THE IMERSPEC METHODOLOGY: PRESENTATION AND PRELIMINARY APPLICATIONS

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Abstract. A new numerical methodology, named IMERSPEC, to solve the Navier-Stokes equations is presented in the present work and applied to solve two kinds of complex flows. It is based on Fourier pseudo-spectral (FPSM) and on immersed boundary methods (IBM). It was developed, initially, for incompressible flows. Wall boundary conditions are modeled using an IBM method. This methodology combines some advantages of high accuracy and low computational cost provided by the FPSM. Another very important characteristic is that, even for incompressible flow, there is no more pressure and velocity coupling. The performance of this new methodology is exemplified in three-dimensional numerical simulations of flows over a backward-facing step geometry and a spatial developing jet. The results are compared with experimental and with numerical results, giving very good agreement.

1. Introduction

In the last two decades a lot of effort has been spent by the fluid dynamic scientific community to address two crucial but conflicting key issues in the science of computational fluid dynamics (CFD). These are associated with the need to model increasingly complex boundary conditions in one hand, and, at the same time, requiring high accuracy (Ferziger & Peric, 2001). The great majority of engineering and geophysical fluid flow problems are characterized by very complex geometries that arise mainly from the irregular domain frontiers. This is often associated with the presence of moving and deformable geometries. In order to be able to solve flows under complex boundary conditions, a whole family of numerical techniques and methods has been developed by the community.

However, increasing topological and geometrical complexity, the computational grid tends to be associated with a decreasing of the overall accuracy and efficiency of the numerical method. For instance, most non-structured Navier-Stokes solvers presents order of convergence smaller than two. Indeed, to produce a non-structured fluid flow code with second order accuracy remains a formidable challenge (Kobayashi et al., 1999). Another greater problem related to these approaches is their high computational cost, both in terms of CPU time and memory.
storage. The quest for high order accuracy has also been the subject of some numerical development (Lele, 1992; Karniadakis & Sherwin, 1999). Spectral methods are characterized by exponential convergence as compared to the exact solution with increasing grid size.

Within the family of spectral methods, the classical Fourier pseudo-spectral collocation method is probably the most impressive, due to its extremely high accuracy and its low computational cost. Moreover, since the pressure terms in the Navier-Stokes equations can be lumped together with the non-linear term, for incompressible flows. So, the Fourier pseudo-spectral collocation method does not require the solution of a pressure Poisson equation. These classical methods, however, are in general not applicable for complex geometries. The Fourier collocation method, in particular, can only be used in flows with periodic boundary conditions. A numerical methodology has been developed in Fluids Mechanic Laboratory of Federal University of Uberlândia, in order to treat very complex and even mobile and deformable geometries, namely, the immersed boundary method (Peskin, 1972).

The goal of the present work is to develop a new methodology for incompressible flows with wall boundary conditions. We look to combines the accuracy and low computational cost of the classical Fourier pseudo-spectral method (Canuto et al., 2007) with flexibility in handling complex geometries allowed by the immersed boundary methods. We introduce, specifically, the IMERSPEC method, which combines a classical Fourier pseudo-spectral method, where any spatial derivative is computed with spectral accuracy, with an immersed boundary method, with the goal of to take into account the effects arising from the presence of complex boundaries.

2. Mathematical model

The present methodology is based on the merging process of the immersed boundary method with a classical Fourier pseudo-spectral method. We start writing the equations in physical space. Then, the pseudo-spectral and immersed boundary methods are described. Finally, the philosophy of coupling methods is presented.

2.1. Mathematical model for the fluid

The present work is restricted to Newtonian fluids and incompressible flows, which are modeled using the Navier-Stokes and the continuity equations. In the physical space and for an inertial reference frame, these equations are:

\[
\frac{\partial u_i}{\partial x_i} = 0, \tag{1}
\]

\[
\frac{\partial u_i}{\partial t} + \frac{\partial}{\partial x_j} (u_i u_j) = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j} \left[ \nu_e \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \right] + f_i, \tag{2}
\]

where \( u_i \) is the filtered velocity component in \([m/s]\); \( (\partial p/\partial x_i) = (1/\rho) (\partial p^*/\partial x_i) \), \( p^* \) being the filtered static pressure in \([N/m^2]\); \( f_i = f_i^* / \rho \), where \( f_i^* \) is the force field per unit of volume \([N/m^3]\); \( \rho \) is the density in \([kg/m^3]\), \( \nu_e = \nu + \nu_t \) is the effective kinematic viscosity, where \( \nu \) is the molecular viscosity and \( \nu_t \) is the kinematic turbulent viscosity, in \([m^2/s]\). The term \( f_i(\vec{x}, t) \) represents a given source term, which is defined in the entire domain \( \Omega_{PED} \), see figure 2.1. It assumes values different from zero only over the Eulerian points that is coincident with the Lagrangean immersed boundary, i.e., \( \Gamma_{PED} \) and \( \Gamma_i \). It is given by equation 3:

\[
f_i(\vec{x}, t) = \begin{cases} F_i(\vec{X}, t) & \text{if } \vec{x} = \vec{X} \\ 0 & \text{if } \vec{x} \neq \vec{X} \end{cases}, \tag{3}
\]

where \( \vec{x} \) is the position of any material particle and \( \vec{X} \) is the position of a material particle that are placed besides an immersed boundary.
The boundary conditions must be periodic in all directions of the Eulerian domain $\Omega_{PeD}$, as shown in figure 2.1, due to the properties of the Fourier pseudo-spectral method. The boundary conditions related to the physical domain $\Omega_{PhD}$ are imposed over the boundary $\Gamma_{PhD}$ and $\Gamma_i$ using the direct forcing methodology. Equation 3 shows that $f_i(\vec{x},t)$ is a discontinuous field. It is a particular case where the domains $\Gamma_{PhD}$ and $\Gamma_i$ are coincident with some collocation points of the periodical domain $\Omega_{PeD}$. When there is no coincidence, between these points, which is very frequent for problem of non Cartesian geometries, it is necessary to distribute the force field $\vec{F}_i$ on its neighbourhoods.

2.2. Mathematical model for immersed interface

The Lagrangean force field is calculated using the direct forcing methodology, which was proposed by Uhlmann (2005). One of the characteristics of this model is that there is no need of ad-hoc constants. It allows, for instance, the no-slip condition modelisation, over the immersed interface, as presented by equation 4:

$$F_i(\vec{X},t) = \frac{U_i(\vec{X},t + \Delta t) - U_i^*(\vec{X},t)}{\Delta t},$$

(4)

where $U_i(\vec{X},t + \Delta t) = U_{FI}$ is the immersed boundary velocity and $U_i^*(\vec{X},t)$ is given by:

$$U_i^*(\vec{X},t) = \begin{cases} u_i^*(\vec{x},t) & \text{if } \vec{x} = \vec{X} \\ 0 & \text{if } \vec{x} \neq \vec{X}. \end{cases}$$

(5)

In equation 5 $u_i^*(\vec{x},t)$ is the estimated velocity, obtained from the solution of Navier-Stokes equations, using $f_i(\vec{x},t) = 0$. Once $U_i^*(\vec{X},t)$ is calculated using equation 5, hence $F_i$ is calculated from equation 4 and $f_i$ is obtained from equation 3. So, the velocity is updated using equation 6:

$$u_i(\vec{x},t + \Delta t) = u_i^*(\vec{x},t) + \Delta t f_i(\vec{x},t).$$

(6)

Velocity and force must be up-dated interactively up to a given residue is attained.
2.3. **Mathematical model in the Fourier spectral space**

Given the mathematical model in the physical space, the next step is to transform it to the Fourier spectral space. For instance, as presented by Mariano et al. (2010),

The transformation of the Navier-Stokes equations gives the estimated velocity:

\[
\frac{\partial \hat{u}_i}{\partial \tau} = i k_j \varphi_{im} \left( \eta_{ef} S_{jm} - \hat{u}_j \hat{u}_m \right),
\]  

(7)

where \( \varphi_{im} \) is the projection tensor presented by Canuto et al. (2006). The non-linear terms that appear at the right hand side of equation 7 can be given by two convolution integrals, which is very expensive to be solved. Otherwise, they can be solved using the pseudo-spectral method as presented by Mariano et al. (2010).

The multi-forcing process, also presented by Mariano et al. (2010), is done up to moment that a given maximum value of the \( L_2 \) norm is attained. Note that this norm measure how good is the modelisation of the boundary condition, which is virtually imposed over the immersed boundary by the multi-forcing process.

3. **Results**

3.1. **The backward-facing step flow simulations**

Figure 2 (a) shows the physical domain \( \Omega_{Ph.D} \), which is immersed inside the periodical domain \( \Omega_{Pe.D} \). The physical domain is bounded by the immersed boundary \( \Gamma_{Ph.D} \) (solid line). The periodical domain is delimited by the boundary \( \Gamma_{Pe.D} \) (dashed line). The “physic boundary conditions” are imposed using the direct forcing method. For instance, the no-slip boundary condition is imposed over the horizontal upper and bottom walls, i.e., over part of \( \Gamma_{Ph.D} \).

![Domains illustration: (a) backward-facing step; (b) round jet.](image)

A turbulent velocity profile \( U_{in}(y,t) \) is imposed at the entrance of the backward-facing step. At the entire boundary \( \Gamma_{Pe.D} \), periodical boundary conditions are imposed. The periodic boundary condition that is imposed at the outlet of the domain make that the physic instabilities, which leave the domain, are re-injected at its entrance. In order to avoid that they affect the boundary conditions, forced at the backward step entrance, a buffer zone (BZ) is used to diffuse and dissipate these instabilities. The forcing zone (FZ) is used in order to make the streamlines aligned to the walls, at the backward-facing step entrance. These procedure are described in details by Mariano (2007) and Mariano et al. (2010).

All simulation presented in this paper were performed using the Runge-Kutta RK46 for temporal integration, which was proposed by Allampalli et al. (2009). The time step changes according to CFL criterion of Courant et al. (1967). In order to validate the methodology,
flow simulations of a backward-facing step were carried out using the domain shown in figure 2 (a). The domain dimensions are normalized by the step height $h = 0.5 \, [m]$, $L_x/h = 73.14$ and $L_y/h = 2.29$. They were divided in $N_x = 2048$ and $N_y = 64$ collocation points, respectively. The aspect ratio is $W/h = 2.0$; $L_{BZ}/h = 3.73$ and $L_{FZ}/h = 0.53$. The kinematic viscosity is given by $[m^2/s]$, where the Reynolds number is taken as $Re_h = 200$, $800$, $1,500$ and $6,000$. $U_1$ in $[m/s]$ is the reference velocity, given by the mean of the velocity profile $U_{in}(y,t)$. For all the simulation of the backward-facing step simulations, no turbulence model was used.

In figure 3 the component $\omega_z$ of the vorticity fields is shown for several values of the Reynolds number, after the statistical steady regime is attained. We note that the flow at $Re_h = 200$ is stable in the entire domain. At $Re_h = 800$ and $Re_h = 1,500$ the flow becomes unstable. In this range of the Reynolds number it is possible to note several vortex moving alternately between the upper and bottom walls. At $Re_h = 6,000$ the flow becomes unstable in all the domain.

Figure 3. The $\omega_z$ vorticity field component, for different values of the Reynolds number, at $tU_1/h = 400$.

In order to validate the methodology we compare the results of the inferior reattachment point, $x_r/h$ with experimental results of Lee & Mateescu (1998). The results of this comparison is presented in table 1, for several values of the Reynolds number, where a very good agreement is obtained for Reynolds number up to $Re_h = 400$. For higher values of the Reynolds number there is very important error of the numerical simulation, as compared with experimental results. As already shown by Armaly et al. (1983), this behaviour was expected, since the simulations presented in the present section are two-dimensional.

In the next paragraphs two main results are presented: the extension of the IMERSPEC methodology to the three dimensional applications and the straightforward parallelization of the numerical code. It is shown that the three dimensional effects is very important as the Reynolds number is increased. A three-dimensional simulation of flow over the backward-facing step was performed at $Re_h = 400$, $h = 0.5 \, [m]$, $L_x/h = 54.0$, $L_y/h = 2.29$ and $L_z/h = 2.29$. The domain was divided in $N_x = 768$, $N_y = 32$ and $N_z = 32$ collocation points, over the directions $(x,y,z)$ respectively. The aspect ratio is $W/h = 2.0$; $L_{BZ}/h = 3.60$ and $L_{FZ}/h = 0.70$, as
illustrated by figure 2.

**Table 1.** Comparison of the mean reattachment point, $x_r/h$, for different values of the Reynolds number.

| $Re_h$ | Lee & Mateescu (1998) | Present work |
|--------|----------------------|--------------|
| 200    | 8.30                 | 8.50         |
| 250    | 9.10                 | 9.71         |
| 300    | 10.30                | 10.64        |
| 350    | 11.10                | 11.39        |
| 400    | 12.90                | 12.18        |
| 450    | 13.20                | 12.61        |
| 500    | 15.50                | 13.50        |

The boundary conditions in spanwise direction are periodic. In order to model the physical noise that exist in the experimental setup (Smirnov et al., 2001), a random perturbations (order of $10^{-4}U_1$) are imposed on the inlet internal boundary condition ($\Gamma_{phD}$) of the velocity field. The results are presented in figure 4 and are compared with experimental profiles of Lee & Mateescu (1998). It is also compared with the two-dimensional results of present work. It is shown a very good agreement of the results of the present work with the experimental results. It is interesting to note that the two-dimensional results are as good as the three-dimensional results. This result was expected, since for $Re_h = 400.0$ the flow over this geometry must be in laminar, stable and almost two-dimensional.

![Figure 4](image_url)

**Figure 4.** Profiles of the longitudinal component of velocity field at $tU_1/h = 100.0$ in (a) $(x/h; z/h) = (7.0; 1.0)$ and (b) $(x/h; z/h) = (15.0; 1.0)$. Three dimensional results, compared with experimental results of Lee & Mateescu (1998) and with two-dimensional results of the present work.

Another simulation of the backward-facing step flow at $Re_h = 1,000$ was performed with $h = 0.5 \ [m]$, $Lx/h = 54.0$, $Ly/h = 2.29$ and $Lz/h = 4.3$, divided in $Nx = 768$, $Ny = 32$ and $Nz = 32$ collocation points, in the $(x, y, z)$ directions respectively. The aspect ratio is $W/h = 2.0$; $L_{BZ}/h = 3.60$ and $L_{FZ}/h = 0.70$, see figure 2 (b). In table 2 on present a
comparison of mean values of the reattachment point of inferior wall \((x_r)\), the detachment point of superior wall \((x_s)\) and the reattachment point of superior wall \((x_{rs})\) with experimental results of Lee & Mateescu (1998) and with the two-dimensional results of the present work. The results of IMERSPEC two-dimensional simulations of the backward-facing step flow, at \(Re_h = 1,000\), presented in table 2, are not in good agreement with experimental data. On the other hand, the three-dimensional simulations results are very closed to the Lee & Mateescu (1998) results, except the \(x_s/h\) which does not agree well, even for the 3D calculation. In general, these results have shown the importance of the three-dimensional effects.

### Table 2. Reattachment point on the inferior wall \(x_r/h\); detachment point on the superior wall \(x_s/h\); and reattachment point on the superior wall, \(x_{rs}/h\), for the backward-facing step flow at \(Re_h = 1,000\).

| Works                          | \(x_r/h\) | \(x_s/h\) | \(x_{rs}/h\) |
|-------------------------------|-----------|-----------|-------------|
| IMERSPEC 2D                   | 18.10     | 15.15     | 36.09       |
| IMERSPEC 3D                   | 12.42     | 16.31     | 19.36       |
| Experimental Lee & Mateescu (1998) | 12.80     | 9.70      | 18.40       |

#### 3.2. Free shear flow: spatial round jet simulations

All simulations were performed in a domain \(Lx/d = 8\), \(Ly/d = 8\) and \(Lz/d = 32\), divided with \(128 \times 128 \times 512\) collocation points in the directions \((x,y,z)\) respectively. A buffer zone and a forcing zone were used, as illustrated in figure 2 (b). The domain of interest is the total domain less the buffer and forcing zones. So, the domain of interest has \(Lx/d = 8\), \(Ly/d = 8\) and \(Lz/d = 24\). The velocity profile imposed on the entrance of the physical domain is the same for all simulations, which is given by:

\[
w(r,\theta, z) = \frac{w_1 + w_2}{2} - \frac{w_1 - w_2}{2} \tanh \left[ \frac{1}{4} \left( \frac{r}{R} - \frac{R}{r} \right) \theta \right],
\]

where \(w_1\) is the input speed of the Jet, \(w_2\) is the speed of the co-flow, \(r\) is the radial coordinate and \(\theta\) is the momentum thickness. The rate \(R/\theta\) defines the slope velocity profile, and has strong influence on the transition process to turbulence. In general, as this rate increases, the instability of the jet also increases (Michalke & Hermann, 2006). In the present work the rate used was \(R/\theta = 20\), \(w_1 = 1.025 \text{ [m/s]}\) and \(w_2 = 0.025 \text{ [m/s]}\). The Reynolds number is given by \(Re_d = (w_1 - w_2) d/\nu\). In all simulations the Reynolds number used is \(Re_d = 1,050\).

In all simulations, a noise is added to the velocity profile at the entrance of the domain, see figure 2 (b), in order to model the residual turbulence. It induces the jet transition to turbulence. The dynamic sub-grid scale Smagorinsky model (Germano et al., 1991) has been used to calculate the turbulent viscosity.

Figure 5 shows the mean dimensionless streamwise velocity component over the centerline of the jet, \(w^* = \langle \bar{w}(0,0,z) - w_2 \rangle / (w_1 - w_2)\). Three mean velocity profiles are shown. Four curves are shown for different levels of residual turbulence injected at the domain entrance. The speed fluctuations are generated using the method of Smirnov et al. (2001) and a white noise method.

Analyzing figure 5, we note that the flow generated under influence of the white noise is almost stable. All the simulation under the Smirnov et al. (2001) model became turbulent. The velocity distribution is very sensible to the kinetic turbulent energy level injected at the entrance of the domain. When a high turbulent intensity is injected, the transition to turbulence
happens early in space. On the contrary, when a low intensity turbulent is injected the transition to turbulence happens later. Using white noise, even with strong turbulence intensity, the jet remains laminar. Similar result was also found in Stanley & Sarkar (1999).

Figure 5. Distribution of the axial component of the velocity, over the axis of the jet, for $Re_d = 1,050$.

The surfaces of the criterion $Q$ are shown in figure 6. It can be observed that inside the physical domain we can found detailed turbulent structures, which was also presented by da Silva & Métais (2002). Strong interactions of longitudinal structures with Kelvin-Helmholtz instabilities can be identified. Far from the entrance the structures becomes chaotic and the turbulent regime can be identified. The coherent structure topology presents the expected behaviour.

Figure 6. Spatially developing round jet; surface of the criterion $Q$; $Re_d = 1,050$.

The spreading rate ($s$), the virtual origin ($z_0$) and the decay constant ($b_u$) of the jet were also
calculated. The table 3 shows these parameters and the comparison with the results of others authors, Todde et al. (2009) and O’Neill et al. (2004). A very good agreement of the present work results compared to the experimental results was obtained, showing the great accuracy of IMERSPEC methodology.

Table 3. Comparison of the virtual origin of jet ($z_0$), the decay constant ($b_u$) and the jet spreading rate ($s$).

| Works                  | $z_0$ | $b_u$ | $s$ |
|------------------------|-------|-------|-----|
| Todde et al. (2009)    | 4.17  | 4.13  | −   |
| O’Neill et al. (2004)  | −     | 5.60  | 0.1 |
| Present work           | 4.05  | 4.13  | 0.1 |

4. Conclusions

The IMERSEPEC methodology (Mariano et al., 2010) was improved and applied to simulate flows over a backward-facing step in two and three dimensional situations. The results obtained are very close to experimental data, even for two-dimensional simulations, for which $Re_h = 400$. At $Re_h = 1,000$ only the results of three-dimensional simulations are in good agreement with the experimental data.

The proposed methodology was also applied to simulate a spatially developing round jet in three dimensional flows. The results obtained are very close to experimental data for $Re_d = 1,050$. It is important to note that the IMERSPEC methodology was developed to incompressible flows and provide good features for Navier-Stokes equations solution, as well as, high accuracy and high convergence order. This is because the pressure linear solver for Poisson equation is replaced by a product of vector-matrix, providing by Fourier pseudo-spectral method.

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