results also supports that explanation so what the maximum error (6) was 5^{th} order of accuracy and mean error was 6^{th} order of accuracy. Both Figs. 5 and 6 showed excellent agreement with the theory. Furthermore, the results showed that the use of a correction terms, by expression (5), didn't affect the order of accuracy of the employed methods.

4. FINAL REMARKS

This work presents a code verification test to the derivative calculations of functions in a structured regular domain with a region limited by jumps. This calculation was done using compact finite difference schemes at 6^{th} order of

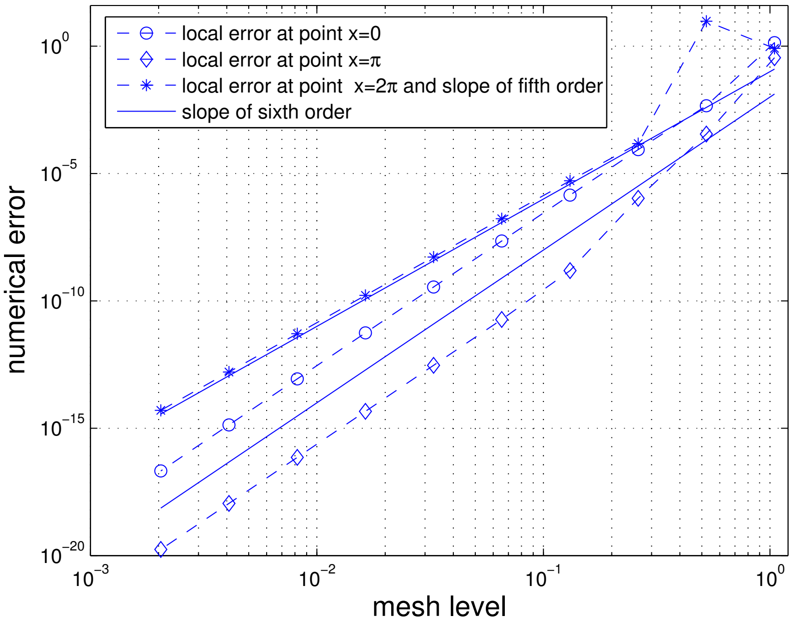

Figure 6. Local error analysis.

accuracy, assuming the corrections of the Taylor's series expansions for near points of the jump. The goal was to evaluate the influence of the jump singularities in the order of accuracy of the calculations. A code test using the Method of Manufactured Solutions (MMS) and a successive mesh refinement was performed.

The results showed that the formal order of accuracy was reached. Therefore, it supported that the finite difference schemes with a Taylor polynomial correction for the calculation near the jump singularities assures the formal order yet implemented in the code.

The conclusion was presented in Linnick and Fasel (2005), however, in the current paper, more details in the verification test using MMS were described. Furthermore, the chosen compact finite difference schemes of 6^{th} order of accuracy, presented in this paper, demands to correct a larger number of points near jump per application than that presented by Linnick and Fasel (2005).

In the future, this calculation will be extended to simulate jumps in a two dimensional domain. Therefore, it can be simulated, for example, a two-dimensional function that presents one region of the domain limited by jump singularities, like an immersed boundary. The methodology will be to double the direction of application of Taylor's correction. This method is called in the literature by Immersed Interface Method (IIM) and is a more recent strategies for the traditional Immersed Boundary Method (IMB).

In the laminar turbulent transition studies, where high accuracy is need to simulate the infinitesimal scales, the IIM could be applied in simulations of the evolution of Tolmien-Schillichting waves in a surface that presents roughness in the domain. This application can help to understand consequences in the nonlinear phenomena of the flow transition.

5. ACKNOWLEDGEMENTS

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7. RESPONSIBILITY NOTICE

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