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# A pressure-corrected Immersed Boundary Method for the numerical simulation of compressible flows

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## Abstract

The development of an improved new IBM method is proposed in the present article. This method roots in efficient proposals developed for the simulation of incompressible flows, and it is expanded for compressible configurations. The main feature of this model is the integration of a pressure-based correction of the IBM forcing which is analytically derived from the set of dynamic equations. The resulting IBM method has been integrated in various flow solvers available in the CFD platform *OpenFOAM*. A rigorous validation has been performed considering different test cases of increasing complexity. The results have been compared with a large number of references available in the literature of experimental and numerical nature. This analysis highlights numerous favorable characteristics of the IBM method, such as precision, flexibility and computational cost efficiency.

*Keywords:* IBM, compressible flows, *OpenFOAM*

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## 1. Introduction

Recent technological progress for aerospace engineering but also ground transportation with magnetic levitation trains (Maglev) promises to reduce the travel time with always increasing speed of the vehicles. Under this perspective,

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5 transport engineering advances are more and more related with compressible  
6 flow configurations.

7 The accurate simulation of the flow evolution around immersed bodies is  
8 arguably one of the most challenging open issues in transport engineering ap-  
9 plications. Success in the flow state prediction allows for precise estimation of  
10 the aerodynamic forces acting on the vehicle, which provides fundamental in-  
11 sight for shape optimization. Gains in drag reduction of the order of percentage  
12 points will result in significantly reduced fuel consumption [1], and they will  
13 allow to remove barriers for consistent green energy usage in the coming years,  
14 in agreement with recent European laws for environment [2]. Additionally, a  
15 precise flow estimation is necessary to estimate other aspects such as the acous-  
16 tic field produced, which may result in improved features of comfort and safety  
17 for the passengers. However, the state-of-the-art in numerical simulation still  
18 needs important development to become an efficient tool for advanced transport  
19 engineering applications. Two main critical issues must be challenged:

- 20 1. **The mesh representation of complex geometric shapes.** The rep-  
21 resentation of fine geometric features in classical body-fitted simulations  
22 may result in overly deformed / stretched elements, and unfavorable char-  
23 acteristics of the mesh quality. This problematic aspect may lead to poor  
24 predictive results.
- 25 2. **Moving immersed bodies.** Even simple prescribed movement laws for  
26 the immersed body may require several computational mesh updates dur-  
27 ing the numerical simulation. These updates entail prohibitive computa-  
28 tional costs.

29 Among the numerous strategies proposed in the literature to overcome these  
30 critical issues, the *Immersed Boundary Method* (IBM) [3, 4] is an established  
31 high-performance tool for the analysis of flow configurations around complex  
32 moving bodies. The characteristic feature of the IBM is the representation of  
33 the body surface via a volume source effect which is integrated in the chosen  
34 mathematical set of equations. Thus, the computational mesh does not need

35 any manipulation in the proximity of the body surface to conform to it. This  
36 implies that negative predictive effects such as mesh element deformation can  
37 be naturally excluded. In addition, body motion can be imposed or determined  
38 without any mesh recalculation. The way these effects are integrated within  
39 the numerical simulation may vary significantly, depending on the strategy em-  
40 ployed. The IBM methods include a large spectrum of tools which operate  
41 using completely different procedures such as fictitious domain approaches [3],  
42 level-set methods [5], Lagrangian multipliers [6] and volume penalization [7].  
43 Depending on the implementation strategy employed to determine the level of  
44 volume forcing representing the body surface, the IBM approaches reported in  
45 the literature are usually classified in two large families, namely the *continuous*  
46 methods and the *discrete* methods. The principal difference in the application  
47 depends on whether the IBM force is integrated in the continuous or discretized  
48 Navier–Stokes equations. The pioneering work proposed by Peskin [3, 8] is the  
49 first continuous forcing method reported in the literature. The flow evolution  
50 is investigated using an Eulerian system of coordinates whereas the immersed  
51 body is represented on a Lagrangian system. In these methods, markers define  
52 the immersed solid boundaries. Interpolation between the two grids is obtained  
53 via approximations of the  $\delta$  delta distribution by smoother functions. Following  
54 this work, other strategies have been investigated. One notable example is the  
55 feedback forcing method, which relies on driving the boundary velocity to rest  
56 [9, 10]. Because of the integration of the IBM forcing in the continuous Navier–  
57 Stokes equations, the continuous methods are not sensitive to the numerical  
58 discretization. However, calibration of the free constants in their formulation is  
59 needed. In addition, they exhibit spurious oscillations and severe CFL restric-  
60 tions, which are associated with the choice of stiffness constants [4]. The direct  
61 forcing method, usually referred to as the discrete approach, provides solutions  
62 to the drawbacks of the continuous forcing approach. In fact, the introduction  
63 of the force term at the discretization stage provides more stable and efficient al-  
64 gorithms [4]. These strategies, which were first investigated by Mohd-Yusof [11],  
65 have been further developed in following original research works [12, 13, 14, 15].

66 The main drawback of these methods is that they exhibit a natural sensitivity to  
67 the numerical discretization, especially for the time derivative for unstationary  
68 flow configurations.

69 In the present work, a discrete IBM method proposed for the analysis of  
70 incompressible flows on curvilinear grids [16, 17, 18] is extended for the anal-  
71 ysis of compressible configurations. As previously discussed, these flows are  
72 a timely subject of investigation because of their relevance in environmental  
73 [19] / industrial [20] studies. To this aim, a pressure-based correction of the  
74 method is introduced, which dramatically improves the numerical prediction  
75 of the flow features. The IBM method developed is assessed via analysis of  
76 test cases exhibiting increasing complexity. In particular, the flow around a  
77 sphere is extensively investigated. This test case represents a classical choice for  
78 studies in aerodynamics around 3D bluff bodies, because a number of realistic  
79 features observed in flows around complex geometries can be here investigated  
80 with reduced computational resources. In addition, moderate Reynolds number  
81 configurations exhibit the emergence of different regimes for subsonic  $Ma$  values,  
82 which are extremely sensitive to fine features of the numerical representation.

83 The article is structured as follows. In Section 2 the mathematical and nu-  
84 merical background, including the analytic derivation of the new IBM method,  
85 is introduced and discussed. In Section 3 the practical implementation in the  
86 flow solvers considered is detailed. In Section 4 the IBM method is validated  
87 via analysis of classical two-dimensional test cases, encompassing a large range  
88 of  $Ma$  values. In Section 5 the flow around a sphere is analyzed. In Section 6  
89 the analysis is extended to a sphere subjected to rotation. Finally, in Section 7  
90 the concluding remarks are drawn.

## 91 **2. Numerical ingredients and Immersed Boundary Method**

92 In this section analytic and numerical details of the IBM algorithm are pro-  
93 vided.

94 *2.1. Governing equations*

95 The general Navier–Stokes equations for a compressible fluid write:

$$\frac{\partial \rho}{\partial t} + \operatorname{div}(\rho \mathbf{u}) = 0 \quad (1)$$

$$\frac{\partial \rho \mathbf{u}}{\partial t} + \mathbf{div}(\rho \mathbf{u} \otimes \mathbf{u}) = -\mathbf{grad} p + \mathbf{div} \bar{\bar{\tau}} + \mathbf{f} \quad (2)$$

$$\frac{\partial \rho e_t}{\partial t} + \operatorname{div}(\rho e_t \mathbf{u}) = -\operatorname{div}(p \mathbf{u}) + \operatorname{div}(\bar{\bar{\tau}} \mathbf{u}) + \operatorname{div}(\lambda(\theta) \mathbf{grad} \theta) + \mathbf{f} \cdot \mathbf{u} \quad (3)$$

96 where  $\rho$  is the density,  $p$  is the pressure,  $\mathbf{u}$  is the velocity,  $\bar{\bar{\tau}}$  is the tensor of the  
 97 viscous constraints,  $e_t$  is the total energy,  $\lambda$  is the thermal conductivity,  $\theta$  is the  
 98 temperature and  $\mathbf{f}$  is a general volume force term. For Newtonian fluids, the  
 99 tensor  $\bar{\bar{\tau}}$  becomes :

$$\bar{\bar{\tau}} = \mu(\theta) \left( (\overline{\operatorname{grad} \mathbf{u}} + {}^t \overline{\operatorname{grad} \mathbf{u}}) - \frac{2}{3} \operatorname{div}(\mathbf{u}) \right) \quad (4)$$

100 where  $\mu$  is the dynamic viscosity. It is here calculated using the Sutherland's  
 101 law as function of temperature  $\theta$ . The total energy  $e_t$  is defined as:

$$e_t = e + \frac{1}{2} \rho \mathbf{u} \cdot \mathbf{u} = C_v \theta + \frac{1}{2} \rho \mathbf{u} \cdot \mathbf{u} \quad (5)$$

102 where  $e$  is the internal energy and  $C_v$  is the heat capacity at constant volume.  
 103 This system is closed by the perfect gas equation of state  $p = \rho r \theta$  where  $r$  is  
 104 the specific gas constant.

105 *2.2. Immersed Boundary Method for compressible flows: numerical formulation*

106 The method here presented roots in previous works proposed by Uhlmann  
 107 [16] and Pinelli et al. [17] which combine strengths of classical continuous forc-  
 108 ing methods [3] and discrete forcing methods [21, 11]. In this framework, the  
 109 numerical results obtained in the Eulerian mesh elements  $x_s$  are modified via  
 110 a body force, which is calculated in a Lagrangian frame of reference defined  
 111 by markers  $X_s$ . These Lagrangian markers describe a discretized shape for the  
 112 immersed body. We will refer to physical quantities in the Lagrangian space  
 113 using capital letters (or via the subscript  $L$  for Greek letters), while low case  
 114 letters will be used for the Eulerian description.

115 *2.2.1. Communication between the Eulerian and Lagrangian systems*

116 Communication between the two frames of reference is performed via two  
 117 steps, namely:

- 118 • the *interpolation*, where physical quantities in the Eulerian mesh are in-  
 119 terpolated on the Lagrangian markers, in order to estimate the volume  
 120 force
- 121 • the *spreading*, where the volume force previously calculated on the La-  
 122 grangian markers is spread back on the Eulerian mesh elements

Physical quantities in the two domains are communicated via interpolation, using  $\delta$  functions originally proposed by Peskin. The case is now exemplified for the physical quantity  $\rho\mathbf{u}$  available on the Eulerian mesh. The corresponding quantity  $\rho_L\mathbf{U}$  on the  $s^{\text{th}}$  Lagrangian marker is determined via the interpolation operator  $\mathcal{I}$  as:

$$\mathcal{I}[\rho\mathbf{u}]_{X_s} = [\rho_L\mathbf{U}](X_s) = \sum_{j \in D_s} (\rho\mathbf{u})_j^n \delta_h(\mathbf{x}_j - \mathbf{X}_s) \Delta\mathbf{x} \quad (6)$$

where  $D_s$  represents the set of points of the Eulerian mesh.  $\Delta\mathbf{x}$  formally refers to an Eulerian quadrature, i.e.  $\Delta\mathbf{x} = \Delta x \Delta y \Delta z$  for the case of a Cartesian uniform mesh. The interpolation kernel  $\delta_h$  is the discretized delta function used in [17] :

$$\delta_h(r) = \begin{cases} \frac{1}{3} \left( 1 + \sqrt{-3r^2 + 1} \right) & 0 \leq r \leq 0.5 \\ \frac{1}{6} \left[ 5 - 3r - \sqrt{-3(1-r)^2 + 1} \right] & 0.5 \leq r \leq 1.5 \\ 0 & \text{otherwise} \end{cases} \quad (7)$$

123 It is centered on each Lagrangian marker  $X_s$  and takes non-zero values inside a  
 124 finite domain  $D_s$ , called the support of the  $s^{\text{th}}$  Lagrangian marker.

The backward communication from the Lagrangian markers to the Eulerian mesh is also performed using delta functions. This is done in the *spreading* step, where the value of the forcing  $F$  is distributed over the surrounding mesh. The

value of the forcing term evaluated on the Eulerian mesh,  $\mathbf{f}(\mathbf{x}_j)$ , is given by:

$$\mathbf{f}(\mathbf{x}_j) = \sum_{k \in D_j} \mathbf{F}_k \delta_h(\mathbf{x}_j - \mathbf{X}_k) \boldsymbol{\epsilon}_k \quad (8)$$

The  $k$ -index refers to a loop over the Lagrangian markers whose support contains the Eulerian node  $j$ .  $\boldsymbol{\epsilon}_k$  is the Lagrangian quadrature, which is calculated by solving a linear system to satisfy a partition of unity condition. As in [17] we have:

$$A\boldsymbol{\epsilon} = \mathbf{1} \quad (9)$$

where the vectors  $\boldsymbol{\epsilon} = (\epsilon_1, \dots, \epsilon_{N_s})^T$  and  $\mathbf{1} = (1, \dots, 1)^T$  have a dimension of  $N_s$ ,  $N_s$  being the number of Lagrangian markers.  $A$  is the matrix defined by the product between the  $k^{\text{th}}$  and the  $l^{\text{th}}$  interpolation kernels such that:

$$A_{kl} = \sum_{j \in D_l} \delta_h(\mathbf{x}_j - \mathbf{X}_k) \delta_h(\mathbf{x}_j - \mathbf{X}_l) \quad (10)$$

### 125 2.2.2. Analytic form of the IBM forcing

126 The novelty of the present approach is represented by i) the extension to  
 127 compressible flow configurations and ii) the addition of a numerical term which  
 128 penalizes deviation from the expected behavior of the pressure gradient close to  
 129 the surface of the body. In numerical simulation, the most classical choice of  
 130 boundary condition for the pressure field is a homogeneous Neumann condition  
 131 i.e. zero gradient in the wall normal direction [22]. The present investigation  
 132 encompasses exclusively this basic condition, which is implemented in most of  
 133 available open source CFD software. However, the proposed algorithm will allow  
 134 for the implementation of more sophisticated and precise pressure boundary  
 135 conditions [23] in future works. This could provide a significant improvement  
 136 for the IBM, which is usually considered less precise in the resolution of near wall  
 137 features when compared with body-fitted approaches. In this case, additional  
 138 information in the form of a wall normal vector  $\vec{e}_{n_s}$  must be provided for each  
 139 Lagrangian marker  $X_s$ .

Let us consider a general discretized form of the momentum equation 2 in the Eulerian frame of reference, represented by the mesh elements  $x_s$ . The time

advancement between the time steps  $n$  and  $n + 1$  is considered:

$$a_s (\rho \mathbf{u})^{n+1} = \phi^{n+1/2} - \mathbf{grad} p^{n+1/2} + \mathbf{f}^{n+1/2} \quad (11)$$

140 where  $a_s$  represents a discretization coefficient which is equal to  $a_s = 1/\Delta t$  if an  
 141 Euler discretization scheme for the time derivative is employed. The three right  
 142 hand terms are calculated at an intermediate time  $n + 1/2$  [16]. In particular,  
 143 the discretized term  $\phi$  includes the convective and viscous terms, as well as the  
 144 part of the discretization of the time derivative related with  $(\rho \mathbf{u})^n$ . So, if we  
 145 indicate with the affix ( $d$ ) the expected value of the solution at the instant  $n + 1$ ,  
 146 the optimal value of the forcing in the Eulerian system is:

$$\mathbf{f}^{n+1/2} = a_s (\rho \mathbf{u})^d - \phi^{n+1/2} + \mathbf{grad} p^{n+1/2} \quad (12)$$

147 In the frame of incompressible flows, Uhlmann [16] showed that the sum of  
 148 the last two terms in the right part of equation 12 corresponds to the Eulerian  
 149 solution  $-a_s (\rho \mathbf{u})^{n+1}$  at the time  $n + 1$  considering  $\mathbf{f} = 0$ . Following the work  
 150 by Uhlmann, we now shift to the Lagrangian system via *interpolation*. Details  
 151 are going to be provided in Section 2.2.1. Assuming that  $a_s$  is unchanged in the  
 152 interpolation step (which is exactly true if  $a_s$  is a function of the time  $t$  only)  
 153 and indicating in capital letters the physical quantities in the Lagrangian space,  
 154 equation 12 is transformed in:

$$\mathbf{F}^{n+1/2} = a_s (\rho_L \mathbf{U})^d - \Phi^{n+1/2} + \mathbf{grad} P^{n+1/2} \quad (13)$$

where  $\rho_L$  is the density field interpolated into the Lagrangian space. We now  
 project the term  $\mathbf{grad} P^{n+1/2}$  in equation 13 in the direction of the Lagrangian  
 wall normal  $\vec{e}_{ns}$ , obtaining

$$\mathbf{grad} P^{n+1/2} = \mathbf{grad} P^{n+1/2} \cdot \vec{e}_{ns} + \mathbf{grad} P^{n+1/2} \cdot \vec{e}_{ts}$$

155  $\vec{e}_{ts}$  represents the direction of the interpolated pressure gradient in the plane  
 156 normal to  $\vec{e}_{ns}$ . In addition, the term  $\mathbf{grad} P^d \cdot \vec{e}_{ns} = 0$  is included to the right  
 157 hand of equation 13. This term represents the expected behavior (superscript

158 *d*) of the pressure field, which supposedly exhibits a zero-gradient condition in  
 159 proximity of a wall. Equation 13 is then recast as:

$$\mathbf{F}^{n+1/2} = a_s (\rho_L \mathbf{U})^d - \Phi^{n+1/2} + \mathbf{grad} P^{n+1/2} \cdot \vec{e}_{ts} - \left( \mathbf{grad} P^d - \mathbf{grad} P^{n+1/2} \right) \cdot \vec{e}_{ns} \quad (14)$$

160 The term  $-\Phi^{n+1/2} + \mathbf{grad} P^{n+1/2} \cdot \vec{e}_{ts} = -a_s \overline{(\rho_L \mathbf{U})}$  is a realistic estimation  
 161 of a first time advancement of the flow field from  $n$  to  $n+1$  using the momentum  
 162 equation only, where the pressure gradient is evaluated using data available at  
 163 the instant  $n$ . On the other hand, the term  $(\mathbf{grad} P^d - \mathbf{grad} P^{n+1/2}) \cdot \vec{e}_{ns}$   
 164 measures the deviation from the expected behavior of the pressure gradient  
 165 following this time advancement. Thus the total forcing in the Lagrangian  
 166 system can be written as:

$$\mathbf{F}^{n+1/2} = a_s \left( (\rho_L \mathbf{U})^d - \overline{(\rho_L \mathbf{U})} \right) - \left( \mathbf{grad} P^d - \mathbf{grad} P^{n+1/2} \right) \cdot \vec{e}_{ns} \quad (15)$$

167 This more elaborated structure of the forcing  $F$  exhibits a number of inter-  
 168 esting aspects:

- 169 1. it naturally fits segregated solvers, where the flow variables are not simul-  
 170 taneously resolved and they can be obtained via corrective loops. The  
 171 new proposals exploits this feature via the separation of the pressure con-  
 172 tribution and thus it is supposed to be efficient over a larger spectrum of  
 173 CFD algorithms;
- 174 2. the calculation of the terms  $\overline{(\rho_L \mathbf{U})}$  and  $\mathbf{grad} P^{n+1/2}$  is integrated within  
 175 the classical formulation of the solver considered, and a full time step  
 176 without the addition of the forcing is not required anymore [16]. This  
 177 implies a significant reduction in the computational costs associated with  
 178 the determination of the Lagrangian forcing  $F$ ;
- 179 3. using this strategy, the behavior of the pressure field is guided towards an  
 180 expected zero-gradient condition in the wall normal direction. This result  
 181 is not granted by the classical integration of the forcing as in [16, 17] and

182 it is essential to capture important features of the flow, as shown in the  
183 following.

### 184 **3. IBM implementation in OpenFOAM numerical solvers**

185 The analytic development described in Section 2.2.2 suggests how the present  
186 formulation of the Lagrangian forcing  $F$  may be suitable for integration in a large  
187 spectrum of algorithmic architectures for fluid mechanics studies. This feature  
188 is extremely relevant for the simulation of compressible flows, where different  
189 resolution approaches must be employed depending on the values of the  $Ma$   
190 number investigated. Thus, in order to validate this important feature of the  
191 proposed method, the implementation of the IBM model has been performed  
192 in the open source library OpenFOAM. With the target to be used further to  
193 investigate industrial configurations, this code provides an efficient coding and  
194 a suitable environment for the implementation of new algorithms. It has been  
195 identified as a convenient and efficient numerical platform because of the sim-  
196 plicity in implementation as well as the availability of numerous routines already  
197 integrated, including IBM for incompressible flows [18]. Two solvers available  
198 in the standard version of the code, which allow for the investigation over a very  
199 large range of  $Ma$  numbers, are considered in the present investigation:

- 200 • the segregated pressure-based solver with PIMPLE loop for compressible  
201 flows for low Mach numbers ( $Ma \leq 0.3$ ) [24], namely *sonicFoam*.
- 202 • the segregated density-based solver with Kurganov and Tadmor divergence  
203 scheme for compressible flows for high Mach numbers ( $Ma > 0.3$ )[24],  
204 namely *rhoCentralFoam*.

205 Details about the algorithmic structure of *sonicFoam* and *rhoCentralFoam*  
206 are provided in the Appendix A. Core differences are observed in the practical  
207 resolution of the equations. These differences stem from ad-hoc strategies de-  
208 veloped with respect to the envisioned range of application of  $Ma$  values. It  
209 will be shown in the following how the IBM method here developed naturally

210 integrates within the structure of the two codes, exhibiting a very high level  
 211 of flexibility. The integration of this new IBM strategy follows recent work by  
 212 Constant et al. [18] dedicated to incompressible flows. The newly generated  
 213 solvers will be referred to in the following as *IBM* versions of the initial solver  
 214 modified and are now presented. A grid convergence analysis of the method is  
 215 provided in the Appendix B.

### 216 3.1. IBM-sonicFoam

217 The structure of the code is very similar to the scheme presented in Appendix  
 218 A. The algorithm goes through the following steps:

- 219 1. The discretized continuity and momentum equations A.1 - A.2 are re-  
 220 solved, providing a first time advancement of  $\rho^*$ ,  $\mathbf{u}^*$ .
- 221 2. A first estimation of the updated pressure field  $p^*$  is obtained via equation  
 222 A.6.
- 223 3. The fields calculated in steps 1 and 2 are *interpolated* on the Lagrangian  
 224 markers in order to obtain the value of the forcing  $\mathbf{F}$ . This value is *spread*  
 225 over the Eulerian mesh, to estimate a forcing term  $\mathbf{f}$  for each mesh cell.
- 226 4. The whole system is resolved again, starting from stored quantities at  
 227 the time step  $n$  and including the forcing term. Equations are resolved  
 228 iteratively until convergence is reached:

$$\rho^{n+1} = \frac{\phi_\rho(\rho^*, \mathbf{u}^*)}{a_\rho} \quad (16)$$

$$\mathbf{u}^{n+1} = \frac{\phi_{\mathbf{u}}(\rho^{n+1}, \mathbf{u}^*)}{a_{\mathbf{u}}} - \frac{\mathbf{grad}p^*}{a_{\mathbf{u}}} + \frac{\mathbf{f}}{a_{\mathbf{u}}} \quad (17)$$

$$e^{n+1} = \frac{\phi_e(\rho^{n+1}, \mathbf{u}^{n+1}, e^*)}{a_e} - \frac{\mathit{div}(p^* \mathbf{u}^{n+1})}{a_e} + \frac{\phi_{fe}(\mathbf{f}, \mathbf{u}^{n+1})}{a_e} \quad (18)$$

$$p^{n+1} = \frac{\phi_p(p^*, \rho^{n+1}, \mathbf{u}^{n+1})}{a_p} + \frac{\phi_{fp}(\mathbf{f})}{a_p} \quad (19)$$

229

230 In this case, the term  $\mathbf{f}$  is not recalculated during the PISO loop and is  
 231 determined only one time at the beginning of the time step.

232 *3.2. IBM-rhoCentralFoam*

233 The integration of the IBM method in the solver rhoCentralFoam presented  
 234 in the Appendix A is performed through the following steps :

- 235 1. The first predictive step resolving equations A.8 , A.9 , A.10 , A.11 and  
 236 A.13 is performed to obtain  $\rho^*$  ,  $p^*$  ,  $e^*$  and  $\mathbf{u}^*$  (and  $p^*$  via state equation).  
 237 The volume forcing is here  $\mathbf{f} = \mathbf{0}$ .  
 238 2. The physical quantities  $\rho^*$  ,  $p^*$  ,  $e^*$  and  $\mathbf{u}^*$  are interpolated in the La-  
 239 grangian space and  $\mathbf{F}$  is calculated. This field is *spread* over to the Eu-  
 240 lerian mesh, so that the value of the forcing term  $\mathbf{f}$  for each mesh cell is  
 241 determined.  
 242 3. Equations A.9 , A.10 , A.11 and A.13 are resolved again including the  
 243 IBM forcing:

$$\rho^{n+1} = \frac{\phi_\rho(\rho^*, \mathbf{u}^*)}{a_\rho} \quad (20)$$

$$(\rho\mathbf{u})^{**} = \frac{\phi'_\mathbf{u}((\rho\mathbf{u})^*)}{a_\mathbf{u}} - \frac{\mathbf{grad}p^*}{a_\mathbf{u}} \quad (21)$$

$$(\mathbf{u})^{**} = (\rho\mathbf{u})^{**}/\rho^{n+1} \quad (22)$$

$$\rho^{n+1}\mathbf{u}^{n+1} = \rho^{n+1}\mathbf{u}^{**} + \frac{\phi_\mathbf{u}(\rho^*, \mathbf{u}^*)}{a_\mathbf{u}} - \frac{\phi'_\mathbf{u}((\rho\mathbf{u})^*)}{a_\mathbf{u}} + \frac{\mathbf{f}}{a_\mathbf{u}} \quad (23)$$

$$(\rho e_t)^{**} = \frac{\phi'_{e_t}((\rho e_t)^*, \mathbf{u}^{**})}{a_{e_t}} - \frac{div(p^*\mathbf{u}^*)}{a_{e_t}} \quad (24)$$

$$e^{**} = (\rho e_t)^{**}/\rho^{n+1} - 0.5((\mathbf{u})^{**} \cdot (\mathbf{u})^{**}) \quad (25)$$

$$\theta^{**} = e^{**}/c_v \quad (26)$$

$$\begin{aligned} \rho^{n+1}e^{n+1} &= \rho^{n+1}e^{**} + \frac{\phi_e(\rho^{n+1}, \mathbf{u}^{n+1}, e^n)}{a_e} - \frac{div(\lambda(\theta^{**})\mathbf{grad}(\theta^{**}))}{a_e} \\ &- \frac{\phi'_{e_t}((\rho e_t)^*, \mathbf{u}^{**})}{a_{e_t}} + \frac{\phi_{fe}(\mathbf{f}, \mathbf{u}^{n+1})}{a_e} \end{aligned} \quad (27)$$

- 244 4. Finally, the temperature  $\theta^{n+1} = e^{n+1}/C_v$  and the pressure  $p^{n+1} = \rho^{n+1} \cdot$   
 245  $(r\theta^{n+1})$  are updated.

246 **4. Numerical validation of the IBM based algorithms**

247 Validation of the new solvers is performed on the 2D flow around a circular  
 248 cylinder. This classical test case has been extensively investigated in the litera-

249 ture for a large spectrum of values of  $Re$  and  $Ma$ , and numerous databases are  
250 available for comparison.

#### 251 4.1. Test case - numerical details

252 The size of the computational domain is chosen to be  $[-16D, 48D]$  in the  
253 streamwise ( $x$ ) direction and  $[-16D, 16D]$  in the vertical ( $y$ )-direction.  $D$  is  
254 the diameter of the cylinder. The physical domain has been determined from  
255 IBM results obtained for incompressible flows [18]. The center of the immersed  
256 circular cylinder is chosen to be in the origin of the frame of reference (Figure 1).  
257 Hexahedral mesh elements have been chosen for the discretization. The physical  
258 domain in the region  $x \times y \in [-D, D] \times [-D, D]$  is discretized in homogeneous  
259 elements of size  $\Delta x = \Delta y = 0.01D$ . Outside this central region, a geometric  
260 coarsening of the elements is imposed (ratio between neighbor elements  $r = 1.05$ )  
261 in both  $x$  and  $y$  directions. The resulting total number of mesh elements is equal  
262 to  $1.5 \times 10^5$ . In addition, the boundary conditions have been carefully selected  
263 for each case accounting for the  $Ma$  number investigated, so that their effect  
264 over the predicted results may be considered negligible. Generally speaking, a  
265 velocity inlet condition is imposed upstream (left side), a mass conserving outlet  
266 condition is imposed downstream and slip / non reflective conditions are chosen  
267 in the normal direction.

268 For each case analyzed, the main physical quantities of interest are compared  
269 with available data of the literature. In particular the bulk flow coefficients are  
270 defined as:

$$C_D = \frac{2F_x}{\rho_\infty U_\infty^2}, \quad C_L = \frac{2F_y}{\rho_\infty U_\infty^2} \quad (28)$$

271 where the forces  $F_x$  and  $F_y$  are directly calculated on the Lagrangian points  
272 and projected in the streamwise direction  $x$  and vertical direction  $y$ , respectively.  
273  $\rho_\infty$  and  $U_\infty$  denote asymptotic physical quantities imposed at the inlet.

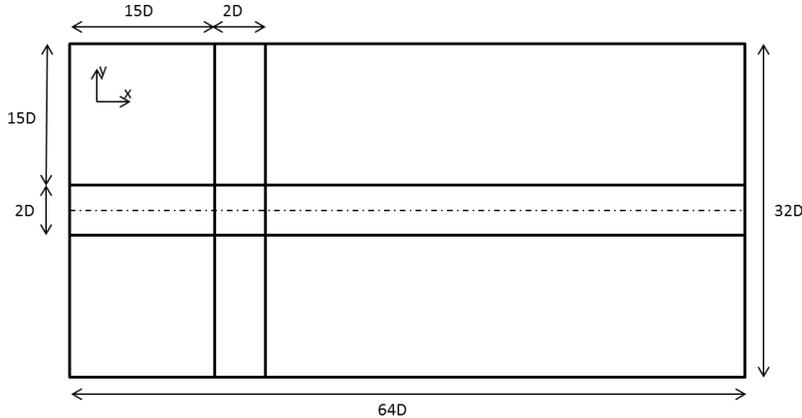


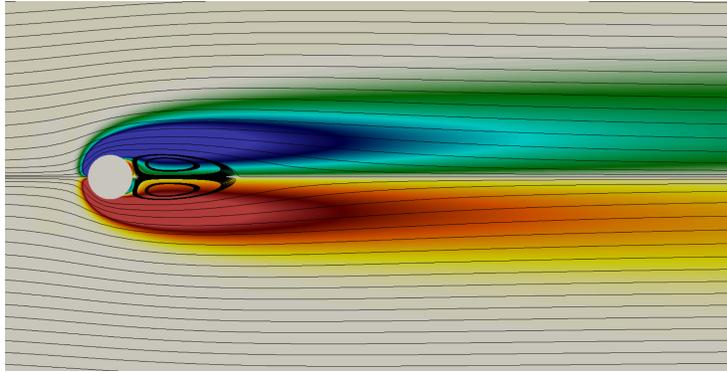
Figure 1: 2D computational domain used for IBM validation.

274 *4.2. Nearly incompressible flow around a circular cylinder case ( $Ma = 0.05$ )*

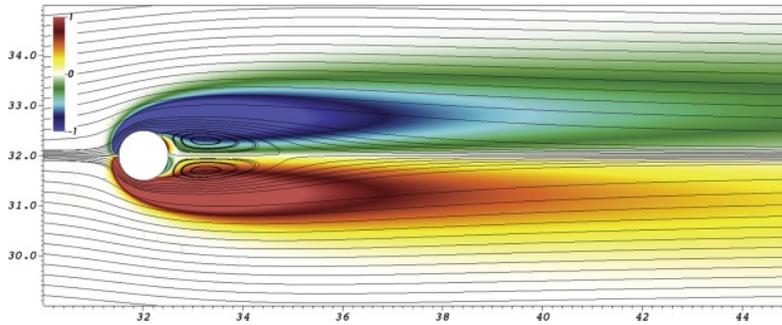
275 Because of the almost negligible contribution of compressibility effects in this  
 276 case, the pressure based solver *IBM – sonicFoam* is chosen for investigation.  
 277 Two configurations are studied for Reynolds numbers  $Re = 40$  and  $Re = 100$ .

278 For  $Re = 40$  the flow is characterized by a laminar steady recirculating re-  
 279 gion (see Figure 2) as the critical point of Bénard - von Kármán instability  
 280 is not reached. Qualitative comparison of the vorticity isocontours with data  
 281 taken from the work of Al-Marouf et al. [29] indicate that the structural orga-  
 282 nization of the flow is well captured. In addition, all characteristic geometrical  
 283 parameters and bulk flow quantities (drag coefficient  $C_D$ ) compare very well  
 284 with the data of literature reported in Table 1, assessing the present results.  
 285 This includes the pressure coefficient  $C_p = \frac{2 \times (p - p_\infty)}{\rho_\infty \times U_\infty^2}$  which is observed to be in  
 286 good agreement with results by Al-Marouf et al. [29] as shown in Figure 3.

287 For  $Re = 100$  an unstationary behavior characterized by a periodic von  
 288 Kármán wake is observed. Results include as well the Strouhal number  $S_t = \frac{fD}{U_\infty}$ ,  
 289 where  $f$  is the shedding frequency computed using the time evolution of the lift  
 290 coefficient  $C_L$ . Comparison shows a very good agreement with results available  
 291 in the literature, see Table 1. For reference, a comparison of the instantaneous



(a)



(b)

Figure 2: Axial vorticity contours and velocity streamlines for the flow past a circular cylinder for  $Ma = 0.05$  and  $Re = 40$ . A zoom around the recirculation region is shown. A qualitative comparison between (a) present IBM simulations and (b) a visualization from the work by Al-Marouf et al. [29] is shown.

292 axial vorticity isocontours obtained via IBM method with similar results re-  
 293 ported in the literature [29] is shown in Figure 4. The time evolution of the  
 294 lift coefficient is shown in Figure 5(a-d), where  $t_a = D/U_\infty$  is the characteristic  
 295 advection time.

| Study                           | $C_D$ | $x_s$ | a    | b    | $\alpha_s$ | $C_l^{rms}$ | $S_t$     |
|---------------------------------|-------|-------|------|------|------------|-------------|-----------|
| <b>Present (Re=40)</b>          | 1.58  | 2.35  | 0.7  | 0.6  | 53.7       | -           | -         |
| Tritton [32] (Exp.)             | 1.59  | -     | -    | -    | -          | -           | -         |
| Le et al. [33] (Num.)           | 1.56  | 2.22  | -    | -    | 53.6       | -           | -         |
| Dennis & Chang [34] (Num.)      | 1.52  | 2.35  | -    | -    | 53.8       | -           | -         |
| Coutanceau & Bouard [35] (Exp.) | -     | 2.13  | 0.76 | 0.59 | 53.5       | -           | -         |
| Gautier et al. [30] (Exp.)      | 1.49  | 2.24  | 0.71 | 0.59 | 53.6       | -           | -         |
| Chiu et al. [36] (Num.)         | 1.52  | 2.27  | 0.73 | 0.6  | 53.6       | -           | -         |
| Taira & Colonius [15] (Num.)    | 1.54  | 2.30  | 0.73 | 0.60 | 53.7       | -           | -         |
| Brehm et al. [37] (Num.)        | 1.51  | 2.26  | 0.72 | 0.58 | 52.9       | -           | -         |
| <b>Present (Re=100)</b>         | 1.35  | -     | -    | -    | -          | 0.237       | 0.164     |
| Berger & Wille [38] (Exp.)      | -     | -     | -    | -    | -          | -           | 0.16-0.17 |
| Le et al. [33] (Num.)           | 1.37  | -     | -    | -    | -          | 0.228       | 0.160     |
| White [39] (Theo.)              | 1.46  | -     | -    | -    | -          | -           |           |
| Stalberg et al. [31] (Num.)     | 1.32  | -     | -    | -    | -          | 0.233       | 0.166     |
| Russell & Wang. [40] (Num.)     | 1.38  | -     | -    | -    | -          | 0.212       | 0.172     |
| Chiu et al. [36] (Num.)         | 1.35  | -     | -    | -    | -          | 0.214       | 0.167     |
| Liu et al. [41] (Num.)          | 1.35  | -     | -    | -    | -          | 0.240       | 0.165     |
| Brehm et al. [37] (Num.)        | 1.32  | -     | -    | -    | -          | 0.226       | 0.165     |

Table 1: Comparison of bulk flow quantities for the flow past a circular cylinder with available data in the literature for  $Ma = 0.05$ .  $C_D$  is the drag coefficient,  $C_l$  is the lift coefficient,  $S_t$  the Strouhal number,  $x_s$  the recirculation length,  $(a, b)$  are the characteristic lengths of the vortex structural organization and  $\alpha_s$  is the separation angle. Data are provided for (top)  $Re = 40$  and (bottom)  $Re = 100$ , respectively.

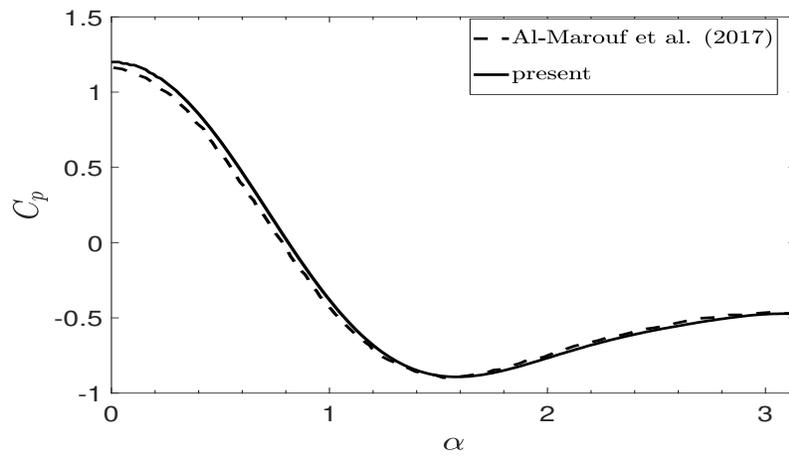
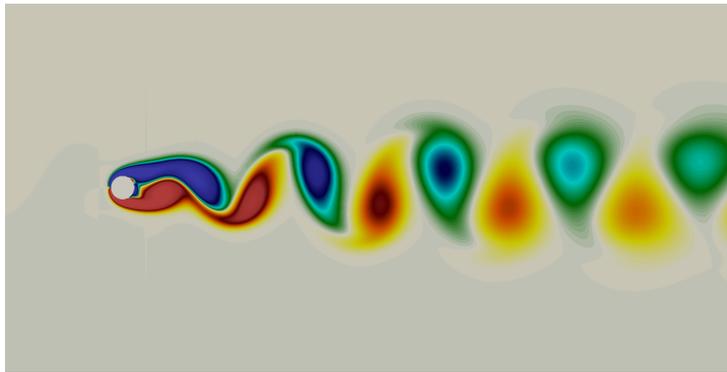
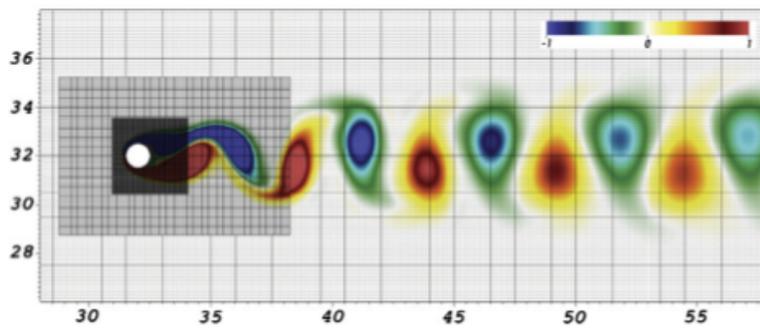


Figure 3: Pressure coefficient  $C_p$  along the cylinder surface, for the angle  $\alpha \in [0, \pi]$ . IBM results are compared with data available in the literature, steady solution for  $Ma = 0.05$  and  $Re = 40$ .



(a)



(b)

Figure 4: Axial vorticity isocontours of the flow around a circular cylinder, unsteady solution for  $Ma = 0.05$  and  $Re = 100$ . A qualitative comparison between (a) present IBM simulations and (b) a visualization from the work by Al-Marouf et al. [29] is shown.

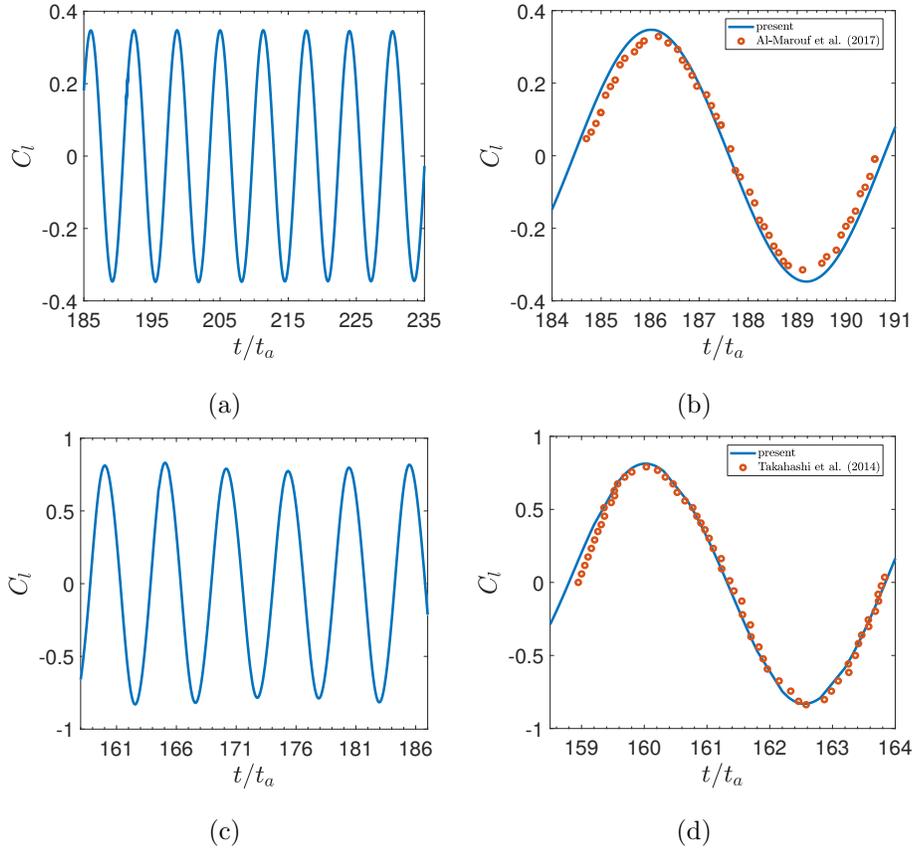


Figure 5: Time evolution of the lift coefficient  $C_l$  for the flow around a circular cylinder for (top row)  $Ma = 0.05$ ,  $Re = 100$  and (bottom row)  $Ma = 0.05$ ,  $Re = 300$ . Present IBM results are shown (left column) over a number of shedding cycles and (right column) compared with data in red markers sampled from the works reported in the literature for a single shedding cycle.

296 4.3. Subsonic flow around around a circular cylinder,  $Ma = 0.3$  and  $Re = 300$

297 The *IBM-sonicFoam* solver is used to perform the present investigation.  
298 For this case compressibility effects are not negligible anymore, albeit they do  
299 not drive the flow evolution. One notable established observation is that the  
300 unstationary vortex shedding does not exhibit a three-dimensional behavior in  
301 this case, contrarily to what is obtained for incompressible flows at the same  $Re$ .  
302 The axial vorticity isocontours are plotted in Figure 6 and the time evolution  
of the lift coefficient is shown in Figure 5 (c-d).

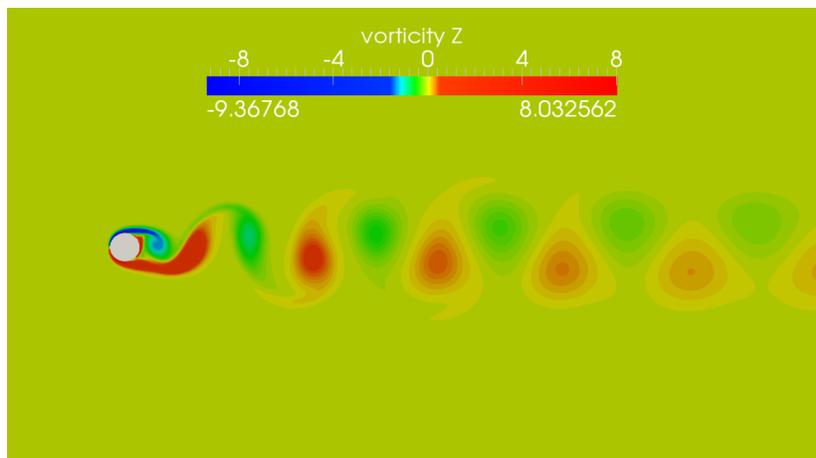


Figure 6: Vorticity isocontours for the flow around a circular cylinder,  $Ma = 0.3$  and  $Re = 300$ .

303

304 Present results for the bulk flow quantities are compared with a classical  
305 body fitted simulation available in the literature [42] in Table 2. The bulk  
306 flow coefficients exhibit a good match with the available reference, assessing the  
307 precision of the IBM solver.

308 4.4. Supersonic flow around cylinder,  $Ma = 2.0$  and  $Re = 300$

309 The strong compressibility effects provide a regularization of the flow, which  
310 is known to be in this case stationary and two-dimensional. The density isocon-  
311 tours in the near field of the cylinder are shown in Figure 7(a) and compared

| Case                         | $C_D$ | $C_l^{rms}$ | $\Delta_{shock}$ |
|------------------------------|-------|-------------|------------------|
| <b>Present (Ma=0.3)</b>      | 1.5   | 0.566       | -                |
| Takahashi et al. [42] (Num.) | 1.444 | 0.573       |                  |
| <b>Present (Ma=2)</b>        | 1.51  | -           | 0.69             |
| Takahashi et al. [42] (Num.) | 1.55  | -           | -                |
| Billig. [43] (Theo.)         | -     | -           | 0.62             |

Table 2: Drag coefficient  $C_D$ , standard deviation of the lift coefficient  $C_l^{rms}$  and standoff distance  $\Delta_{shock}$ , computed for the flow around a circular cylinder for  $Re = 300$ ,  $Ma = 0.3$  and  $Ma = 2$ . Present IBM results are compared with data available in the literature.

312 with a similar representation by Takahashi et al.[42] (Figure 7(b)). The IBM-  
313 rhoCentralFoam solver successfully captures the physical behavior of the flow,  
314 which exhibits a stationary and symmetric behavior. In addition, a bow shock  
315 before the circular cylinder is clearly obtained as shown in Figure 7 (c).

316 The comparison of the drag coefficient  $C_D$  and standoff distance  $\Delta_{shock}$  with  
317 available data in the literature [42, 43] reported in Table 2 again indicates that  
318 a successful prediction of the flow is obtained. The standoff distance  $\Delta_{shock}$  is  
319 the minimum separation from the shock and the immersed body. Additionally,  
320 the pressure coefficient distribution is compared with data from Takahashi et  
321 al. [42] in Fig. 8, showing again, a very good match with available reference.

#### 322 4.5. Effects of the pressure gradient correction in the IBM forcing

323 At last, the effects of the newly introduced term in the IBM formulation are  
324 assessed. To do so, three different numerical settings have been considered:

- 325 • Complete IBM forcing as in equation 15
- 326 • IBM forcing without pressure correction (i.e. first term of equation 15)
- 327 • Body fitted

328 The three strategies have been applied to the analysis of the flow around  
329 a circular cylinder for different values of  $Ma \in [0.05, 2]$  and  $Re \in [40, 300]$ .

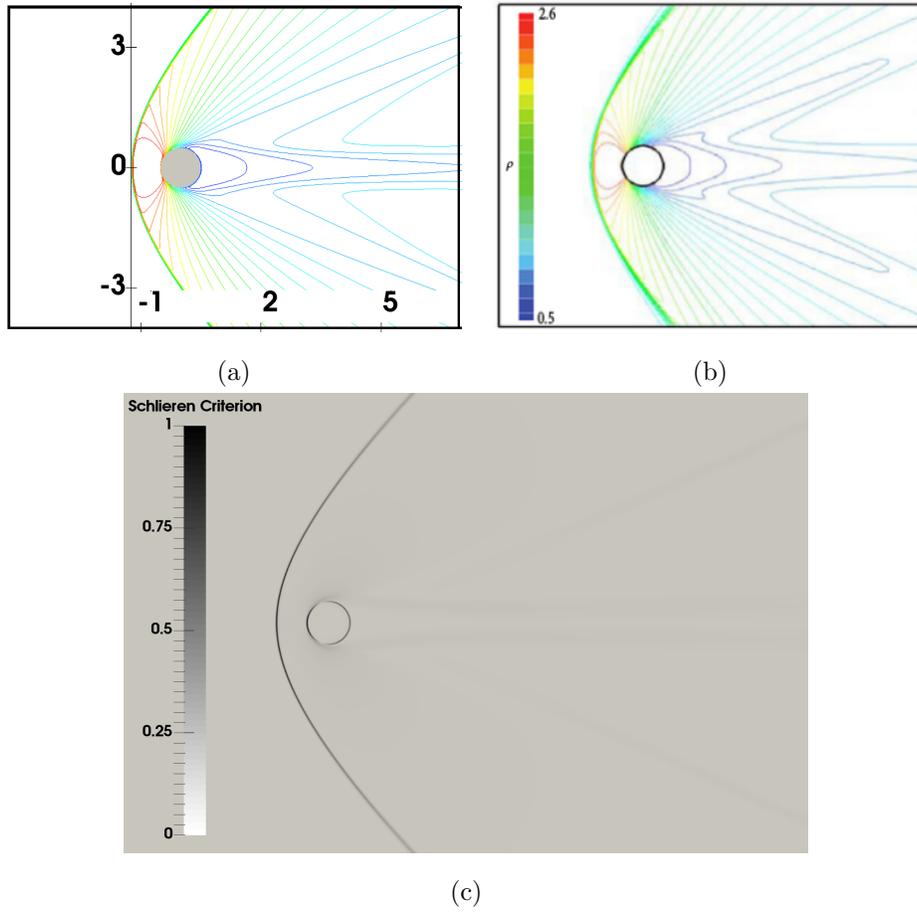


Figure 7: Density  $\rho$  isocontours for the flow around a circular cylinder for  $Ma = 2.0$  and  $Re = 300$ . (a) Present **normalized** IBM results are compared with (b) visualizations taken from the work of Takahashi et al.[42]. **The legend for  $\rho$  is the same for the two figures and the size of the zoom in  $D$  units is almost identical, allowing for direct qualitative comparison.** (c) Visualization via the **normalized** Schlieren criterion of the bow shock.

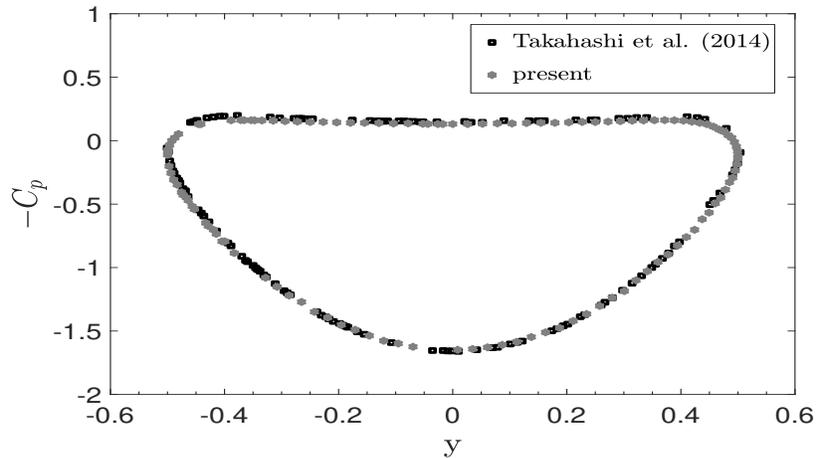


Figure 8: Pressure coefficient distributions for the case  $Ma = 2.0$ ,  $Re = 300$ . Present IBM results are compared with data available in the literature.

330 The mesh resolution around the cylinder and in the wake area is roughly the  
 331 same for the three simulations and it was verified that convergence of the re-  
 332 sults was reached. In addition, the time step for the simulations is the same  
 333 and it has been set to comply with the relation  $\max(Co) = 0.1$ , where  $Co$  is  
 334 the Courant number. Results are shown in figure 9 for two different simulations  
 335 for  $Re = 40$ ,  $Ma = 0.05$  and  $Ma = 2$ . The comparison of the surface distribu-  
 336 tion of the pressure coefficient  $C_p$  is shown. The two configurations have been  
 337 chosen to highlight the behavior of the IBM forcing over the parametric space  
 338 investigated. Counter-intuitively, the configuration for  $Ma = 2$  is the easiest  
 339 to predict, because the presence of the bow shock regularizes the wall pressure  
 340 behavior. In this case, as shown in figure 9(a), the three simulations obtain an  
 341 almost identical behavior for  $C_p$ . For more complex configurations, such as the  
 342 case for  $Ma = 0.05$  in figure 9(b), one can observe that the IBM without pres-  
 343 sure correction exhibits accuracy issues. On the other hand, the quality of the  
 344 prediction using the IBM pressure corrected scheme systematically matches the  
 345 body-fitted prediction for every configuration investigated. Thus, the inclusion  
 346 of this term provides a beneficial effect in particular for complex configurations,  
 347 preventing a degradation of the IBM performance for these applications. The

348 analysis of the database did not indicate that the pressure correction is more  
349 beneficial for low or high  $Ma$  configurations. It just prevents loss of accuracy for  
350 complex applications. Thus, the inclusion of the pressure correction term in the  
351 IBM formalism dramatically improves the robustness for the calculation of the  
352 pressure field in the near wall region. The precise calculation of the wall pres-  
353 sure distribution is an essential feature governing the emergence and evolution of  
354 different dynamic regimes, which are going to be studied for three-dimensional  
355 immersed bodies in the next sections.

## 356 5. Compressible flow regimes around a sphere

357 The three-dimensional flow around a sphere is now investigated. As previ-  
358 ously mentioned, this investigation encompasses a large range of  $Ma$  and  $Re$   
359 values, representing a challenging test case for validation.

### 360 5.1. Computational grids

361 The computational domain is here set to  $x \times y \times z = [-16D, 48D] \times$   
362  $[-16D, 16D] \times [-16D, 16D]$  where  $D$  is the diameter of the sphere. Again,  
363 the center of the body is set in the origin of the system. Two computa-  
364 tional meshes have been employed to investigate this test case. A first coarser  
365 mesh, which will be referred to as *sphereA*, is made by hexahedral uniform  
366 elements which are progressively refined approaching the sphere region (see fig-  
367 ure 10). The size of the elements is refined by a factor two in each space  
368 direction when crossing the prescribed interfaces between regions at differ-  
369 ent resolution. The central most refined region is defined by the coordinates  
370  $x \times y \times z = [-1.25D, 1.25D] \times [-1.25D, 1.25D] \times [-1.25D, 1.25D]$ . Within this  
371 region, the mesh resolution is  $\Delta x = \Delta y = \Delta z = 1/64D$ . This mesh is composed  
372 by a total of  $5 \times 10^6$  elements.

373 A second more refined mesh, which will be referred to as *sphereB*, has been  
374 employed to perform a more accurate analysis of the near wall features for a  
375 limited number of targeted values of  $Ma$ ,  $Re$ . The mesh is almost identical to

376 *sphereA*, but a higher resolution region is included for  $x \times y \times z = [-D, D] \times$   
 377  $[-D, D] \times [-D, D]$ . Within this region, a resolution  $\Delta x = \Delta y = \Delta z = 1/128D$   
 378 has been imposed. The total number of mesh elements is in this case  $16 \times 10^6$ .

The size of the mesh elements in the near wall region has been selected accordingly to the recommendations of Johnson and Patel [46]:

$$\Delta x_{min} = \Delta y_{min} = \Delta z_{min} \approx \frac{1.13}{\sqrt{Re} \times 10.0} \quad (29)$$

379 In order to provide a suitable representation of the physical features of the  
 380 flow, the *IBM-sonicFoam* solver is used for  $Ma \leq 0.3$  and conversely the *IBM-*  
 381 *rhoCentralFoam* solver is employed for  $Ma > 0.3$ .

382 The numerical simulations have been performed using the native mpi paral-  
 383 lelization software available in OpenFOAM and the physical domain has been  
 384 partitioned in 40 and 64 sub-domains for *SphereA* and *SphereB*, respectively.  
 385 For the simulation of steady cases, flow convergence is obtained after approx-  
 386 imately 90 scalar hours for simulations using mesh *sphereA* and 150 hours for  
 387 simulations using mesh *sphereB*. For unsteady simulations, the CFL number  
 388 has been fixed to 0.1. The computational resources demanded to perform a full  
 389 shedding cycle in an established regime is on average equal to 48 - 84 scalar  
 390 hours for the mesh *sphereA* and for the mesh *sphereB*, respectively.

## 391 5.2. Physical regimes observed for moderate $Re$

392 This test case has been chosen because of the emergence of different regimes  
 393 which exhibit a very high sensitivity to the asymptotic values of  $Ma$  and  $Re$   
 394 prescribed at the inlet, representing a challenging test case of validation. In  
 395 particular, if very low  $Ma$  configurations are considered, the flow undergoes a  
 396 transition from a steady axisymmetric state to a steady planar-symmetric con-  
 397 figuration and finally an unsteady regime with progressively higher Reynolds  
 398 numbers. The two transitions are observed for  $Re \approx 210$  and  $Re \approx 280$ , respec-  
 399 tively. For  $Ma$  progressively higher, the two threshold  $Re$  values increase but  
 400 they get progressively closer, finally superposing for  $Ma \approx 1$ . For higher  $Ma$

401 values, a steady planar-symmetric regime is not observed anymore. A represen-  
402 tation of the qualitative features of these three regimes ( $Ma = 0.4$ ) is shown in  
403 Figure 11 using vorticity isocontours.

404 In order to perform a rigorous investigation of this test case, a database of 120  
405 numerical simulations has been performed in the parametric space  $[Ma] \times [Re] =$   
406  $[0.3, 2] \times [50, 600]$  using the coarser mesh *sphereA*. Results are compared with  
407 recent data reported in the literature for body-fitted numerical simulations using  
408 high order discretization schemes [44, 45].

### 409 5.3. Emergence of different characteristic regimes: a parametric study

410 The emergence of different flow regimes with variations in the prescribed  
411 values of  $(Ma, Re)$  is here investigated. The resulting regimes observed via  
412 analysis of the database of 120 simulations performed using the mesh *sphereA*  
413 are summarized in Figure 12. The comparison with high precision data by San-  
414 sica et al. [45] indicates that very similar thresholds for the transition between  
415 dynamic regimes are obtained as shown in Figure 13. Maximum differences  
416 observed are of the order of  $\approx 8\%$  of the Reynolds number. These maximum  
417 differences are observed for  $Ma \approx 0.8$ ,  $Re \approx 250$  where Sansica et al. [45] hy-  
418 pothetised a linear evolution of the threshold value which was determined via  
419 stability analysis from a limited number of simulations. Thus, it is arguable that  
420 this relatively small difference in the results could simply be associated with the  
421 strategy of investigation. In particular, the very larger number of IBM numer-  
422 ical simulations here performed around the parameter value  $Ma \approx 1$  suggests  
423 that the disappearance of the steady planar-symmetric regime is rather abrupt  
424 and not linearly progressive.

425 The database results have been employed to perform as well quantitative  
426 analyses of the main bulk quantities characterizing the flow regimes. A map of  
427 the drag coefficient  $C_d$ , the separation angle  $\alpha_s$  and the recirculation length  $x_s$   
428 as a function of  $Re$  and  $Ma$  are shown in Figures 14. The comparison of the  
429 present results with data by Nagata et al. [44] further assesses the precision of  
430 the proposed IBM method.

|                | Studies                                | $\overline{C_D}$ | $x_s$ | $St$  | $\Delta_{shock}$ |
|----------------|--|------------------|-------|-------|------------------|
| <b>Ma=0.3</b>  | <b>Present (Re=300) <i>sphereA</i></b> | 0.72             | 2.15  | 0.118 | -                |
|                | <b>Present (Re=300)</b>                | 0.703            | 2.05  | 0.123 | -                |
|                | Nagata [44] (Num.)                     | 0.68             | 2     | 0.128 | -                |
|                | <b>Present (Re=600) <i>sphereA</i></b> | 0.605            | 2.2   | 0.135 | -                |
|                | <b>Present (Re=600)</b>                | 0.58             | 2.1   | 0.143 | -                |
|                | Krumins [47] (Exp.)                    | 0.54             | -     | -     | -                |
| <b>Ma=0.95</b> | <b>Present. (Re=50)</b>                | 2.116            | 1.15  | -     | -                |
|                | <b>Present (Re=600)</b>                | 0.91             | 4.1   | 0.138 | -                |
|                | Krumins [47] (Exp.)                    | 0.9              | -     | -     | -                |
| <b>Ma=2</b>    | <b>Present (Re=300)</b>                | 1.39             | 1     | -     | 0.2              |
|                | Nagata [44] (Num.)                     | 1.41             | 1     | -     | 0.2              |
|                | <b>Present (Re=600)</b>                | 1.27             | 1.1   | -     | 0.18             |
|                | Krumins [47] (Exp.)                    | 1.17             | -     | -     | -                |

Table 3: Bulk flow quantities for the flow past a sphere, obtained via IBM simulation. The refined grid *sphereB* is used for all but two cases, where *sphereA* has been chosen. Present results are compared with available data in the literature.  $C_D$  is the time-averaged drag coefficient,  $x_s$  is the recirculation length,  $St$  is the Strouhal number and  $\Delta_{shock}$  is the shock distance.

431 *5.4. Investigation of the subsonic flow around a sphere*

432 The unsteady flow configurations are analysed using the mesh *sphereB* for  
433 the two sets of parameters  $(Ma, Re)=(0.3, 300)$  and  $(0.3, 600)$ . For these two  
434 cases, an unsteady behavior is obtained as shown by the time evolution of the  
435 lift coefficient  $C_l$  shown in Figure 15. The drag coefficient  $C_d$  and the Strouhal  
436 number  $St$  are reported in Table 3. The comparison of these quantities with  
437 data from the literature [44, 47] assesses the high level of performance of the  
438 proposed IBM-solver. In addition, the comparison with results using the coarse  
439 grid *sphereA* highlights very limited differences, which assesses the robustness  
440 of the criteria employed to determine the mesh refinement.

### 441 5.5. *Finer analysis of transonic regimes*

442 A limited number of numerical simulations have been performed using the  
443 mesh *sphereB* to further investigate the emergence of different dynamic regimes  
444 for  $Ma = 0.95$ . We remind that this threshold value for the  $Ma$  number cor-  
445 responds to an abrupt transition from the steady axisymmetric state to the  
446 unsteady regime. Two higher-resolution numerical simulation are performed  
447 for  $Re = 50$  and  $Re = 600$ . Isocontours of  $Ma$  are shown in Figure 16 (a-b)  
448 for the two cases. For the latter, a detached shock can be clearly observed via  
449 Q-criterion and Schlieren criterion, which is reported in Figure 16 (c-d). In  
450 addition, the comparison of the bulk flow quantities with data from the litera-  
451 ture [44, 47], which are reported in table 3, again assesses the precision of the  
452 proposed IBM method.

### 453 5.6. *Investigation of the supersonic flow around a sphere*

454 The supersonic flows for  $Ma = 2$  are investigated using the refined mesh. In  
455 this case, the numerical simulations are performed for  $Re = 300$  and  $Re = 600$ .  
456 In this case compressibility effects are very strong and a steady axisymmetric  
457 configuration is observed in both cases. The analysis of the main bulk flow  
458 quantities, which is reported in table 3, indicates that all the physical features  
459 are accurately captured, when compared with data in the literature [47, 44].  
460 Qualitative representations via isocontours of the  $Ma$  number and the Schlieren  
461 criterion are shown in Figure 17(a) and in Figure 17(b), respectively. These  
462 results assess the correct representation of the physical features of the flow via  
463 IBM.

## 464 6. Flow around a sphere under rotation

465 In this section, a flow configuration including an immersed moving body is  
466 studied. In order to consistently advance with respect to the analyses in the  
467 previous sections, the flow around a rotating sphere is investigated. The sphere  
468 rotates with constant angular velocity  $\omega$  around the  $z$  axis. The asymptotic inlet

469 Mach number  $Ma_\infty$  of the flow in the streamwise  $x$  direction and the rotational  
470 Mach number  $Ma_\omega = \omega D/2$  characterizing rotation are:

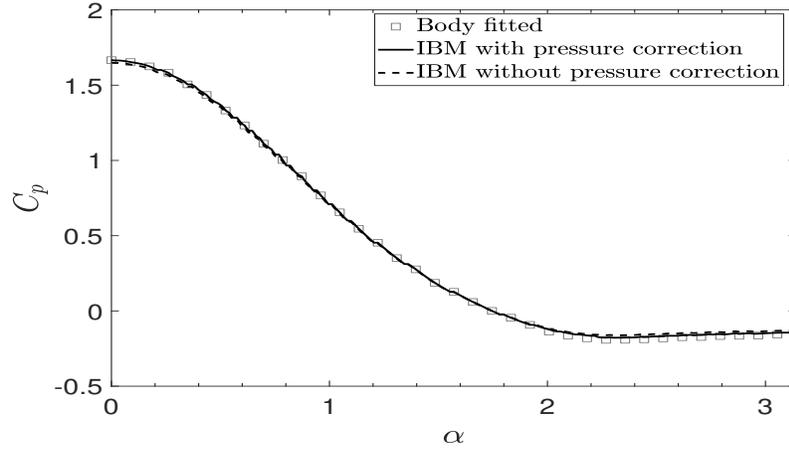
$$Ma_\infty = 0.5 \tag{30}$$

$$Ma_\omega = 0.5 \tag{31}$$

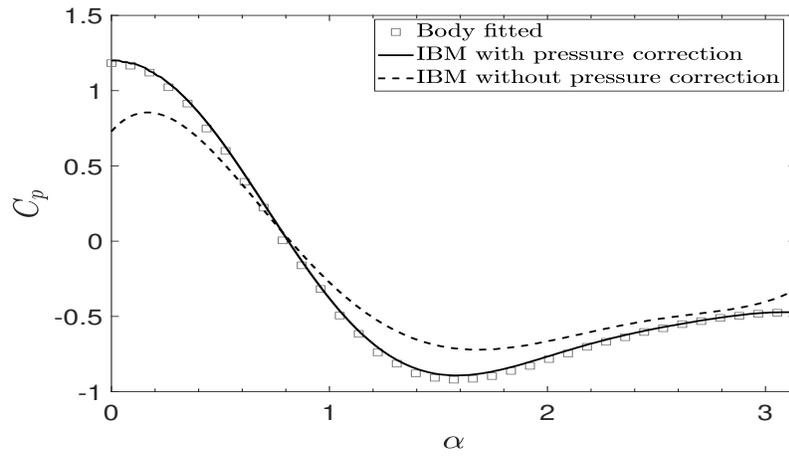
471 Two simulations are performed for  $Re = 200$  and  $Re = 300$ , respectively.  
472 They are compared with correspondent IBM simulations of the flow around a  
473 fixed sphere i.e.  $Ma_\omega = 0$ . The comparison between the four simulations is re-  
474 ported in Figures 18 , 19 and 20 using the Q criterion, velocity streamlines and  
475  $Ma$  isocontours. For the case  $Re = 200$ , the flow without imposed rotation is  
476 stationary. However, the sphere rotation triggers the emergence of an unsteady  
477 regime, where coherent structures are periodically advected downstream. Addi-  
478 tionally, the streamlines behind the sphere lose their symmetric behavior. For  
479  $Re = 300$ , both flow configurations are unstationary. However, the effect of  
480 the rotation is clearly visible in the evolution of the flow quantities. In partic-  
481 ular, the recirculation bubble is not symmetrical anymore, and a lift effect is  
482 obtained. More interesting features can be deduced by the analysis of the bulk  
483 flow coefficients reported in table 4. Generally speaking, the rotation is respon-  
484 sible for an increased value of the drag coefficient  $C_D$  and the Strouhal number  
485  $S_t$ . However, the generation of a lift force is as well observed, which is usually  
486 referred to as Magnus effect. The analysis of the present results indicates that  
487 the IBM model successfully captures this physical feature.

| Studies           | $C_D$ | $C_l$ | $C_l^{rms}$ | $S_t$ |
|-------------------|-------|-------|-------------|-------|
| <b>Re = 200</b>   |       |       |             |       |
| $Ma_\omega = 0$   | 0.87  | 0     | -           | -     |
| $Ma_\omega = 0.5$ | 1.02  | 0.5   | 0.46        | 0.17  |
| <b>Re = 300</b>   |       |       |             |       |
| $Ma_\omega = 0$   | 0.77  | 0.08  | 0.068       | 0.12  |
| $Ma_\omega = 0.5$ | 0.92  | 0.47  | 0.45        | 0.22  |

Table 4: Bulk flow quantities for the flow around a sphere under rotation.



(a)



(b)

Figure 9: Distribution of the pressure coefficient  $C_p$  obtained via body-fitted and IBM numerical simulations. Data are visualized with respect to the angle  $\alpha \in [0, \pi]$ . The case of the stationary flow around a circular cylinder for  $Re = 40$  is investigated. Configurations for (a)  $Ma = 2$  and (b)  $Ma = 0.05$  are shown, respectively.

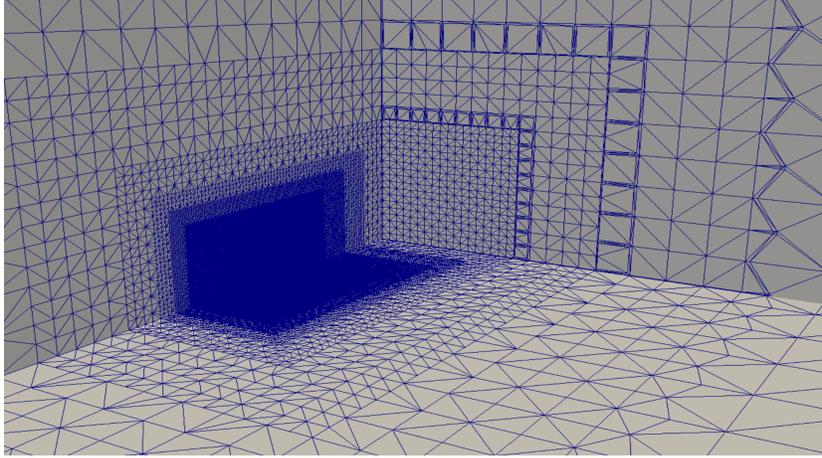


Figure 10: Visualization of cutting planes inside the 3D mesh used for the calculation of the flow around a sphere.

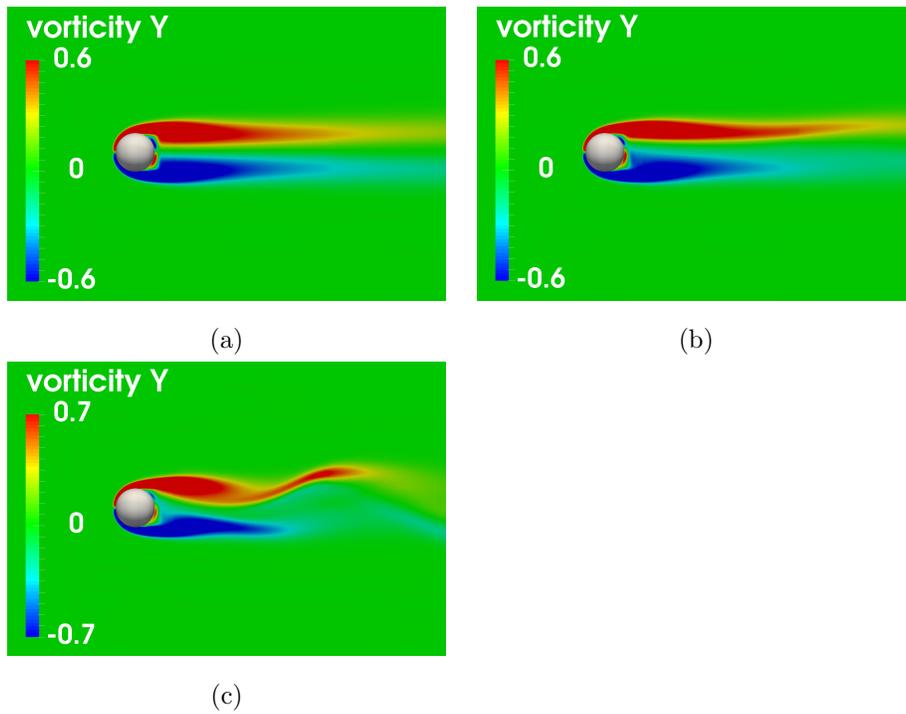


Figure 11: Vorticity contours for the flow around a sphere for  $Ma = 0.4$ , (a)  $Re = 205$  (steady axisymmetric state), (b)  $Re = 250$  (steady planar-symmetric configuration) and (c)  $Re = 300$  (unsteady regime). The vorticity component around the  $y$  axis is shown.

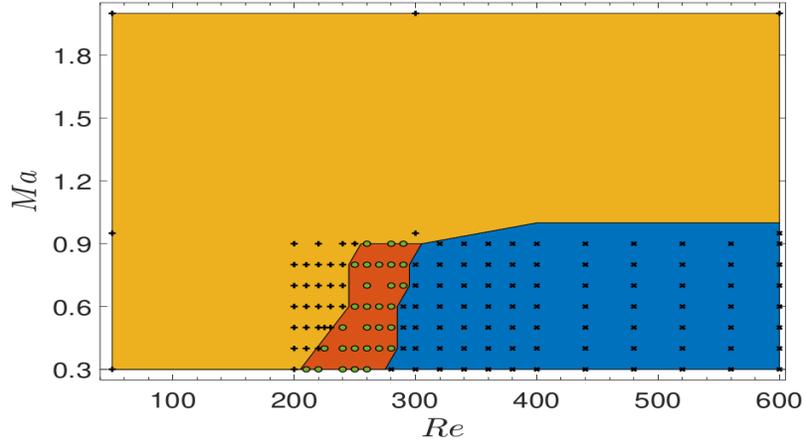


Figure 12: Emergence of different characteristic regimes for the flow around a sphere, as a function of  $Re$  and  $Ma$ : (+) steady axisymmetric flow, (●) steady planar-symmetric flow, (x) unsteady periodic flow.

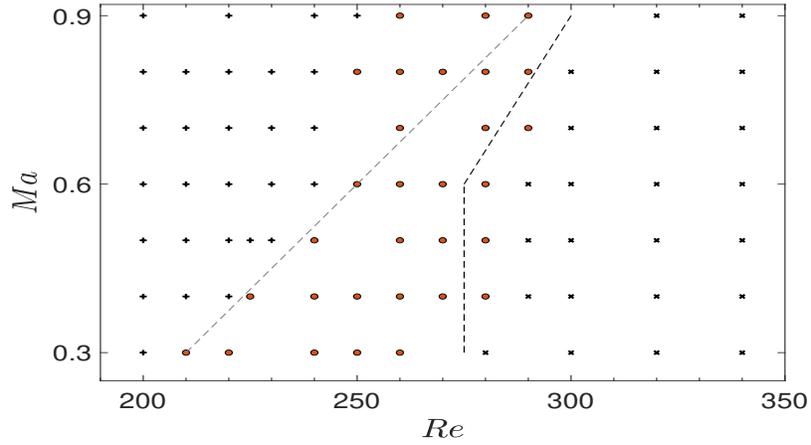


Figure 13: Type of flow field for subsonic regime: (+) Steady axisymmetric flow, (●) Steady planar-symmetric flow, (x) Unsteady periodic flow. Dashed lines represent threshold values for the change in dynamic regime, as calculated via stability analysis by Sansica et al. [45].

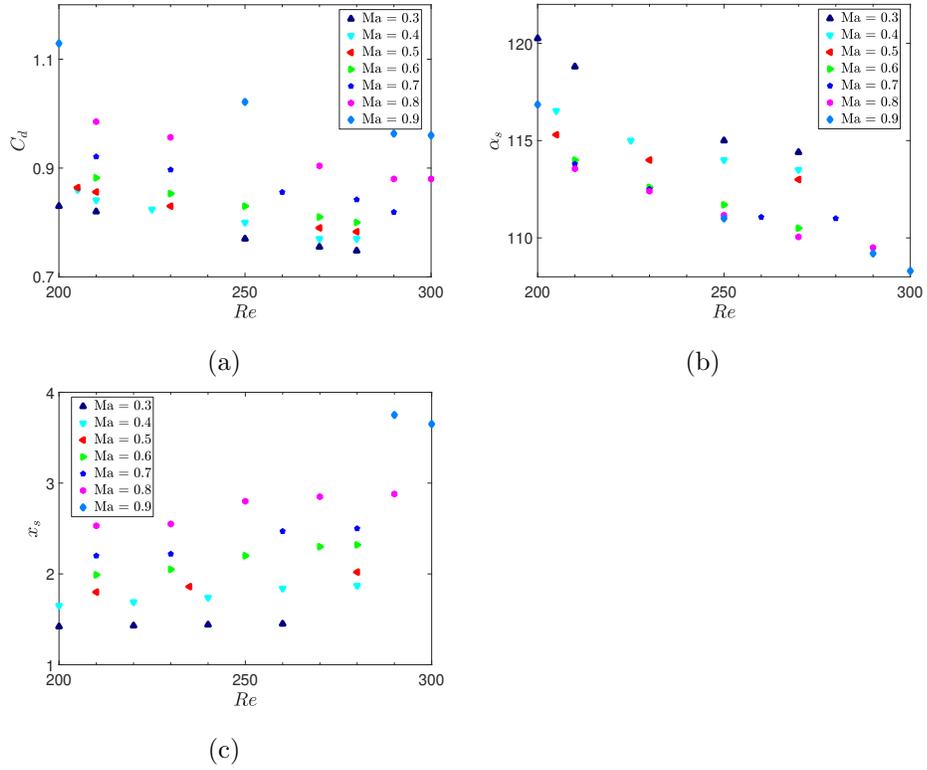


Figure 14: (a) Drag coefficient  $C_d$ , (b) separation angle  $\alpha_s$  and (c) recirculation length  $x_s$  as a function of  $Re$  and  $Ma$ . Data are sampled from a database of 120 simulations.

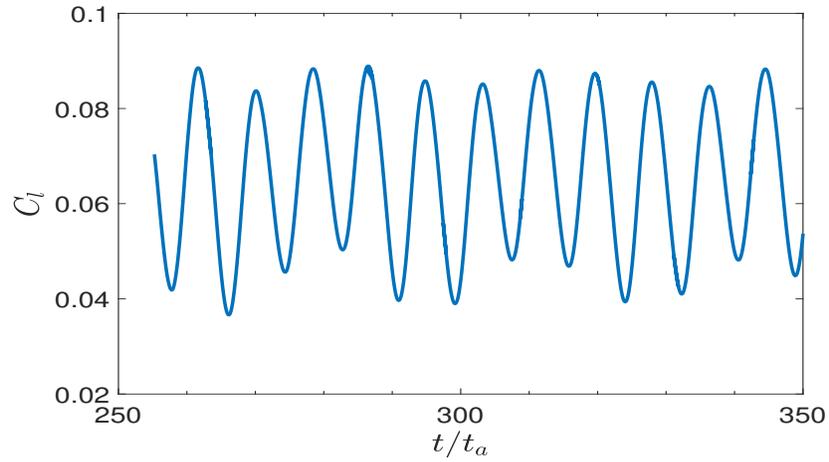


Figure 15: Time evolution of the lift coefficient  $C_l$  for the flow around a sphere for  $Ma = 0.3$  and  $Re = 300$ .

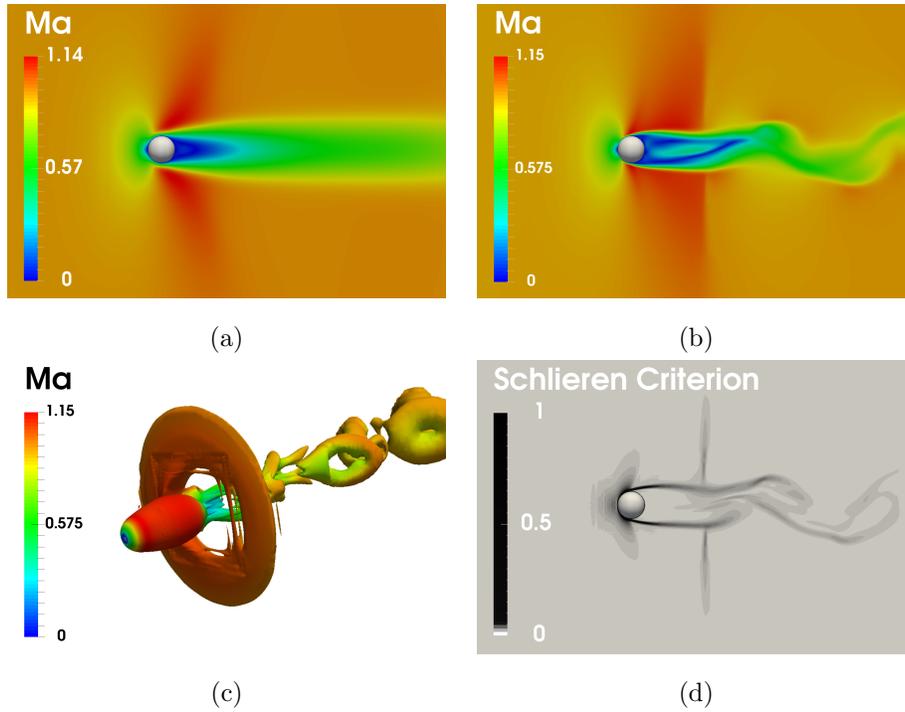


Figure 16: Numerical simulation of the transonic flow around a sphere for  $Ma = 0.95$ , using the high resolution mesh *sphereB*. Isocontours of the  $Ma$  number are shown for (a)  $Re = 50$  and (b)  $Re = 600$ , respectively. For the latter case, a detached shock is observed via (c) Q-criterion and (d) [normalized](#) Schlieren criterion is shown.

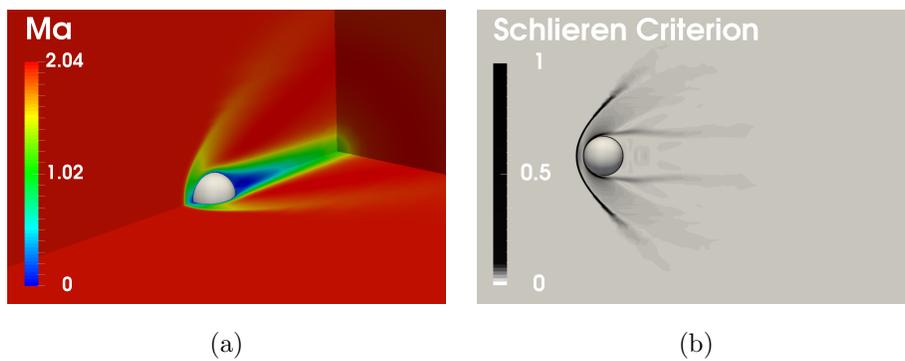


Figure 17: Numerical simulation of the supersonic flow around a sphere for  $Ma = 2$ , using the high resolution mesh *sphereB*. (a) Isocontours of the  $Ma$  number are shown for  $Re = 300$  and (b) the [normalized](#) Schlieren criterion is presented for  $Re = 600$ .

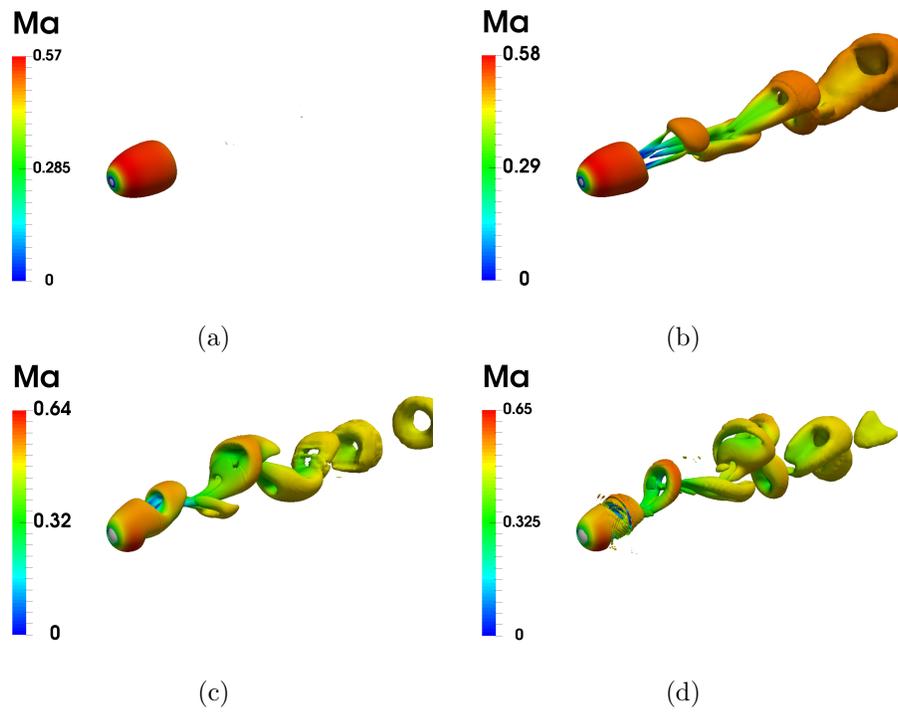


Figure 18: Vortex structures for the flow around a sphere under rotation for  $Ma_\infty = 0.5$ . The configurations (a)  $Ma_\omega = 0$ ,  $Re = 200$ , (b)  $Ma_\omega = 0$ ,  $Re = 300$ , (c)  $Ma_\omega = 0.5$ ,  $Re = 200$  and (d)  $Ma_\omega = 0.5$ ,  $Re = 300$  are investigated, respectively.

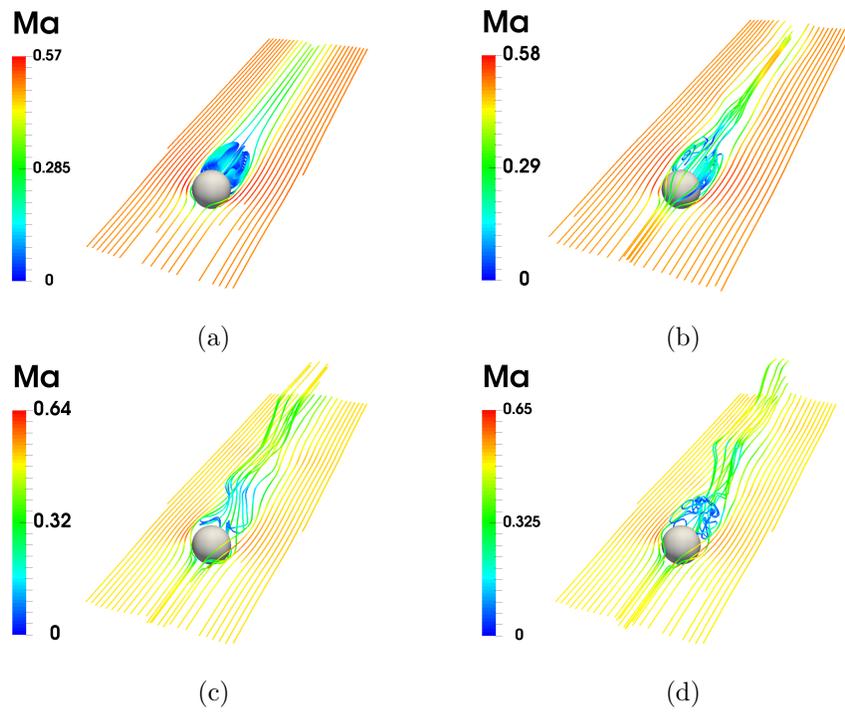


Figure 19: Streamlines for the flow around a sphere under rotation for  $Ma_\infty = 0.5$ . The configurations (a)  $Ma_\omega = 0$ ,  $Re = 200$ , (b)  $Ma_\omega = 0$ ,  $Re = 300$ , (c)  $Ma_\omega = 0.5$ ,  $Re = 200$  and (d)  $Ma_\omega = 0.5$ ,  $Re = 300$  are investigated, respectively.

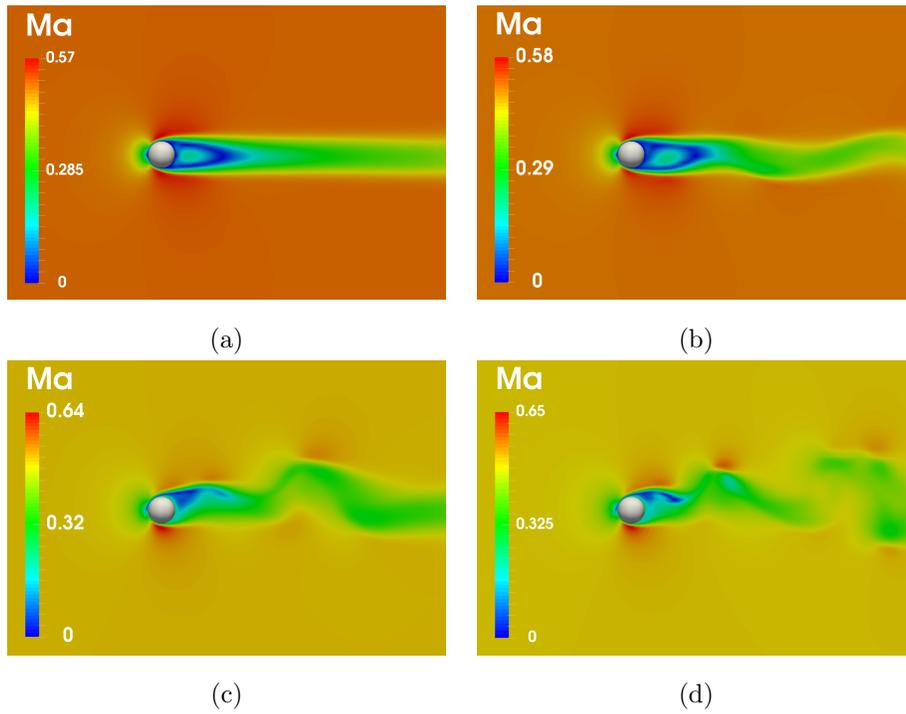


Figure 20: Isocontours of the Mach number for the flow around a sphere under rotation for  $Ma_\infty = 0.5$ . The configurations (a)  $Ma_\omega = 0$ ,  $Re = 200$ , (b)  $Ma_\omega = 0$ ,  $Re = 300$ , (c)  $Ma_\omega = 0.5$ ,  $Re = 200$  and (d)  $Ma_\omega = 0.5$ ,  $Re = 300$  are investigated, respectively.

488 **7. Conclusions**

489 The development of an improved IBM method is proposed in the present  
490 article. This method is based on previous works for incompressible flows and  
491 it is expanded towards the analysis of compressible configurations. The most  
492 essential feature of this model is the integration of a pressure-based correction  
493 of the IBM forcing which is analytically derived from the dynamic set of equa-  
494 tions. The resulting IBM method has been integrated in different flow solvers  
495 available in the CFD platform *OpenFOAM*. A rigorous validation has been per-  
496 formed considering different test cases of increasing complexity. The results  
497 have been compared with a large number of references available in the litera-  
498 ture of experimental and numerical nature. The analysis highlights numerous  
499 favorable characteristics of the IBM method:

- 500 • **precision.** The validation process has encompassed different test cases  
501 over a large spectrum of dynamic regimes in the range of investigation  
502  $Ma \in [0.05, 2]$ ,  $Re \in [40, 600]$ . For each case investigated, the IBM  
503 simulation successfully predicted the physical quantities investigated. This  
504 level of precision is intimately tied with the pressure correction term, which  
505 allows for prescribing more sophisticated condition in the near wall region.  
506 Even if classical choices have been employed in the present research work,  
507 this observation open new research paths for IBM advancement.
- 508 • **flexibility.** The IBM method proved to work remarkably well when im-  
509 plemented in two completely different flow solvers. This aspect indicates  
510 that an efficient performance should be granted even with implementation  
511 to other codes available for CFD investigation.
- 512 • **computational costs.** The determination of the IBM forcing exploits  
513 the recursive calculation features of the numerical algorithms, so that a  
514 whole time advancement without IBM forcing is not needed anymore.  
515 This aspect provides a computational advancement with respect to early  
516 development of similar IBM strategies.

517 The application of the proposed IBM method to the analysis of three-  
518 dimensional flows confirmed its capabilities to capture fine physical features  
519 of the emerging wake dynamic regimes. Comparison of the present results  
520 with body-fitted DNS using high order schemes highlighted minimal differences,  
521 which is a signature of the precision of the proposed method in the represen-  
522 tation of flow configurations exhibiting flow separation. This class of flow is  
523 observed in a large number of industrial flows and transport engineering appli-  
524 cations.

525 The research work has been developed employing computational resources  
526 within the framework of the project gen7590-A0012A07590 DARI-GENCI and  
527 Mesocentre of Poitiers.

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## 658 **Appendix A. Native OpenFOAM solvers - algorithmic structure**

659 The solver *sonicFoam* is described first. As previously mentioned, this tool is  
660 a segregated, pressure-based solver relying on implicit discretization of the time  
661 derivative and a pressure implicit step using a splitting of operators (PISO) and  
662 an iterative resolution [25, 26]. The different steps of the algorithm are now  
663 described for the time evolution from the time step  $n$  to  $n + 1$ . First estimations  
664 of the quantities  $\rho^*$ ,  $U^*$  and  $e^*$  are derived via finite volume discretization of  
665 equations 1 , 2 and 3 , respectively:

$$\rho^* = \frac{\phi_\rho(\rho^n, \mathbf{u}^n)}{a_\rho} \quad (\text{A.1})$$

$$\mathbf{u}^* = \frac{\phi_{\mathbf{u}}(\rho^*, \mathbf{u}^n)}{a_{\mathbf{u}}} - \frac{\mathbf{grad}p^n}{a_{\mathbf{u}}} \quad (\text{A.2})$$

$$e_t^* = \frac{\phi_{et}(\rho^*, \mathbf{u}^*, e_t^n)}{a_{et}} - \frac{div(p^n \mathbf{u}^*)}{a_{et}} \quad (\text{A.3})$$

666 Here, the terms  $\phi_\rho$ ,  $\phi_{\mathbf{u}}$  and  $\phi_e$  represent the results of the finite volume  
667 discretization for every term with the exception of the pressure related terms  
668 and the volume forcing term (which is for the moment considered to be zero  
669 for sake of clarity). The terms  $a_\rho$ ,  $a_{\mathbf{u}}$  and  $a_e$  include coefficients resulting from  
670 the time discretization and possibly turbulence / subgridscale modeling. Two  
671 important aspects must be highlighted:

- 672 • equations A.1, A.2 and A.3 are not solved simultaneously, but they are  
673 strictly resolved in the presented order because of their nested structure;
- 674 • the equations are solved using the pressure field calculated at the previous  
675 time step  $n$ . This feature will be exploited for IBM implementation, as  
676 already indicated in the decomposition presented in equations 13 - 15.

677 The prediction of the new pressure field is obtain via manipulation of the  
678 vectorial momentum equation 2 via application of divergence operator. The  
679 resulting Poisson equation for the pressure field is:

$$div(\mathbf{grad}p) = -\frac{\partial}{\partial t}div(\rho\mathbf{u}) - div(\mathbf{div}(\rho\mathbf{u} \otimes \mathbf{u})) \quad (\text{A.4})$$

680 The term  $\partial div(\rho\mathbf{u})/\partial t$ , which is equal to zero in incompressible flows, can  
681 be manipulated using equation 1:

$$\frac{\partial}{\partial t}div(\rho\mathbf{u}) = -\frac{\partial\rho}{\partial t} = -\frac{\partial\rho}{\partial p}\frac{\partial p}{\partial t} = -\Psi\frac{\partial p}{\partial t} \quad (\text{A.5})$$

682 where the normalized compressibility coefficient  $\Psi = \partial\rho/\partial p$  is included.  
683 Combining equations A.4 and A.5 provides an evolution equation for  $p$ , which  
684 can be discretized in the following form:

$$p^* = \frac{\phi_p(p^n, \rho^*, \mathbf{u}^*)}{a_p} \quad (\text{A.6})$$

685 Equation A.6 provides a time advancement for  $p$ . The PISO loop consists  
686 of:

- 687 1. a resolution of equation A.6, which allows to update the pressure field to  
688 a state  $p^*$
- 689 2. equations A.1, A.2 and A.3 are solved using the updated value  $p^*$ . The  
690 new flow quantities are used to provide a new estimation for the pressure  
691 field

692 This loop continues until a suitable convergence criterion set by the user is  
693 satisfied. Because of the use of a quasi-Poisson equation to determine the pres-

694 sure  $p$ , this algorithm works best for lower  $Ma$  numbers, where compressibility  
 695 effects are not dominant.

The solver *rhoCentralFoam* is now described. Here KT [27] and KNP [28] numerical schemes are employed, which allow for capturing discontinuity / shock features while conserving a general second order central scheme formulation. The numerical scheme allows the transport of fluid properties by both the flow and the acoustic waves. The integration of the convective term on a control volume  $V$  is written:

$$\sum_f \pi_f \sigma_f = \sum_f \beta \pi_{f+} \sigma_{f+} + (1 - \beta) \pi_{f-} \sigma_{f-} + \omega_f (\sigma_{f-} - \sigma_{f+}) \quad (\text{A.7})$$

696 with:

- 697 1. the mass flux  $\pi_f$
- 698 2. the volumetric unknown  $\sigma = (\rho \mathbf{u}); (\mathbf{u}(\rho \mathbf{u})); (\mathbf{u}(\rho e_t))$
- 699 3.  $f_+$  and  $f_-$  indicate the two directions of incoming flux and outgoing flux,  
 700 respectively
- 701 4.  $\beta$  the weighted coefficient of  $f_+$  and  $f_-$
- 702 5. the diffusive mass flux of the maximum speed of propagation of any dis-  
 703 continuity  $\omega_f$

704 The numerical resolution is here performed following a nested cycle. Initially,  
 705 weak terms of the evolution equations are neglected. Following this first pre-  
 706 diction, progressively more complete evolution equations are considered. With  
 707 respect to this point, the matrices  $\phi'_{\mathbf{u}}$ ,  $\phi_{\mathbf{u}}$ ,  $\phi'_{e_t}$  and  $\phi_e$  used below represent the  
 708 finite volume discretization for:

- 709 1. the momentum equation excluding the viscous term, the pressure term  
 710 and the volume forcing term
- 711 2. the momentum equation excluding the pressure term and the volume forc-  
 712 ing term
- 713 3. the total energy equation excluding the heat flux term, the pressure-  
 714 velocity term and the volume forcing-velocity term

715 4. the internal energy equation excluding the pressure-velocity term and the  
716 volume forcing-velocity term

717 As previously explained, the coefficient  $a_{\mathbf{u}}$ ,  $a_{e_t}$  and  $a_e$  result from the numerical  
718 discretization. The governing equations are solved from the time step  $n$  to the  
719 time step  $n + 1$  in the following order:

1. The continuity equation 1 for the density  $\rho^{n+1}$ :

$$\rho^{n+1} = \frac{\phi_{\rho}(\rho^n, \mathbf{u}^n)}{a_{\rho}} \quad (\text{A.8})$$

2. The momentum equation 2 for an intermediate estimate of the momentum  
( $\rho\mathbf{u}$ ) $^*$ . In this step, viscous stresses are excluded:

$$(\rho\mathbf{u})^* = \frac{\phi'_{\mathbf{u}}((\rho\mathbf{u})^n)}{a_{\mathbf{u}}} - \frac{\mathbf{grad}p^n}{a_{\mathbf{u}}} \quad (\text{A.9})$$

720 3. The velocity field is calculated as  $\mathbf{u}^* = (\rho\mathbf{u})^*/\rho^{n+1}$

4. The momentum equation, including the viscous stresses, is solved again  
by combining with equation A.9 :

$$\rho^{n+1}\mathbf{u}^{n+1} = \rho^{n+1}\mathbf{u}^* + \frac{\phi_{\mathbf{u}}(\rho^n, \mathbf{u}^n)}{a_{\mathbf{u}}} - \frac{\phi'_{\mathbf{u}}((\rho\mathbf{u})^n)}{a_{\mathbf{u}}} \quad (\text{A.10})$$

721 5. Update momentum :  $(\rho\mathbf{u})^{n+1} = \rho^{n+1}\mathbf{u}^{n+1}$

6. The energy equation 3 for the total energy  $(\rho e_t)^*$  is resolved excluding the  
heat flux term.

$$(\rho e_t)^* = \frac{\phi'_{e_t}(\mathbf{u}^{n+1}, (\rho e_t)^n)}{a_{e_t}} - \frac{div(p^n \mathbf{u}^n)}{a_{e_t}} \quad (\text{A.11})$$

7. Update of an intermediate estimate of internal energy  $e^*$  associated with  
( $\rho e_t$ ) $^*$ :

$$e^* = \frac{(\rho e_t)^*}{\rho^{n+1}} - 0.5(\mathbf{u}^{n+1} \cdot \mathbf{u}^{n+1}) \quad (\text{A.12})$$

722 and an intermediate estimation of the temperature  $\theta^* = e^*/c_v$

8. Resolution of the energy equation for the internal energy  $e^{n+1}$  including  
the heat flux term:

$$\rho^{n+1}e^{n+1} = \rho^{n+1}e^* + \frac{\phi_e(\rho^{n+1}, \mathbf{u}^{n+1}, e^n)}{a_e} - \frac{div(\lambda(\theta^*)\mathbf{grad}(\theta^*))}{a_e} - \frac{\phi'_{e_t}(\mathbf{u}^{n+1}, (\rho e_t)^n)}{a_{e_t}} \quad (\text{A.13})$$

723 9. Then final update of the temperature  $\theta^{n+1} = e^{n+1}/c_v$  and the pressure  
724  $p^{n+1} = \rho^{n+1} \cdot (r\theta^{n+1})$ .

725 **Appendix B. Grid convergence analysis**

726 The accuracy of the proposed IBM method is assessed via the analysis of  
727 the flow around a circular cylinder for  $Ma = 0.05$  and  $Re = 300$ . Details of the  
728 test case investigated are reported in section 4. Data from the work of Gautier  
729 et al. [30] is used as a reference solution. The precision of the IBM method  
730 is investigated using  $L_2$  and  $L_\infty$  norms so that, for a physical quantity  $\phi$ , the  
731 error is estimated as:

$$e_{\phi_{L_2}} = \|\phi_{ref} - \phi_G\|_2 \quad (\text{B.1})$$

$$e_{\phi_{L_\infty}} = \|\phi_{ref} - \phi_G\|_\infty \quad (\text{B.2})$$

732 where  $\phi_G$  is the reference solution [30]. The grid convergence analysis is  
733 performed evaluating results from four different grids. The mesh resolution in  
734 the near cylinder region is imposed to be  $\Delta x = \Delta y = \{\frac{D}{80}; \frac{D}{96}; \frac{D}{112}; \frac{D}{128}\}$  where  
735  $D$  is the diameter of the cylinder. The corresponding number of Lagrangian  
736 markers employed is  $\{252; 302; 352; 402\}$ , respectively.

737 Results for the streamwise velocity  $u$  are shown in Figure B.21. The error is  
738 calculated selecting points at a distance of  $0.52 D$  from the center of the cylinder.  
739 One can observe that order of the grid convergence is almost 2 for the  $L_2$  norm  
740 and 1 for the  $L_\infty$  norm. These results indicate that the precision of the original  
741 method [17] is conserved via the current implementation and it is perhaps even  
742 improved when compared with previous analyses using the initial OpenFOAM  
743 formulation [18].

744 The behavior of error in the prediction of the drag coefficient  $C_D$  is shown  
745 in Figure B.22. In the framework of this IBM method, the drag coefficient is  
746 directly calculated using information available on the Lagrangian markers. For  
747 this quantity, the rate of convergence is slightly faster than first order.

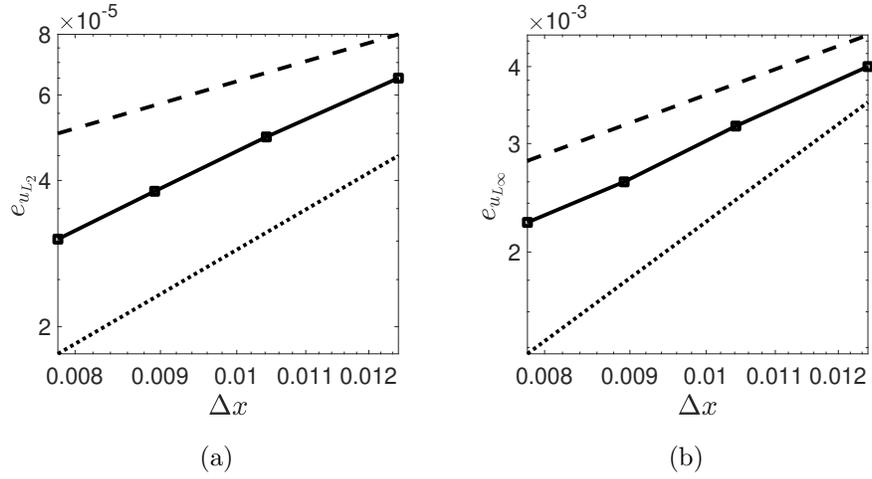


Figure B.21: Convergence rate in the prediction of the streamwise velocity  $u$  via the pressure-corrected IBM method. The error is calculated using (a) a  $L_2$  norm and (b) a  $L_\infty$  norm, respectively. Dashed lines (first order accuracy) and dotted lines (second order accuracy) are included to highlight the error behavior.

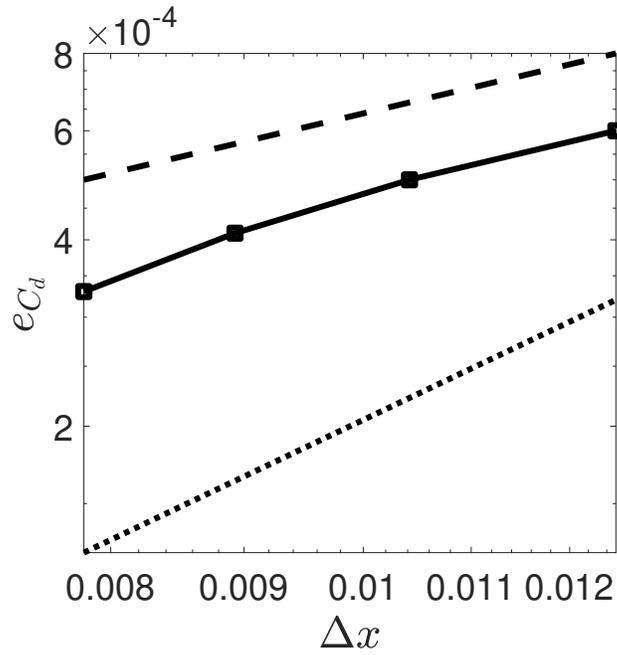


Figure B.22: Convergence rate in the prediction of the drag coefficient  $C_D$  via the pressure-corrected IBM method.