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A study on using an immersed boundary technique for modeling 3D incompressible fluids with internal fluid-body interface

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Abstract. This work investigates the outcomes of using an immersed boundary technique for the mixed finite element formulation of tridimensional incompressible fluid flows governed by the Navier-Stokes equations with internal fluid-body interfaces. A classical Eulerian approach is followed to describe the fluid. A Newton-Raphson scheme is devised to solve the resulting non-linear equations within a time step. The fluid-body interface is treated by the Nitsche's method, which is an immersed boundary technique whereby the fluid boundary conditions over the contact with the bodies are imposed weakly. In order to ascertain the accuracy and efficiency of the adopted method, numerical simulations of tridimensional flows of an incompressible fluid are analyzed and compared against reference solutions. This work refers to an intermediate stage of a PhD research that aims to model problems of fluid-particle interaction (FPI) and particle-laden fluids.

Keywords: immersed boundary technique, Navier-Stokes equations, finite element method, 3D incompressible fluid flows.

1 Introduction

In the fluid-body interaction realm, if we restrict only to the way how the numerical method handles the interface between the fluid and the body phases, the most common numerical approaches currently available may be categorized into two major groups. The first one is called coincident boundary methods, being those in which the computational grid of the fluid ends exactly where the computational grid of the solid begins (see Donea et al. [1]). The second one is the so-called immersed boundary method in which the fluid and body meshes are totally independent from each other, and overlapped (see Benk, Ulbrich and Mehl [2]).

In this work, the objective is to evaluate the performance of an immersed boundary technique for 3D computational simulations of incompressible fluid flows governed by Navier-Stokes equations. In particular, we are interested in the Nitsche's method (Nitsche [3]) since, among other issues, it does not increase the system's degrees of freedom and has a rather straightforward implementation. A Newmark scheme (Newmark [4]) is used to time-integrate the governing equations. For the spatial discretization, a mixed finite element formulation within a standard Galerkin framework is used with a special 3D Taylor-Hood tetrahedral element which satisfies the LBB-condition (see e.g. Wieners [5] and Bruman and Fernández [6]). The fluid problem is treated through an Eulerian description, which avoids re-meshing or mesh adaptation throughout the solution. A Newton-Raphson procedure is iteratively performed within the Newmark time integration scheme to deal with the non-linearities. Numerical instability that may potentially arise from convective-dominated problems is handled considering low to moderate Reynolds numbers.

We point out that this work reports only partial results from a broader research, in which we are developing a numerical framework to deal with 3D fluid-particle interaction problems.

2 Governing equations and finite element formulation

2.1 Fluid

Let us considerer the incompressible viscous flow formulation for the Navier-Stokes equations:

$$\rho \frac{d\boldsymbol{u}}{dt} = \text{div}\boldsymbol{T} + \rho \boldsymbol{b} \quad \text{in } \Omega, \tag{1}$$

$$\text{div } \boldsymbol{u} = 0 \quad \text{in } \Omega. \tag{2}$$

Eq. (1) is the well-known conservation of linear momentum of a material point of the fluid and eq. (2) is the mass conservation principle (it is equal to zero due to the incompressibility assumption). The problem domain is referred to as Ω, whereas $\rho, \boldsymbol{u}, \boldsymbol{T}$ and $\boldsymbol{b}$ are the fluid's density, velocity field, Cauchy stress and volumetric force per unit mass, respectively.

Considering an Eulerian description and Newtonian material law for the fluid, the following system of differential equations arise from eq. (1) and eq. (2):

$$\begin{aligned} &\dot{\boldsymbol{u}} + (\nabla \boldsymbol{u})\boldsymbol{u} - 2\nu \text{div}(\nabla^s \boldsymbol{u}) + \nabla p = \boldsymbol{b} \quad \text{in } \Omega, \\ &\text{div } \boldsymbol{u} = 0 \quad \text{in } \Omega, \end{aligned} \tag{3}$$

wherein $\dot{\boldsymbol{u}} = d\boldsymbol{u}/dt$ (material time derivative), ν is the fluid's kinematic viscosity, $\nabla^s \boldsymbol{u}$ is the strain rate tensor and p the fluid's kinematic pressure.

Boundary conditions are either of Dirichlet (essential) or Neumann (natural) types. They are defined as

$$\begin{aligned} &\boldsymbol{u} = \bar{\boldsymbol{u}} \quad \text{in } \Gamma_u, \\ &\boldsymbol{T}\boldsymbol{n} = \bar{\boldsymbol{t}} \quad \text{in } \Gamma_t, \end{aligned} \tag{4}$$

where $\boldsymbol{n}$ is the unit outward normal vector to the boundary, and $\bar{\boldsymbol{u}}$ and $\bar{\boldsymbol{t}}$ are the prescribed traction and velocity vectors, respectively. The initial conditions can be written in function of the initial velocity $\boldsymbol{u}_0$ as

$$\boldsymbol{u} = \boldsymbol{u}_0 \quad \text{in } \Omega \quad (t = 0). \tag{5}$$

The weak form of (3) is

$$(\boldsymbol{w}, \dot{\boldsymbol{u}})_\Omega + c(\boldsymbol{u}; \boldsymbol{w}, \boldsymbol{u})_\Omega + a(\boldsymbol{w}, \boldsymbol{u})_\Omega - (\text{div}\boldsymbol{w}, p)_\Omega + (q, \text{div}\boldsymbol{u})_\Omega - (\boldsymbol{w}, \bar{\boldsymbol{t}})_{\Gamma_t} = (\boldsymbol{w}, \boldsymbol{b})_\Omega \quad \forall \boldsymbol{w}, q, \tag{6}$$

where $\boldsymbol{w}$ and q are arbitrary test functions for the velocity and pressure fields, respectively. The trilinear and bilinear forms of the convective and viscous terms are

$$c(\boldsymbol{u}; \boldsymbol{w}, \boldsymbol{u})_\Omega = \int_\Omega \boldsymbol{w} \cdot (\nabla \boldsymbol{u})\boldsymbol{u} d\Omega \text{ and } a(\boldsymbol{w}, \boldsymbol{u})_\Omega = \int_\Omega \nabla \boldsymbol{w} : \nu \nabla \boldsymbol{u} d\Omega. \tag{7}$$

2.2 Time discretization and integration

The time variable is discretized into time instants $(t_0, t_1, t_2, \ldots, t_n, t_{n+1}, \ldots, t_f)$, with the time-step size $\Delta t = t_{n+1} - t_n$ for the integration. In the present work we used the Newmark's method (see Newmark [4]) to integrate the eq. (6). The fluid's acceleration at time t_{n+1} is given by

$$\dot{\boldsymbol{u}}^{n+1} = \frac{1}{\gamma}\left(\frac{\boldsymbol{u}^{n+1} - \boldsymbol{u}^n}{\Delta t}\right) - \left(\frac{1-\gamma}{\gamma}\right)\dot{\boldsymbol{u}}^n, \tag{8}$$

where γ is the Newmark's integration parameter, and the notation with a superscript means the time instant at which the corresponding variable is referred. To enforce second-order accuracy in the integration, we adopt $\gamma = 1/2$. By introducing eq. (8) into eq. (6), we get the semi discrete weak form as follows

$$
\begin{aligned}
& \boldsymbol{w},\boldsymbol{u}\ _{\Omega} + \gamma\Delta t\Big[c\ \ \boldsymbol{u};\boldsymbol{w},\boldsymbol{u}\ _{\Omega} + a\ \ \boldsymbol{w},\boldsymbol{u}\ _{\Omega} - \ \mathrm{div}\boldsymbol{w},p\ _{\Omega} + \ q,\mathrm{div}\boldsymbol{u}\ _{\Omega} \\
& -\ \boldsymbol{w},\bar{\boldsymbol{t}}\ _{\Gamma_t} - \ \boldsymbol{w},\boldsymbol{b}\ _{\Omega}\Big]^{n+1} = \ \boldsymbol{w},\boldsymbol{u}^n\ _{\Omega} + \ 1-\gamma\ \ \Delta t\ \ \boldsymbol{w},\dot{\boldsymbol{u}}^n\ _{\Omega}\quad \forall \boldsymbol{w},q,
\end{aligned} \tag{9}
$$

2.3 Spatial discretization

For spatial discretization, a standard mixed finite element scheme is applied. The velocity and pressure fields are the primitive variables of the problem and the fluid's domain is discretized with the Taylor-Hood tetrahedral finite element (see Taylor and Hood [7]). Such element uses quadratic shape functions for the velocity field and linear shape functions for the pressure field to overcome the numerical instability (LBB compatibility condition). The finite element approximation can be written as

$$
\begin{aligned}
\boldsymbol{u} \approx \mathbf{N}_u\mathbf{u}_e \ \text{ and } \ p \approx \mathbf{N}_p\mathbf{p}_e, \\
\boldsymbol{w} \approx \mathbf{N}_u\mathbf{w}_e \ \text{ and } \ q \approx \mathbf{N}_p\mathbf{q}_e,
\end{aligned} \tag{10}
$$

where $\mathbf{N}_u$ and $\mathbf{N}_p$ are matrices that contain the element's shape functions of the velocity and pressure fields, respectively, and $\mathbf{u}_e$ and $\mathbf{p}_e$ are the vectors that collect the element's nodal degrees of freedom. The fully discrete weak form is obtained by introducing eq. (10) into the semi discrete weak form (9) and after some algebra we reach the matrix form of the fluid problem as below

$$
\begin{cases}
\dfrac{1}{\gamma\Delta t}\mathbf{M}\mathbf{u}^{n+1} + \mathbf{C}\ \ \mathbf{u}^{n+1}\ \ \mathbf{u}^{n+1} + \mathbf{K}\mathbf{u}^{n+1} + \mathbf{G}\mathbf{p}^{n+1} = \mathbf{f}^{n+1} + \dfrac{1}{\gamma\Delta t}\mathbf{M}\mathbf{u}^{n} + \dfrac{1-\gamma}{\gamma}\mathbf{M}\dot{\mathbf{u}}^{n} \\
\mathbf{G}^{\mathrm{T}}\mathbf{u}^{n+1} = \mathbf{0}
\end{cases}, \tag{11}
$$

where $\mathbf{M}$, $\mathbf{C}$, $\mathbf{K}$, $\mathbf{G}$ and $\mathbf{G}^{\mathrm{T}}$ are the mass, convective, viscous, gradient operator and divergent operator matrices, respectively. Still in (11), $\mathbf{f}^{n+1}$ is the vector that contains the field forces and boundary conditions. The system of equations (11) is non-linear due to the convective term, and its solution is achieved using a Newton-Raphson scheme in which complete quadratic convergence is guaranteed. For more details about the numerical derivation and implementation, the interested reader is referred to Gomes and Pimenta [8].

3 Enforcement of interface constraints

In the realm of fixed grid methods, the Nitsche's method (Nitsche [3]) has continually gained great attention in the context of implicit interfaces modeled by the XFEM (Dolbow and Harari [9]), also with imposition of constraints along non-matching surface grids (Bazilevs and Hughes [10]). In this work, the Nitsche's method is used to enforce the interface constraints (Dirichlet boundary conditions) for treating the mechanical interactions of overlapping finite element meshes, as depicted in Figure 1. One of the great advantages of this method is the fact that it does not add new degrees of freedom except from those of the original mesh.

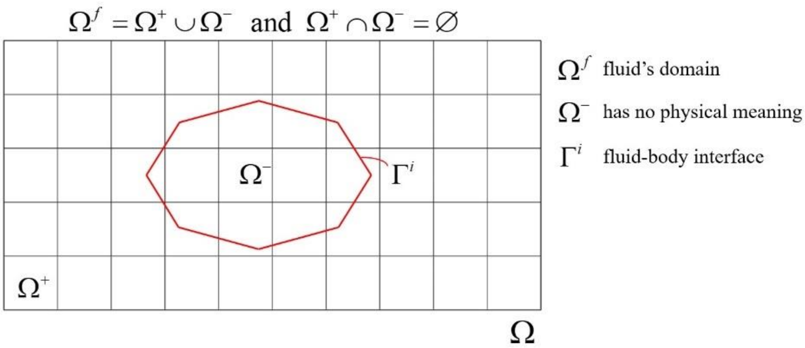

Figure 1. Embedded fluid-body interface.

Applying Nitsche's method to the Navier-Stokes problem for incompressible fluid flow, the weak form is given as

$$\begin{aligned}&\Big[\frac{1}{\gamma\Delta t}\left(\boldsymbol{w},\boldsymbol{u}\right)_{\Omega}+c\left(\boldsymbol{u};\boldsymbol{w},\boldsymbol{u}\right)_{\Omega}+a\left(\boldsymbol{w},\boldsymbol{u}\right)_{\Omega}-\left(\mathrm{div}\boldsymbol{w},p\right)_{\Omega}+\left(q,\mathrm{div}\boldsymbol{u}\right)_{\Omega}\\&-\nu\left\langle\partial_n\boldsymbol{u},\boldsymbol{w}\right\rangle_{\Gamma^i}-\nu\left\langle\partial_n\boldsymbol{w},\boldsymbol{u}\right\rangle_{\Gamma^i}+\left\langle p\boldsymbol{n},\boldsymbol{w}\right\rangle_{\Gamma^i}-\left\langle q\boldsymbol{n},\boldsymbol{u}\right\rangle_{\Gamma^i}+\nu\frac{\alpha_1}{h}\left\langle\boldsymbol{u},\boldsymbol{w}\right\rangle_{\Gamma^i}\\&+\frac{\alpha_2}{h}\left\langle\boldsymbol{u}\cdot\boldsymbol{n},\boldsymbol{w}\cdot\boldsymbol{n}\right\rangle_{\Gamma^i}\Big]^{n+1}=\Big[\left(\boldsymbol{w},\bar{\boldsymbol{t}}\right)_{\Gamma_t}+\left(\boldsymbol{w},\boldsymbol{b}\right)_{\Omega}-\nu\left\langle\partial_n\boldsymbol{w},\bar{\boldsymbol{u}}\right\rangle_{\Gamma^i}-\left\langle q\boldsymbol{n},\bar{\boldsymbol{u}}\right\rangle_{\Gamma^i}\\&+\nu\frac{\alpha_1}{h}\left\langle\bar{\boldsymbol{u}},\boldsymbol{w}\right\rangle_{\Gamma^i}+\frac{\alpha_2}{h}\left\langle\bar{\boldsymbol{u}}\cdot\boldsymbol{n},\boldsymbol{w}\cdot\boldsymbol{n}\right\rangle_{\Gamma^i}\Big]^{n+1}+\frac{1}{\gamma\Delta t}\left(\boldsymbol{w},\boldsymbol{u}^n\right)_{\Omega}+\frac{1-\gamma}{\gamma}\left(\boldsymbol{w},\dot{\boldsymbol{u}}^n\right)_{\Omega}\quad\forall\boldsymbol{w},q,\end{aligned}\tag{12}$$

where h denotes the local mesh size on the boundary Γ^i, $\partial_n(\cdot)$ is the normal derivative of $(\cdot)$, and α_1 and α_2 are penalty coefficients. The interested reader is referred to Benk, Ulbrich and Mehl [2] for more details on the Nitsche's method applied to the Navier-Stokes equations. The fully discrete weak form of eq. (12) in matrix form is given by

$$\begin{cases}\dfrac{\mathbf{M}}{\gamma\Delta t}\mathbf{u}^{n+1}+\mathbf{C}\left(\mathbf{u}^{n+1}\right)\mathbf{u}^{n+1}+\mathbf{K}^{*}\mathbf{u}^{n+1}+\mathbf{G}^{*}\mathbf{p}^{n+1}=\mathbf{f}^{n+1}+\mathbf{H}\bar{\mathbf{u}}^{n+1}\dfrac{\mathbf{1}}{\gamma\Delta t}\mathbf{M}\mathbf{u}^{n}+\dfrac{1-\gamma}{\gamma}\mathbf{M}\dot{\mathbf{u}}^{n}\\ \mathbf{G}^{\mathrm{T}*}\mathbf{u}^{n+1}=\mathbf{0}\end{cases},\tag{13}$$

where

$$\begin{aligned}&\mathbf{K}^{*}=\mathbf{K}+\mathbf{B}+\mathbf{B}^{\mathrm{T}}+\mathbf{E}+\mathbf{F},\ \mathbf{G}^{*}=\mathbf{G}_e+\mathbf{D},\ \mathbf{G}^{\mathrm{T}*}=\mathbf{G}_e^{\mathrm{T}}+\mathbf{D}^{\mathrm{T}},\ \text{and}\ \mathbf{H}=\mathbf{B}^{\mathrm{T}}+\mathbf{E}+\mathbf{F},\\&\mathbf{B}=\sum_e\mathbf{A}_e^{\mathrm{T}}\int_{\Gamma^i}-\nu\mathbf{N}_u^{\mathrm{T}}\left[\mathbf{N}_{u,j}\left(\boldsymbol{e}_j^{\mathrm{T}}\boldsymbol{n}\right)\right]d\Gamma^i\mathbf{A}_e,\ \mathbf{D}=\sum_e\mathbf{A}_e^{\mathrm{T}}\int_{\Gamma^i}\left[\boldsymbol{n}^{\mathrm{T}}\mathbf{N}_u\right]^{\mathrm{T}}\mathbf{N}_p d\Gamma^i\mathbf{A}_e,\\&\mathbf{E}=\sum_e\mathbf{A}_e^{\mathrm{T}}\left(\nu\frac{\alpha_1}{h}\right)\int_{\Gamma^i}\mathbf{N}_u^{\mathrm{T}}\mathbf{N}_u d\Gamma^i\mathbf{A}_e\ \text{and}\ \mathbf{F}=\sum_e\mathbf{A}_e^{\mathrm{T}}\left(\frac{\alpha_2}{h}\right)\int_{\Gamma^i}\left[\boldsymbol{n}^{\mathrm{T}}\mathbf{N}_u\right]^{\mathrm{T}}\left[\boldsymbol{n}^{\mathrm{T}}\mathbf{N}_u\right]d\Gamma^i\mathbf{A}_e,\end{aligned}\tag{14}$$

in which $\mathbf{A}_e$ is the assembling matrix relative to the elements of the interface i.

4 Numerical examples

The formulation above was implemented in our in-house FEM code, which is written in FORTRAN language. In the next subsections we show two numerical examples to ascertain its validity and robustness.

4.1 3D Steady laminar flow around a fixed particle

This example consists of a three-dimensional laminar flow around a fixed particle (spherical geometry) within a narrow channel governed by Stokes equations. The geometry, the boundary conditions and the finite element mesh used are illustrated in Figure 2.

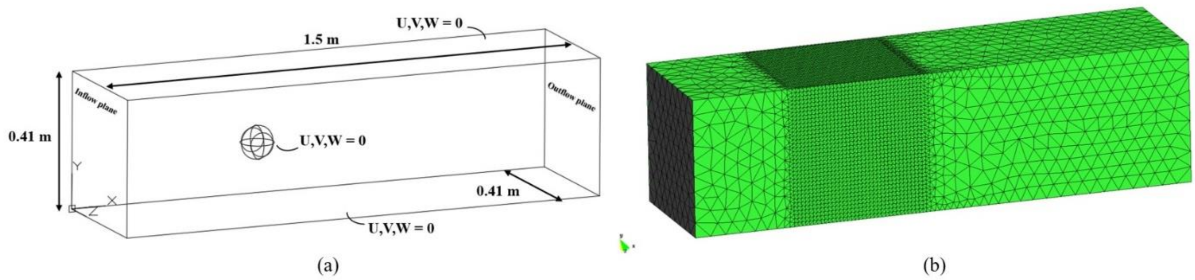

Figure 2. (a) Geometry and boundary conditions for 3D steady laminar flow around a fixed particle; (b) Finite element mesh used, 292553 tetrahedral elements and 403705 nodes.

The fluid velocity at the entrance (inflow plane) of the channel is purely horizontal (x-direction) and flows a parabolic distribution along the cross-section of the channel, given by

$$U\left(0,y,z\right)=\frac{16U_m yz\left(H-y\right)\left(H-z\right)}{H^4},V=W=0, \quad (15)$$

where $U_m = 0.45\,m/s$ and $H = 0.41m$ with $\mathrm{Re} = 45$ (Reynolds number). The fluid's density is $\rho = 1.0\,kg/m^3$ and the kinematic viscosity is $\nu = 10^{-3}\,m^2/s$. The coordinates of the center of the sphere are $C = \left(0.5, 0.2, 0.205\right)$ and its diameter is $D = 0.1m$. Notation for the velocity components is $\left(u_1, u_2, u_3\right) = \left(U, V, W\right)$ and the boundary condition at outflow plane is zero traction. The penalty coefficients used were $\alpha_1 = \alpha_2 = 10^4$. Figure 3(a) shows velocity and pressure results using a conventional simulation (i.e., applying the Dirichlet boundary condition over the fluid-body interface in a strong way). Figure 3(b) are the results in velocity and pressure fields using the immersed boundary technique with Nitsche's method. As we can see, our results are in very good agreement with the conventional simulation.

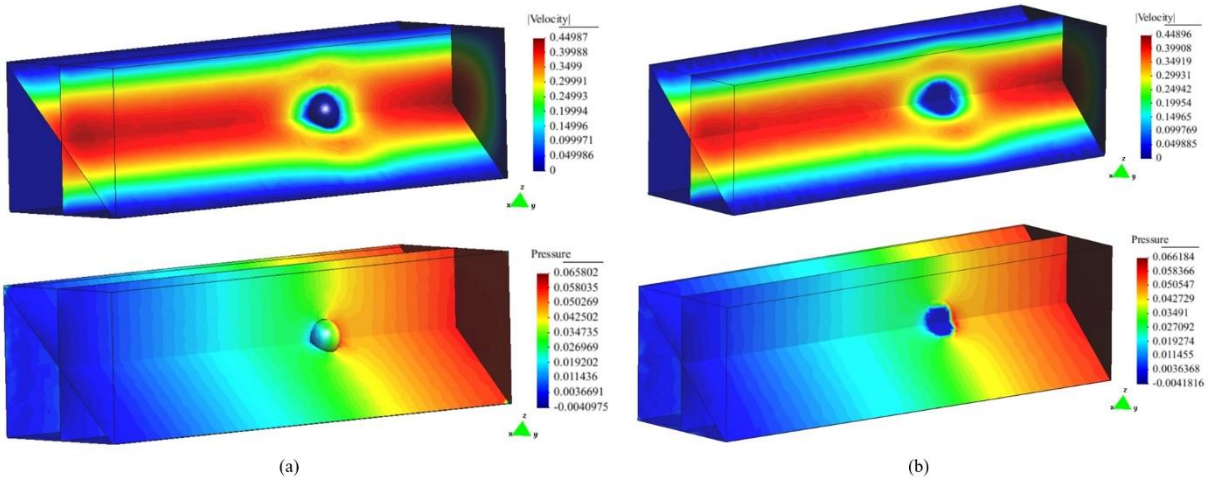

Figure 3. (a) Velocity and pressure isocurves from conventional simulation; (b) Velocity and pressure isocurves from Nitsche's method.

4.2 3D Unsteady laminar flow around two fixed particles

This example consists of a three-dimensional unsteady laminar flow around two particles (also spherical geometry) within a narrow channel governed by the Navier-Stokes equations. Figure 4 shows the geometry and boundary conditions used in this example.

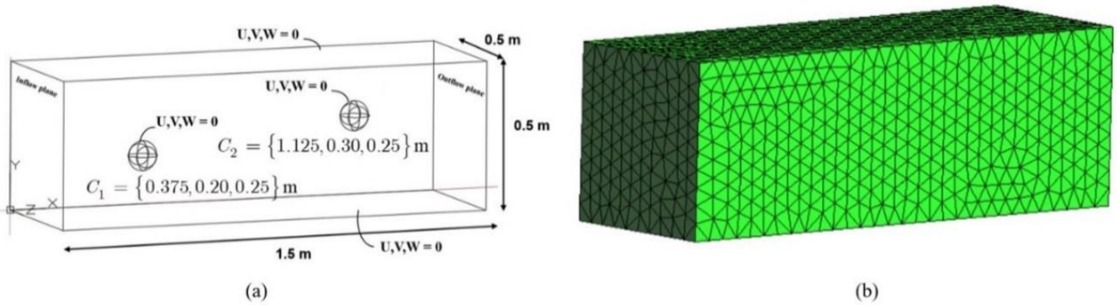

Figure 4. (a) Geometry and boundary conditions for 3D unsteady laminar flow around two fixed particles; (b) Finite element mesh used, 158057 tetrahedral elements and 213992 nodes.

The velocity profile used in this example is the same defined by eq. (15) with $U_m = 1.0\,m/s$ and

$H = 0.5m$. The fluid's density, the kinematic viscosity and the penalty coefficients are the same used in the previous example. The time interval adopted is $0 \le t \le 4.0s$ with $\Delta t = 0.01s$ and $\gamma = 1/2$. The convergence tolerance used within the Newton-Raphson interactions is $\text{TOL} = 10^{-6}$.

Figure 5 and Figure 6 show the results in velocity and pressure fields. It is possible to observe that the velocity results show again very good agreement in relation to the conventional simulation. The pressure results, in turn, are slightly different than the conventional simulation. The Nitsche's method is a kind of penalty method and when it is used to enforce the Dirichlet boundary conditions on Γ^i, it would trigger various artifacts in the pressure field in the vicinity of Γ^i that may change the final results (specially for drag and lift forces). Thus, the choice of the penalty coefficients (α_1 and α_2) and the mesh resolution around the Γ^i is of great importance in such simulations.

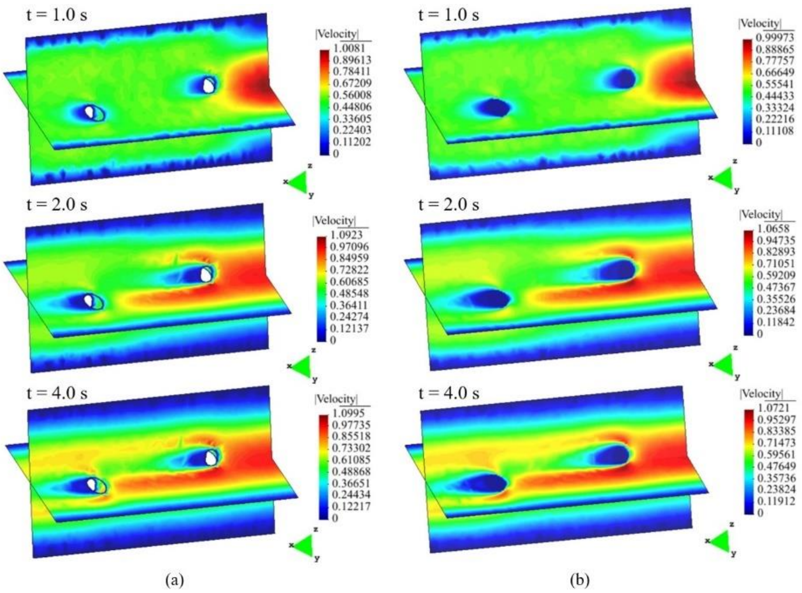

Figure 5. (a) Velocity isocurves from conventional simulation; (b) Velocity isocurves from Nitsche's method.

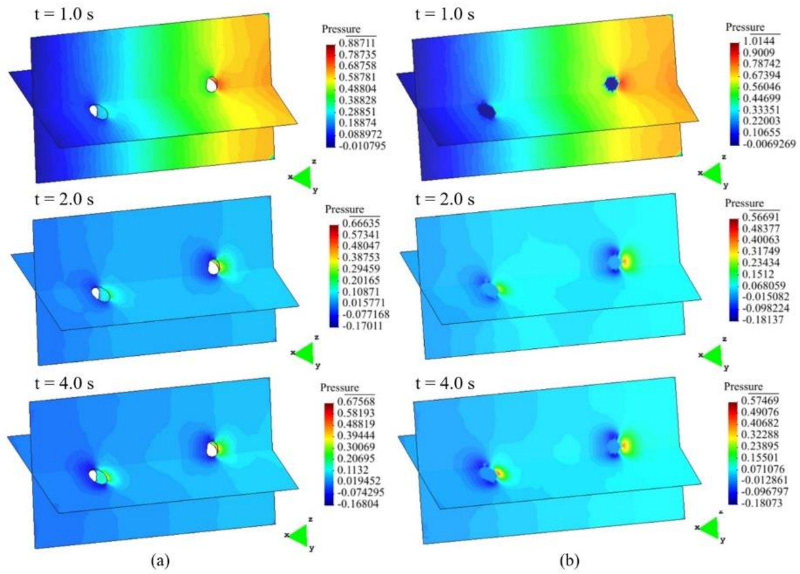

Figure 6. (a) Pressure isocurves from conventional simulation; (b) Pressure isocurves from Nitsche's method.

5 Conclusions

The main purpose of this work was to present a 3D computational simulation using an immersed boundary technique based on the Nitsche´s method for the mixed finite element formulation of incompressible fluid flows governed by Navier-Stokes equations with internal fluid-body interfaces. This is our first results for 3D simulations using such technique (i.e., Nitsche's method). Regarding only the Nitsche's method, the results showed a good agreement with the reference solutions, however, there is still some effort to understand how to correctly choose the penalty coefficients and appropriate mesh refinement in the vicinity of Γ^i to produce better results. This work is still in progress and the next step is to evaluate the drag and lift forces on each body´s surface Γ^i, with which we hope to be able to solve fluid-particle interaction problems of particle-laden fluids.

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