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A Moving-Least-Squares Immersed Boundary Method for simulating the fluid-structure interaction of elastic bodies with arbitrary thickness

M. D. de Tullio*, G. Pascazio

*Dipartimento di Meccanica, Matematica e Management, DMMM
Centro di Eccellenza in Meccanica Computazionale, CEMeC
Politecnico di Bari, Via Re David 200, 70125, Bari, Italy*

Abstract

A versatile numerical method for the fluid-structure-interaction of bodies with arbitrary thickness, immersed in an incompressible fluid, is presented, with the aim of simulating different biological engineering applications. A discrete-forcing immersed boundary method is adopted, based on a moving least squares approach to reconstruct the solution in the vicinity of the immersed surface. A simple spring-network model is considered for describing the dynamics of deformable structures, in order to have the freedom of easily model and simulate different biological systems that can not always be described by simple continuum models, without affecting the computational time and simplicity of the overall method. The fluid and structures are coupled in a strong way, in order to avoid instabilities related to large accelerations of the bodies. The method gives accurate results comparable with that of sharp direct-forcing approach, and can manage pressure differences across the surface in one grid cell, still obtaining very smooth forces. The effectiveness of the method has been validated by means of several test cases involving: rigid bodies, either falling in a quiescent fluid, fluttering or tumbling, or transported by a shear flow; infinitely thin elastic structures with mass, such as a two-dimensional flexible filament and an inverted flexible filament in a free stream; a three-dimensional model of a bio-prosthetic aortic valve opening and closing under a pulsatile flowrate. A very good agreement is obtained in all cases, comparing with available experimental

*Corresponding author. E-mail address: marcodonato.detullio@poliba.it

data and numerical results obtained by different methods.

Keywords: Immersed Boundary Method, Fluid-Structure Interaction, Network Spring Model, Direct Forcing with Moving Least Squares, Elastic Zero-thickness Body, Flexible Filament

1. Introduction

Fluid-structure interaction (FSI) problems are found in many engineering areas. The three-dimensional computational modeling is particularly challenging and has recently encountered the interest of several research groups. Among different FSI problems, biological applications are becoming of ever increasing interest in the scientific community and their accurate and efficient numerical simulation provides an essential means in understanding the fundamental physics and reducing the time needed for experiments. The accurate description of FSI can not ignore the fact that moving and/or deforming bodies act on the surrounding fluid that is forced to move accordingly (no-slip condition), and reacts with pressure and velocity gradients distribution that, in turn, produces the surface forces that cause the motion of the body. This poses several challenges for the numerical approaches adopted. With no intent of being exhaustive, one can mention: rigid particle of arbitrarily shape transported by the fluid; deformable particles in shear flows (capsules, vesicles, cells), constituted by a liquid droplet enclosed by a structure with thickness much smaller than the particle size; elastic slender bodies immersed in a fluid, such as flags, insect wings, jellyfishes, bioprosthetic heart valves, where a thin surface is significantly deformed by the fluid. In the mentioned cases, describing the dynamics of the interaction between the body and the fluid is not a trivial task, since the numerical method needs to be able to handle in an efficient way complex and very thin geometries undergoing large deformations, without losing accuracy.

Given the large displacements/deformations of the bodies, body-fitted approaches [1, 2], both structured and unstructured, are not the optimal choice. They need the time-consuming regeneration or deformation of the mesh and the successive projection of the flow field solution from previous mesh to new one, which can lead to a decrease of accuracy. Immersed Boundary (IB) methods [3, 4] are more suitable, since the governing equations are solved on a fixed grid, covering the whole domain, thus including points that rely inside the closed boundaries (if any). Continuous forcing IB methods de-

32 rived by the classical approach proposed by Peskin [3] have been widely used,
33 considering different biological and engineering applications involving elastic
34 slender bodies [5, 6, 7, 8]. An advantage of these monolithic approaches is the
35 inherent strong coupling for fluid-structure-interaction and their simplicity.
36 On the other hand, they have a fundamental difficulty in handling structures
37 with mass and the immersed interface is smeared by distributing the forcing
38 terms over several grid nodes in the vicinity of the solid boundary. An alter-
39 native is to consider partitioned algorithms, in which the fluid and structures
40 are solved independently and then coupled, as done in [9] for studying flex-
41 ible filaments, adopting a feedback forcing approach[10], but with a severe
42 limitation on the numerical integration time-step. On the other hand, direct
43 forcing methods [11] are particularly attractive, for their moderate limita-
44 tion of the computational time step [12, 4]. They give very good results
45 for fixed boundaries, but their extension to FSI problems needs particular
46 attention in order to attenuate spurious oscillation of hydrodynamic forces
47 that are potential source of instabilities [13, 14, 15, 16, 17]. The alterna-
48 tive direct-forcing scheme of Uhlmann [13], computing the forcing term on
49 Lagrangian markers (laying on the immersed body), provides smooth hydro-
50 dynamic forces, with the requirement of a uniform distribution of the markers
51 on the body. Vanella and Balaras [15] improved Uhlmann’s approach [13],
52 by using a versatile moving-least-squares (MLS) approximation to build the
53 transfer functions between the Eulerian and Lagrangian grids for rigid bodies.
54 Discrete-forcing IB method have been used for studying deformable bodies
55 [18, 19, 20, 21, 22] with good accuracy.

56 The aim of this work is to build a numerical tool for simulating the fluid-
57 structure-interaction of arbitrarily shaped, very thin surfaces, both rigid and
58 deformable, so as to be able to describe the dynamics of either closed (en-
59 closing a volume) particles, both solid and deformable, such as capsules or
60 biological cells [23, 24], or open, describing zero-thickness slender bodies. In
61 order to achieve such a goal, several ingredients are coupled together form-
62 ing an accurate, efficient and simple code. A partitioned, discrete-forcing IB
63 method is adopted, based on a MLS approach, similar to [15], in order to re-
64 construct the solution in the vicinity of the immersed surface and to convert
65 the Lagrangian forcing back to the Eulerian grid for the case of thin surfaces
66 that can be rigid or undergo large deformations. With the aim of describing
67 different biological systems that may consist of diversely scaled elements (e.g.
68 cells, organ tissues) and that can not always be described by simple contin-
69 uum models, for the case of non rigid bodies we adopted a simple but very

70 versatile methodology based on spring-network models. The surface is dis-
71 cretized by a triangulated mesh and the mass is assumed to be distributed on
72 the nodes of the triangles; these are connected by in-plane and out-of-plane
73 (bending) springs in order to model the structural elastic behavior [25]. For
74 both rigid and deformable bodies, the fluid and structures are coupled in a
75 strong way, in order to avoid instabilities related to strong accelerations of
76 the mass-points. A 4-th order predictor-corrector method is adopted, based
77 on Hamming’s method with mop-up correction [26]. Particular attention is
78 required in determining the hydrodynamic loading on the structure, consider-
79 ing the thinness of the bodies. The method gives accurate results comparable
80 with that of sharp direct-forcing approach, and can manage pressure differ-
81 ences across the surface in one grid cell. Moreover, the method is able to
82 obtain very smooth forces, needed by the FSI approach. The only restriction
83 to the computational time step is related to the flow solver stability condition
84 and to the accuracy needed in determining the body dynamics, depending on
85 the specific problem under study. The tool has been validated by means of
86 several test cases of increasing complexity, involving closed surfaces, enclos-
87 ing a volume, and rigid particles: the sedimentation of an elliptic particle in
88 a quiescent fluid, the fluttering and tumbling dynamics of a falling plate and
89 a single sphere settling under gravity, as well as a circular particle transport
90 in a planar Couette flow are considered. On the other hand, open surfaces
91 representing infinitely thin elastic structures with mass are considered: a
92 two-dimensional flexible filament and an inverted flexible filament in a free
93 stream. Finally, a three-dimensional model of a bio-prosthetic aortic valve
94 is considered, with nonlinear and anisotropic mechanical properties, open-
95 ing and closing during the pulsatile cardiac cycle. A good agreement has
96 been obtained in the cases where numerical and/or experimental results are
97 available in the literature, considering both the rigid motion as well as the
98 deformation dynamics.

99 It is important to note that the procedure is very general, and both fluid
100 and structure solvers can be replaced by more suitable ones, depending on
101 the problem of interest. A straightforward extension is the use of a finite-
102 element structural solver for describing the dynamics of deformable slender
103 surfaces (e.g. membrane solver of [27]) maintaining the same data structure
104 and formalism, with just an increase of the computational cost due to the
105 structural solver. Moreover, the presented methodology has been adopted
106 on non-uniform structured Cartesian grids, but it can be easily extended to
107 unstructured meshes, provided that the minimum number of Eulerian grid

108 points in the support domain, needed by the MLS procedure is provided.

109 2. Numerical method

110 2.1. Flow solver

111 Under the assumption of incompressible flow, the governing equations for
112 the fluid dynamics are the Navier–Stokes and continuity equations:

$$\rho_f \left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) = -\nabla p + \mu \nabla^2 \mathbf{u} + \rho_f \mathbf{f} \quad (1)$$

$$113 \quad \nabla \cdot \mathbf{u} = 0 \quad (2)$$

114 where ρ_f is the fluid density, \mathbf{u} is the fluid velocity, p is the pressure, μ is the
115 fluid dynamic viscosity and \mathbf{f} contains the forcing terms, such as that of the
116 IB technique. The above equations are non-dimensionalized, introducing the
117 Reynolds number $Re = \frac{\rho_f U L}{\mu}$, with U and L a reference velocity and length,
118 respectively. The non-linear terms are discretized by an explicit Adams–
119 Bashforth scheme and the linear viscous terms by an implicit Crank–Nicolson
120 scheme, yielding the following semi-discrete equation:

$$\frac{\hat{\mathbf{u}} - \mathbf{u}^n}{\Delta t} = -\alpha \nabla p^n + \gamma H^n + \rho H^{n-1} + \frac{\alpha}{2 Re} \nabla^2 (\hat{\mathbf{u}} + \mathbf{u}^n), \quad (3)$$

121 where \mathbf{u}^n denotes the velocity at the time level n , $\hat{\mathbf{u}}$ is the intermediate
122 solution, Δt is the time step, H contains the non-linear terms, α , γ and ρ
123 are the constants of the Adam–Bashforth/Crank–Nicolson scheme [28, 29].
124 Equation (3) can be written in delta-form as:

$$(1 - \beta \nabla^2) \Delta \hat{\mathbf{u}} = [-\alpha \nabla p^n + \gamma H^n + \rho H^{n-1}] \Delta t + 2 \beta \nabla^2 \mathbf{u}^n \quad (4)$$

125 with $\Delta \hat{\mathbf{u}} = \hat{\mathbf{u}} - \mathbf{u}^n$ and $\beta = \Delta t \alpha / (2 Re)$. Employing a second-order-accurate
126 space discretization with centered finite differences on a Cartesian staggered
127 grid, the matrix associated with the left-hand-side of the equation (4) is
128 sparse and its direct inversion requires, by standard methods, a huge num-
129 ber of operations. Thus, an approximate factorization technique allows the
130 computation of the intermediate non-solenoidal velocity field $\hat{\mathbf{u}}$ by means
131 of the solution of simple tri-diagonal matrices [28, 29]. In order to get a
132 divergence-free velocity field, a scalar quantity φ is introduced, such that:

$$\mathbf{u}^{n+1} = \hat{\mathbf{u}} - \alpha \Delta t \nabla \varphi. \quad (5)$$

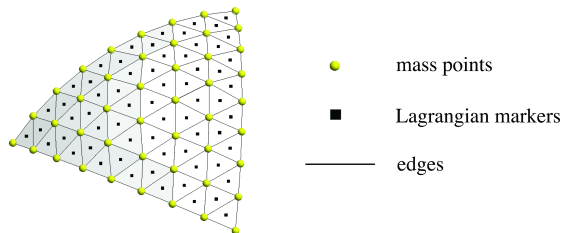


Figure 1: Geometry description by means of triangular elements, whose centroids coincide with the Lagrangian markers.

133 If the discrete divergence operator is applied to the above equation and the
 134 velocity field \mathbf{u}^{n+1} is required to be solenoidal, an elliptic equation for φ is
 135 obtained,

$$\nabla^2 \varphi = \frac{\nabla \cdot \hat{\mathbf{u}}}{\alpha \Delta t}. \quad (6)$$

136 The large-banded matrix associated with this equation is reduced to a penta-
 137 diagonal matrix using trigonometric expansions (FFTs) in the spanwise di-
 138 rection, and the resulting Helmholtz equations are then inverted using the
 139 FISHPACK package [30]. Finally, the pressure field is computed as

$$p^{n+1} = p^n + \varphi - \frac{\alpha \Delta t}{2 Re} \nabla^2 \varphi. \quad (7)$$

140 2.2. Immersed boundary treatment

141 In order to overcome the presence of large fluctuations in the hydrody-
 142 namic forces arising when extending the direct-forcing formulation of [11]
 143 to cases with moving objects, a MLS approach similar to [15] is employed.
 144 Following the idea of [13], the forcing is computed on Lagrangian markers
 145 laying on the immersed surface, so as to satisfy the boundary condition,
 146 and then transferred to the Eulerian grid-points. The structure surface is
 147 discretized by means of N_t triangular elements and the Lagrangian markers
 148 coincide with the triangles' centroids (figure 1). Given a Lagrangian marker,
 149 first the closest Eulerian node is identified, which is centered in a cell with
 150 dimension Δx_i in each i -th direction (see figure 2). Then, a support do-
 151 main is created, centered on the Lagrangian point and extending to $\pm r_i$,
 152 with $r_i = 1.5 \Delta x_i$. In this way N_e Eulerian points are enclosed in the support
 153 domain and associated to the selected marker (27 in three dimensions). A

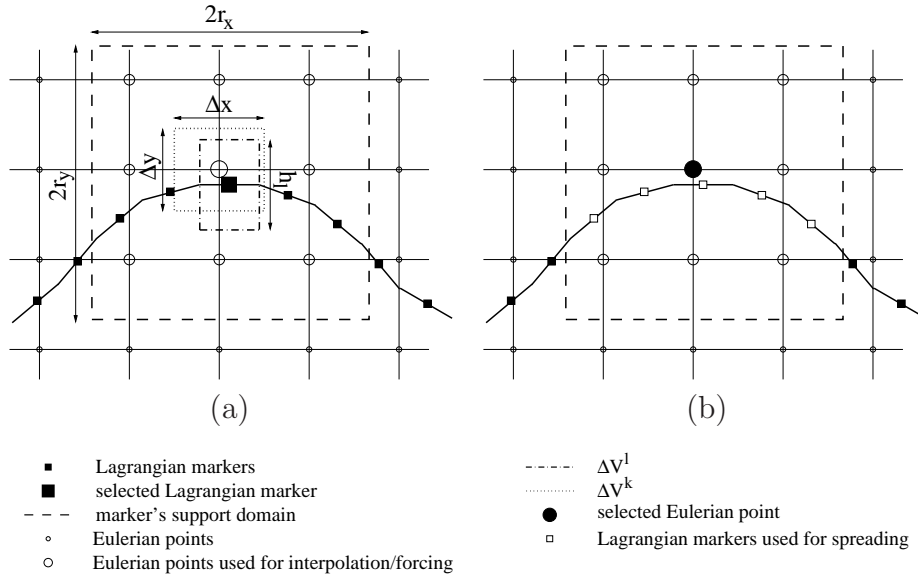


Figure 2: Scheme for IB forcing. (a) Definition of the support domain for a Lagrangian marker. The Eulerian points are involved in the interpolation of the variables at the Lagrangian marker. (b) Lagrangian points associated to a selected Eulerian point. The Lagrangian points are involved in the spreading of the forcing to the Eulerian node.

154 volume $\Delta V^l = A_l h_l$ is associated to the marker, where A_l is the l -th trian-
 155 gle area and h_l is the local thickness, equal to the average mesh size at the
 156 marker location. The MLS approximation is the key ingredient to build a
 157 transfer function between the Eulerian and Lagrangian grids, that is able to
 158 provide a smooth solution also when applied to arbitrary moving bodies [15].
 159 The reconstruction procedure consists in the following steps:

- 160 1. Compute the intermediate velocity $\hat{\mathbf{u}}$ from equation (3) in all the Eule-
 161 rian grid points; this involves also the N_e points of the support domain
 162 surrounding a Lagrangian point.
 163 2. Compute the velocity component, \hat{U}_i , at each Lagrangian grid point,
 164 l , corresponding to the non-solenoidal velocity field. Using the MLS
 165 approach, it can be approximated in the support domain as:

$$\hat{U}_i(\mathbf{x}) = \mathbf{p}^T(\mathbf{x})\mathbf{a}(\mathbf{x}) = \sum_{j=1}^4 p_j(\mathbf{x})a_j(\mathbf{x}), \quad (8)$$

166 where $\mathbf{p}^T(\mathbf{x}) = [1, x, y, z]$ is the linear basis function vector (a cost-
 167 efficient choice able to represent the field variation of the variable up

168 to the accuracy of the adopted spatial discretization scheme [15]), $\mathbf{a}(\mathbf{x})$
 169 is a vector of coefficients and \mathbf{x} is the Lagrangian point position. The
 170 coefficient vector $\mathbf{a}(\mathbf{x})$ is obtained minimizing, with respect to $\mathbf{a}(\mathbf{x})$,
 171 the weighted L2-norm defined as:

$$J = \sum_{k=1}^{N_e} W(\mathbf{x} - \mathbf{x}^k) [\mathbf{p}^T(\mathbf{x}^k)\mathbf{a}(\mathbf{x}) - \hat{u}_i^k]^2, \quad (9)$$

172 where \hat{u}_i^k and \mathbf{x}^k are the intermediate velocity component and position
 173 vector, respectively, at Eulerian point k in the support domain and
 174 $W(\mathbf{x} - \mathbf{x}^k)$ is a given weight function. This operation leads to

$$\mathbf{A}(\mathbf{x})\mathbf{a}(\mathbf{x}) = \mathbf{B}(\mathbf{x})\hat{\mathbf{u}}_i^k, \quad (10)$$

175 with

$$\mathbf{A}(\mathbf{x}) = \sum_{k=1}^{N_e} W(\mathbf{x} - \mathbf{x}^k)\mathbf{p}(\mathbf{x}^k)\mathbf{p}^T(\mathbf{x}^k), \quad (11)$$

$$\mathbf{B}(\mathbf{x}) = [W(\mathbf{x} - \mathbf{x}^1)\mathbf{p}^T(\mathbf{x}^1) \dots W(\mathbf{x} - \mathbf{x}^{N_e})\mathbf{p}^T(\mathbf{x}^{N_e})] \quad (12)$$

177 and

$$\mathbf{B} = [\hat{u}_i^1 \dots \hat{u}_i^{N_e}]^T. \quad (13)$$

178 Combining the equations, \hat{U}_i can be rewritten as:

$$\hat{U}_i(\mathbf{x}) = \mathbf{\Phi}^T(\mathbf{x})\hat{\mathbf{u}}_i^k = \sum_{k=1}^{N_e} \phi_k^l(\mathbf{x}) \hat{u}_i^k, \quad (14)$$

179 where $\mathbf{\Phi} = \mathbf{p}(\mathbf{x})\mathbf{A}^{-1}(\mathbf{x})\mathbf{B}(\mathbf{x})$ is the transfer operator containing the
 180 shape function values for marker point l . In this work, the exponential
 181 function [31] is used, written as:

$$W(\mathbf{x} - \mathbf{x}^k) = \begin{cases} e^{-(r_k/\alpha)^2} & r_k \leq 1 \\ 0 & r_k > 1 \end{cases} \quad (15)$$

182 where $\alpha = 0.3$ and r_k is given by

$$r_k = \frac{|\mathbf{x} - \mathbf{x}^k|}{r_w} \quad (16)$$

183 with r_i the size of the support domain previously defined. Note that the
 184 shape functions reproduce exactly the linear polynomial contained in
 185 their basis and possess the partition of unity property $\sum_{k=1}^{N_e} \phi_k(\mathbf{x}) = 1$.
 186 Moreover, the field approximation is continuous on the global domain
 187 as the MLS shape functions are compatible [31, 15].

188 3. Calculate the volume force component F_i at all Lagrangian grid points:

$$F_i = \frac{V_i^b - \hat{U}_i}{\Delta t}, \quad (17)$$

189 where V_i^b is the velocity component on the marker to be imposed as a
 190 boundary condition.

191 4. Transfer back F_i to the k Eulerian grid points associated with each
 192 Lagrangian grid point, using the same shape functions employed in
 193 the interpolation procedure, properly scaled by a factor c_l , which is
 194 determined by imposing that the total force acting on the fluid is not
 195 changed by the transfer [15]:

$$f_i^k = \sum_{l=1}^{N_t} c_l \phi_k^l F_i^l; \quad (18)$$

196 in the above equation f_i^k is the volume force component in the Eulerian
 197 point k and N_t indicates the number of Lagrangian points associated
 198 with the Eulerian point k (i.e. Lagrangian point whose support domain
 199 contains the selected Eulerian point, as shown on the right in figure 2).
 200 The scaling factor c_l is obtained considering a forcing volume associated
 201 with each Eulerian point equal to the Eulerian cell volume, ΔV^k , and
 202 the forcing volume associated with the Lagrangian marker previously
 203 defined, and imposing that the total force acting on the fluid is not
 204 changed by the transfer:

$$\sum_{k=1}^{N_{e,tot}} f_i^k \Delta V^k = \sum_{l=1}^{N_t} F_i^l \Delta V^l. \quad (19)$$

205 Rearranging the terms, one has:

$$c_l = \frac{\Delta V^l}{\sum_{k=1}^{N_e} \phi_k^l \Delta V^k} \quad (20)$$

206 The transfer operators conserve momentum on both uniform and stretched
 207 grids, while the equivalence of total torque between the Eulerian and
 208 Lagrangian grids are guaranteed for uniform grids, with minimal errors
 209 for low stretched grids (about 10%) [15].

210 5. Correct the intermediate velocity so as to impose the correct boundary
 211 conditions on the immersed body:

$$\mathbf{u}^* = \hat{\mathbf{u}} + \Delta t \mathbf{f}, \quad (21)$$

212 where \mathbf{f} is the volume force at Eulerian cells, obtaining a velocity field
 213 that is not divergence-free and that will be projected into a divergence-
 214 free space by applying the pressure correction which satisfies the Pois-
 215 son equation (6).

216 2.3. Rigid body equations

217 The motion of the rigid body immersed in the fluid is governed by the
 218 Newton–Euler equations imposing the equilibrium of translation and rota-
 219 tion:

$$M \frac{d\mathbf{V}}{dt} = \mathbf{F}_{tot}, \quad \mathbf{V} = \frac{d\mathbf{X}}{dt}, \quad (22)$$

$$[I] \frac{d\mathbf{\Omega}}{dt} = \mathbf{T}_{tot}, \quad \mathbf{\Omega} = \frac{d\mathbf{\Theta}}{dt}. \quad (23)$$

221 In the equations above, M and $[I]$ are the mass and inertia tensor of the
 222 body, \mathbf{V} and \mathbf{X} its baricentre’s velocity and position, $\mathbf{\Omega}$ and $\mathbf{\Theta}$ its angu-
 223 lar velocity and position, respectively, and \mathbf{F}_{tot} and \mathbf{T}_{tot} are the total force
 224 and moment acting on the body. The total force and moment include the
 225 hydrodynamics contributions, the gravity forces, if present, and any other
 226 additional force depending on the problem. Concerning the hydrodynam-
 227 ics loadings, the overall contribution is obtained integrating over the body’s
 228 surface the pressure and viscous stresses as explained in section 2.5.

229 2.4. Spring network model for deformable bodies

230 A simple spring network model is adopted for describing the dynam-
 231 ics of deformable bodies, based on the minimum energy concept [25]. The
 232 structural model is built considering the triangulated network of N_s springs
 233 (edges), forming N_t triangles. The mass of the structure is concentrated on
 234 the N_v vertices of the triangles, uniformly distributed on the surface. The
 235 potential energy of the system includes in-plane elastic terms, combined with

236 bending energy and additional constraints for surface area and volume con-
 237 servations.

238 The simplest elastic energy model is described by:

$$W^e = \frac{1}{2}k_e x^2 \quad (24)$$

239 where W^e is the related potential energy, $x = l - l_0$, l is the length of the
 240 stretched spring, l_0 is the length of the spring in the *stress-free* configuration
 241 and k_e is the elastic constant. The elastic constant for a given edge of length
 242 l is obtained by the model of [32]:

$$k_e = \frac{Eh \sum_i A_i}{l^2}, \quad (25)$$

243 where E is the Young's modulus for the material, h is the membrane thickness
 244 (here assumed uniform for all triangles), i identifies the triangles sharing the
 245 selected edge (here two triangles) and A_i is the triangle area. Taking the
 246 derivative of the potential energy with respect to displacements, the nodal
 247 forces corresponding to the elastic energy for nodes 1 and 2 connected by an
 248 edge (figure 3) are obtained by:

$$\mathbf{F}_1^e = -k_e(l - l_0) \frac{\mathbf{r}_{12}}{l} \quad (26)$$

249

$$\mathbf{F}_2^e = -k_e(l - l_0) \frac{\mathbf{r}_{21}}{l} \quad (27)$$

250 where $\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$, with \mathbf{r}_i position vector of the node i and $l = |\mathbf{r}_{21}|$ is the
 251 actual edge length.

252 The out-of-plane deformation of two adjacent faces sharing an edge is
 253 modeled by means of a bending spring, as shown in figure 3. Four nodes are
 254 involved in the energy term. Considering a null reference curvature of the
 255 local surface, the free elastic energy in discrete form is given by [33]:

$$W^b = k_b(1 - \mathbf{n}_1 \cdot \mathbf{n}_2) = k_b[1 - \cos(\theta)] \quad (28)$$

256 where \mathbf{n}_1 and \mathbf{n}_2 are the surface vectors normal to the triangular elements
 257 shared by the edge, θ is the angle between \mathbf{n}_1 and \mathbf{n}_2 and k_b is the bending
 258 constant. In case of a surface with non-zero reference curvature in the stress-
 259 free configuration, the bending energy can be written as

$$W^b = k_b[1 - \cos(\theta - \theta_0)] \quad (29)$$

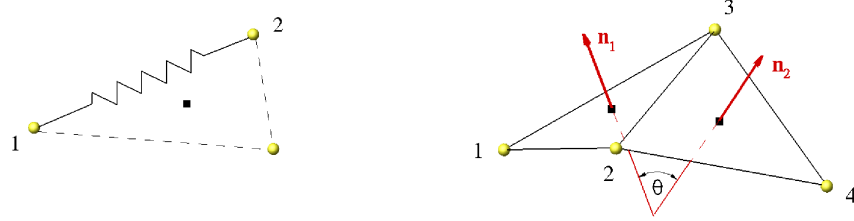


Figure 3: Left: sketch of the two nodes (vertices of an edge) involved in the elastic spring model. Right: four nodes (belonging to the two triangles sharing an edge) involved in the bending spring model.

260 where θ_0 is the value of θ in the stress-free configuration. The bending
 261 constant k_b is related to the equivalent averaged bending modulus of the
 262 structure, B , as [34]:

$$k_b = B \frac{2}{\sqrt{3}}. \quad (30)$$

263 The nodal forces corresponding to the bending energy are obtained as (see
 264 figure 3):

$$\mathbf{F}_1^E = \beta_b [b_{11} (\mathbf{n}_1 \times \mathbf{r}_{32}) + b_{12} (\mathbf{n}_2 \times \mathbf{r}_{32})] \quad (31)$$

$$\mathbf{F}_2^E = \beta_b [b_{11} (\mathbf{n}_1 \times \mathbf{r}_{13}) + b_{12} (\mathbf{n}_1 \times \mathbf{r}_{34} + \mathbf{n}_2 \times \mathbf{r}_{13}) + b_{22} (\mathbf{n}_2 \times \mathbf{r}_{34})] \quad (32)$$

$$\mathbf{F}_3^E = \beta_b [b_{11} (\mathbf{n}_1 \times \mathbf{r}_{21}) + b_{12} (\mathbf{n}_1 \times \mathbf{r}_{42} + \mathbf{n}_2 \times \mathbf{r}_{21}) + b_{22} (\mathbf{n}_2 \times \mathbf{r}_{42})] \quad (33)$$

$$\mathbf{F}_4^E = \beta_b [b_{11} (\mathbf{n}_1 \times \mathbf{r}_{23}) + b_{22} (\mathbf{n}_2 \times \mathbf{r}_{23})] \quad (34)$$

268 with

$$b_{11} = -\frac{\cos(\theta)}{|\mathbf{n}_1|^2}; \quad b_{12} = \frac{1}{|\mathbf{n}_1||\mathbf{n}_2|}; \quad b_{22} = -\frac{\cos(\theta)}{|\mathbf{n}_2|^2}; \quad (35)$$

269 and

$$\beta_b = k_b \frac{\sin(\theta)\cos(\theta_0) - \cos(\theta)\sin(\theta_0)}{\sqrt{1 - \cos^2(\theta)}} \quad (36)$$

270 Additional energy terms can be added, in order to give a constraint on the
 271 area (of each triangle and/or global area) and enclosed volume (if the surface
 272 is closed) changes [25, 35].

273 For each node of the structure the dynamic equation of motion is solved,
 274 considering the internal and external forces:

$$m_p \ddot{\mathbf{x}} = \mathbf{F}^{\text{ext}} + \mathbf{F}^{\text{int}} = \mathbf{F} \quad (37)$$

275 where m_p is the mass of the node, \mathbf{F}^{ext} are the external forces on the nodes
276 (i.e. hydrodynamic loads, gravity forces) and \mathbf{F}^{int} are the internal forces
277 previously defined. A damping term could be added on the left hand side in
278 order to take into account for the viscoelasticity of the structure.

279 A comment is necessary regarding the adopted structural model. Spring
280 network models are discrete, defining the elastic forces on the vertices based
281 on edges' length and triangles' reciprocal angle variations, as well as other
282 constraints such as area and volume variations. This makes the models far
283 from the continuum model, which assumes the homogeneity of the mechanical
284 properties throughout the membrane surface. Therefore, the evaluation
285 of the spring constants, in order to mimic the continuum model, may not
286 be trivial. There are several studies in literature aiming at defining a link
287 between spring networks and continuum mechanics. Gelder [32] showed that
288 such models can not represent a continuum membrane model exactly, but
289 proposed an alternative formulation to evaluate the spring constant in order
290 to accurately represent an isotropic continuum membrane. Delingette [36]
291 introduced a novel spring type (bi-quadratic spring with tensile and angular
292 stiffness), based on finite strain mechanics and with great potential for
293 accurate non-linear membrane simulations. In [37], the effect of network
294 parameters, i.e. mesh, spring type and surface constraint have been studied,
295 with particular attention to the modeling of a red blood cell's (RBC)
296 membrane. They showed that an isotropic spring network is mechanically
297 isotropic in small deformation while a spring network with high randomness
298 tend to be mechanically isotropic even in large deformation and that the
299 network elasticity is independent of the density of the network mesh. All
300 spring networks are indeed vulnerable against surface area dilation. In
301 conclusion, the mechanical behavior of such models is conditionally equivalent
302 to that of continuum-based membrane models [37]. Different spring models
303 can be used, e.g., linear, truss, neo-Hookean, worm-like-chains. Several
304 applications have been presented in literature, especially for RBC mechanics
305 [38, 39, 34, 40, 35, 37, 41], showing that the model can give sufficiently
306 accurate results in modeling the RBC membrane. Here, we decided to adopt a
307 spring network model for its very simple formulation and reduced computational
308 cost. Moreover, one has to take into account that in several biological
309 applications the uncertainty in determining material properties could be
310 larger than the discrepancies between spring network and continuum models.
311 In any case, there is no limitation of the proposed method in replacing this
312 simplified solver by a more accurate, and computationally more expensive,

313 finite element membrane solver [27].

314 As an example of a more complex biological tissue, the simulation of
315 the dynamics of a bioprosthetic aortic valve in a pulsatile flow is presented
316 in section 3.8. During the cardiac cycle, the aortic valve leaflets open and
317 close by bending, undergoing large deformation with change of curvature,
318 and resist diastolic pressure experiencing in-plane stresses. This complex be-
319 havior is strictly related to the leaflet internal structure, therefore a proper
320 specification of the material properties combined with a realistic mechanical
321 model are crucial. Three layers compose the aortic leaflet tissue, each hav-
322 ing different characteristics. The different fiber orientation is responsible of
323 mechanical anisotropy: the circumferential elastic modulus of human aortic
324 valve tissue can be 6-8 times larger than the one evaluated in the radial direc-
325 tion [42]. Moreover, the material response to large strains is highly nonlinear
326 and hyperelastic. Here, the presented banding model is adopted, along with
327 a simplified nonlinear anisotropic material behavior for the in-plane stress.
328 As shown in [43], using a continuum model, the in-plane response of the
329 aortic valve tissue can be described by means of Fung-type constitutive law:

$$S_{ij} = \frac{\partial W}{\partial E_{ij}} \quad (38)$$

330 where S_{ij} and E_{ij} are the components of the second Piola–Kirchhoff stress
331 tensor and Green strain tensor, respectively, i and j are the indices repre-
332 senting the two principal directions, and W is the strain energy density. W
333 can be formulated as [44]:

$$W = \frac{c}{2}(e^Q - 1) \quad (39)$$

334 with

$$Q = A_1 E_{11}^2 + A_2 E_{22}^2 + 2A_3 E_{11} E_{22} + A_4 E_{12}^2 + 2A_5 E_{11} E_{12} + 2A_6 E_{22} E_{12} \quad (40)$$

335 The values of the constants are obtained by fitting previously published bi-
336 axial experiments on normal aortic valve tissue [43], and are here reported for
337 reference, $c = 9.7 Pa$, $A_1 = 49.558$, $A_2 = 5.2871$, $A_3 = -3.124$, $A_4 = 16.031$,
338 $A_5 = -0.004$ and $A_6 = -0.02$. With the aim of using a network spring
339 model instead of a continuum one, as done in [43] (where the only structural
340 solver is considered), the anisotropic behavior is simplified considering only
341 two stress-strain curves, corresponding to equibiaxial loading (one curve for

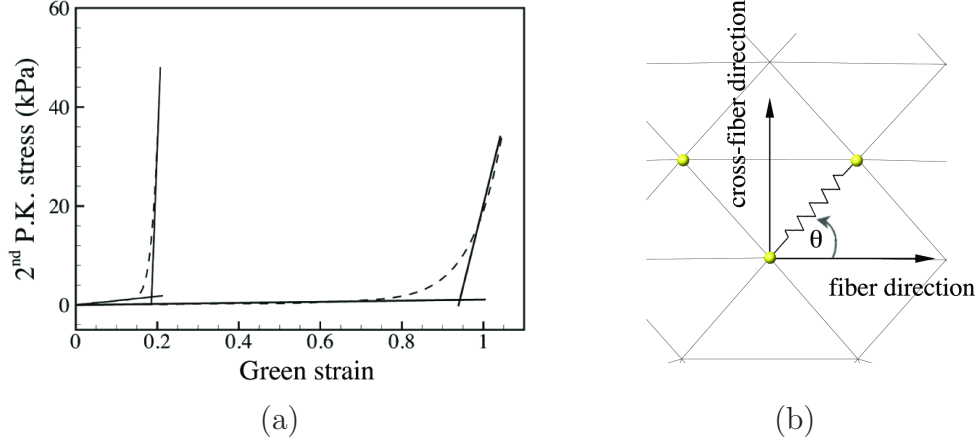


Figure 4: Bilinear relationship approximating the hyperelastic behavior of aortic valve material, as in [43].

342 the fiber fiber direction and one for the cross-fiber direction) of the aortic
 343 valve tissue (see figure 4a). The nonlinear behavior in both directions is fur-
 344 ther simplified approximating the curves by means of a piecewise linear fit
 345 consisting of a segment of slope m_1 passing through the origin and a second
 346 segment of slope m_2 intersecting the first segment at some critical value of
 347 Green strain (indicated as stretch ratio λ^*). The undeformed (stress-free)
 348 configuration of the valve leaflet is taken as a reference for evaluating the
 349 angle between the single spring (edge) direction with respect to the material
 350 fiber direction (horizontal direction in this work), θ , as indicated in figure 4b.
 351 Then, for each edge at a given angle θ , intermediate between the the fiber and
 352 cross-fiber directions, the slope parameter is calculated by (m_1 for example):

$$m_1(\theta) = \sqrt{m_{1f}^2 \cos^2 \theta + m_{1c}^2 \sin^2 \theta} \quad (41)$$

353 where m_{1f} and m_{1c} are the initial slopes in the fiber and cross-fiber direc-
 354 tions, respectively. The same formulation is adopted to evaluate the other
 355 parameters, m_2 and λ^* , based on the angle θ in the stress-free configura-
 356 tion of the mesh. In such a way, the line slopes as well as the stretch ratio is
 357 stored for each spring. The Van Gelder [32] approach is employed for calcu-
 358 lating elastic constant, k_e , where in place of Young's modulus, the evaluated
 359 slopes of the bilinear model, m_1 or m_2 are used, depending on whether the
 360 actual deformation of the spring corresponds to a value of stretch less than

361 or greater than λ^* [43]. Two elastic constants are obtained (form small and
 362 large displacements, k_{e1} and k_{e2}). The elastic force on one node of the spring
 363 (e.g. node 1 in figure 3) is evaluated by:

$$\mathbf{F}_1^E = -k_{e1}(l - l_0)\frac{\mathbf{r}_{12}}{l} \quad (42)$$

364 for springs with stretch magnitude less than λ^* , or

$$\mathbf{F}_1^E = -[k_{e1}l_0(\lambda^* - 1) + k_{e2}(l - \lambda^*l_0)]\frac{\mathbf{r}_{12}}{l} \quad (43)$$

365 for springs with stretch magnitude freater than λ^* .

366 2.5. Force and moment evaluation

367 The forces and moments in equations (22),(23) and (37) are calculated by
 368 considering the pressure and viscous stresses over the immersed body surface.
 369 Given the triangular discretization of the surface, the local force contribution
 370 is evaluated for each triangular element.

371 For the case of a closed surface, representing a rigid or deformable solid,
 372 the single contributions to the force and moment are evaluated for each tri-
 373 angular element, l :

$$\mathbf{F}_l(t) = (\boldsymbol{\tau}_l \cdot \mathbf{n}_l - p_l \mathbf{n}_l) S_l, \quad (44)$$

$$\mathbf{M}_l(t) = [(\boldsymbol{\tau}_l \cdot \mathbf{n}_l - p_l \mathbf{n}_l) \times \mathbf{r}_l] S_l, \quad (45)$$

375 where $\boldsymbol{\tau}_l$ and p_l are the viscous stress tensor and pressure, evaluated at the
 376 centroid of each triangle (location of the Lagrangian marker, l), \mathbf{n}_l and S_l
 377 are the unit outward normal vector and area of each triangle, while \mathbf{r}_l is
 378 the position vector of the marker with respect to its baricentre. In order
 379 to evaluate the pressure p_l and the velocity derivatives, for each Lagrangian
 380 marker a probe is created along its normal direction, at a distance h_l , equal
 381 to the averaged local grid size. Using the same MLS formulation described
 382 above, pressure and velocity are evaluated at the probe location. Then, the
 383 pressure on the markers is calculated as:

$$p_l = p_l^* + \frac{D\mathbf{u}_l}{Dt} \cdot \mathbf{n}_l \quad (46)$$

384 where p_l^* is the pressure on the probe and the second term of the right hand
 385 side, involving the acceleration of the marker, $D\mathbf{u}_l/Dt = d\mathbf{v}_l/dt$, comes
 386 from the evaluation of the pressure gradient in the normal direction by the

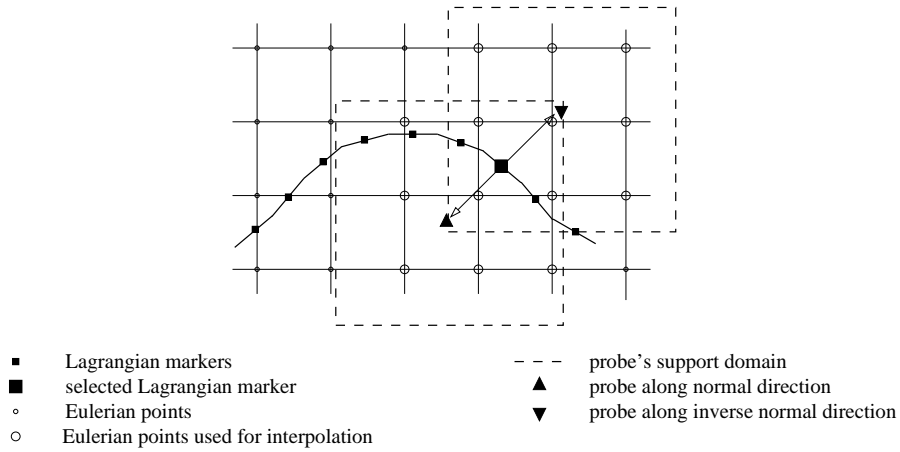


Figure 5: Scheme for IB forces evaluation.

387 momentum equation [14]. Concerning the velocity derivatives on the body
 388 surface, these are considered equal to the velocity derivatives evaluated at the
 389 probes, that is equivalent to assume a linear variation of the velocity near
 390 the body. This is consistent with the second-order accuracy of the space
 391 discretization scheme and turns out to be a good approximation provided
 392 that the grid is sufficiently refined near the body. For the case of rigid bodies,
 393 the total force and moment to be considered in equations (22) and (23) are
 394 obtained by summing all the contributions of equations (44) and (45) over
 395 the N_t triangles describing the immersed surface; on the other hand, in case
 396 of deformable bodies, the $\mathbf{F}_l(t)$ is equally distributed among the three nodes
 397 of the l -th triangle: the total hydrodynamic force acting on each triangle
 398 vertex is obtained summing all the contributions of the triangles sharing that
 399 node.

400 In the case of vesicles or open surfaces, one has to account for the forces
 401 due to the presence of the fluid on both sides of the surface, namely, also in
 402 the opposite normal direction, for each triangle, in order to obtain the total
 403 force:

$$404 \quad \mathbf{F}_l(t) = S_l [(\boldsymbol{\tau}_l^+ - \boldsymbol{\tau}_l^-) \cdot \mathbf{n}_l - (p_l^+ - p_l^-)\mathbf{n}_l] , \quad (47)$$

$$405 \quad \mathbf{M}_l(t) = S_l [(\boldsymbol{\tau}_l^+ - \boldsymbol{\tau}_l^-) \cdot \mathbf{n}_l - (p_l^+ - p_l^-)\mathbf{n}_l] \times \mathbf{r}_l , \quad (48)$$

406 where $+$ and $-$ quantities are evaluated on the probes along the positive and
 407 negative \mathbf{n}_l directions, respectively (see figure 1). It is worth noting that
 with the present method one can sustain large pressure differences across

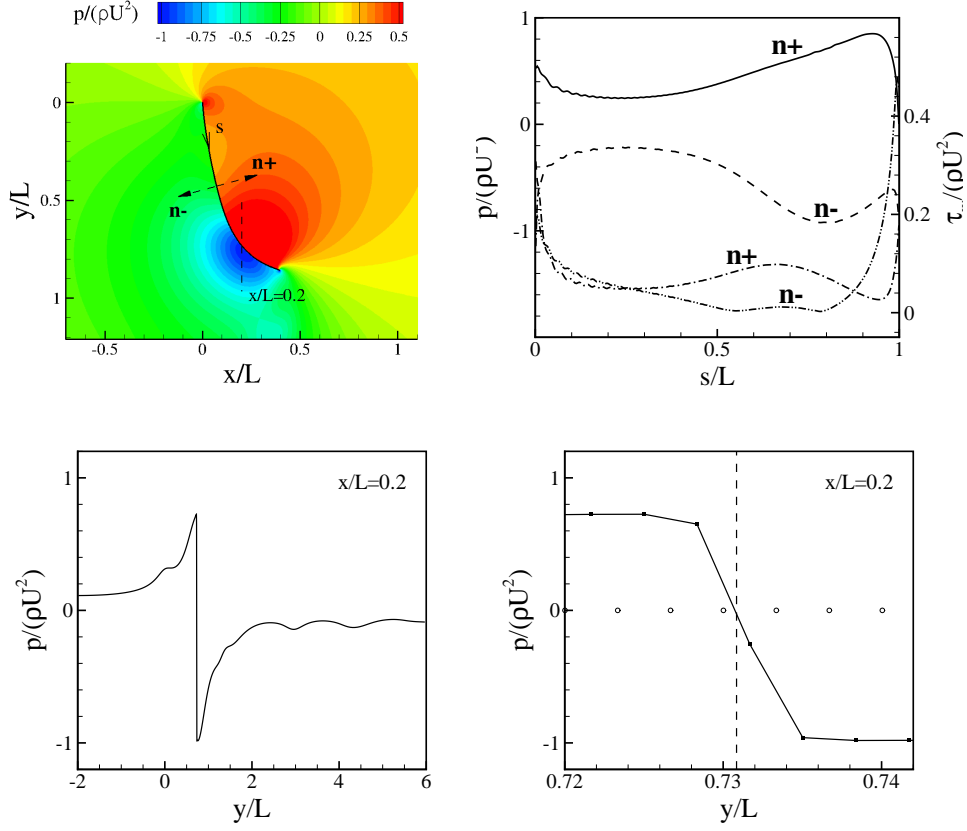


Figure 6: Pressure (red lines) and streamwise velocity (blue lines) distributions on the centerline of the computational domain for the case of a uniform flow past a fixed vertical plate.

408 one Eulerian cell.

409 As an example, the results for the flow past a fixed, *zero-thickness* vertical
 410 plate is shown in figure 6. The flow comes from left to right with velocity U
 411 and impacts on a plate of height L , with $Re = \rho_f UL / \mu = 200$. The compu-
 412 tational domain is $[-2L, 6L] \times [-4L, 4L]$. The center of the plate is placed at
 413 $[0.5L, 0]$. Inlet and outlet boundary conditions are imposed on the vertical
 414 boundaries, while free-shear wall conditions are imposed for the horizontal
 415 boundaries. A non uniform grid of 671×747 nodes is used with a uniform
 416 grid spacing of $0.01L$ in the vicinity of the plate. The Lagrangian markers
 417 are distributed uniformly onto the plate surface, with a spacing of about 0.7
 418 the local Eulerian grid size in that area. Figure 6 shows the pressure and

419 streamwise velocity distributions on the centerline of the computational do-
 420 main. The pressure difference across the plate is shown, captured in one grid
 421 cell along the streamwise direction (figure 6, left). Figure 6 shows an instan-
 422 taneous field of the pressure contours and the pressure distribution along the
 423 plate considering the upstream and downstream normal probe directions.

424 2.6. Fluid-structure-interaction strategy

425 The evaluation of the flow and body motion at each time step is carried
 426 out by means of an implicit strongly coupled approach to ensure convergence
 427 and to allow the use of larger time steps, since the prediction of the flow field
 428 and of the hydrodynamic loads requires the knowledge of the motion of the
 429 bodies and vice-versa [45]. The adopted approach is based on Hamming’s
 430 4th order modified predictor-corrector method with mop-up correction [26].
 431 For the case of a rigid body, $\ddot{\mathbf{x}}$, $\dot{\mathbf{x}}$ and \mathbf{x} represent the acceleration, velocity
 432 and position, respectively, of the body’s baricentre (in that case $m = M$ is
 433 the mass of the entire body), and the same approach is adopted to evaluate
 434 angular acceleration, velocity and position (considering the inertial tensor).
 435 On the other hand, for the case of deformable body, $\ddot{\mathbf{x}}$, $\dot{\mathbf{x}}$ and \mathbf{x} represent
 436 acceleration, velocity and position, respectively, of each triangle’s vertex and
 437 $m = m_p$ is the mass on each node, obtained by uniformly distributing the
 438 total mass of the structure over the N_v nodes. Subscripts indicate the time
 439 instant.

440 For each time step,

441 1. Predictor:

- 442 • $\ddot{\mathbf{x}}_n = \mathbf{F}_n/m$
- 443 • $\dot{\mathbf{x}}_{n+1}^p = \dot{\mathbf{x}}_{n-3} + \frac{4}{3}\Delta t (2\ddot{\mathbf{x}}_n - \ddot{\mathbf{x}}_{n-1} + 2\ddot{\mathbf{x}}_{n-2})$
- 444 • $\dot{\mathbf{x}}_{n+1}^m = \dot{\mathbf{x}}_{n+1}^p - \frac{112}{121} (\dot{\mathbf{x}}_n^p - \dot{\mathbf{x}}_n^c)$
- 445 • $\mathbf{x}_{n+1}^p = \mathbf{x}_{n-3} + \frac{4}{3}\Delta t (2\dot{\mathbf{x}}_n - \dot{\mathbf{x}}_{n-1} + 2\dot{\mathbf{x}}_{n-2})$
- 446 • $\mathbf{x}_{n+1}^m = \mathbf{x}_{n+1}^p - \frac{112}{121} (\mathbf{x}_n^p - \mathbf{x}_n^c)$
- 447 • Solve flow and structure (if deformable body) equations, using the
 448 predicted structural node position and velocity and evaluate \mathbf{F}_{n+1}^1

449 2. Corrector: do loop on k , while convergence is achieved:

- 450 • $\ddot{\mathbf{x}}_{n+1}^k = \mathbf{F}_{n+1}^k/m$
- 451 • $\dot{\mathbf{x}}_{n+1}^c = \frac{1}{8} (9\dot{\mathbf{x}}_n - \dot{\mathbf{x}}_{n-2}) + \frac{3}{8}\Delta t (2\ddot{\mathbf{x}}_{n+1}^k + 2\ddot{\mathbf{x}}_n - \ddot{\mathbf{x}}_{n-1})$

- 452 • $\mathbf{x}_{n+1}^c = \frac{1}{8}(9\mathbf{x}_n - \mathbf{x}_{n-2}) + \frac{3}{8}\Delta t(2\dot{\mathbf{x}}_{n+1}^k + 2\dot{\mathbf{x}}_n - \dot{\mathbf{x}}_{n-1})$
- 453 • Check for converge of the structure equations: $|\mathbf{x}_{n+1}^{k+1} - \mathbf{x}_{n+1}^k| < \epsilon$
- 454 • If converged,
 - 455 – $\dot{\mathbf{x}}_{n+1} = \dot{\mathbf{x}}_{n+1}^c + \frac{9}{121}(\dot{\mathbf{x}}_{n+1}^p - \dot{\mathbf{x}}_{n+1}^c)$
 - 456 – $\mathbf{x}_{n+1} = \mathbf{x}_{n+1}^c + \frac{9}{121}(\mathbf{x}_{n+1}^p - \mathbf{x}_{n+1}^c)$
 - 457 – Solve flow and structure equations (if deformable body), using
 - 458 the new structural node position and velocity and evaluate
 - 459 \mathbf{F}_{n+1}
- 460 • If not converged,
 - 461 – Solve flow and structure equations (if deformable body), using
 - 462 the actual structural node position and velocity and evaluate
 - 463 \mathbf{F}_{n+1}^{k+1}
 - 464 – repeat the corrector procedure until convergence

465 In order to provide the previous time steps solutions needed, lower-order
 466 method are employed for the first time steps of integration. The tolerance ϵ
 467 considered in this work is equal to 10^{-7} , and the method converges in 2 – 8
 468 iterations, depending on the problem complexity and structure mass and
 469 elastic properties. In the case of large accelerations, under-relaxation could
 470 be considered in order to maintain the system stable.

471 3. Results

472 3.1. Sedimentation of an elliptic particle

473 The dynamics of a single two-dimensional elliptic particle sedimenting
 474 in a confined channel is considered here to validate the FSI procedure. A
 475 systematic verification study is also performed to check the order of accuracy
 476 of the algorithm. The problem is configured as an elliptic particle with
 477 aspect ratio $\alpha = a/b = 2$, where a and b are the major and minor axes,
 478 respectively, as shown in Figure 7. The confined channel has width L , with
 479 a blockage ratio $\beta = L/a = 4$. The density ratio, $\gamma = \rho_s/\rho_f$ is set equal to
 480 1.1, where ρ_s and ρ_f are the particle and fluid densities, respectively. The
 481 computational domain is $[0, L] \times [0, 7L]$ in X and Y directions, respectively,
 482 with the gravity g pointing in the negative Y direction. The particle starts
 483 falling with the centroid in $(0.5L, 6L)$, with an initial angle of $\theta_0 = 45^\circ$,
 484 to break the symmetry. Considering the terminal settling velocity of the

485 particle, V_T , the major axis of the ellipse and the fluid kinematic viscosity,
 486 ν , the Reynolds number is $Re_T = V_T a / \nu = 12.5$, while the Froude number
 487 is $Fr_T = V_T / \sqrt{ga} = 0.126$. In physical units, the major axis of the ellipse is
 488 0.1 cm and the kinematic viscosity of the fluid is $0.01 \text{ cm}^2/\text{s}$ [46]. A slip wall
 489 boundary condition is applied at the top boundary and all other boundaries
 490 are treated as no-slip wall boundaries. Eight uniform Cartesian grids are
 491 used with nodes: 81×561 , 101×701 , 134×934 , 161×1121 , 201×1401 ,
 492 267×1867 , 401×2801 , 801×5601 , corresponding to an Eulerian grid spacing,
 493 $\Delta h/a$, of 0.05, 0.04, 0.03, 0.025, 0.02, 0.015, 0.01, 0.005, respectively. A
 494 uniform Lagrangian marker spacing is adopted for all the cases, equal to 0.77
 495 the Eulerian grid size. With the aim of investigating the overall numerical
 496 accuracy in both space and time, the time steps for each grid is chosen
 497 in order to maintain a constant ratio between the grid spacing and time
 498 step, $\Delta h / \Delta t = 5U_t$. In Figure 7 the present results in terms of particle
 499 settling velocity, trajectory (location of center of mass) and orientation for
 500 the grids with $\Delta h/a$ equal to 0.04, 0.02 and 0.01 are shown, compared with
 501 the numerical results obtained by [46] by means of a finite-element method.
 502 The particle settles into the center of the channel ($x/L = 0.5$) with a constant
 503 velocity, and sediments in a horizontal configuration ($\theta = 0$). The agreement
 504 of the results is very good for the three grids considered. For the accuracy
 505 study, the solution from the finest grid, 801×5601 , is used as reference. Three
 506 relative errors are defined, for the terminal position and velocity at time $t =$
 507 0.8 s , namely $\epsilon_P = [(Y - Y^{ref})/Y^{ref}]_{t=0.8s}$ and $\epsilon_V = [(V_Y - V_Y^{ref})/V_Y^{ref}]_{t=0.8s}$,
 508 respectively, and for the time averaged value of the terminal velocity in the
 509 interval $t = [0.8, 1.6] \text{ s}$, namely $\epsilon_{\langle V_Y \rangle} = (\langle V_Y \rangle - \langle V_Y^{ref} \rangle) / \langle V_Y^{ref} \rangle$.
 510 The relative errors are reported versus grid spacing in Figure 8, showing
 511 a first-order convergence rate for the coarser grids and an evident overall
 512 second-order accuracy on finer grids.

513 3.2. Fluttering and tumbling of a plate

514 The falling dynamics of a plate is considered in order to test the ability
 515 of the proposed technique to capture the transition between tumbling and
 516 fluttering. Previous experimental studies [47] on thin flat strips falling in
 517 a vertical cell have shown that the transition is regulated by the Reynolds
 518 and Froude numbers. A two-dimensional elliptical plate is considered, with
 519 a thickness-to-length ratio h/L equal to 0.125, as shown in Figure 9a. The
 520 Reynolds number, defined as $Re = U_0 L / \nu$, is equal to 140 for the flutter-
 521 ing and to 420 for the tumbling case, where $U_0 = \sqrt{2(\rho_s/\rho_f - 1)hg}$ is the

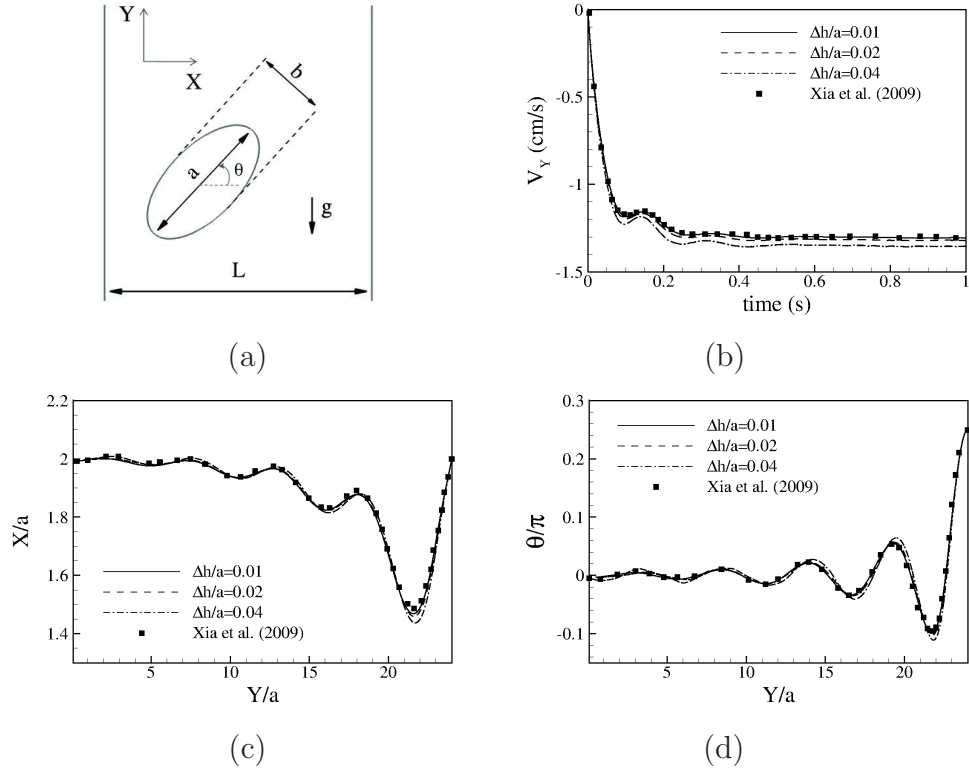


Figure 7: (a) Geometrical parameters for the elliptic particle sedimenting in a confined channel, with $Re_T = 12.5$, $Fr_T = 0.126$, $\alpha = 2$, $\beta = 4$, $\gamma = 1.1$; (b) sedimentation velocity; (c) location of center of mass; (d) orientation of the particle. Present numerical results (lines) are compared with finite-elements numerical results of [46] (symbols).

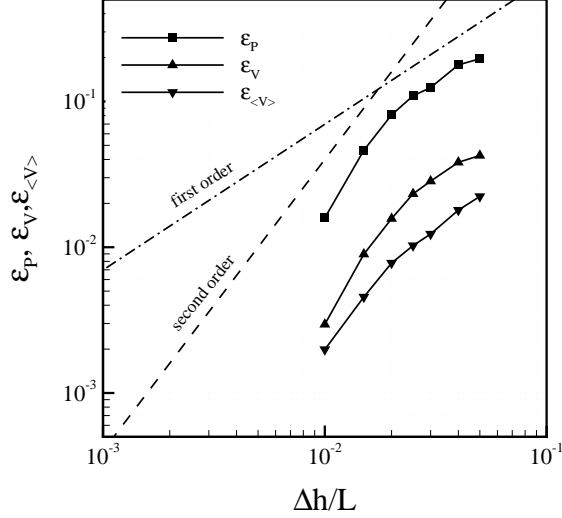


Figure 8: Systematic study of accuracy for an elliptic particle sedimenting in a confined channel, with $Re_T = 12.5$, $Fr_T = 0.126$, $\alpha = 2$, $\beta = 4$, $\gamma = 1.1$.

522 characteristic speed and g the module of gravitational acceleration, the latter
523 pointing in the negative Y direction. The modified Froude number, defined as
524 $Fr = \sqrt{M/(\rho_f L^2)}$ for a two-dimensional body, with M the mass of the plate
525 per unit width, is equal to 0.45 and 0.89 for the fluttering and tumbling cases,
526 respectively, as done in the computational work of [48]. The computational
527 domain considered is $[0, 30L] \times [0, 30L]$ in X and Y directions, respectively.
528 The particle starts falling with the centroid in $(15L, 28L)$ for the fluttering
529 cases, and in $(25L, 28L)$ for the tumbling ones, with two different initial
530 angles per case, θ_0 , of 45° and -75° . Slip wall boundary conditions are ap-
531 plied at the top boundary and at the vertical boundaries of the domain, while
532 a no-slip boundary condition is imposed at the bottom boundary. A uniform
533 computational grid is used, with 2300×2300 nodes, with an Eulerian grid
534 spacing of about $0.013L$, and a uniform Lagrangian marker spacing of $0.01L$.
535 A constant time step of $\Delta t = 5 \cdot 10^{-3} L/U_0$ is used. The trajectories of the
536 plates are reported in figure 9. The two plates show a very similar steady
537 fluttering, regardless their initial angle, with a different transient process for
538 the case with $\theta_0 = -75^\circ$. Concerning the tumbling behavior, the plate with
539 $\theta_0 = 45^\circ$ shows a longer transient period in which it starts fluttering and
540 then falls tumbling. The descending angle with respect to the horizontal

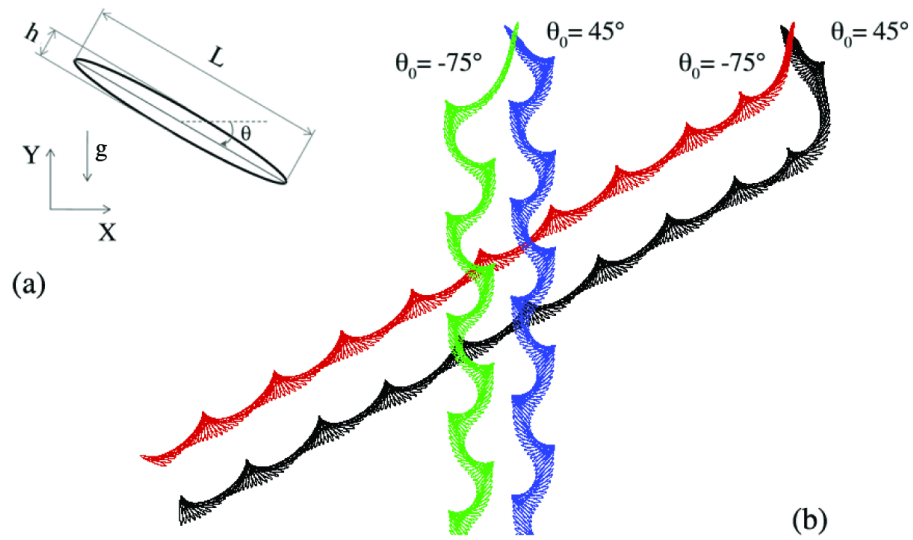


Figure 9: (a) Geometrical parameters for the plate falling in a quiescent fluid. (b) Overlapping of plate positions for fluttering ($Re = 140$, $Fr = 0.45$) and tumbling ($Re = 420$, $Fr = 0.89$) plates. Black: tumbling case, $\theta_0 = 45^\circ$; red: tumbling case, $\theta_0 = -75^\circ$; blue: fluttering case, $\theta_0 = 45^\circ$; green: fluttering case, $\theta_0 = -75^\circ$ (Colour online).

541 direction is the same in the two tumbling cases. Figure 10 shows the hori-
 542 zontal and vertical force coefficients, calculated by $C_i = 2F_i/\rho_f U^2 L$, where
 543 F_i is the hydrodynamic force acting on the plate in the i -th direction, as
 544 well as the two velocity components for the fluttering and tumbling cases
 545 with $\theta_0 = 45^\circ$, compared with the numerical results of [48]. A very good
 546 agreement is obtained for all the cases.

547 3.3. Particle migration in a planar Couette flow

548 The two-dimensional motion of a single circular particle in a shear flow is
 549 considered, in order to evaluate the sensibility of the code in capturing the
 550 particle lateral migration, which is due to a vertical velocity component that
 551 is very small compared with the horizontal one (slow migration). The differ-
 552 ence in the relative velocity across a solid particle may drive it to move later-
 553 ally since the side with a higher relative velocity may lead to a lower pressure.
 554 In [49, 50], the authors suggested that three mechanisms are responsible for
 555 the motion in a linear shear flows: wall lubrication repulsion; inertial lift due
 556 to shear slip and lift due to particle rotation. An accurate evaluation of the
 557 forces is necessary to properly evaluate the correct dynamics. The circular
 558 particle has radius r and the width of the channel is $h = 8r$. The computa-
 559 tional domain considered is $[-100r, 100r] \times [0, 8r]$ in the x and y directions,
 560 respectively. Periodic boundary conditions are imposed in the horizontal di-
 561 rection. In the vertical direction, no-slip wall is imposed at the lower surface
 562 of the domain, while the upper surface has an imposed velocity, U_h (see fig-
 563 ure 11). The bulk Reynolds number considered is $Re_b = U_h h/\nu = 40$, which
 564 corresponds to a particle Reynolds number $Re_p = U_h r^2/(\nu h) = 0.625$ that
 565 does not satisfy the small- Re_p condition required for validity of perturbation
 566 theories of the viscous type or inertial type [49]. The particle is considered
 567 neutrally buoyant. Two initial conditions are considered, with the particle
 568 vertical position equal to $h/4$ and $3h/4$. Here we consider the initial value of
 569 the difference between the particle streamwise velocity and the undisturbed
 570 velocity at the center of the particle, namely *slip velocity* (δU), $\delta U_{init} = 0$.
 571 Ho and Leal [51] and later Vasseur and Cox [52] showed that in conditions
 572 of low Reynolds number, neutrally buoyant particles in a simple shear Cou-
 573 ette flow will migrate toward the center plane because of the influence of
 574 the walls (agreeing with experimental observations by Halow and Wills [53]).
 575 In the present simulations for the Couette flow, the particles are observed
 576 to migrate toward the median plane of the channel, as shown in Figure 12,
 577 regardless of their initial position, with a good agreement with the results

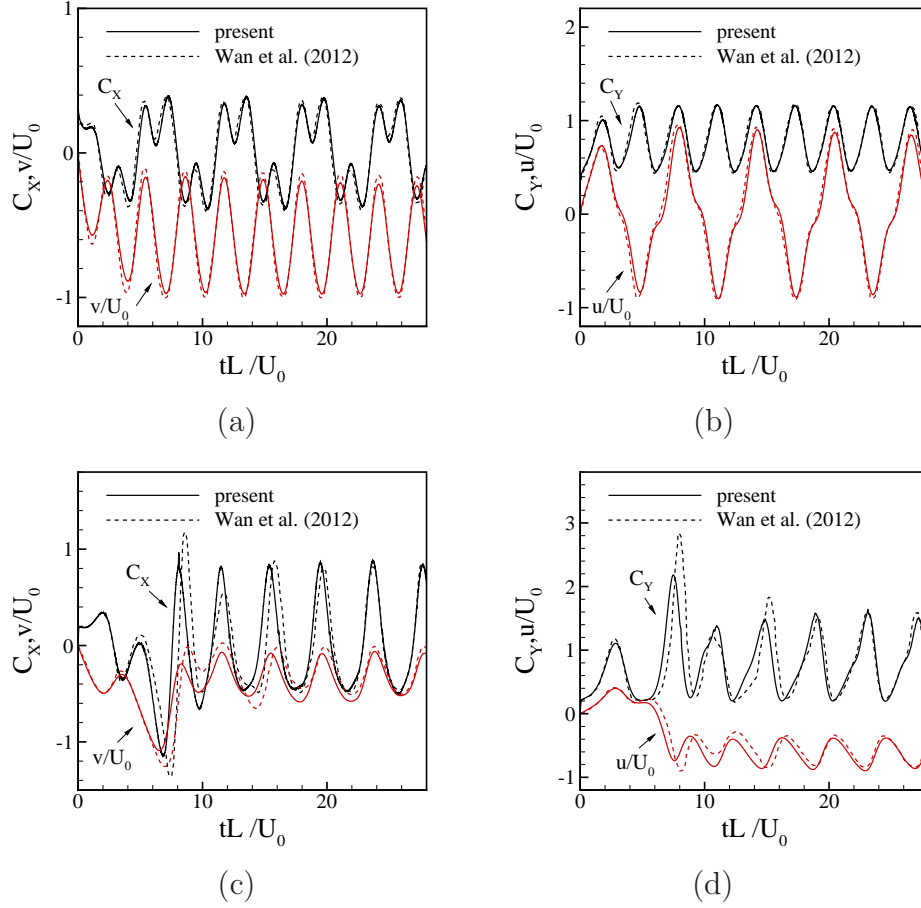


Figure 10: Top: fluttering case with $Re = 140$, $Fr = 0.45$, $\theta_0 = 45^\circ$. (a) Horizontal force coefficient, C_x , and vertical velocity component, v ; (b) vertical force coefficient, C_y , and horizontal velocity component, u . Bottom: tumbling case with $Re = 420$, $Fr = 0.89$, $\theta_0 = 45^\circ$. (c) Horizontal force coefficient, C_x , and vertical velocity component, v ; (d) vertical force coefficient, C_y , and horizontal velocity component, u . Continuous lines indicate present results, while dashed lines indicate numerical results of [48].

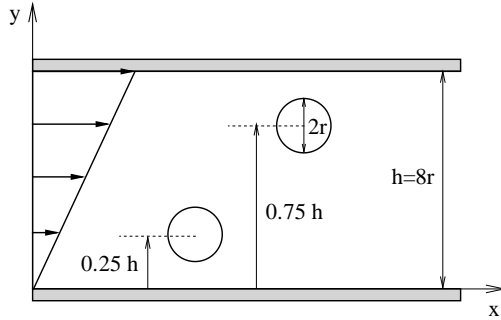


Figure 11: Sketch of the configuration for a circular particle transported in a shear flow between walls, at $Re_b = 40$.

578 obtained by [50]. Note that the migration velocity of the particles depends
 579 on the initial conditions at the early migration stage. Figure 12 reports the
 580 particle vertical position and migration velocity in function of time. With
 581 the prescribed initial slip velocity, the particle migrates gradually toward the
 582 equilibrium position, rotating with an instantaneous angular velocity that
 583 reaches an equilibrium value of about the 47% of the constant shear rate of
 584 the undisturbed flow field. This means that the particles rotate with the
 585 angular velocity of the flow field to within a small correction, as found also
 586 by Feng et al. [50].

587 3.4. Single sphere settling under gravity

588 To further validate the method, a three-dimensional case involving fluid-
 589 structure interaction with a rigid body is considered, by simulating the mo-
 590 tion of a sphere falling under gravity in a closed container. Experimental
 591 investigations have been performed by [54], by means of particle image ve-
 592 locimetry, providing an accurate measure of both the sphere trajectory and
 593 velocity from the moment of its release until rest at the bottom of the channel.
 594 Given the relative small ratio between the box width and the particle diam-
 595 eter, the full flow field can be simulated under identical conditions. A sphere
 596 with diameter $d = 15\text{ mm}$ is considered. The Froude and Reynolds numbers
 597 are defined as $Re = u_\infty d / \nu$ and $Fr = u_\infty / \sqrt{gd}$, where $g = 9.81\text{ m/s}^2$ is the
 598 module of the gravity acceleration and u_∞ is the sedimentation velocity of a
 599 sphere in an infinite medium. In order to determine u_∞ , the relation for the

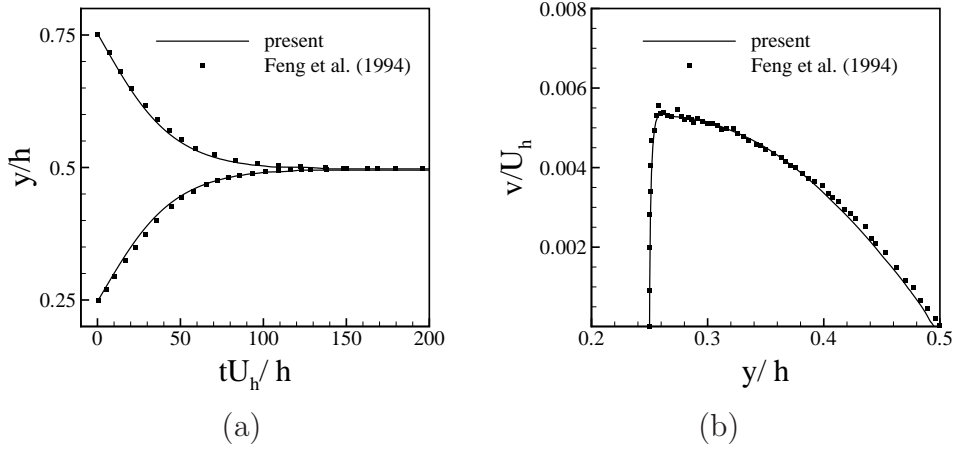


Figure 12: Lateral migration of a circular neutrally buoyant particle in a shear flow between walls, at $Re_h = 40$. The particle is released at $y_0 = h/4$ and $y_0 = 3h/4$, with $\delta U_{init} = 0$. (a) Vertical baricentre position, y , versus time. (b) Migration vertical velocity, v , versus vertical baricentre position, y . Continuous lines indicate present results, symbols indicate numerical results of [50].

600 drag coefficient of Abraham [55] is used:

$$C_d = C_0 \left(1 + \frac{\delta_0}{\sqrt{Re}} \right)^2 \quad (49)$$

601 with $C_0 \delta_0^2 = 24$ and $\delta_0 = 9.06$, obtaining

$$u_\infty = \sqrt{\frac{4gd}{3C_d}(\gamma - 1)} \quad (50)$$

602 Four different conditions are considered, with different density ratios, $\gamma =$
603 ρ_s/ρ_f , and parameters, as reported in Table 1. The computational domain
604 considered is $[0, 6.67d] \times [0, 6.67d] \times [0, 10.67d]$, where the last is the grav-
605 ity acceleration direction. The particle starts falling with the centroid in
606 $(3.33d, 3.33d, 8d)$. No-slip wall conditions are imposed at all the boundary
607 surfaces of the domain. A uniform grid of $241 \times 241 \times 385$ nodes is used with
608 a grid spacing of about $0.028d$. The Lagrangian markers are distributed uni-
609 formly onto the sphere surface, with a spacing of $0.02d$, that is equal to 0.71
610 the Eulerian grid size. The constant time step used depends on the case con-
611 sidered and is reported in Table 1. The sphere sedimentation velocity and
612 trajectory are reported in Figure 13, where the present results are compared

Re_∞	γ	u_∞ (m/s)	Fr_∞	$\Delta t u_\infty / d$
1.5	1.155	0.038	0.0991	0.0001
4.1	1.161	0.060	0.156	0.0005
11.6	1.164	0.091	0.237	0.0007
31.2	1.167	0.128	0.334	0.001

Table 1: Reynolds number, density ratio, settling velocity in an infinite medium, Froude number and non-dimensional time step used in the simulation for the case of a sphere settling under gravity in a closed channel.

613 with the experimental data of [54]. A very good agreement is obtained for
614 all the configurations considered.

615 3.5. Two-dimensional flexible filament in a free stream

616 A flexible filament motion in a free stream is simulated in order to test
617 the ability of the simplified structural model to capture the dynamics of
618 deformable bodies. Also in this case, a systematic verification study is per-
619 formed to check the order of accuracy of the algorithm in the deformable-
620 geometry case. The geometry of the problem is reported in figure 14. A
621 zero-thickness filament of length L is pinned at the leading edge and freely
622 moves under the effect of incoming flow and gravity. The initial orientation
623 angle of the filament with respect to the flow is $\theta_0 = 0.1\pi$. The filament is
624 considered inextensible ($k_e = 250000$) and flexible ($k_b = 0.15$) in order to
625 replicate the test of [21] and [9]. The ratio of solid and fluid densities, γ is
626 equal to 150. The Reynolds number, based on the filament length, L , the fluid
627 density, ρ_f and the inflow velocity, U is equal to 200. The Froude number is
628 equal to 0.5. The computational domain considered is $[-4L, 4L] \times [-2L, 6L]$
629 in the x and y directions respectively, with the filament leading edge in the
630 origin of the domain and the gravity acting in the flow direction (negative
631 y direction). No-slip wall boundary conditions are imposed at the vertical
632 boundaries, while inlet and outlet boundary conditions are imposed at the
633 horizontal ones, as indicated in figure 14. The filament has no thickness
634 in the present simulation. Pressure and viscous forces acting on the fila-
635 ment are obtained considered two probes from each Lagrangian marker, in
636 both directions, as explained in section 2.5. The mass of the nodes of the
637 filament is calculated considering a thickness of $0.01L$. Seven non uniform

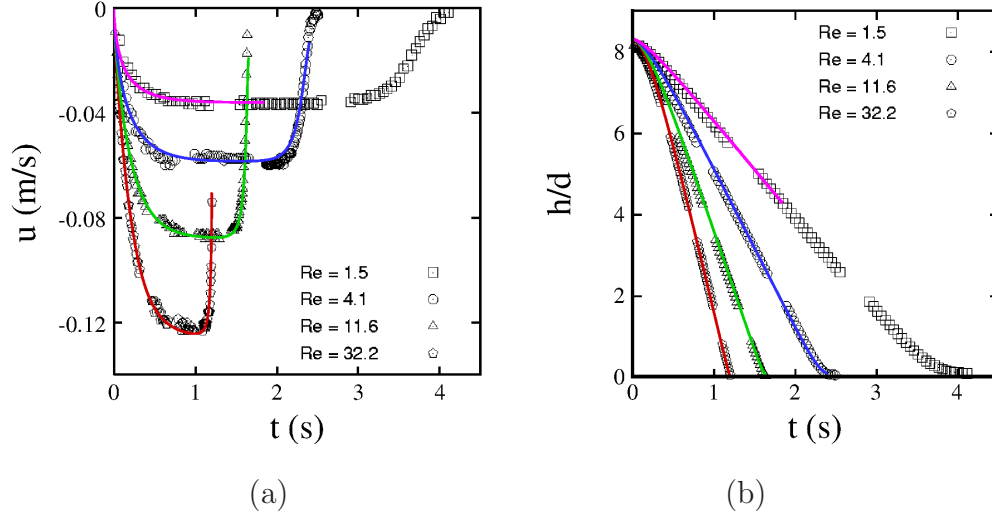


Figure 13: Single sphere settling under gravity in a small container. (a) Spere sedimentation velocity; (b) sphere trajectory. Numerical results (continuous lines) are compared with experimental results (symbols) of ten Cate et al. [54] at four Reynolds numbers.

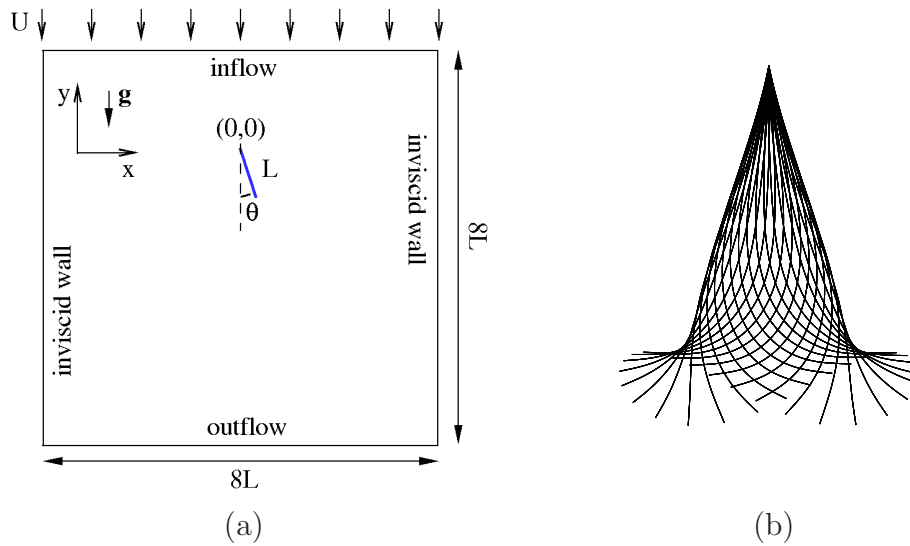


Figure 14: (a) Scheme of the computational setup for the simulation of the flow around a flexible filament in a free stream. (b) Flapping filament configuration at several time points along its flapping cycle; $Re = 300$, $\gamma = 1$, $k_b = 0.1$.

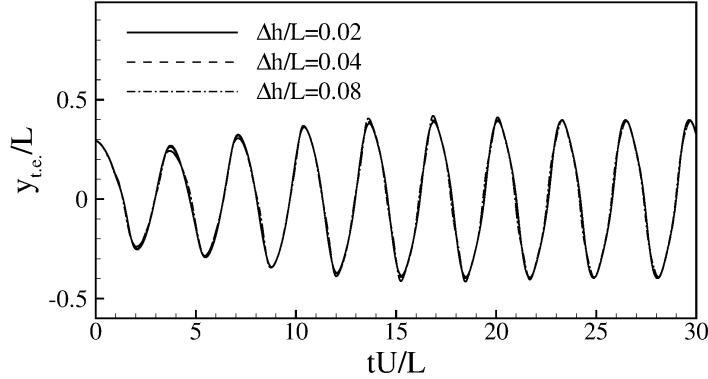


Figure 15: Comparison of trailing-edge transverse location time traces for a flexible filament in a free stream, with $Re = 200$, $\gamma = 150$ and $k_b = 0.15$.

638 Cartesian grids are used, refined in the vicinity of the filament, with nodes:
639 81×561 , 101×701 , 134×934 , 161×1121 , 201×1401 , 267×1867 , 401×2801 ,
640 The grid spacing is maintained uniform in a box containing the filament of
641 $[-1.2L, 1.2L] \times [-L, 4L]$ in the x and y directions respectively, correspond-
642 ing to an Eulerian grid spacing, $\Delta h/L$, of 0.05, 0.04, 0.03, 0.025, 0.02, 0.015,
643 0.01, respectively. A uniform Lagrangian marker spacing is adopted for all
644 the cases, equal to 0.7 the Eulerian grid size. With the aim of investigating
645 the overall numerical accuracy in both space and time, the time steps for
646 each grid is chosen in order to maintain a constant ratio between the grid
647 spacing and time step, $\Delta h/\Delta t = 10U_t$. The filament shows a periodic flap-
648 ping state after few cycles. The filament configuration during the periodic
649 flapping is reported in figure 14b for the finest case, showing the symmetric
650 behavior of the structure deformation. In Figure 15 the present results in
651 terms of time traces of the trailing edge transverse location of the flexible
652 filament for the grids with local $\Delta h/L$ equal to 0.04, 0.02 and 0.01 are shown,
653 showing very similar results, with some discrepancies of the coarse mesh with
654 respect to the finer ones. For the accuracy study, the solution from the finest
655 grid, 801×5601 , is used as reference. Two relative errors are defined, for
656 the maximum value of the filament trailing-edge transverse location, x_{max} ,
657 namely $\epsilon_A = (x_{max} - x_{max}^{ref})/x_{max}^{ref}$ and for the oscillation period, T , namely
658 $\epsilon_T = (T - T^{ref})/T^{ref}$. The relative errors are reported versus grid spacing
659 in Figure 16, showing an overall second-order accuracy on finer grids. The
660 instantaneous vorticity contours at four time points along the flapping cycle

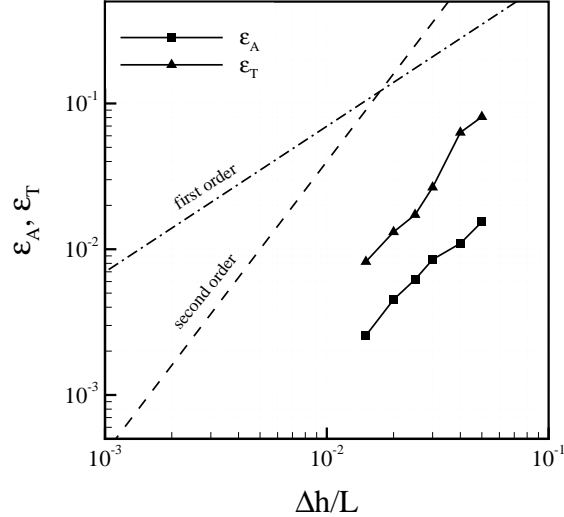


Figure 16: Systematic study of accuracy for a flexible filament in a free stream, with $Re = 200$, $\gamma = 150$ and $k_b = 0.15$.

661 are reported in figure 17. In Figures 18 and 19, the present results on the
 662 finest grid, in terms of time traces of the trailing-edge transverse location and
 663 drag and lift coefficients, respectively, are compared with numerical results
 664 of [21] and [9]. The results are in good agreement, with slight phase differ-
 665 ences. The force coefficients are calculated by $C_F = 2F/\rho_f U^2 L$, where F is
 666 the hydrodynamic force acting on the filament in the streamwise (drag) and
 667 transverse (lift) directions, respectively. It is worth noting that no spurious
 668 oscillations are present even in the presence of deforming geometries for all
 669 the grids.

670 3.6. Three-dimensional flow around a flapping flag

671 As a three-dimensional test-case considering a deformable body, the flow
 672 around a flapping flag in a free stream is considered. The schematic of the
 673 problem is reported in figure 20, where a square flag of length L is considered.
 674 The computational domain is a rectangular box with $[-L, L] \times [-4L, 4L] \times$
 675 $[-L, 7L]$ in the x, y and z directions, respectively. The center of the leading
 676 edge of the flag is positioned at the origin. The initial shape of the flag
 677 is a flat plate, inclined of $\theta_0 = 0.1\pi$ with respect to the xz -plane, z being
 678 the streamwise direction and x the vertical one. The leading-edge of the

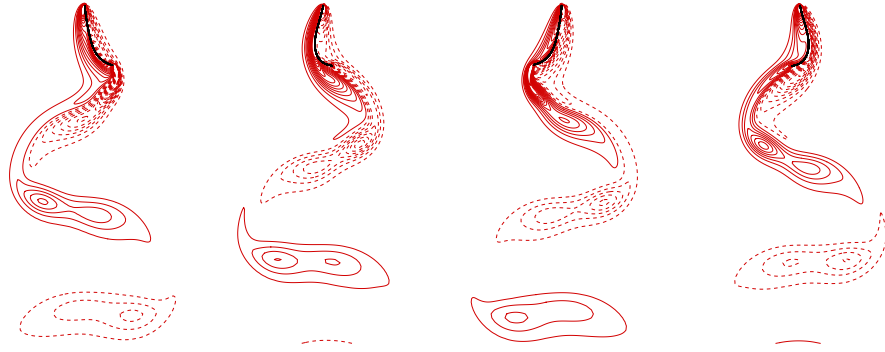


Figure 17: Instantaneous vorticity contours for the simulation of the flow around a flexible filament in a free stream, with $Re = 200$, $\gamma = 150$, $k_b = 0.15$. From left to right $t/T = 6$, $t/T = 6.25$, $t/T = 6.5$ and $t/T = 6.75$.

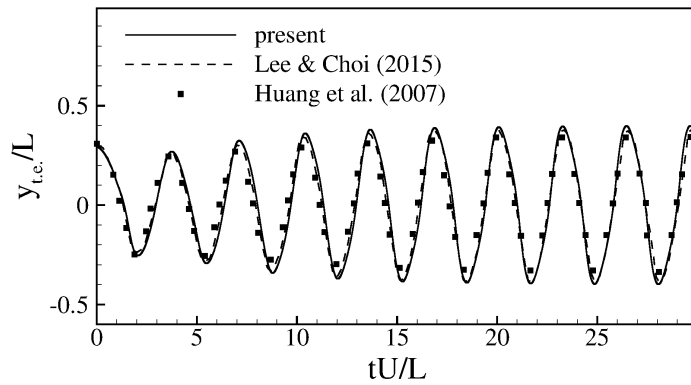


Figure 18: Comparison of trailing-edge transverse location time traces for a flexible filament in a free stream, with $Re = 200$, $\gamma = 150$ and $k_b = 0.15$. Present results (—), Lee and Choi [21] (---), Huang et al. [9] (■).

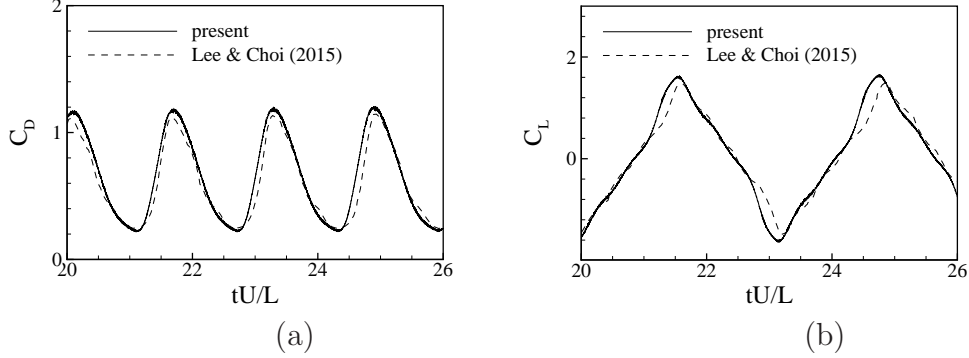


Figure 19: Time histories of the drag (a) and lift (b) coefficients for a flexible filament in a free stream, with $Re = 200$, $\gamma = 150$ and $k_b = 0.15$. Present results (—), Lee and Choi [21] (---).

679 flag is pinned, while the other three edges are free to move. The simula-
680 tion is performed on a nonuniform grid, refined around the flag and in the
681 wake, with $101 \times 228 \times 260$, nodes and a uniform maximum resolution of
682 $\Delta x = \Delta y = \Delta z = 0.02L$ near the flag. The flag is considered inextensi-
683 ble (the elastic constant is taken sufficiently large, $k_e = 2500$), and flexible
684 ($k_b = 0.15$) in order to replicate the test of [9]. The ratio of solid and fluid
685 densities, γ is equal to 100. The Reynolds number, based on L , the inflow
686 velocity, U , and the fluid kinematic viscosity is equal to 200. No gravity is
687 considered ($Fr = 0$). A constant time step is used of $\Delta t = 10^{-3} L/U$. Fig-
688 ure 21 shows the time traces of the middle point transverse location at the
689 trailing edge of the flapping flag (filled circle in figure 20), compared with
690 the numerical results of [20],[21] and [9]. A good agreement is obtained. The
691 peak-to-peak excursion amplitude as well as the Strouhal number, defined
692 as $St = fL/U$, for the middle trailing edge point, are reported in table 2, f
693 being the oscillation frequency. Moreover, the time traces of force coefficients
694 (drag and lift), obtained as $C_F = 2F/\rho_f U^2 L^2$, F being the hydrodynamic
695 force in z (drag) or y (lift) direction, are shown in figure 22, compared with
696 numerical results of [20] and [21]. The agreement is satisfactory. Finally, the
697 instantaneous vortical structures, identified by Q -criterion [56] (iso-surface
698 of $Q = 0.1$) around the flapping flag at $t/T = 2.41$ are reported in figure 23,
699 showing the characteristic jairpin-like structure shed at each flapping [9].

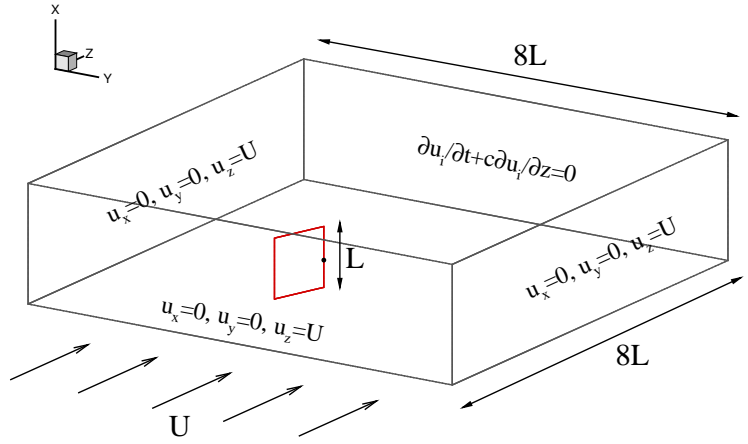


Figure 20: Problem description for the simulation of the flow around a flapping flag in a free stream.

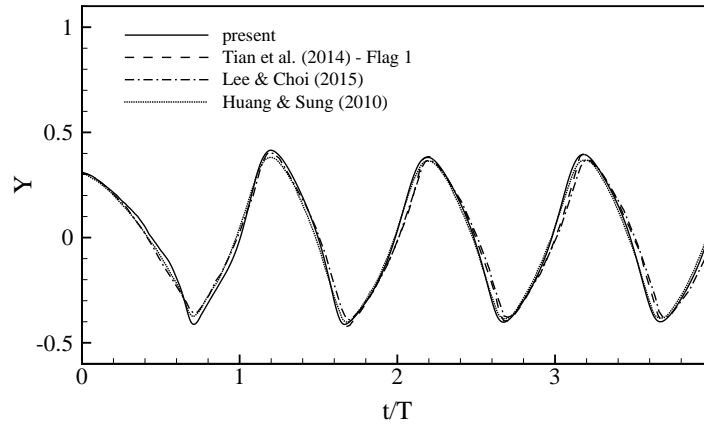


Figure 21: Time traces of the trailing-edge transverse location (middle point) of the flapping flag, for $Re = 200$, $Fr = 0$ and $\gamma = 100$.

	Amplitude A/L	Strouhal number St
present	0.795	0.265
Tian et al. (2014) - Flag 1	0.812	0.263
Lee & Choi (2015)	0.752	0.265
Huang & Sung (2010)	0.780	0.260

Table 2: Flapping flag in uniform flow with $Re = 200$, $Fr = 0$ and $\gamma = 100$. Comparison of peak-to-peak excursion amplitude, A/L , and the Strouhal number, St , for the middle trailing-edge point.

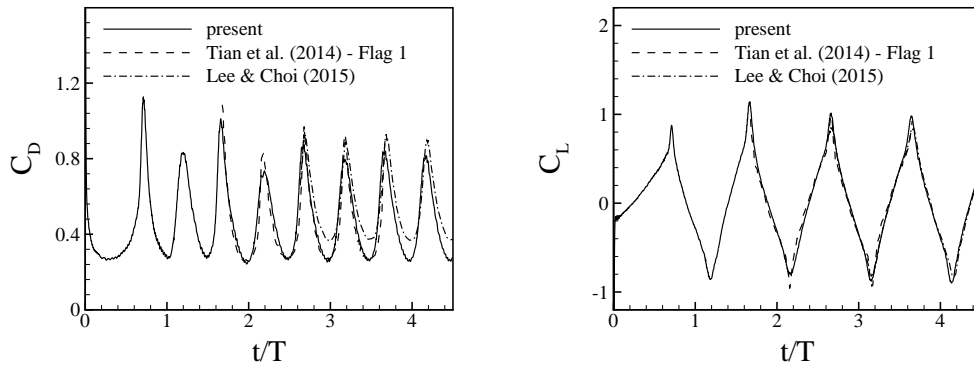


Figure 22: Time traces of the drag and lift coefficients of the flapping flag, for $Re = 200$, $Fr = 0$ and $\gamma = 100$.

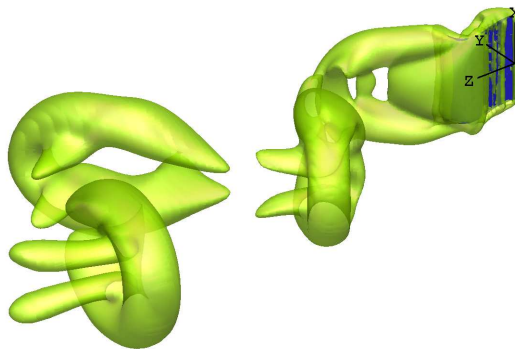


Figure 23: Vortical structures (q-criterion) around the flapping filament at $t/T = 2.41$, for $Re = 200$, $Fr = 0$ and $\gamma = 100$.

700 *3.7. Three-dimensional inverted flag in a free stream*

701 The dynamics of an inverted flag is considered in order to test the sim-
 702 plified structural model in the case of very large deformation and to test the
 703 sensitivity of the model to the bending stiffness parameter. With the aim
 704 of harvesting fluid kinetic energy, flow-induced flapping of an elastic sheet
 705 has recently been proposed. However, an efficient system for energy har-
 706 vesting has to easily become unstable, even at low velocities, and have high
 707 excitation amplitude [57]. The configuration adopted is that of an inverted
 708 filament, with a free leading edge and a clamped trailing edge. Experimental
 709 investigations by [57] on the flapping dynamics of an inverted elastic sheet,
 710 have shown that the sheet response can be largely divided in three modes,
 711 depending on the bending stiffness of the plate. A straight mode is observed
 712 for high bending, with the sheet that remains straight or flutters with very
 713 small amplitudes around the equilibrium position; a periodic flapping from
 714 side to side, with large amplitudes is found for intermediate bending; an-
 715 other quasi-steady behavior is observed for low bending, with the sheet that
 716 bends in one direction and maintains a highly curved shape, fluttering with
 717 small amplitudes around this deflected configuration. The proposed method
 718 is therefore used to capture the different dynamics varying the bending coeffi-
 719 cient of the network-spring model. The schematic of the problem is the same
 720 used in the flapping flag case 20, where a square flag of length L is considered
 721 in a computational domain with size $[-L, L] \times [-4L, 4L] \times [-L, 7L]$ in the
 722 x, y and z directions, respectively, with the center of the leading edge of the
 723 flag positioned at the origin. The initial shape of the flag is a flat plate, with
 724 no inclination with respect to the xz -plane, z being the streamwise direction
 725 and x the vertical one. The trailing-edge of the flag is clamped, while the
 726 other three edges are free to move. No gravity is considered. The simula-
 727 tion is performed on a nonuniform grid, refined around the flag and in the
 728 wake, with $101 \times 228 \times 260$, nodes and a uniform maximum resolution of
 729 $\Delta x = \Delta y = \Delta z = 0.02L$ near the flag. In order to compare the results
 730 with the experiments of [57], two non-dimensional dynamical parameters are
 731 considered, the bending-stiffness, β , and the mass ratio, γ , here defined as:

$$\beta = \frac{B}{\rho_f U^2 L^3} \quad \text{and} \quad \gamma = \frac{\rho_s h}{\rho_f L}, \quad (51)$$

732 where B is the flexural rigidity of the sheet, ρ_f and ρ_s are the fluid and
 733 sheet densities, respectively, U is the undisturbed flow velocity and h is the

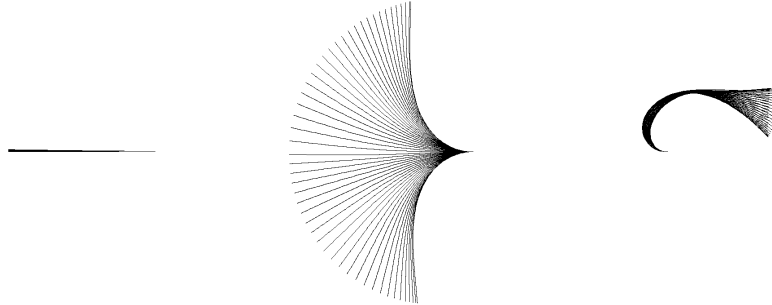


Figure 24: Inverted flexible filament in a free stream at $Re = 200$, $\gamma = 1$. From left to right, the bending rigidity decreases, showing a *straight mode* (left), a *flapping mode* (middle) and a *deflected mode* (right). No gravity is considered.

734 sheet thickness. The flag is considered inextensible (the elastic constant is
 735 taken sufficiently large, $k_e = 5000$), while the bending constant is calculated
 736 by equation ??, assuming different values to replicate the abovementioned
 737 three different behaviors. The Reynolds number, based on L , the inflow
 738 velocity, U , and the fluid kinematic viscosity, ν is considered equal to 200
 739 (lower than that in the experiments of [57]). A constant time step is used of
 740 $\Delta t = 10^{-3} L/U$.

741 Figure 24 reports the superimposed filament positions in time, showing
 742 straight, flapping and deflected modes, respectively, as the bending rigidity
 743 of the model is reduced. Additionally, the free leading edge vertical position
 744 in time is shown in figure 25, with a clear periodic behavior for the flapping
 745 mode and a more complex reduced fluttering with a non clear periodicity for
 746 the deflected mode and (with smaller amplitude) straight mode. Finally, the
 747 free leading edge vertical position in time for the case with $Re = 250$, $\gamma = 2$,
 748 $k_b = 20$, is compared with the corresponding experimental results of [57]
 749 with a bending stiffness parameter β equal to 0.1. A very good agreement is
 750 obtained also in this test.

751 3.8. Three-dimensional flow through a bio-prosthetic aortic valve

752 Finally, a three-dimensional test case is presented in order to test the
 753 thin-structure dynamics under high pressure gradients. The case considered
 754 is that of a bioprosthesis aortic valve, with three deformable cusps that open
 755 and close under a pulsatile flowrate. The flow domain considered reproduces
 756 the initial tract of the ascending aorta, with a geometry similar to that used

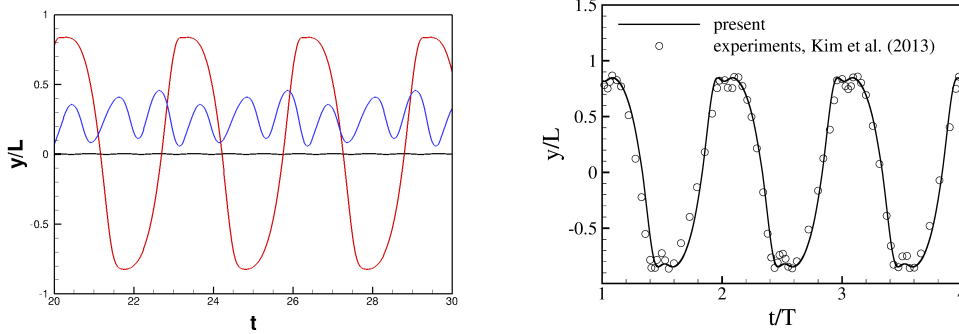


Figure 25: Left: inverted flexible filament in a free stream at $Re = 200$, $\gamma = 1$. Time history of the y -coordinate of the tip. Right: comparison of the y -coordinate of the filament tip for the case with $Re = 250$, $\gamma = 2$, $k_b = 20$; symbols indicate experimental results of [57] with $\beta = 0.1$.

757 in [58]. It is considered rigid and composed of i) an inflow circular tube
758 upstream of the valve, with the same diameter of the valve and length h_1 ; ii)
759 a tract with three sinuses of Valsalva reproducing the physiological case, with
760 length h_s ; iii) a larger tube after the sinuses, with larger diameter, D , and
761 length h_3 . All the geometrical parameters are given in figure 26a, along with
762 a schematic of the problem. The valve considered wants to mimic the Trifecta
763 valve model (St Jude Medical Inc., Minneapolis), which is a trileaflet tissue
764 valve constructed using a polyester and tissue-covered titanium stent. The
765 leaflets are made of pericardial tissue and are attached to the exterior of the
766 stent in order to mimic the hemodynamics performance of a healthy aortic
767 heart valve. The valve has a diameter $d_0 = 23mm$, and height h_l , as shown in
768 figure 26a. The leaflet geometry is obtained reproducing the real valve stress-
769 free geometry, as reported in figure 26b. The leaflets nodes corresponding to
770 the stent position (thick black lines in figure 26b) are constrained to be fixed
771 in time. Moreover, a geometrical constraint is adopted considering three
772 vertical planes at 120° and passing through the center of the orifice, allowing
773 only sliding of the structural nodes on the planes and preventing the leaflets
774 from passing through each other. It is worth noting that contact between two
775 nodes of different structures could be easily modeled using properly defined
776 interaction potentials and adding a repulsion force to the total forces acting
777 on a single node, but here a geometrical approach has been adopted for
778 simplicity. The elastic behavior of the pericardial tissue is modeled with
779 the simplified, nonlinear anisotropic model described in section 2.4. Bending

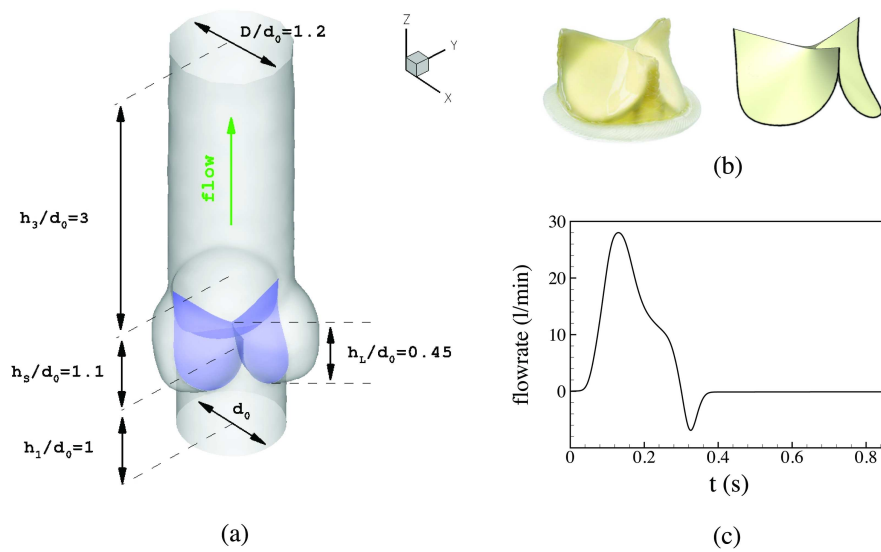


Figure 26: (a) Scheme of the configuration for the three-dimensional flow through a bio-prosthetic aortic valve. The main geometrical parameters are shown, related to the valve diameter, $d_0 = 23 \text{ mm}$. (b) Trifecta aortic valve real model (St Jude Medical Inc., Minneapolis) and stress-free computational model (on the left) of the three leaflets. Thick black lines indicate the constrained edges. (c) Pulsatile flowrate adopted in the simulations.

780 stiffness is also added to the model, using a bending constant $k_b = 0.01$. The
 781 material density is set equal to that of the fluid and a constant thickness of
 782 0.5 mm is considered. A nonuniform grid with $257 \times 257 \times 372$ nodes is used
 783 in x, y and z directions, respectively, z being the streamwise direction, with
 784 an Eulerian grid spacing near the valve $0.01d_0$, and an averaged Lagrangian
 785 marker spacing of $0.007d_0$ on the leaflets. A constant CFL value of 0.25 is
 786 adopted, leading to a variable temporal resolution ranging from 200 to $2\mu\text{s}$
 787 during the simulation. A pulsatile flowrate is imposed in the inlet section
 788 of the domain, with a cardiac output of approximately 5 l/min , at a fixed
 789 beat rate of 70 beats/min (see figure 26c), while standard convective outflow
 790 conditions are imposed at the outlet section. The blood density is set to
 791 1060 kg/m^3 . The peak Reynolds number is about 6700, based on the inlet
 792 velocity, the inflow tube diameter and the blood kinematic viscosity.

793 Figure 27 shows a comparison between the real valve in in-vitro exper-
 794 iments (St. Jude Medical Inc., www.sjm.com) and the present numerical
 795 results, at two different time instants during the opening phase, indicated
 796 with open circles in figure 28a. Moreover, the comparison of numerical and
 797 experimental projected valve area (PVA) seen from the top of the domain
 798 in the xy plane, divided by its maximum value assumed during the cardiac
 799 cycle, PVA_{max} , is shown in figure 28a. The agreement with experiments of
 800 the valve leaflets dynamics and projected area is very good, considering the
 801 complexity of the model and the uncertainty in the material properties. Fur-
 802 thermore, it is important to stress that experimental data are obtained by
 803 valve visualization from the valve manufacturer website, with no information
 804 about the exact flowrate waveform. Figure 28b reports one leaflet config-
 805 uration at some instants during the cycle indicated by symbols in figure
 806 28a. Finally, the valve configuration and the streamwise velocity contours,
 807 along with the instantaneous vortical structures, identified by Q -criterion [56]
 808 (iso-surface of $Q = 0.1$), at three different instants of the cardiac cycle are re-
 809 ported in figures 29-31. The jet-like flow that emerges from the central orifice
 810 of the valve is clearly shown, with high shear stresses occurring at the edge of
 811 the jet during the deceleration phase. Large-scale vortical structures form,
 812 starting from the leaflet commissures and in the three sinuses of Valsalva
 813 during the acceleration phase. After peak systole, instabilities occur at the
 814 edge of the jet and smaller scale structures are developed, still maintaining
 815 a clear central jet, as shown in figure 30. The flow appears more disordered
 816 during the deceleration phase at late systole, with decreasing flowrate and
 817 small scale vortical structures that fill completely the domain. It is impor-

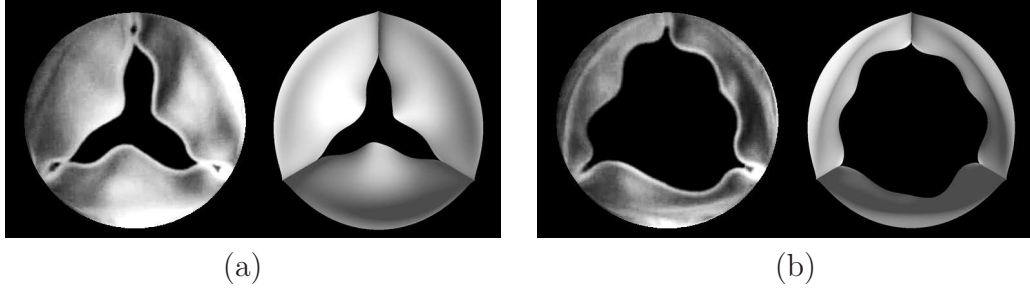


Figure 27: Instantaneous snapshots of the valve leaflets dynamics from an experimental visualization (on the left of each figure) and numerical results (on the right of each figure), at two instants during the opening phase, indicated with open circles in figure 28a.

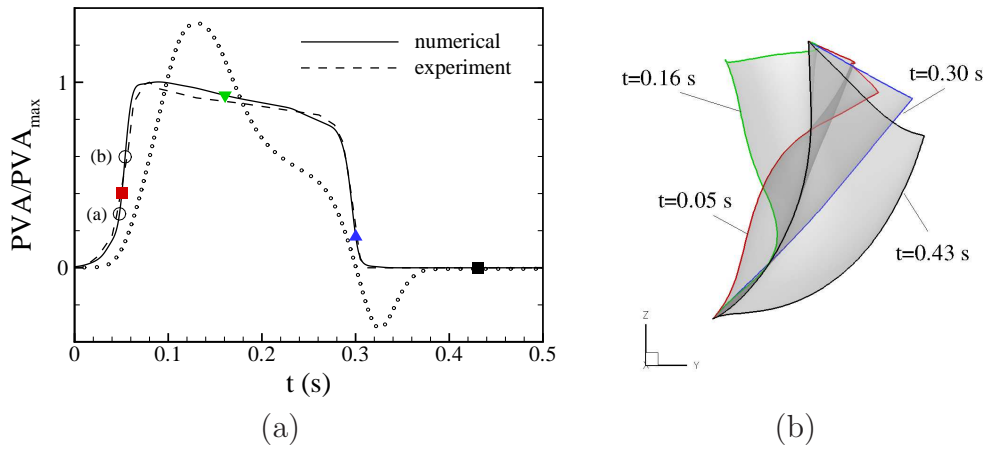


Figure 28: (a) Projected valve area PVA divided by its maximum value assumed on the cycle, PVA_{max} for a cardiac cycle for numerical simulations (continuous line) and experiments (dashed lines). (b) Leaflet configuration at some instants during the cycle indicated by symbols in figure 28a.

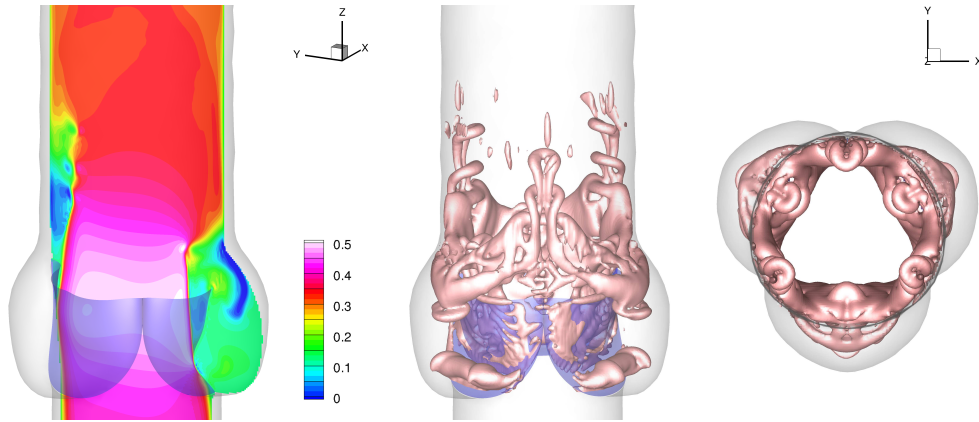


Figure 29: Peak of flowrate ($t = 0.13$ s). Left: streamwise velocity contours (in m/s) in the yz plane. Right: instantaneous vortical structures identified by Q-criterion (isosurfaces of $Q = 0.1$).

818 tant to note that the structural model performance are promising and the
 819 valve dynamics is reasonably accurate, with a very reduced computational
 820 cost (about 1%) with respect to the fluid solver one.

821 4. Conclusions

822 A versatile numerical method for the fluid-structure-interaction of bod-
 823 dies of arbitrary thickness, immersed in an incompressible fluid, is presented,
 824 with the aim of simulating different biological engineering applications. A
 825 partitioned, discrete-forcing immersed boundary method is adopted, based
 826 on a moving least squares method to reconstruct the solution in the vicini-
 827 ty of the immersed surface and to convert the Lagrangian forcing back to
 828 the Eulerian grid. A simple spring-network model is considered for describ-
 829 ing the dynamics of non-rigid bodies and structures, in order to have the
 830 freedom of easily model and simulate different biological systems that can
 831 not always be described by simple continuum models, without affecting the
 832 computational time and simplicity of the overall method. The surfaces can
 833 be rigid or deformable, and can be either closed, in order to describe solid
 834 bodies or capsules and biological cells, or open, describing slender bodies,
 835 such as filaments or organ tissues. Fluid and structures are coupled in a
 836 strong way, in order to avoid instabilities related to large accelerations due
 837 to the deformations of the surfaces. The evaluation of the hydrodynamic

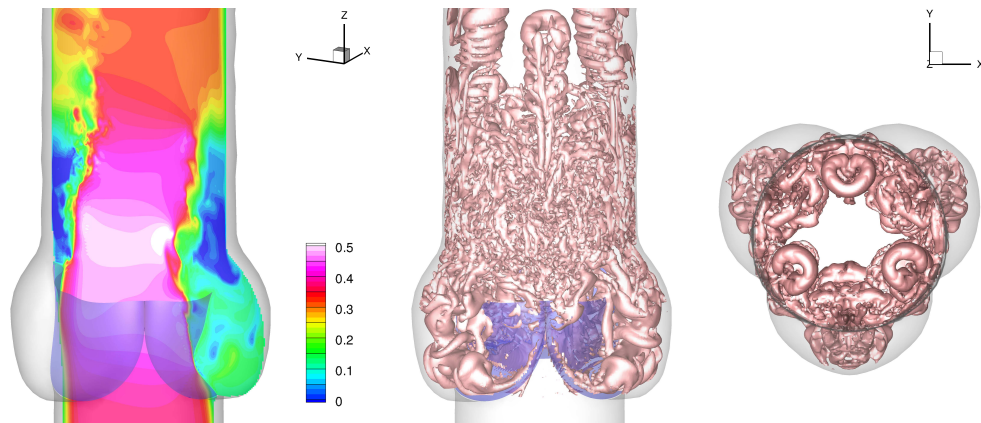


Figure 30: Early systole ($t = 0.16 s$). Left: streamwise velocity contours (in m/s) in the yz plane. Right: instantaneous vortical structures identified by Q-criterion (isosurfaces of $Q = 0.1$).

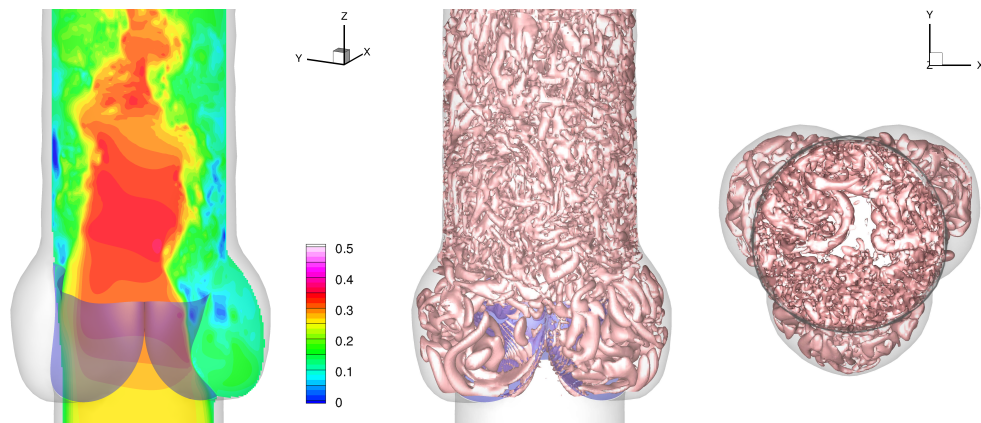


Figure 31: Late systole ($t = 0.23 s$). Left: streamwise velocity contours (in m/s) in the yz plane. Right: instantaneous vortical structures identified by Q-criterion (isosurfaces of $Q = 0.1$).

838 loadings on the structure requires particular attention, in particular of the
839 case of structures of zero-thickness. In this case, two probes are sent from
840 each location at which the forces need to be calculated, along both sides
841 of the normal-to-surface direction, evaluating the pressure and velocity gra-
842 dient near the body. The method gives accurate results comparable with
843 that of sharp direct-forcing approach, and can manage pressure differences
844 across the surface in one grid cell, still obtaining very smooth forces. The
845 immersed boundary technique as well as the structural solver do not im-
846 pose any restriction to the computational time step, which is determined
847 based on stability conditions of the flow solver. The accuracy of the method
848 has been validated by means of several test cases of increasing complexity.
849 Several testcases with rigid bodies falling in a quiescent fluid, fluttering or
850 tumbling, or transported by a shear flow are presented, showing a very good
851 agreement with available experimental data and numerical results obtained
852 by different approaches. In the abovementioned cases, the surface is closed
853 and undeformable, enclosing a volume and thus representing a rigid particle.
854 Then, open surfaces representing infinitely thin elastic structures with mass
855 are considered: a two-dimensional flexible filament and an inverted flexible
856 filament in a free stream. A very good agreement has been obtained in all
857 the cases, as shown by comparison with numerical and experimental results
858 available in the literature. Therefore, in all the test considered, the method
859 proves to be accurate and efficient in handling both rigid and deformable
860 bodies, even using a simplified description of the mechanical properties of
861 the structure. Finally, a three-dimensional model of a bio-prosthetic aortic
862 valve is considered, with nonlinear and anisotropic mechanical properties,
863 opening and closing during a pulsatile cardiac cycle, showing a good quali-
864 tative agreement with respect to in-vitro data, considering the complexity of
865 both the geometry and the material properties of the biological tissue.

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