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The immersed boundary method for simulating structure-fluid interaction

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Abstract

The immersed boundary (IB) method is the method for studying flexible structure-fluid interaction. In this article, we present the mathematical structure of the method which aims to simulate mostly the problems in biofluid dynamics. The philosophy of the IB method is to make the communication between the Eulerian variables that are used in fluid dynamics and the Lagrangian variables that are used to describe the elasticity of the material through the Dirac delta function. Since the method was introduced in 1972, it has been used widely in various structure-fluid interactions. Some applications are mentioned in this article.

Keywords: biofluid dynamics, immersed boundary method, Lagrangian, Eulerian

Introduction

The immersed boundary (IB) method was first proposed by Charles S. Peskin [1] and it has been used to study various flexible material-fluid interactions, such as deformation of red blood cells under shear flow [2], DNA coiling [3], and cellular growth [4]. The method is both a mathematical formulation and numerical simulation. In this article, a brief review of the method and some applications will be given. The mathematical formulation of the IB method and descriptions of the numerical algorithm will be presented. Some applications to structure-fluid interactions will be mentioned as well.

Mathematical Formulation

The spirit of the IB method is the connection between the Lagrangian and Eulerian variables through the Dirac delta function. Roughly speaking, the structure is described by Lagrangian variables (curvilinear coordinates). Since the structure is deformed throughout the process, the key step is to introduce the Eulerian variables (Cartesian coordinates) describing the fluid velocity along the way. The Dirac delta function is then introduced in order to make the communication between the structure and the fluid.

Let us consider an incompressible elastic material embedded in a three-dimensional space. The curvilinear coordinates attached on the material is specified by $\mathbf{q} = (q_1, q_2, q_3)$. At time t, the material's Cartesian coordinates $\mathbf{X} = (X_1, X_2, X_3)$ are related to $\mathbf{q}$ through;

$$\begin{aligned} X_1 &= X_1(q_1, q_2, q_3, t), \\ X_2 &= X_2(q_1, q_2, q_3, t), \\ X_3 &= X_3(q_1, q_2, q_3, t). \end{aligned} \tag{1}$$

Let $M(q_1,q_2,q_3)$ be the mass density of the material. Then, the integration $\int M dq_1 dq_2 dq_3$ gives the mass occupied in the volume $dq_1 dq_2 dq_3$. Please note that M is not a function of time because mass is conserved. We further assume that the elastic energy stored in the material is a functional of $\mathbf{X} = (X_1, X_2, X_3)$ at time t such that $E[\mathbf{X}(q_1,q_2,q_3,t)]$. The elastic force density $\mathbf{F}(q_1,q_2,q_3)$ can be calculated from;

$$\mathbf{F} = -\frac{\delta E}{\delta \mathbf{X}}. \tag{2}$$

Note that Eq. (2) is completely in Lagrangian form. The equations of fluid are given by the Navier-Stokes equations which can be described in Eulerian form;

$$\rho\left(\frac{\partial}{\partial t} + \mathbf{u}(\mathbf{x},t)\cdot\nabla\right)\mathbf{u}(\mathbf{x},t) = -\nabla P(\mathbf{x},t) + \mu\nabla^2\mathbf{u}(\mathbf{x},t) + \mathbf{f}(\mathbf{x},t), \tag{3}$$

and

$$\nabla\cdot\mathbf{u}(\mathbf{x},t) = 0, \tag{4}$$

where ρ is the density of the fluid, $\mathbf{u}(\mathbf{x},t)$ is the fluid velocity, $P(\mathbf{x},t)$ is the pressure, μ is the dynamic viscosity of the fluid, and $\mathbf{f}(\mathbf{x},t)$ is the external force per unit volume acting on the fluid element. Eq. (3) describes the conservation of momentum. While, Eq. (4) is the conservation of mass which is the condition of incompressible fluid. The connection between the Lagrangian and Eulerian variables is done through the Dirac delta function;

$$\rho(\mathbf{x},t) = \int M(q_1,q_2,q_3)\delta(\mathbf{x}-\mathbf{X})dq_1dq_2dq_3,$$
$$\mathbf{f}(\mathbf{x},t) = \int \mathbf{F}(q_1,q_2,q_3,t)\delta(\mathbf{x}-\mathbf{X})dq_1dq_2dq_3.$$

These equations show the density $\rho(\mathbf{x},t)$ and the elastic force density $\mathbf{f}(\mathbf{x},t)$ in the Eulerian variables. The velocity of the material point is given by;

$$\frac{\partial \mathbf{X}}{\partial t} = \int \mathbf{u}(\mathbf{x},t)\delta(\mathbf{x}-\mathbf{X})d\mathbf{x}. \tag{5}$$

The point on the boundary will move with the local fluid velocity associated to that point. This enforces the no-slip boundary condition.

Numerical IB Method

In this section, we shall first discuss the spatial discretization by employing two independent grids, i.e., the fluid and structure grids. Next, the approximate form of the Dirac delta function is discussed. We then describe the temporal discretization. Finally, we will give the numerical algorithm used for numerical IB method.

Spatial discretization

The fluid grid for the Eulerian variables (simply called the Eulerian grid) is denoted by g_e. It is a 3-vector in Cartesian coordinates with integer components of the form $\mathbf{x} = h\mathbf{e}$, where $\mathbf{e} = (e_1, e_2, e_3)$ and h is the size of the spatial step. Similarly, the structure grid (or the Lagrangian grid) denoted by G_l is the set of $(k_{q_1}\Delta q_1, k_{q_2}\Delta q_2, k_{q_3}\Delta q_3)$, where k_{q_1}, k_{q_2}, and k_{q_3} are integers. The discretization of the elastic energy can be written as;

$$E_h = \sum_{k'_{q_1},k'_{q_2},k'_{q_3}} \varepsilon_{k'_{q_1},k'_{q_2},k'_{q_3}} \left(\mathbf{X}_{k_{q_1},k_{q_2},k_{q_3}}\right) \Delta q_1 \Delta q_2 \Delta q_3, \tag{6}$$

where $\varepsilon_{k'_{q_1},k'_{q_2},k'_{q_3}}$ is the local energy density. Then, the discrete elastic force density associated with the point $(k_{q_1}\Delta q_1, k_{q_2}\Delta q_2, k_{q_3}\Delta q_3)$ is of the form;

$$\mathbf{F}_{k_{q_1},k_{q_2},k_{q_3}} = -\sum_{k'_{q_1},k'_{q_2},k'_{q_3}} \frac{\partial \varepsilon_{k'_{q_1},k'_{q_2},k'_{q_3}}}{\partial \mathbf{X}_{k_{q_1},k_{q_2},k_{q_3}}}. \tag{7}$$

Now, we can write the discrete form of the equations of motion described in Sec. II as;

$$\rho(\mathbf{x},t) = \sum_{(q_1,q_2,q_3)\in G_l} M(q_1,q_2,q_3)\delta_h(\mathbf{x}-\mathbf{X})\Delta q_1 \Delta q_2 \Delta q_3,$$

$$\mathbf{f}(\mathbf{x},t) = \sum_{(q_1,q_2,q_3)\in G_l} \mathbf{F}(q_1,q_2,q_3,t)\delta_h(\mathbf{x}-\mathbf{X})\Delta q_1 \Delta q_2 \Delta q_3,$$

and

$$\frac{d\mathbf{X}}{dt} = \sum_{\mathbf{x}\in g_e} \mathbf{u}(\mathbf{x},t)\delta_h(\mathbf{x}-\mathbf{X})h^3. \tag{8}$$

The approximate Dirac delta function

The three-dimensional Dirac delta function in a discrete form with the spatial width h can be written as;

$$\delta_h(\mathbf{x}) = \frac{1}{h^3}\varphi\left(\frac{x_1}{h}\right)\varphi\left(\frac{x_2}{h}\right)\varphi\left(\frac{x_3}{h}\right), \tag{9}$$

where $\mathbf{x} = (x_1, x_2, x_3)$ is a three-dimensional vector in Cartesian coordinates. Peskin and McQueen [5] give the choice of the delta function by the simple formula;

$$\varphi(r) = \begin{cases} \frac{1}{4}\left(1+\cos\left(\frac{\pi r}{2}\right)\right), & |r| \le 2, \\ 0, & \text{otherwise}, \end{cases} \tag{10}$$

where $\varphi(r) = \varphi(x_i/h), i = (1,2,3)$. Other choices for the successfully approximate delta function are in [8].

Temporal discretization

In order to make the temporal discretization, we use the midpoint method (also known as the second-order Runge-Kutta method). Let us consider the differential equation of the form;

$$\frac{dy}{dt} = \mathrm{f}(\mathrm{y}), \tag{11}$$

with the initial condition $y(t_0) = y_0$. We define;

$$y_{n+1} - y_n = (\Delta t) f\left(y_{n+\frac{1}{2}}\right),$$

$$t_{n+1} = t_n + \Delta t,$$

for $n = 0,1,2,3,\ldots$. From this scheme, we can move the material point from the position $\mathbf{X}_n$ to $\mathbf{X}_{n+1}$;

$$\mathbf{X}_{n+1} - \mathbf{X}_n = (\Delta t)\sum_{\mathbf{x}\in g_e} \mathbf{u}_{n+\frac{1}{2}}(\mathbf{x})\,\delta_h\left(\mathbf{x}-\mathbf{X}_{n+\frac{1}{2}}\right)h^3. \tag{12}$$

Numerical algorithm

The numerical algorithm is described as follows. For each time step;

1. Calculate the elastic force density $\mathbf{F}(q_1, q_2, q_3, t)$ on Lagrangian grid
2. Spread the force density from the Lagrangian grid to the Eulerian grid:$\mathbf{f}(\mathbf{x}, t) = \sum_{(q_1,q_2,q_3)\in G_l} \mathbf{F}(q_1, q_2, q_3, t)\delta_h(\mathbf{x} - \mathbf{X})\Delta q_1 \Delta q_2 \Delta q_3$,
3. Solve the Navier-Stokes equations on the Cartesian coordinates
4. Update the material point position: $\frac{d\mathbf{X}}{dt} = \sum_{\mathbf{x}\in g_e} \mathbf{u}(\mathbf{x}, t)\delta_h(\mathbf{x} - \mathbf{X})h^3$.

Applications

Many authors have used the IB method for studying various structure-fluid interactions. Since it was introduced to study the fluid dynamics of heart valves by Peskin [1], the diverse phenomena and systems such as modeling of the whole heart [5], the deformation of red blood cells under shear flows [2], and fluid-interaction of flexible bacterial flagella [6] have been studied. Recently, the method has been used to simulate the dynamics of growth vesicles with permeability [7].

Conclusions

The immersed boundary method is the method for simulating incompressible elastic bodies immersed in viscous incompressible fluid. The main idea of the method is to spread the elastic energy stored in the material from the curvilinear coordinates to the Cartesian coordinates with the help from the Dirac delta function. Since the IB method was introduced in 1972, a wide range of applications has been demonstrated. This assures the robustness of the method.

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