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Fast immersed interface Poisson solver for 3D unbounded problems around arbitrary geometries

T. Gillis *, G. Winckelmans, P. Chatelain

Institute of Mechanics, Materials and Civil Engineering, Université catholique de Louvain 1348 Louvain-la-Neuve, Belgium

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ABSTRACT

We present a fast and efficient Fourier-based solver for the Poisson problem around an arbitrary geometry in an unbounded 3D domain. This solver merges two rewarding approaches, the lattice Green's function method and the immersed interface method, using the Sherman-Morrison-Woodbury decomposition formula. The method is intended to be second order up to the boundary. This is verified on two potential flow benchmarks. We also further analyse the iterative process and the convergence behavior of the proposed algorithm. The method is applicable to a wide range of problems involving a Poisson equation around inner bodies, which goes well beyond the present validation on potential flows.

1. Introduction

Solving the Poisson equation is ubiquitous in many computational disciplines such as electromagnetism, fluid mechanics and theoretical physics. Therefore, the problem has been deeply studied and is a recurrent subject within the literature. Still, two major challenges remain: solving the problem in an unbounded framework, and taking into account the presence of a body within the computational domain. These two remaining challenges are widespread and often coupled in many applications, such as computational fluid dynamics applied to the simulation of flows past bodies, like blades and wings.

One may solve the first challenge, i.e. computing unbounded solutions, using two classes of methods. The first kind, based on James [1] and Lackner [2] ideas, solves two problems to determine coherent outer boundary conditions, as proposed by McCorquodale et al. [3], Marichal et al. [4,5]. In this work, we use a second type of method based on the convolution of a kernel function. This convolution is performed using fast summation algorithms: Fast Multipole Methods (FMM) [6–11], Fourier transforms (Hockney–Eastwood technique) [12–15], or a combination of both [16–18] (see [19] for a comparison between the FMM and FFT-based methods). The kernel function is either built through a regularization of the Green's function [11,13,14], or by using the lattice Green's function [9,10,16–18,20].

The second challenge, i.e. taking an immersed body and the discontinuities at its interface into account, can be solved using several methods. We will not attempt to provide an exhaustive review of all of them; instead, we highlight some of the prominent techniques. One of the earliest approach is known as the capacitance matrix method. For example, Proskurowski and Widlund [21] and O'Leary and Widlund [22] embed the irregular domain of interest into a regular one and impose the boundary condition using single layer and double layer potentials. The Helmholtz equation is then solved using iterative methods and algebraic decompositions, like the Sherman–Morrison–Woodbury formula (also known as the Woodbury

* Corresponding author.
E-mail address: thomas.gillis@uclouvain.be (T. Gillis).

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formula), as proposed earlier in a similar context by George [23] and Buzbee et al. [24]. Over the same period of time, Peskin [25] introduced the Immersed Boundary (IB) method, still widely used and renowned for its robustness [18,26,27]. It discretizes the additional sources due to the body on several grid points using discrete delta functions, thus mollifying the body interface. Some recent developments propose a harmonic extension in the body to allow the use of a symmetric discrete delta function and therefore increase the order of convergence of the method [28]. However, this harmonic extension requires additional Poisson equation resolutions. Let us also mention the works based on the potential layer theory from Mayo [29], McKenney et al. [30], Mayo and Greenbaum [31] and a recent contribution from Askham and Cerfon [32], which is also based on the potential layer method, but reuses the harmonic expansion proposed earlier in the contexts of the IB technique [28]. In a similar way, the Boundary Element Methods (BEM) [33,34], relies on panels and FMM acceleration to take the inner obstacle into account. They solve the integral equation associated to the panels and then compute a new Poisson equation including the additional source terms. Finally, let us present the Immersed Interface Method (IIM) [4,35–38], which uses modified Taylor series to take the inner body into account. The IIM offers a proven high order and sharp treatment of boundaries, does not require the introduction of a mollification or any extension in the body and the introduced perturbation has a tiny support around the boundary. Originally developed in a multidimensional way [35] but subject to stability issues, it has been modified to work with one-dimensional dimensions splitting [36,37] and recently applied to 2D problems [4,36].

However, within a regular grid framework, coupling a fast summation based solver and immersed bodies still remains an open challenge. Apart from the fast BEM methods which do not take advantage of the structured grid, none of the above techniques achieves a fast, accurate and grid-based solution of the unbounded Poisson problem around a body. For example, the Miller iteration [39], applied by Marichal et al. [4] to the IIM framework, needs to compute the outer boundary conditions iteratively, together with the inner boundary conditions: this tends to increase dramatically the computational cost. Furthermore, recent fast 3D Poisson solvers, like the FMM-based lattice Green's function convolution [16] or the FTT-based regularized kernel convolution [14], were never coupled with the immersed interface method.

In this work, we consider the inner body as a local perturbation of an unbounded body-free Poisson problem. The Sherman–Morrison–Woodbury (SMW) formula [40, p. 50] efficiently couples the Immersed Interface Method (IIM), used to impose the boundary condition, with a fast Poisson solver. This approach draws inspiration from existing works, such as the capacitance matrix method applied with a direct solver [23,24] or the work on hybrid grid-particle methods and penalization performed by Chatelin and Poncet [41]. To be consistent in the coupling, we use lattice Green's function (LGF) kernel [16], equivalent to inverting the standard 3-points Laplacian stencil considered in the IIM.

In this paper, we first present the three different technologies (LGF, IIM and SMW) and further explain how to couple them together (Section 2). Secondly, we investigate the rate of convergence on two benchmarked potential flow applications and validate its second order behavior (Section 3). Finally, we close this work by a short conclusion and perspectives for future work.

2. Methodology

We consider the unbounded 3D scalar Poisson problem around a body, Ω_b:

$$\nabla^2 u(\mathbf{x}) = f(\mathbf{x}), \quad \mathrm{supp}(f) \in \Omega \setminus \Omega_b \ , \tag{1}$$

where $\mathbf{x} \in \mathbb{R}^3$, Ω is the computational domain which encapsulates the body and the support of the source term, $f(\mathbf{x})$, and the unbounded solution, $u(\mathbf{x})$, decays at least as $1/|\mathbf{x}|$ at infinity. Without loss of generality we assume a Neumann boundary condition on $\partial\Omega_b$. Using a standard 3-point grid discretization for the Laplacian operator, ∇_h^2, we aim at a second order solver, which uses IIM in order to take the inner boundary condition into account.

We decompose the problem (1) into two sub-problems. The first one is the body-free problem, expressed by the unbounded elliptic operator, ∇_h^2. The second one is the boundary problem, the perturbation of this operator by the body contribution, expressed as an additional source term, f_b. In this section we successively address these two problems and the method used to couple them.

2.1. A second order unbounded, body-free, 3D Poisson solver

The straightforward inversion of ∇_h^2 operator is challenging and computationally intensive [1,2,39,42]. For the sake of efficiency, we rather follow an approach of grid-based fast convolution of the Green's function with the source term. Because the IIM tools, discussed in Section 2.2, consist in finite differences modifications, we use the Green's function associated with the standard second order cross stencil (3 × 3 × 3). As proposed by Liska and Colonius [16], the body-free Poisson equation, expressed in wave space, $(k_x\, ;\, k_y\, ;\, k_z) \in [-\pi/h_x\, ;\, \pi/h_x] \times [-\pi/h_y\, ;\, \pi/h_y] \times [-\pi/h_z\, ;\, \pi/h_z]$, becomes

$$\frac{1}{h^2}\left[4\sin^2(k_x h_x/2) + 4\sin^2(k_y h_y/2) + 4\sin^2(k_z h_z/2)\right]\hat{u} \triangleq \sigma(\mathbf{k}h)\,\hat{u} = \hat{f} \ , \tag{2}$$

where $\hat{u}$ and $\hat{f}$ are the Fourier transforms of u and f. In this work, we consider a structured grid with $h = h_x = h_y = h_z$. The associated lattice Green's function (LGF) is given by the unbounded inverse Fourier transform of $1/(\sigma(\mathbf{k}h))$ [16]: