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Over-determined formulation of the immersed boundary conditions method

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ABSTRACT

The over-determined formulation of the immersed boundary conditions (IBC) method is proposed. The method relies on the Fourier expansions in the periodic direction and Chebyshev expansions in the transverse direction. The boundaries of the physical domain are immersed inside a regular computational domain and the boundary conditions enter the algorithm in the form of constraints. Construction of these constraints provides degrees of freedom in excess of that required to formulate a closed system of algebraic equations. Use of the additional degrees of freedom that leads to an over-determined system is explored in order to improve the accuracy of the IBC method and to expand its applicability to more extreme geometries. The over-constraint formulation has been tested on three model problems that lead to the Laplace, biharmonic and Navier–Stokes equations and thus cover the most commonly encountered types of operators. In all cases tested the over-determined formulation was found to improve the performance of the IBC method.

1. Introduction

'Immersed boundary' (IB) methods refer to a class of methods where the computational domain extends beyond the physical domain resulting in edges of the physical domain immersed inside the computational domain. The name has been coined by Peskin [1] in the context of cardiac mechanics problems. The concept is very attractive as one can work with a fixed, regular computational domain regardless of the shape of the physical domain, i.e., the cost of generating boundary conforming grid has been completely eliminated. Field equations can be discretized using a simple reference coordinate system and are never changed regardless of the geometry of the physical domain. The main challenge associated with this method is the development of procedures that result in the enforcement of physical boundary conditions along the physical boundaries located inside of the computational domain. There are no conditions to be imposed along the edges of the computational domain (unless the edges of the physical and computational domains coincide) and thus the problem formulation needs to be closed by a set of constraints rather then by the classical boundary values. The IB method has been developed primarily in the context of fluid flow problems. The prevailing procedure for imposition of constraints replacing physical boundary conditions involves introduction of additional forcing that makes the fluid to move along the physical boundary. This methodology has roots in the physics of the problem, requires good understanding of the problem, and algorithm calibration involves elements of trial and error. Details of procedures based on the so-called continuous and discrete forcing are reviewed in [2,3].

Fictitious domain methods [4,5] offer an alternative approach for handling boundary irregularities where problems formulated on a complicated domain are solved on a simpler domain that contains the complicated domain. Use of simple domain enables efficient computational grid generation. The fictitious domain method is very suitable for moving boundary problems as it does not require regeneration of grid to account for the changing boundary geometries [5].

A separate group of methods has its roots in the methodology developed for handling the moving boundary problems and has been reviewed in [6]. Here one should focus on the fixed grid methods where the motion of the interface is tracked through a reference fixed grid. The most popular methods are based on the fluid fluxes and are known as the volume of the fluid (VOF) method. More recent methods rely on the concept of level set [7,8]. All these methods are of low-order in terms of spatial accuracy as they are based on the low-order finite-difference and/or finite-volume discretizations, and the interface tracking procedures result in smearing of the interface.

An alternative direction for handling boundary irregularities has been proposed by Szumbarski and Floryan [9] and is referred to as the immersed boundary conditions (IBC) method in the present work. The IBC method is conceptually similar to the IB methods as the physical field of interest is immersed inside the computational domain. However, unlike the IB method, the IBC method does not use additional forcing to impose the physical boundary

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conditions rather transforms the original boundary value problem into an internal value problem. The concept behind the IBC method is also different from the fictitious domain method as it does not simplify the geometry of the problem to enforce the boundary conditions [4]. The IBC method leads to a formal construction of boundary constraints that provide the required closing relations. Spatial discretization relies on the spectral expansions and thus provides ability to reach machine level accuracy. The boundary constraints rely on the representation of physical boundary in the spectral space and nullifying the relevant Fourier modes. Such implementation is limited to geometries that can be represented by Fourier expansions but results in a gridless algorithm as all possible variations of boundary geometries are described in terms of the Fourier coefficients only. The programming effort associated with modeling of changes of geometry has been essentially removed as the only information required for specifying the new geometry is reduced to a set of Fourier coefficients provided as input to the code. The additional attractiveness of this concept is associated with the precise mathematical formalism, high accuracy and sharp identification of the location of physical boundaries. This method has been successfully extended to unsteady problems [10] as well as moving boundary problems [11,12] where the boundary geometries are time-dependent. The computational advantage of this approach over conventional mapping-based spectral algorithm is more evident for the moving boundary problems [11,12], because only the entries in the coefficient matrix corresponding to the discretized boundary conditions are required to be computed at each time step while part of the coefficient matrix corresponding to the discretized field equations needs to be constructed only once. The special structure of the coefficient matrices resulting from the algorithm also provides opportunities for devising more efficient iterative solution methods [10–12]. While the IBC method has been successfully employed for various classes of problems, it has limitations in terms of severity of boundary geometry that can be handled accurately. Various tests have shown that if either the wave number of the physical boundary corrugation or the amplitude of this corrugation is too large, the method fails to provide an acceptable accuracy [9–12].

The present work addresses the limitations of the IBC method discussed above. The IBC method relies on the Galerkin projection for the construction of discretized analog of the field equations. Some of the projection equations are eliminated to provide "space" for the boundary conditions, which are imposed in the Tau-like manner. The boundary conditions are "discretized' using the IBC concept resulting in a number of boundary constraints that is far in excess of that required to formulate a closed system of algebraic equations. In the "classical" formulation of the IBC method [9], only the number of boundary constraints required to form a closed system is retained and boundary constraints corresponding to the lowest (dominant) Fourier modes are used for this purpose. Use of additional available constraints could lead to an increase in the accuracy of the IBC method and could extend its applicability to more extreme geometries, but leads to an over-determined formulation of the problem. Since we have chosen to work with the over-determined formulation, we can also explore whether the use of all available projection equations offers any computational advantage.

The possible gains associated with the over-determined formulation of the IBC method could be problem dependent. In order to provide a definite answer, we have tested this formulation on three model problems involving most commonly found operators, i.e., the Laplace operator, the biharmonic operator and the Navier–Stokes equations. In each case, we have used the same class of geometries for testing purposes so that the reader can identify issues associated with the progressively more complicated operators. Section 2 discusses model geometry. Section 3 provides description of the method for the Laplace equation. Section 4 is devoted to the solution of a model problem that leads to a biharmonic operator. Section 5 provides discussion of the solution of the Navier–Stokes equations. Section 6 provides a short summary of the main conclusions. In order to provide reliable testing of the accuracy of the over-determined formulation, we have determined reference solutions by solving all three model problems using the mapping method that leads to the classical treatment of boundary conditions. A brief outline of the relevant algorithms is given in Appendices A, B, C for the Laplace, biharmonic and Navier–Stokes problems, respectively.

2. Model geometry

We select model geometry in the form of a two-dimensional slot extending to $\pm\infty$ in the x-direction and periodic with the wavelength $\lambda = 2\pi/\alpha$ (see Fig. 1). The slot is bounded by walls whose geometry is expressed in terms of Fourier expansions in the form

$$y_L(x) = -1 + \sum_{n=-N_A}^{n=+N_A} H_L^{(n)} e^{in\alpha x}, \quad y_U(x) = 1 + \sum_{n=-N_A}^{n=+N_A} H_U^{(n)} e^{in\alpha x}, \qquad (2.1\text{a, b})$$

where $H_L^{(n)} = \left(H_L^{(-n)}\right)^*, H_U^{(n)} = \left(H_U^{(-n)}\right)^*$ and the asterisk denotes complex conjugate. Such geometries are of interest in simulations of various physical phenomena where surface roughness plays important role, e.g., electrical micro-capacitors, micro-heat exchangers, laminar-turbulent transition, electrostatic filters, etc. We have selected three types of field equations that the reader might encounter in such applications, i.e., the Laplace equation (discussed in Section 3), the biharmonic equation (discussed in Section 4) and the Navier–Stokes equations (discussed in Section 5). These equations are linear second-order, linear fourth-order and nonlinear fourth-order, respectively, and thus provide ample opportunity for illustration of the performance of the algorithm.

3. Problems described by the Laplace equation

The Laplace equation governs different types of practical flow problems, e.g., conductive heat flow, ground-water hydrology, potential flow, etc. In our case we shall consider the Laplace equation to be describing the conductive heat flow in a corrugated slot whose geometry has been defined in Section 2.

3.1. Problem formulation

The dimensionless field equation describing heat flow at steady state has the form

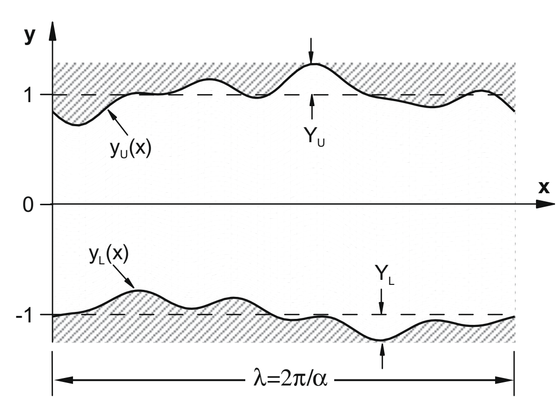

Fig. 1. Sketch of the domain of interest in the physical plane.