FOURIER PSEUDO SPECTRAL-IMMERSED BOUNDARY METHOD APLIED NON-PERIODICS FLOWS

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Abstract. *Pseudo spectral methods provide an excellent numerical accuracy and it becomes very efficient when Fast Fourier Transform algorithm is used. It presents a low computational cost when compared to anothers high-order methods. Nevertheless this method can be only applied to solve periodic flows. Aiming to solve this restriction, the immersed boundary method is being used with pseudo spectral method. It will be presented in the present work the Green-Taylor Vortex flow, in order to validate the computational code, and the Lid Driven Cavity Flow with differents Reynolds' numbers, demonstrating the possibility of solving non-periodic flows through the Fourier pseudo spectral method.*

Keywords*: Fourier pseudo-spectral method, immersed boundary method, driven cavity, Taylor-Green vortex*

1. INTRODUCTION

Phenomena involving aeroacustic, transition to turbulence and combustion are problems that modern engineering aim to understand, among other manners, using techniques of the Computational Fluids Dynamics (CFD). In the case of the aeroacustic is important to use a method that captures the sound pressure waves. In phenomena involving transition to turbulence is necessary to study the small instabilities that become the flows turbulent. In the combustion, exists processes that involve the small edges of the turbulent flow. In these problems the CFD uses methods of high order accuracy to obtain results for analyses which represent the in fact physics phenomena mentioned.

The high order methods provide an excellent accuracy, for example: the methods of high order finite differences and the compact schemes, but, on the other hand, they have as disadvantaged the computational expensive cost in comparison to the conventional methodologies. With the advent of the spectral methods joining high accuracy with low computational cost became possible. This low cost is given by the Fast Fourier Transformed (FFT), since the cost of a problem resolution with finite differences is the order of $O(N^2)$, where N is the number of the grid points, the cost of the FFT is of $O(N\log_2 N)$ (Canuto *et al*, 1988). In addition, it was also developed the projection method (Silveira-Neto, 2002; Souza, 2005 and Mariano, 2007), which disentails pressure field of the Navier-Stokes equation calculates in the spectral space. Using the projection process is not necessary to calculate the Poisson equation, like it is done by the conventional methodologies. Normally, solving this equation is the most expensive part of a CFD code. The disadvantage of the spectral methodology is the difficulty to work with complex geometries and boundary conditions.

One of the most practical methodologies to work with complex geometries is the Immersed Boundary (IB) (Peskin, 1972). It is distinguished by the imposition of a term source, which has the role of a body force imposed in the Navier-Stokes equation to represent a virtual immersed body in the flow (Goldstein *et al*, 1993). This facilitates for represent any geometry, whether it is complex or in movement.

A new methodology, presented in this paper, uses the Fourier pseudo-spectral method connected in the immersed boundary method. It is proposed to simulate flows with non-periodic boundary conditions making use of the term source of the immersed boundary.

First, it will be demonstrated the transformation of the Navier-Stokes equations for the Fourier spectral space, as well as the imposition of the source term. In the second part, the details of numerical implementation of the computational code developed will demonstrated. Finally, the results of two validation problems will be shown: the first one is the Taylor-Green flow (Souza, 2005) and the second is the lid driven cavity, that is a non-periodic problem solved by the Fourier spectral method, where the boundary conditions had been imposed through of the force field of the immersed boundary.

2. MATHEMATICAL MODELING

In this session will be presented the classic mathematical model of the immersed boundary proposed by Lima e Silva (2003), which calculates the term source through the Virtual Physical Model, after that, the equations that govern the problem will be transformed for the Fourier spectral space using the properties of the discrete Fourier transformed and, finally, the methodology proposed by this paper will be presented, which connect the two methodologies.

2.1. Mathematic model for the fluid

The Immersed Boundary methodology (Peskin, 1972) consists in working with two independents meshes: the eulerian mesh, where the fluid equations are solved and the lagrangian mesh, which represents the solid interface immersed in fluid. The eulerian mesh is cartesian and fixed, and is simulate as if it was completely full of fluid. The flow is governed by conservation momentum equation and the continuity equation. The information of the fluid/solid interface is passed to the eulerian mesh for the addition of the term source to the Navier-Stokes equations. This term play a role of a body force that represents the boundary conditions of the immersed geometry (Goldstein, 1993). The equations that govern the problem are presented in its tensorial form:

$$\frac{\partial u_l}{\partial t}+\frac{\partial(u_l u_j)}{\partial x_j}=-\frac{\partial p}{\partial x_l}+\nu\frac{\partial^2 u_l}{\partial x_j \partial x_j}+f_l \qquad (1)$$

$$\frac{\partial u_j}{\partial x_j}=0 \qquad (2)$$

where $\frac{\partial p}{\partial x_l}=\frac{1}{\rho}\frac{\partial p^*}{\partial x_l}$; p^* is the static pressure in [N/m^2]; u_l is the velocity in the l direction in [m/s]; $f_l=\frac{f_l^*}{\rho}$; f_l^* is the term source in [N/m^3]; ρ is the density; ν is the cinematic viscosity in [m^2/s]; x_l is the spatial component (*x,y*) in [*m*] and *t* is the time in [*s*]. The boundary conditions are imposed in a classical way and the initial condition is any velocity field that satisfies the continuity equation.

The source term is defined in all domain, but presents values different from zeros only in the points that coincides with the immersed geometry, enabling that the eulerian field perceives the presence of the solid interface (Enriquez-Remigio, 2000).

$$f_l(\vec{x},t)=\begin{cases}F_l(\vec{x}_k,t) & \text{if } \vec{x}=\vec{x}_k\\ 0 & \text{if } \vec{x}\neq\vec{x}_k\end{cases} \qquad (3)$$

where $\vec{x}$ is the position of the particle in the fluid and $\vec{x}_k$ is the position of the a point on the solid interface (Figure 1).

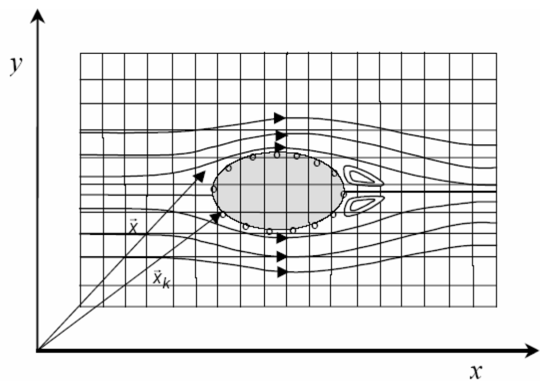

Figure 1. Schematically representation of eulerian and lagrangian domain

Using this definition can be concluded that the field $f_l\left(\vec{x},t\right)$ is discontinuous, which can be numerically solved only when there are coincidence between the points that compose the interface domain with the points that compose the fluid domain. In cases that there are not coincidence between this points, very frequently in the complex geometries, it is necessary to distribute the function $f_l\left(\vec{x},t\right)$ on its neighborhoods (Unverddi and Triggvason, 1992). Just by calculating the lagrangian force field $F_l\left(\vec{x}_k,t\right)$, it can be distribute and thus, to transmit the information geometry presence for the eulerian meshes.

2.2. Mathematic Model for the immersed interface

In this paper, the lagrangian force field is calculate by the Virtual Physical Model, which was proposed by Lima e Silva et al. (2003). One of the characteristics of this model is that is not necessary the use of ad-hoc constants. It is based in the Newton second law and allows the modeling non-slip condition on the immersed interface. The lagrangian force $F_l\left(\vec{x}_k,t\right)$ is available by momentum conservation equation over a fluid particle that is joined in the fluid-solid interface, equation (4):

$$F_l\left(\vec{x}_k,t\right)=\frac{\partial u_l}{\partial t}\left(\vec{x}_k,t\right)+\frac{\partial}{\partial x_j}(u_l u_j)\left(\vec{x}_k,t\right)+\frac{\partial p}{\partial x_l}\left(\vec{x}_k,t\right)-\nu\frac{\partial^2 u_l}{\partial x_j \partial x_j}\left(\vec{x}_k,t\right) \tag{4}$$

The values of $u_l\left(\vec{x}_k,t\right)$ and $p\left(\vec{x}_k,t\right)$ are done by interpolation of the velocities and pressure, respectively, of the eulerian points near the immersed interface.

2.3 Fourier Transforms

By defining the equations that governs the flow through immersed boundary method, the next step is to transform them to the Fourier spectral space. First applies the Fourier transform in the continuity equation (2):

$$ik_j\hat{u}_j=0 \tag{5}$$

From the analytic geometry is known that the scalar product between two vectors is null, just if both are orthogonal. Therefore, from the equation (5), we have that the wave number vector k_j is orthogonal to transform velocity $\hat{u}_j$. So, is defining the plane π (Silveira-Neto, 2002), perpendicular to wave number vector $\vec{k}$ and thus, the transformed velocity vector $\hat{\vec{u}}\left(\vec{k},t\right)$, belongs to the plane π.

Now applies the Fourier transform in the momentum equation (2):

$$\frac{\partial\hat{u}_l}{\partial t}+ik_j\widehat{u_l u_j}=-ik_l\hat{p}-\nu k^2\hat{u}_l+\hat{f}_l \tag{6}$$

where k^2 is the square norm of the wave number vector, i.e. $k^2=k_jk_j$.

In agreement of the plane π definition, each one of the terms of the equation (6) assume a position related to it: the transient term $\frac{\partial\hat{u}_l}{\partial t}$ and the viscous term $\nu k^2\hat{u}_l$ belong to the plane π. The gradient pressure term is perpendicular to the plane π, and the non-linear, $ik_j\widehat{u_l u_j}$, and the force filed, $\hat{f}_l$, a priori, it is not known in which position it can be found in relation to plane π. By jointing the terms of the equation (6) and observing the definition of plane π, we have that:

$$\underbrace{\left[\frac{\partial\hat{u}_l}{\partial t}+\nu k^2\hat{u}_l\right]}_{\in\pi}+\underbrace{\left[ik_j\widehat{u_l u_j}-\hat{f}_l+ik_l\hat{p}\right]}_{\in\pi}=0 \quad \Rightarrow \tag{7}$$

To satisfy the equation (7), it is needed that the non-linear and the force field terms are over the plane π. For that, it is utilized the projection tensor definition (Canuto *et al*, 2002), which projects any vector over it. Therefore, by applying this definition on the right hand side of the sum done in the equation (7):

$$\left[ik_j\widehat{u_l u_j} + ik_l\hat{p} - \hat{f}_l\right] = \wp_{lm}\left[ik_j\widehat{u_m u_j} - \hat{f}_m\right] \tag{8}$$

It must be noticed that the parcel of the pressure field is orthogonal to the plane π, so, it is null after to be projected, disentailing from the calculates of Navier-Stokes equations in the spectral space. The pressure field can be recovered at the pos-processing manipulating the equation (7) (Mariano *et al*, 2007).

Other important point is about the non-linear term, in which appears the product of transformed functions, in agreement with the Fourier transformed properties, this operation is a convolution product and its solution is given by convolution integral. Therefore the momentum equation in the Fourier space, using the method of the projection, assumes the following form:

$$\frac{\partial\hat{u}_l\left(\vec{k}\right)}{\partial t} + \nu k^2\hat{u}_l\left(\vec{k}\right) = \wp_{lm}\hat{f}_m - ik_j\wp_{lm}\int_{\vec{k}=\vec{r}+\vec{s}}\hat{u}_m\left(\vec{r}\right)\hat{u}_j\left(\vec{k}-\vec{r}\right)d\vec{r} \tag{9}$$

2.4 Coupling of the methods in the Fourier spectral space

The necessary derivatives for the solver of the lagrangian force, equation (4), are make generating a new field of velocity

$$u_l^F = \begin{cases} u_l \text{ se } \vec{x} \neq \vec{x}_k, \\ u_k \text{ se } \vec{x} = \vec{x}_k, \end{cases} \tag{10}$$

where u_k is the fluid velocity in the points of the immersed boundary and, u_l^F is the eulerian velocity field modified by imposed boundary conditions. After, this field is transformed to Fourier space and it is calculate the derivatives of the langrangian force field using the Fourier transformed propeties:

$$\widehat{F}_l\left(\vec{k},t\right) = \frac{\partial\widehat{u_l^F}}{\partial t} + \frac{\widehat{\partial(u_l^F u_j^F)}}{\partial x_j} + ik_l\widehat{p^F} - \nu k^2\widehat{u_l^F} \tag{11}$$

After calculate $\hat{F}_l\left(\vec{k},t\right)$ make the inverse Fourier transformed in this field using the definition done in the equation (3) it get eulerian force field, $f_l\left(\vec{x},t\right)$, in the physic space. Last, transformed it for the spectral space, $\widehat{f}_l\left(\vec{k},t\right)$ and added it in the equation (9).

3. NUMERICAL METHOD

When solved numerically the Navier-Stokes equations with the Fourier spectral method using the Discrete Fourier Transform (DFT), which is define by Briggs and Henson (1995) how:

$$\widehat{f}_k = \sum_{n=-N/2+1}^{N/2} f_n e^{\frac{-i2\pi kn}{N}} \tag{12}$$

when k is the wave number, N is the number of meshes points, n get the position x_n of the collocation points ($x_n = n\Delta x$) and $i = \sqrt{-1}$.

The DFT has the restriction of the using periodics boundary conditions, by limiting the use of Fourier spectral transformed for the problems that satisfy this boundary conditions.

Same with this restriction, the Fourier spectral method is very used for example in the simulations of temporal jets and turbulence isotropic, because its low computational cost gives by Fast Fourier Transform (FFT) (Cooley and Tukey, 1965). This algorithm solver the DFT with of the way very efficiently $O(N\log_2 N)$, whereas the calculation of (12) is of

$O(N^2)$, where N is the collocation points number. For the systems with many collocation points, for example: tridimensionals problems, the spectral method is very cheap when compared with another conventional high order methodologies.

3.1. Treatment of the non-linear term

The non-linear term can be handing by different forms: advective, divergent, skew-symmetric, or rotational. (Canuto *et al* (1988) and Souza (2005), in spite of being the same mathematically, they present different properties when discrteized. The skew-symmetric form is more stable and present the best results, but is twice more onerous that the rotational form. However this inconvenience can be solved using the alternate skew-simétric form, this is consists in aternate between the advective and divergent forms in each time step (Zang, 1987), this is proceeding adopted for this paper.

For all forms of the handing the non-linear term is necessary solve the convolution integral, but the numerical solution of this integral is computational expensive. So, using by to solver this problem, the pseudo-spectral method, which calculates the velocity product in the physical space and transformed this product for the spectral space Souza (2005).

3.2. Filtering

The Fourier spectral method is influenced by discontinuous fields, because they yield the Gibbs phenomenon. It introduces errors in the high frequencies losing the spectral accuracy. In two steps of the methodology proposed by the present work, equations (3) and (10), appear the discontinuous fields, aiming to avoid the Gibbs phenomenon utilize filters:

$$\hat{f}\left(\vec{k},t\right)_{filtered} = \sigma(\theta)\hat{f}\left(\vec{k},t\right) \tag{13}$$

where $\sigma(\theta)$ is the filter function. In this paper use the sharpened raised cosine filter (14) proposed by Kopriva (1986):

$$\sigma(\theta) = \sigma_0^4\left(35 - 84\sigma_0 + 70\sigma_0^2 - 20\sigma_0^3\right) \tag{14}$$

where σ_0 is done by (15).

$$\sigma_i = 1/4\left(1+\cos\theta_i\right) \tag{15}$$

where: $\theta_i = Lk_i / N$;

4. RESULTS

To validate the proposed methodology and developed code, two classical problems used in CFD was chosen, the first one are the Taylor-Green flow (Souza, 2005), which has an analytic solution to incompressible two-dimensional Navier-Stokes equations, with periodic boundary conditions. This case was useful to validate the developed pseudo-spectral code. The second one is the lid driven cavity (Ghia *et al*, 1982), that is a classical problem very used due to its simple geometry and its well established boundary conditions (prescribe velocities). This case allowed to validate the solution of incompressible two-dimensional Navier-Stokes equations, which are using Fourier pseudo-spectral method with non-periodic boundary conditions imposed by immersed boundary.

4.1. Taylor-Green Flows

Given the analytics equations to velocities components (*u* and *v*) and the pressure fields, conditioned to spatial coordinates (*x* and *y*) and time (*t*) (Taylor and Green, 1937):

$$u\left(x,y,t\right) = -U_\infty \cos(x).\sin(y).e^{-2t\nu} \tag{16}$$

$$\mathrm{v}\left(x,y,t\right) = U_\infty \sin(x).\cos(y).e^{-2t\nu} \tag{17}$$

$$p\left(x,y,t\right)=U_{\infty}/4\left[\cos(2x)+\cos(2y)\right]e^{-4t\nu} \tag{18}$$

Where U_{∞} is the flow velocity amplitude in [*m/s*]. Can be observed in the equations (16) and (17) satisfies the continuity equation and the equation (18) allows the validation of the pressure field solver (Mariano, 2007). Three different cases were simulated, increasiling the number of collocation points (*32x32, 64x64 e 128x128*). The error between analytic and numerical solution was calculate by L_2 norm, purposesing to contrast with the result obtained by Souza (2005).

$$L_2=\sqrt{\frac{1}{N_x}\frac{1}{N_y}\sum_{i=1}^{N_x}\sum_{j=1}^{N_y}\left\|u_N\left(x_i,y_j,t\right)-u_a\left(x_i,y_j,t\right)\right\|^2} \tag{19}$$

In all cases $U_{\infty}=1.0\ m/s$ and $\nu=\pi/500\ m^2/s$. The time step is $\Delta t=0.0005\ s$ using the third order Adams-Bashforth scheme for the temporal evolution. For comparison, the problem were admensionalized utilizing as parameters: $L^*=L/2\pi$, where $L=Lx=Ly=2\pi$, $u^*=2\pi u/\nu$, $\mathrm{v}^*=2\pi\mathrm{v}/\nu$ and $t^*=t\nu/4\pi^2$.

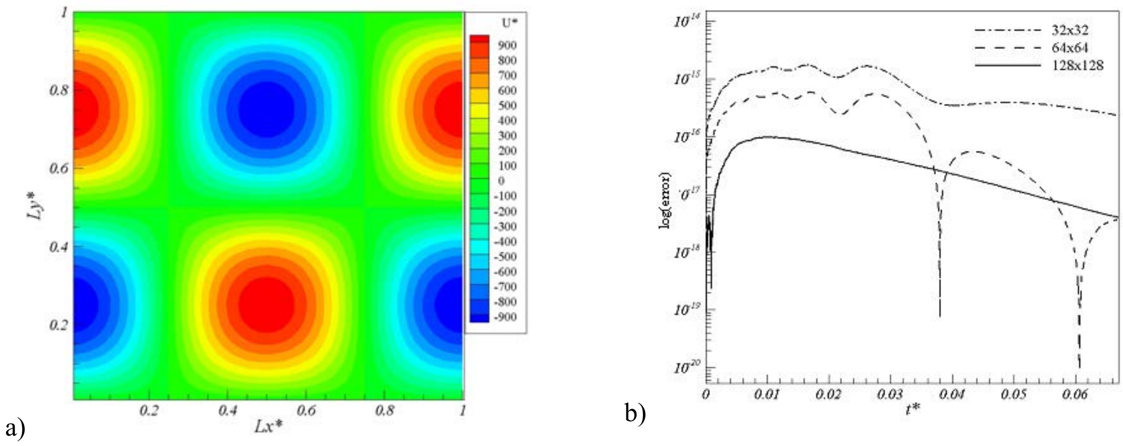

Figure 2: a) Horizontal component of velocity b) L_2 norm, according to time for different collocation points.

The figure 2 (a) presents the horizontal velocity field to case with *128x128* collocation points. The figure 2 (b) shows the L_2 norm in function of the time to different simulated cases. The simulations of the figure 2 were done with a code written in Fortran 90 with double precision. It is possible to note the high accuracy that pseudo-spectral method can reach, once that the L_2 norm reaches values of 10^{-16}, that means the machine accuracy.

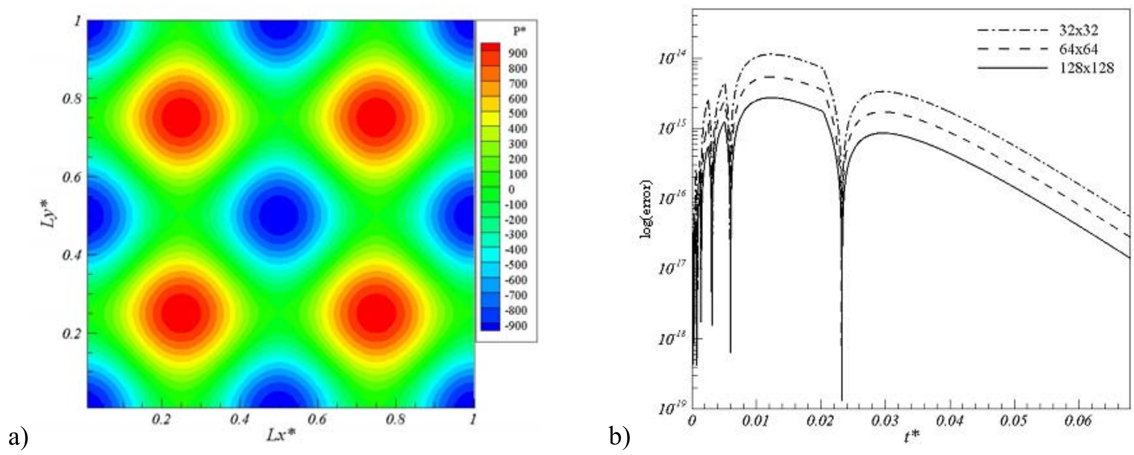

Figure 3: a) Pressure field with *128x128* collocation points; b) Comparison the L_2 norm in function of the time to different collocation points to the pressure field.

At the figure 3 (a) is shown the pressure field for simulation with *128x128* collocation points and at the figure 3 (b) is the presented the L_2 norm of pressure field. At this figure the L_2 norm reaches the same order that the velocity components, which means, 10^{-16}. The same order were reached by Souza (2005) simulating the same case. Due to the logarithmic scale the graphics at the figures 2(b) and 3 (b) seem to present great oscillations, but these are minors than the machine precision.

4.2. Lid driven cavity

It was also validated the methodology for non-periodic boundary conditions problems simulating the lid driven cavity. This is a classic CFD problem, since it presents a simple geometric configuration with well defined boundary conditions. Besides that, it presents the development of the primary vortex that induces the secondary vortex.

The cavity can be understood as rectangular section geometry, where at the superior face is imposed a constant velocity (Arruda, 2004). The calculus domain is divided in two parts: an external domain, where is imposed periodicity conditions, and a second one (internal domain), which represents the cavity itself, like show in figure 4. The boundary conditions of the internal domain are imposed, virtually, through the force field of immersed boundary methodology. An horizontal velocity is set on the cavity (lid) superior wall named U_T, for all the simulation in this paper $U_T = 1.0\ m/s$ and null velocity for every other walls. The Reynolds number is defined as $Re=U_T l_x/\nu$.

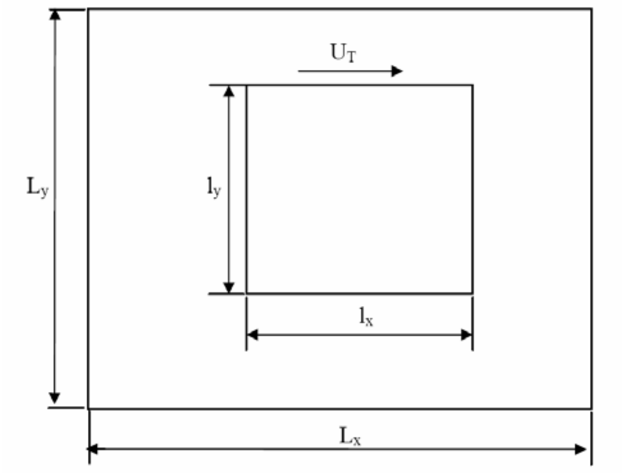

Figure 4: Domain of the calculus used at lid driven cavity for the simulations.

To test the internal domain influence related to the external, it was established a new variable called $\lambda=L/l$ realizing three simulations with different λ values (*4, 2* and *1.3*), fixing the value of $Lx=Ly=2\pi$, and varying the *lx* and *ly* values, according to λ, maintaining the collocation points constant at the external domain with *256x256*, and the points density length constant, $\Delta t=0.0005\ s$ and $Re=100$. The horizontal velocity fields are shown at figure 6.

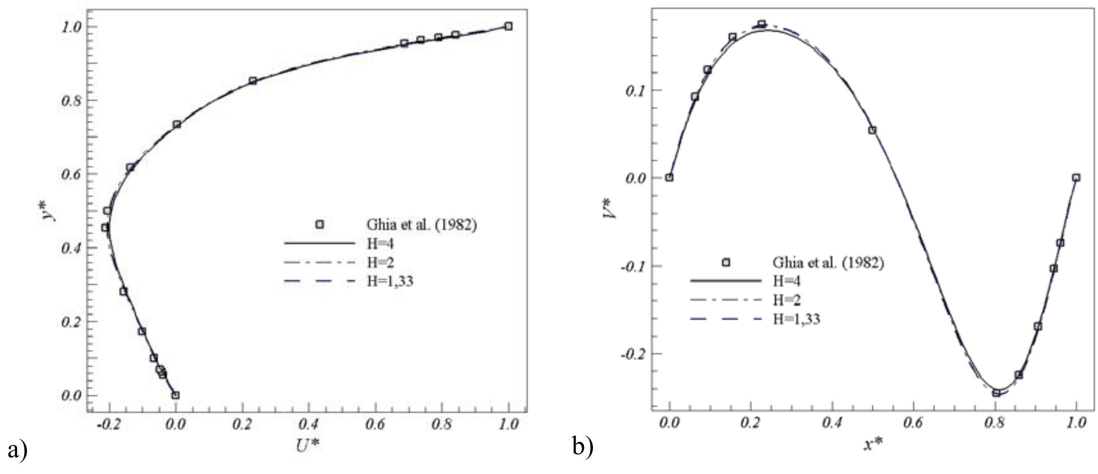

Figure 5: Velocity profiles a) horizontal component in $y=0.5\ m$; b) vertical component in $x=0.5\ m$.

At figure 5 (a) and (b) is showed the velocity profiles in the center of cavity of the simulations presented at figure 6. Note that both are very closed from Ghia *et al*. (1982).

By analyzing of the figure 6 (a) (*λ =4*) it is possible notice that the secondary vortex is not formed, this is happen because of the external domain flow influence, which is very complex, no provide the force sufficient in the boundary. Due the external vortex formation instabilities emerges in the calculates at figure 6 (c) can be observed that the secondary recirculation is not positioned correctely, because it had been dislocated by the boundary periodicity condition influence. The case simulate in figure 6 (b) is the best representation of the secondary vortex position in the cavity.

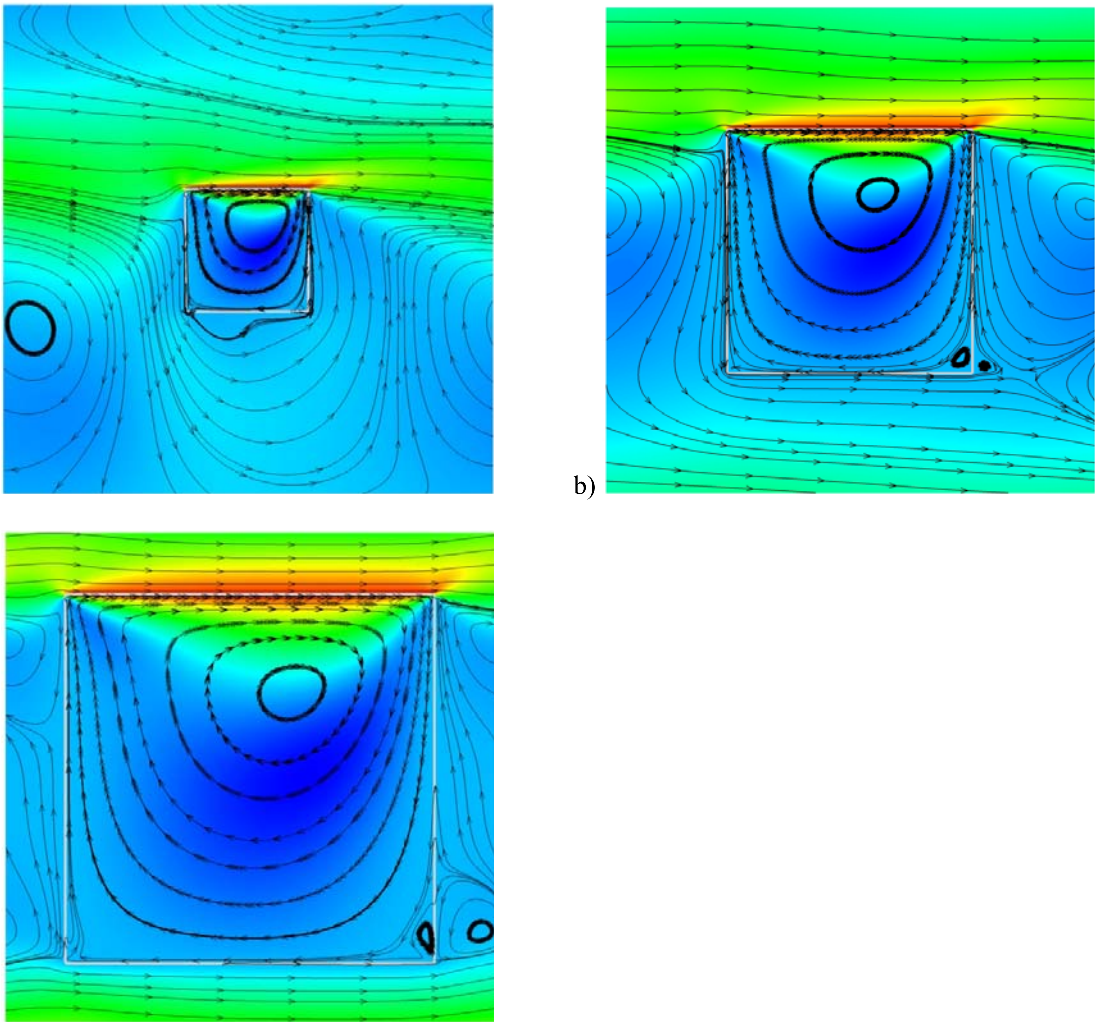

Figure 6: Horizontal velocity component a) λ=4, b) λ=2 e c) λ=1.3.

The table 1 shows the comparison geometric centre position of primary and secondary recirculation for different authors for the case showed at figure 6 (b) (λ=2).

Table 1. Recirculation centre position formed at lid driven cavity.

Authors	Centre Vorticity		Left Vorticity		Right Vorticity	
	x (m)	*y (m)*	*x (m)*	*y (m)*	*x (m)*	*y (m)*
Arruda (2004)	0.62	0.78	-	-	-	-
Ghia *et al* (1982)	0.6172	0.7344	0.0313	0.0391	0.9453	0.0625
Present work	0.6172	0.7365	-	-	0.9525	0.0634
% error in relation to Ghia *et al* (1982)	0.00	0.29	-	-	0.76	1.44

The table 1 shows a good agreement for the compared parameter (vortex geometric centre position) with others authors (Ghia *et al*, 1982 and Arruda, 2004). It can be observed that primary recirculation position results are quite close from Ghia *et al* (1982), presenting errors near from 1.00%. The right vortex is also well positioned when compared to others authors. Secondary left vortex was not captured, because of the use of the filtering, which is necessary to stable the code, but provide the dissipation of small edges (Canuto et al, 1988).

The table 2 demonstrates the vortex values at centre of the primary vortex in comparison to different authors for the case showed at figure 6 (b) (λ=2). The results is very closed to the others authors (Ghia *et al*, 1982 and Arruda, 2004), The relative error is the 1.89% in comparison with data of Ghia *et al* (1982).

Table 2. Vorticity value at primary recirculation.

Authors	Vorticity
Ghia *et al* (1982)	3.17
Arruda (2004)	3.30
Present work	3.11
% error in relation to Ghia *et al* (1982)	1.89

5. CONCLUSIONS

The motivations of this paper are improve the pseudo-spectral methodology, that is high order method and low computational cost, but restrained to periodic boundary conditions. Looking forward this aim a fusion of immersed boundary and the classic Fourier pseudo-spectral method was made.

The Fourier pseudo-spectral method allows solver the incompressible Navier-Stokes equations with the high order accuracy. In case where the equations to be solved are periodic and steady the methodology accuracy order is restrained to machine accuracy (10^{-16} for double precision). This is viewed in the Taylor-Green flows in the comparison between the analytical and numerical solution. Other great vantage is the computational cost when compared another high order methods, because the pressure disentail and the use FFT algorithm.

The connection between the Fourier pseudo-spectral and immersed boundary methodologies allow simulate non-periodic-flows, in the simulations of the driven lid cavity it is possible observe the velocities, pressure fields and the classic coherent structures of this flow. In the future, it will hope solver the problems with non coincidence between lagrangian and eulerian points, allowing solver the complex and movel geometries.

6. ACKNOWLEDGEMENTS

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