



# Spectrally-accurate immersed boundary conditions method for three-dimensional flows



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## ABSTRACT

A three-dimensional, spectrally accurate algorithm based on the immersed boundary conditions (IBC) concept has been developed for the analysis of flows in channels bounded by rough boundaries. The algorithm is based on the velocity–vorticity formulation and uses a fixed computational domain with the flow domain immersed in its interior. The geometry of the boundaries is expressed in terms of double Fourier expansions and boundary conditions enter the algorithm in the form of constraints. The spatial discretization uses Fourier expansions in the stream-wise and span-wise directions and Chebyshev expansions in the wall-normal direction. The algorithm can use either the fixed-flow-rate constraint or the fixed-pressure-gradient constraint; a direct implementation of the former constraint is described. An efficient solver which takes advantage of the structure of the coefficient matrix has been developed. It is demonstrated that the applicability of the algorithm can be extended to more extreme geometries using the over-determined formulation. Various tests confirm the spectral accuracy of the algorithm.

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## 1. Introduction

The immersed boundary (IB) method provides a general conceptual basis for developing efficient computational tools to solve flow problems involving complex boundary geometries. The concept can be traced to algorithms developed for the analysis of moving boundary problems, especially fixed grid Eulerian methods [1–8]. The term “immersed boundary” has been attributed to Peskin [9] who used it in the context of cardiac mechanics problems. The method works by discretizing the governing equations within a regular computational domain that surrounds the complex flow domain. Special procedures are then used to enforce the boundary conditions along the physical boundaries, immersed within the computational domain. This is analogous to imposing interfacial boundary conditions on an interface moving through a fixed grid. The computational efficiency of this class of methods stems from the elimination of the cost of generating boundary conforming grids but leads to challenges in enforcing the flow boundary conditions.

The essence of the IB method is to impose forcing at the edge of the computational domain so that the flow quantities evaluated along the edge of the physical domain assume values specified by the boundary conditions. Various implementations have been developed over the past few decades [10,11] with the forcing applied in either a continuous or discrete manner. Most of implementations apply either low-order finite-difference, or finite-volume or finite-element techniques for the spatial discretization [12–14] resulting in limited spatial accuracy. Some of the recent implementations

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employ either the spectral discretization [15,16] or higher-order finite-differencing [17] for the field equations, however, it remains to be shown that the complete solution delivers the same accuracy.

A fully spectrally-accurate version of the IB method, referred to as the Immersed Boundary Conditions (IBC) method, was proposed in [18] for two-dimensional flow problems. We use a distinct name for this method, IBC method, as its theoretical bases are completely different from the typical IB methods. The discretization relies on two types of Fourier expansions, one for the field variables and one for the boundary conditions. The boundary relations responsible for the enforcement of the boundary conditions involve an overlap of these two expansions which is constructed formally and provides the means to enforce boundary conditions with spectral accuracy. The use of Chebyshev expansions in the non-periodic direction makes the algorithm effectively gridless and, thus, allows quick adaptation to different geometries.

The spectral discretization of the field equations in the IBC method begins by representing the unknowns in terms of Fourier expansions, leading to a system of modal equations coupled through nonlinear terms [19]. Typical solution procedures remove this coupling by using nonlinear terms from the previous iteration. This permits to solve each modal equation separately as is the case when simulating flows in smooth channels [20]. The modal equations are discretized using Chebyshev expansions [21]. The construction of boundary relations involves representing values of Chebyshev polynomials at the boundaries in terms of another set of Fourier expansions (“Boundary Fourier Expansions” or BFE) which yields more constraints than required to form a closed system of algebraic equations [22]. The “classical” formulation gives priority to constraints corresponding to the lowest Fourier modes from the BFE’s and retains enough of them to form a closed algebraic system. These constraints provide coupling between the modal equations resulting in a need to solve a very large algebraic system. The cost of the solution can be lowered by two orders of magnitude as far as memory requirements and computational time are concerned using linear solvers which take advantage of the structure of the coefficient matrix [23]. The number of required Fourier modes increases very rapidly with increasing boundary complexities as the rate of convergence of the BFE’s decreases. This cost may be lowered by using the over-determined formulation where the number of boundary relations is increased to counter-balance the smaller convergence rates of BFE’s while the number of modal equations remains unchanged [22]. The resulting system has a rectangular coefficient matrix with a very peculiar structure but can be solved very efficiently using an algorithm which takes advantage of this structure. The best solution strategy involves solving the part of the system resulting from the field equations exactly and the part resulting from the boundary relations in the least squares sense [24].

The above discussion shows that the existing spectrally-accurate algorithms for the Navier–Stokes equation based on the concept of immersed boundaries deal only with two-dimensional problems. There is therefore a need to develop an extension of the IBC method suitable for the analysis of three-dimensional flows. One needs to pay attention to the memory management as the size of the problem increases rapidly when more Fourier modes are required to deal with the increased three-dimensional geometric complexity.

This paper describes the three-dimensional version of the IBC method with applications focused on the analysis of flows in domains bounded by rough walls. Section 2 introduces the model problem. Section 3 describes the numerical formulation of the problem; Section 3.1 discusses the velocity–vorticity formulation and Section 3.2 presents the numerical discretization. Here, Section 3.2.1 presents the discretization of the field equations, Section 3.2.2 discusses the discretization of the boundary conditions and Section 3.2.3 presents the discretization of the flow constraints. Section 4 is focused on the solution process; Section 4.1 describes the specialized linear solver used repeatedly during the iterative solution process while Section 4.2 discusses efficiencies resulting from taking advantage of the complex conjugate property of the unknowns. Section 5 discusses the evaluation of the pressure field. Section 6 discusses testing of the algorithm. Section 7 presents the over-determined formulation of this algorithm and discusses the range of its applicability. Section 8 provides a short summary of the main conclusions.

## 2. Problem formulation

### 2.1. Geometry of flow domain

Consider a channel formed by rough walls extending to  $\pm\infty$  in the  $x$ - and  $z$ -directions. The upper and lower walls are located at  $y_U(x, z)$  and  $y_L(x, z)$ , respectively. It is assumed that the roughness is periodic in the  $x$ - and  $z$ -directions with wavelengths  $\lambda_x = 2\pi/\alpha$  and  $\lambda_z = 2\pi/\beta$  where  $\alpha$  and  $\beta$  stand for the wave numbers in the  $x$ - and  $z$ -directions (Fig. 1), respectively, resulting in the flow domain defined as  $\mathcal{S}_f = [0, \lambda_x] \times [y_L, y_U] \times [0, \lambda_z]$ . The channel geometry can be described using Fourier expansions of the form

$$y_U(x, z) = 1 + \sum_{n=-N_A}^{N_A} \sum_{m=-M_A}^{M_A} H_U^{(n,m)} e^{i(n\alpha x + m\beta z)}, \quad y_L(x, z) = -1 + \sum_{n=-N_A}^{N_A} \sum_{m=-M_A}^{M_A} H_L^{(n,m)} e^{i(n\alpha x + m\beta z)} \quad (2.1)$$

where half of the mean channel opening  $L$  has been used as the length scale and  $N_A$  and  $M_A$  denote the number of Fourier modes required for the description of the roughness geometry in the  $x$ - and  $z$ -directions. The expansion coefficients satisfy the reality conditions of the form  $H_U^{(n,m)} = H_U^{(-n,-m)*}$  and  $H_L^{(n,m)} = H_L^{(-n,-m)*}$  where star denotes the complex conjugates.

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