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

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### 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

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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 1. Introduction

Fluid-structure interaction (FSI) problems are found in many engineering 2 areas. The three-dimensional computational modeling is particularly chal-3 lenging and has recently encountered the interest of several research groups. 4 Among different FSI problems, biological applications are becoming of ever 5 increasing interest in the scientific community and their accurate and efficient 6 numerical simulation provides an essential means in understanding the fundamental physics and reducing the time needed for experiments. The accurate 8 description of FSI can not ignore the fact that moving and/or deforming 9 bodies act on the surrounding fluid that is forced to move accordingly (no-10 slip condition), and reacts with pressure and velocity gradients distribution 11 that, in turn, produces the surface forces that cause the motion of the body. 12 This poses several challenges for the numerical approaches adopted. With 13 no intent of being exhaustive, one can mention: rigid particle of arbitrarily 14 shape transported by the fluid; deformable particles in shear flows (capsules, 15 vesicles, cells), constituted by a liquid droplet enclosed by a structure with 16 thickness much smaller than the particle size; elastic slender bodies immersed 17 in a fluid, such as flags, insect wings, jellyfishes, bioprosthetic heart valves, 18 where a thin surface is significantly deformed by the fluid. In the mentioned 19 cases, describing the dynamics of the interaction between the body and the 20 fluid is not a trivial task, since the numerical method needs to be able to han-21 dle in an efficient way complex and very thin geometries undergoing large 22 deformations, without loosing accuracy. 23

Given the large displacements/deformations of the bodies, body-fitted 24 approaches [1, 2], both structured and unstructured, are not the optimal 25 choice. They need the time-consuming regeneration or deformation of the 26 mesh and the successive projection of the flow field solution from previous 27 mesh to new one, which can lead to a decrease of accuracy. Immersed Bound-28 ary (IB) methods [3, 4] are more suitable, since the governing equations are 29 solved on a fixed grid, covering the whole domain, thus including points that 30 rely inside the closed boundaries (if any). Continuous forcing IB methods de-31

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

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

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

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

<sup>108</sup> points in the support domain, needed by the MLS procedure is provided.

## 109 2. Numerical method

#### 110 2.1. Flow solver

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

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

113

$$\boldsymbol{\nabla} \cdot \boldsymbol{u} = 0 \tag{2}$$

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

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

where  $\boldsymbol{u}^n$  denotes the velocity at the time level n,  $\hat{\boldsymbol{u}}$  is the intermediate solution,  $\Delta t$  is the time step, H contains the non-linear terms,  $\alpha$ ,  $\gamma$  and  $\rho$ are the constants of the Adam–Bashforth/Crank–Nicolson scheme [28, 29]. Equation (3) can be written in delta-form as:

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

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

$$\boldsymbol{u}^{n+1} = \hat{\boldsymbol{u}} - \alpha \,\Delta t \,\boldsymbol{\nabla}\varphi \,. \tag{5}$$



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

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

$$\nabla^2 \varphi = \frac{\boldsymbol{\nabla} \cdot \hat{\boldsymbol{u}}}{\alpha \,\Delta t} \,. \tag{6}$$

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

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

#### 140 2.2. Immersed boundary treatment

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



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.

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

1. Compute the intermediate velocity  $\hat{u}$  from equation (3) in all the Eulerian grid points; this involves also the  $N_e$  points of the support domain surrounding a Lagrangian point.

163 164

165

2. Compute the velocity component,  $\hat{U}_i$ , at each Lagrangian grid point, l, corresponding to the non-solenoidal velocity field. Using the MLS approach, it can be approximated in the support domain as:

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

where  $p^{T}(x) = [1, x, y, z]$  is the linear basis function vector (a costefficient choice able to represent the field variation of the variable up to the accuracy of the adopted spatial discretization scheme [15]), a(x)is a vector of coefficients and x is the Lagrangian point position. The coefficient vector a(x) is obtained minimizing, with respect to a(x), the weighted L2-norm defined as:

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

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

3.7

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

175 with

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

176

$$\boldsymbol{B}(\boldsymbol{x}) = \left[ W(\boldsymbol{x} - \boldsymbol{x}^{1}) \boldsymbol{p}^{T}(\boldsymbol{x}^{1}) \dots W(\boldsymbol{x} - \boldsymbol{x}^{N_{e}}) \boldsymbol{p}^{T}(\boldsymbol{x}^{N_{e}}) \right]$$
(12)

177 and

$$\boldsymbol{B} = \begin{bmatrix} \hat{u}_i^1 \dots \hat{u}_i^{N_e} \end{bmatrix}^T .$$
(13)

Combining the equations,  $\hat{U}_i$  cab be rewritten as:

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

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

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

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

$$r_k = \frac{|\boldsymbol{x} - \boldsymbol{x}^k|}{r_w} \tag{16}$$

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

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

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

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

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

$$f_i^k = \sum_{l=1}^{N_t} c_l \, \phi_k^l F_i^l \,; \tag{18}$$

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

$$\sum_{k=1}^{N_e,tot} f_i^k \Delta V^k = \sum_{l=1}^{N_t} F_i^l \Delta V^l \,. \tag{19}$$

Rearranging the terms, one has:

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

<sup>206</sup> 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].

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

$$\boldsymbol{u}^* = \hat{\boldsymbol{u}} + \Delta t \, \boldsymbol{f} \,, \tag{21}$$

where f is the volume force at Eulerian cells, obtaining a velocity field that is not divergence-free and that will be projected into a divergencefree space by applying the pressure correction which satisfies the Poisson equation (6).

# 216 2.3. Rigid body equations

The motion of the rigid body immersed in the fluid is governed by the Newton-Euler equations imposing the equilibrium of translation and rotation:

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

220

$$[I] \frac{d\Omega}{dt} = T_{tot}, \qquad \Omega = \frac{d\Theta}{dt}.$$
(23)

In the equations above, M and [I] are the mass and inertia tensor of the 221 body, V and X its baricentre's velocity and position,  $\Omega$  and  $\Theta$  its angu-222 lar velocity and position, respectively, and  $F_{tot}$  and  $T_{tot}$  are the total force 223 and moment acting on the body. The total force and moment include the 224 hydrodynamics contributions, the gravity forces, if present, and any other 225 additional force depending on the problem. Concerning the hydrodynam-226 ics loadings, the overall contribution is obtained integrating over the body's 227 surface the pressure and viscous stresses as explained in section 2.5. 228

### 229 2.4. Spring network model for deformable bodies

A simple spring network model is adopted for describing the dynamics of deformable bodies, based on the minimum energy concept [25]. The structural model is built considering the triangulated network of  $N_s$  springs (edges), forming  $N_t$  triangles. The mass of the structure is concentrated on the  $N_v$  vertices of the triangles, uniformly distributed on the surface. The potential energy of the system includes in-plane elastic terms, combined with <sup>236</sup> bending energy and additional constraints for surface area and volume con-<sup>237</sup> servations.

<sup>238</sup> The simplest elastic energy model is described by:

$$W^e = \frac{1}{2}k_e x^2 \tag{24}$$

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

$$k_e = \frac{Eh\sum_i A_i}{l^2},\tag{25}$$

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

$$\mathbf{F}_{1}^{e} = -k_{e}(l-l_{0})\frac{\mathbf{r}_{12}}{l}$$
(26)

249

$$\mathbf{F}_{2}^{e} = -k_{e}(l-l_{0})\frac{\mathbf{r}_{21}}{l}$$
(27)

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 actual edge length.

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

$$W^{b} = k_{b}(1 - \mathbf{n}_{1} \cdot \mathbf{n}_{2}) = k_{b}[1 - \cos(\theta)]$$
(28)

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

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



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.

where  $\theta_0$  is the value of  $\theta$  in the stress-free configuration. The bending constant  $k_b$  is related to the equivalent averaged bending modulus of the structure, B, as [34]:

$$k_b = B \frac{2}{\sqrt{3}} \,. \tag{30}$$

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

$$\mathbf{F}_{1}^{E} = \beta_{b} \left[ b_{11} \left( \mathbf{n}_{1} \times \mathbf{r}_{32} \right) + b_{12} \left( \mathbf{n}_{2} \times \mathbf{r}_{32} \right) \right]$$
(31)

267

$$\mathbf{F}_{2}^{E} = \beta_{b} \left[ b_{11} \left( \mathbf{n}_{1} \times \mathbf{r}_{13} \right) + b_{12} \left( \mathbf{n}_{1} \times \mathbf{r}_{34} + \mathbf{n}_{2} \times \mathbf{r}_{13} \right) + b_{22} \left( \mathbf{n}_{2} \times \mathbf{r}_{34} \right) \right]$$
(32)

$$\mathbf{F}_{3}^{E} = \beta_{b} \left[ b_{11} \left( \mathbf{n}_{1} \times \mathbf{r}_{21} \right) + b_{12} \left( \mathbf{n}_{1} \times \mathbf{r}_{42} + \mathbf{n}_{2} \times \mathbf{r}_{21} \right) + b_{22} \left( \mathbf{n}_{2} \times \mathbf{r}_{42} \right) \right]$$
(33)

$$\mathbf{F}_{4}^{E} = \beta_{b} \left[ b_{11} \left( \mathbf{n}_{1} \times \mathbf{r}_{23} \right) + b_{22} \left( \mathbf{n}_{2} \times \mathbf{r}_{23} \right) \right]$$
(34)

268 with

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

269 and

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

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

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

$$m_p \ddot{\mathbf{x}} = \mathbf{F}^{\mathbf{ext}} + \mathbf{F}^{\mathbf{int}} = \mathbf{F} \tag{37}$$

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

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

 $_{313}$  finite element membrane solver [27].

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

$$S_{ij} = \frac{\partial W}{\partial E_{ij}} \tag{38}$$

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

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

334 with

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

The values of the constants are obtained by fitting previously published biaxial esperiments on normal aortic valve tissue [43], and are here reported for reference, c = 9.7 Pa,  $A_1 = 49.558$ ,  $A_2 = 5.2871$ ,  $A_3 = -3.124$ ,  $A_4 = 16.031$ ,  $A_5 = -0.004$  and  $A_6 = -0.02$ . With the aim of using a network spring model instead of a continuum one, as done in [43] (where the only structural solver is considered), the anisotropic behavior is simplified considering only 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].

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

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

where  $m_{1f}$  and  $m_{1c}$  are the initial slopes in the fiber and cross-fiber direc-353 tions, respectively. The same formulation is adopted to evaluate the other 354 parameters,  $m_2$  and  $\lambda^*$ , based on the angle  $\theta$  in the stress-free configuration 355 of the mesh. In such a way, the line slopes as well as the stretch ratio is 356 stored for each spring. The Van Gelder [32] approach is employed for calcu-357 lating elastic constant,  $k_e$ , where in place of Young's modulus, the evaluated 358 slopes of the bilinear model, m1 or m2 are used, depending on whether the 359 actual deformation of the spring corresponds to a value of stretch less than 360

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

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

for springs with stretch magnitude less than  $\lambda^*$ , or

$$\mathbf{F}_{1}^{E} = -\left[k_{e1}l_{0}(\lambda^{*}-1) + k_{e2}(l-\lambda^{*}l_{0})\right]\frac{\mathbf{r}_{12}}{l}$$
(43)

for springs with stretch magnitude freater than  $\lambda^*$ .

## 366 2.5. Force and moment evaluation

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

For the case of a closed surface, representing a rigid or deformable solid, the single contributions to the force and moment are evaluated for each triangular element, l:

$$\boldsymbol{F}_{l}(t) = \left(\boldsymbol{\tau}_{l} \cdot \boldsymbol{n}_{l} - p_{l}\boldsymbol{n}_{l}\right) S_{l}, \qquad (44)$$

374

$$\boldsymbol{M}_{l}(t) = \left[ \left( \boldsymbol{\tau}_{l} \cdot \boldsymbol{n}_{l} - p_{l} \boldsymbol{n}_{l} \right) \times \boldsymbol{r}_{l} \right] S_{l} \,, \tag{45}$$

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

$$p_l = p_l^* + \frac{D\boldsymbol{u}_l}{Dt} \cdot \boldsymbol{n}_l \tag{46}$$

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



Figure 5: Scheme for IB forces evaluation.

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

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

$$\boldsymbol{F}_{l}(t) = S_{l} \left[ \left( \boldsymbol{\tau}_{l}^{+} - \boldsymbol{\tau}_{l}^{-} \right) \cdot \boldsymbol{n}_{l} - (p_{l}^{+} - p_{l}^{-}) \boldsymbol{n}_{l} \right] , \qquad (47)$$

$$\boldsymbol{M}_{l}(t) = S_{l} \left[ \left( \boldsymbol{\tau}_{l}^{+} - \boldsymbol{\tau}_{l}^{-} \right) \cdot \boldsymbol{n}_{l} - (p_{l}^{+} - p_{l}^{-}) \boldsymbol{n}_{l} \right] \times \boldsymbol{r}_{l} , \qquad (48)$$

where  $^+$  and  $^-$  quantities are evaluated on the probes along the positive and negative  $n_l$  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.

As an example, the results for the flow past a fixed, *zero-thickness* vertical 409 plate is shown in figure 6. The flow comes from left to right with velocity U410 and impacts on a plate of height L, with  $Re = \rho_f UL/\mu = 200$ . The compu-411 tational domain is  $[-2L, 6L] \times [-4L, 4L]$ . The center of the plate is placed at 412 [0.5L, 0]. Inlet and outlet boundary conditions are imposed on the vertical 413 boundaries, while free-shear wall conditions are imposed for the horizontal 414 boundaries. A non uniform grid of  $671 \times 747$  nodes is used with a uniform 415 grid spacing of 0.01L in the vicinity of the plate. The Lagrangian markers 416 are distributed uniformly onto the plate surface, with a spacing of about 0.7417 the local Eulerian grid size in that area. Figure 6 shows the pressure and 418

streamwise velocity distributions on the centerline of the computational domain. The pressure difference across the plate is shown, captured in one grid cell along the streamwise direction (figure 6, left). Figure 6 shows an instantaneous field of the pressure contours and the pressure distribution along the plate considering the upstream and downstream normal probe directions.

#### 424 2.6. Fluid-structure-interaction strategy

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

440 For each time step,

## 441 1. Predictor:

442 443

444 445

446

447

448

450

451

•  $\ddot{\mathbf{x}}_n = \mathbf{F}_n/m$ 

• 
$$\dot{\mathbf{x}}_{n+1}^p = \dot{\mathbf{x}}_{n-3} + \frac{4}{3}\Delta t \left( 2 \ddot{\mathbf{x}}_n - \ddot{\mathbf{x}}_{n-1} + 2 \ddot{\mathbf{x}}_{n-2} \right)$$

• 
$$\dot{\mathbf{x}}_{n+1}^m = \dot{\mathbf{x}}_{n+1}^p - \frac{112}{121} (\dot{\mathbf{x}}_n^p - \dot{\mathbf{x}}_n^c)$$

• 
$$\mathbf{x}_{n+1}^p = \mathbf{x}_{n-3} + \frac{4}{3}\Delta t \left( 2\dot{\mathbf{x}}_n - \dot{\mathbf{x}}_{n-1} + 2\dot{\mathbf{x}}_{n-2} \right)$$

• 
$$\mathbf{x}_{n+1}^m = \mathbf{x}_{n+1}^p - \frac{112}{121} (\mathbf{x}_n^p - \mathbf{x}_n^c)$$

• Solve flow and structure (if deformable body) equations, using the predicted structural node position and velocity and evaluate  $\mathbf{F}_{n+1}^1$ 

)

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

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

452	• $\mathbf{x}_{n+1}^c = \frac{1}{8} \left( 9\mathbf{x}_n - \mathbf{x}_{n-2} \right) + \frac{3}{8} \Delta t \left( 2\dot{\mathbf{x}}_{n+1}^k + 2\dot{\mathbf{x}}_n - \dot{\mathbf{x}}_{n-1} \right)$
453	• Check for converge of the structure equations: $ \mathbf{x}_{n+1}^{k+1} - \mathbf{x}_{n+1}^{k}  < \epsilon$
454	• If converged,
455	$- \; \dot{\mathbf{x}}_{n+1} = \dot{\mathbf{x}}_{n+1}^c + rac{9}{121} \left( \dot{\mathbf{x}}_{n+1}^p - \dot{\mathbf{x}}_{n+1}^c  ight)$
456	$-  \mathbf{x}_{n+1} = \mathbf{x}_{n+1}^c + rac{9}{121} \left( \mathbf{x}_{n+1}^p - \mathbf{x}_{n+1}^c  ight)$
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

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

## 471 **3. Results**

## 472 3.1. Sedimentation of an elliptic particle

The dynamics of a single two-dimensional elliptic particle sedimenting 473 in a confined channel is considered here to validate the FSI procedure. A 474 systematic verification study is also performed to check the order of accuracy 475 of the algorithm. The problem is configured as an elliptic particle with 476 aspect ratio  $\alpha = a/b = 2$ , where a and b are the major and minor axes, 477 respectively, as shown in Figure 7. The confined channel has width L, with 478 a blockage ratio  $\beta = L/a = 4$ . The density ratio,  $\gamma = \rho_s/\rho_f$  is set equal to 470 1.1, where  $\rho_s$  and  $\rho_f$  are the particle and fluid densities, respectively. The 480 computational domain is  $[0, L] \times [0, 7L]$  in X and Y directions, respectively, 481 with the gravity q pointing in the negative Y direction. The particle starts 482 falling with the centroid in (0.5L, 6L), with an initial angle of  $\theta_0 = 45^\circ$ , 483 to break the symmetry. Considering the terminal settling velocity of the 484

particle,  $V_T$ , the major axis of the ellipse and the fluid kinematic viscosity, 485  $\nu$ , the Reynolds number is  $Re_T = V_T a/\nu = 12.5$ , while the Froude number 486 is  $Fr_T = V_T / \sqrt{ga} = 0.126$ . In physical units, the major axis of the ellipse is 487  $0.1 \, cm$  and the kinematic viscosity of the fluid is  $0.01 \, cm^2/s$  [46]. A slip wall 488 boundary condition is applied at the top boundary and all other boundaries 489 are treated as no-slip wall boundaries. Eight uniform Cartesian grids are 490 used with nodes:  $81 \times 561$ ,  $101 \times 701$ ,  $134 \times 934$ ,  $161 \times 1121$ ,  $201 \times 1401$ , 491  $267 \times 1867, 401 \times 2801, 801 \times 5601$ , corresponding to an Eulerian grid spacing, 492  $\Delta h/a$ , of 0.05, 0.04, 0.03, 0.025, 0.02, 0.015, 0.01, 0.005, respectively. A 493 uniform Lagrangian marker spacing is adopted for all the cases, equal to 0.77494 the Eulerian grid size. With the aim of investigating the overall numerical 495 accuracy in both space and time, the time steps for each grid is chosen 496 in order to mantain a constant ratio between the grid spacing and time 497 step,  $\Delta h/\Delta t = 5U_t$ . In Figure 7 the present results in terms of particle 498 settling velocity, trajectory (location of center of mass) and orientation for 499 the grids with  $\Delta h/a$  equal to 0.04, 0.02 and 0.01 are shown, compared with 500 the numerical results obtained by [46] by means of a finite-element method. 501 The particle settles into the center of the channel (x/L = 0.5) with a constant 502 velocity, and sediments in a horizontal configuration ( $\theta = 0$ ). The agreement 503 of the results is very good for the three grids considered. For the accuracy 504 study, the solution from the finest grid,  $801 \times 5601$ , is used as reference. Three 505 relative errors are defined, for the terminal position and velocity at time t =506 0.8 s, namely  $\epsilon_P = [(Y - Y^{ref})/Y^{ref}]_{t=0.8s}$  and  $\epsilon_V = [(V_Y - V_Y^{ref})/V_Y^{ref}]_{t=0.8s}$ , 507 respectively, and for the time averaged value of the terminal velocity in the 508 interval t = [0.8, 1.6] s, namely  $\epsilon_{\langle V \rangle} = (\langle V_Y \rangle - \langle V_Y^{ref} \rangle) / \langle V_Y^{ref} \rangle$ . 509 The relative errors are reported versus grid spacing in Figure 8, showing 510 a first-order convergence rate for the coarser grids and an evident overall 511 second-order accuracy on finer grids. 512

### <sup>513</sup> 3.2. Fluttering and tumbling of a plate

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



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  $Re_T = 12.5$ ,  $Fr_T = 0.126$ ,  $\alpha = 2$ ,  $\beta = 4$ ,  $\gamma = 1.1$ .

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



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).

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

#### 547 3.3. Particle migration in a planar Couette flow

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



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  $Re_b = 40$ .

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

## <sup>587</sup> 3.4. Single sphere settling under gravity

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



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].

drag coefficient of Abraham [55] is used:

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

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

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

Four different conditions are considered, with different density ratios,  $\gamma =$ 602  $\rho_s/\rho_f$ , and parameters, as reported in Table 1. The computational domain 603 considered is  $[0, 6.67d] \times [0, 6.67d] \times [0, 10.67d]$ , where the last is the grav-604 ity acceleration direction. The particle starts falling with the centroid in 605 (3.33d, 3.33d, 8d). No-slip wall conditions are imposed at all the boundary 606 surfaces of the domain. A uniform grid of  $241 \times 241 \times 385$  nodes is used with 607 a grid spacing of about 0.028d. The Lagrangian markers are distributed uni-608 formly onto the sphere surface, with a spacing of 0.02d, that is equal to 0.71609 the Eulerian grid size. The constant time step used depends on the case con-610 sidered and is reported in Table 1. The sphere sedimentation velocity and 611 trajectory are reported in Figure 13, where the present results are compared 612

$Re_{\infty}$	$\gamma$	$u_{\infty} (\mathrm{m/s})$	$Fr_{\infty}$	$\Delta t  u_{\infty}/d$
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.

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

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

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



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  $k_b = 0.15$ .

Cartesian grids are used, refined in the vicinity of the filament, with nodes: 638  $81 \times 561, 101 \times 701, 134 \times 934, 161 \times 1121, 201 \times 1401, 267 \times 1867, 401 \times 2801, 201 \times 1401, 201 \times 1807, 401 \times 2801, 401 \times 1807, 40$ 639 The grid spacing is maintained uniform in a box containing the filament of 640  $[-1.2L, 1.2L] \times [-1L, 4L]$  in the x and y directions respectively, correspond-641 ing to an Eulerian grid spacing,  $\Delta h/L$ , of 0.05, 0.04, 0.03, 0.025, 0.02, 0.015, 642 0.01, respectively. A uniform Lagrangian marker spacing is adopted for all 643 the cases, equal to 0.7 the Eulerian grid size. With the aim of investigating 644 the overall numerical accuracy in both space and time, the time steps for 645 each grid is chosen in order to mantain a constant ratio between the grid 646 spacing and time step,  $\Delta h/\Delta t = 10U_t$ . The filament shows a periodic flap-647 ping state after few cycles. The filament configuration during the periodic 648 flapping is reported in figure 14b for the finest case, showing the symmetric 649 behavior of the structure deformation. In Figure 15 the present results in 650 terms of time traces of the trailing edge transverse location of the flexible 651 filament for the grids with local  $\Delta h/L$  equal to 0.04, 0.02 and 0.01 are shown, 652 showing very similar results, with some discrepancies of the coarse mesh with 653 respect to the finer ones. For the accuracy study, the solution from the finest 654 grid,  $801 \times 5601$ , is used as reference. Two relative errors are defined, for 655 the maximum value of the filament trailing-edge transverse location,  $x_{max}$ , 656 namely  $\epsilon_A = (x_{max} - x_{max}^{ref})/x_{max}^{ref}$  and for the oscillation period, T, namely  $\epsilon_T = (T - T^{ref})/T_{ref}$ . The relative errors are reported versus grid spacing 657 658 in Figure 16, showing an overall second-order accuracy on finer grids. The 659 instantaneous vorticity contours at four time points along the flapping cycle 660



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

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

## 670 3.6. Three-dimensional flow around a flapping flag

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



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] ( $\blacksquare$ ).



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] (- - -).

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



Figure 20: Problem description for the simulation of the flow arounf 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  $\gamma = 100$ .

#### <sup>700</sup> 3.7. Three-dimensional inverted flag in a free stream

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

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

where B is the flexural rigidity of the sheet,  $\rho_f$  and  $\rho_s$  are the fluid and 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.

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

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

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

Finally, a three-dimensional test case is presented in order to test the thin-structure dynamics under high pressure gradients. The case considered is that of a bioprosthetic aortic valve, with three deformable cusps that open and close under a pulsatile flowrate. The flow domain considered reproduces 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  $\beta = 0.1$ .

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



Figure 26: (a) Scheme of the consiguration for the three-dimensional flow through a bioprosthetic aortic valve. The main geometrical parameters are shown, related to the valve diameter,  $d_0 = 23 \, mm$ . (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) Pulstile flowrate adopted in the simulations.

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

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



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).

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

# 821 4. Conclusions

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



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).

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

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