Computing Jump Conditions for the Immersed Interface Method Using Triangular Meshes

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Abstract

The immersed interface method (IIM) can be employed to solve many interface problems on fixed Cartesian grids by incorporating necessary interface-induced *Cartesian* jump conditions into numerical schemes. In this paper, we present a method to compute the necessary Cartesian jump conditions from given *principal* jump conditions using triangular mesh representation of an interface. The triangular mesh representation is simpler and robuster than interface parametrization for a complex or non-smooth interface. We test our method by using the computed Cartesian jump conditions in the IIM to solve a Poisson equation subject to an interface with the shape of a sphere, cube, cylinder or cone. The results demonstrate the expected second-order accuracy of the solution in the infinity norm.

Keywords: the immersed interface method, triangular meshes, jump conditions, Poisson solvers, complex geometries, non-smooth interfaces, Cartesian grid methods

1. Introduction

The immersed interface method (IIM) was first proposed by LeVeque and Li [2] to solve elliptic equations with discontinuous coefficients and singular sources. Since then it has been developed to be a general methodology for solving various interface problems and irregular-domain problems [3].

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The key idea of the IIM is to incorporate interface-induced jump conditions into discretization schemes to achieve desired solution accuracy and solving efficiency. To give an example on how jump conditions are incorporated into a numerical scheme, we consider the central finite difference approximation of a derivative of a discontinuous function. Let $g(s)$ be a function with jump discontinuities at $s = l$ and $s = r$ that fall within a three-node stencil as $s_{i-1} < l < s_i \leq r < s_{i+1}$, where s_{i-1} , s_i and s_{i+1} are the stencil nodes satisfying $s_{i+1} - s_i = s_i - s_{i-1} = h$. The central finite difference scheme for $g''(s_i)$ on this stencil reads [5, 6]

$$\frac{d^2 g(s_i)}{ds^2} = \frac{g(s_{i+1}) - 2g(s_i) + g(s_{i-1}))}{h^2} + O(h^2) - \frac{1}{h^2} \left(\sum_{n=0}^3 \frac{-[g^{(n)}(l)]}{n!} (s_{i-1} - l)^n + \sum_{n=0}^3 \frac{[g^{(n)}(r)]}{n!} (s_{i+1} - r)^n \right), \quad (1)$$

where $[g^{(n)}(l)] = g^{(n)}(l^+) - g^{(n)}(l^-)$ denotes the jump conditions of the n -th derivatives of $g(s)$ at $s = l$, and similarly $[g^{(n)}(r)]$ the jump conditions at $s = r$. This example shows that we can modify a *standard* finite difference scheme to approximate derivatives of a discontinuous function by adding some extra terms that involve necessary jump conditions. In particular, a PDE for an interface problem can be discretized on a fixed Cartesian grid by incorporating into standard discretization schemes the jump conditions of the solution and its derivatives with respect to Cartesian coordinates. We name these jump conditions *Cartesian* jump conditions.

For the function p , we call

$$[p], \quad \left[\frac{\partial p}{\partial \mathbf{n}} \right], \quad [\Delta p]$$

the *principal* jump conditions, which are the jump conditions of p , the normal derivative of p and the Laplacian of p across an interface, respectively, where $\mathbf{n}$ denotes a unit normal vector for the interface, and a jump condition is hereafter defined as $[\cdot] = (\cdot)_{\mathbf{n}^+} - (\cdot)_{\mathbf{n}^-}$ with $\mathbf{n}^+$ and $\mathbf{n}^-$ denoting right and left limits respectively. These principal jump conditions can often be derived from the physics of a problem. The goal of this paper is to obtain from the given principal jump conditions the following Cartesian jump conditions

$$[p], \quad \left[\frac{\partial p}{\partial x_i} \right], \quad \left[\frac{\partial^2 p}{\partial x_i \partial x_j} \right]$$

where x_i and x_j ($i, j \in \{1, 2, 3\}$) are Cartesian coordinates in 3D.

In [6], a systematic approach based on interface parametrization was proposed to derive the Cartesian jump conditions from the principal jump conditions. However, interface parametrization is practically difficult for complex or non-smooth interfaces. In this paper, we propose a method to compute the Cartesian jump conditions using triangular mesh representation of an interface, which is more flexible and robust to deal with complex or non-smooth interfaces.

To test our method, we use the Cartesian jump conditions computed by the method in the IIM to solve the Poisson equation $\Delta p = f$ subject to the given principal jump conditions across a closed interface in 3D. Based on Eqn. (1), the Poisson equation can be discretized on a uniform Cartesian grid as

$$\Delta_h p_{ijk} = f_{ijk} + C_{ijk},$$

where Δ_h is the standard seven-point discrete Laplacian at the grid point (i, j, k) , h is the spatial step of the grid, and C_{ijk} denotes the extra terms involving the necessary Cartesian jump conditions. The jump contribution C_{ijk} is nonzero only if the interface cuts through the seven-point Laplacian stencil at the grid point (i, j, k) .

According to Eqn. (1), the local truncation error of the seven-point discrete Laplacian is $O(h)$ if the jump conditions of the third-order Cartesian derivatives are not included. However, it is difficult or costly to obtain the jump conditions of the third-order or higher Cartesian derivatives. Fortunately, second-order accuracy of the solution in the infinity norm can still be achieved in solving a Poisson equation subject to an interface if the local truncation error is reduced from $O(h^2)$ to $O(h)$ only for stencils cut by the interface [1]. So we only need to compute the Cartesian jump conditions listed above. Realizing that $(s_{i-1} - l)$ and $(s_{i-1} - r)$ in Eqn. (1) is at most $O(h)$, we need to compute $\left[\frac{\partial p}{\partial x_i}\right]$ with $O(h^2)$ accuracy and $\left[\frac{\partial^2 p}{\partial x_i \partial x_j}\right]$ with $O(h)$ accuracy.

One motivation of the work in this paper is to solve a fluid flow around moving rigid objects on a fixed Cartesian grid using the IIM with boundary condition capturing [8, 10]. The flow is formulated such that the rigid objects are replaced by the virtual fluid enclosed by singular forces concentrating on the surfaces of the objects via the Dirac delta function, which induce jump discontinuities in the velocity and the pressure across the interfaces between

the virtual and real fluids. The principal jump conditions for the velocity and the pressure are related with the singular forces [6], which can be determined explicitly in the boundary condition capturing approach [8, 9, 10]. Using the method proposed in this paper, we can obtain the Cartesian jump conditions explicitly. They appear at the right-hand sides of linear systems resulting from the discretization of the Navier-Stokes equations without modifying the coefficient matrices corresponding to the background standard numerical schemes, so standard fast solvers such as FFT solvers can be employed to solve the linear systems. Linnick and Fasel [4] presented a high-order IIM in which Cartesian jump conditions are directly computed from unknown solutions using one-sided finite difference schemes. Since their Cartesian jump conditions are solution-dependent, the coefficient matrices of their linear systems are modified and iterative solvers are required.

2. Cartesian Jump Conditions

Suppose that a triangular mesh representation of a closed interface is given. See Fig. 1 for examples. Suppose that the edge lengths of the triangular mesh is of $O(h)$. Suppose that the principal jump conditions $[p]$, $\left[\frac{\partial p}{\partial \mathbf{n}}\right]$, and $[\Delta p]$ are given at appropriate locations (specified later) on the triangular mesh. The Cartesian jump condition $[p]$ is given as a principal jump condition. We compute the Cartesian jump conditions $\left[\frac{\partial p}{\partial x_i}\right]$ and $\left[\frac{\partial^2 p}{\partial x_i \partial x_j}\right]$ at each vertex of the triangular mesh.

According to Eqn. (1), we need to compute $\left[\frac{\partial p}{\partial x_i}\right]$ with at least $O(h^2)$ accuracy and $\left[\frac{\partial^2 p}{\partial x_i \partial x_j}\right]$ with at least $O(h)$ accuracy such that the local truncation error of the seven-point discrete Laplacian is at most $O(h)$ for stencils cut by the interface, as already stated in Section 1.

To facilitate later presentation, we consider an arbitrarily chosen triangular panel $\triangle ABC$ in Fig. 2 (a) and an arbitrarily chosen vertex A in Fig. 2 (b).

2.1. $O(h^2)$ computation of $\left[\frac{\partial p}{\partial x_i}\right]$

For an arbitrary triangular panel $\triangle ABC$ shown in Fig. 2 (a), we first introduce some notations in the computation of $\left[\frac{\partial p}{\partial x_i}\right]$. We denote the middle points of the edges AB , BC and CA as D , E and F , respectively, and the intersection of AE and DF as M (which is the middle point of AE and DF).

Figure 1: Triangular meshes for a sphere, a cube, a cylinder and a cone.

Figure 2: (a) A triangular panel $\triangle ABC$ and various points, lines and vectors associated with it. (b) A vertex A shared by $n_A = 5$ surrounding triangular panels.

We let $\ell_\alpha = |ME|$, $\ell_\beta = |MF|$ (ℓ_α and ℓ_β are of $O(h)$), s_α and s_β be the axes along ME and MF with unit vectors $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$, respectively, and $\mathbf{n}$ be the unit normal vector of the panel $\triangle ABC$ pointing outside of the closed interface. We suppose that the vertices A , B and C are ordered such that $\mathbf{n}$ is in the direction of $\boldsymbol{\alpha} \times \boldsymbol{\beta}$.

Assume that we know the principal jump conditions $[\frac{\partial p}{\partial \mathbf{n}}]$ at the point M with at least $O(h^2)$ accuracy and the principal jump conditions $[p]$ at the points A , B , C , D , E and F with at least $O(h^3)$ accuracy. Our first step is to compute $[\frac{\partial p}{\partial x_i}]$ at the point M with $O(h^2)$ accuracy. We have

$$\boldsymbol{\alpha} \cdot [\nabla p]_M = \left[\frac{\partial p}{\partial s_\alpha} \right]_M = \frac{[p]_E - [p]_A}{2\ell_\alpha} + O(h^2), \quad (2)$$

$$\boldsymbol{\beta} \cdot [\nabla p]_M = \left[\frac{\partial p}{\partial s_\beta} \right]_M = \frac{[p]_F - [p]_D}{2\ell_\beta} + O(h^2), \quad (3)$$

$$\mathbf{n} \cdot [\nabla p]_M = \left[\frac{\partial p}{\partial \mathbf{n}} \right]_M. \quad (4)$$

Eqs. (2,3,4) form the following linear system

$$\begin{pmatrix} \alpha_1 & \alpha_2 & \alpha_3 \\ \beta_1 & \beta_2 & \beta_3 \\ n_1 & n_2 & n_3 \end{pmatrix} \begin{pmatrix} \left[\frac{\partial p}{\partial x_1} \right] \\ \left[\frac{\partial p}{\partial x_2} \right] \\ \left[\frac{\partial p}{\partial x_3} \right] \end{pmatrix} = \begin{pmatrix} \frac{[p]_E - [p]_A}{2\ell_\alpha} \\ \frac{[p]_F - [p]_D}{2\ell_\beta} \\ \left[\frac{\partial p}{\partial \mathbf{n}} \right] \end{pmatrix}. \quad (5)$$

This linear system can be solved analytically to give $[\nabla p]$ at the point M with $O(h^2)$ accuracy. We apply this process for all the panels on our mesh.

Next, we use $[\nabla p]$ at the interior point M of each panel to compute $[\nabla p]$ at all the vertices. For the single panel shown in Fig.2 (a), linear interpolation gives

$$2[\nabla p]_A + [\nabla p]_B + [\nabla p]_C = 4[\nabla p]_M + O(h^2). \quad (6)$$

So by repeating the linear interpolation for all the adjacent panels to the vertex A and then doing summation of the results, we can form a linear

equation

$$2n_A[\nabla p]_A + 2[\nabla p]_B + 2[\nabla p]_C + \cdots = 4 \sum_{i=1}^{n_A} [\nabla p]_{M_i}, \quad (7)$$

where n_A is the number of the adjacent vertices (or panels) to the vertex A , as demonstrated in Fig.2 (b), and the factor 2 in front of $[\nabla p]_B$ and $[\nabla p]_C$ comes from the fact that the edge BC is shared by two neighboring panels. Assembling such linear equations for all the vertices forms the linear system

$$\begin{pmatrix} n_A & 1 & 1 & \cdots \\ 1 & n_B & 1 & \cdots \\ 1 & 1 & n_C & \cdots \\ & & \vdots & \end{pmatrix} \begin{pmatrix} [\nabla p]_A \\ [\nabla p]_B \\ [\nabla p]_C \\ \vdots \end{pmatrix} = 2 \begin{pmatrix} \sum_{i=1}^{n_A} [\nabla p]_{M_i} \\ \sum_{i=1}^{n_B} [\nabla p]_{M_i} \\ \sum_{i=1}^{n_C} [\nabla p]_{M_i} \\ \vdots \end{pmatrix}, \quad (8)$$

which can be solved using the conjugate gradient (CG) method as its coefficient matrix is symmetric positive definite (SPD). The solution is $[\nabla p]$ at all the vertices with $O(h^2)$ accuracy. This linear system is not coupled with p if the given principal jump conditions are explicitly known and not coupled with p , which is the case in the IIM with boundary condition capturing for fluid-solid interaction [8, 10].

Denote the coefficient matrix as G . To compute the matrix-vector product $Gq = d$ for a known approximation q of the solution in the CG method, we do not need to construct or store G or find surrounding panels for each vertex. Write down $Gq = d$ as

$$\begin{pmatrix} n_A & 1 & 1 & \cdots \\ 1 & n_B & 1 & \cdots \\ 1 & 1 & n_C & \cdots \\ & & \vdots & \end{pmatrix} \begin{pmatrix} q_A \\ q_B \\ q_C \\ \vdots \end{pmatrix} = \begin{pmatrix} d_A \\ d_B \\ d_C \\ \vdots \end{pmatrix}. \quad (9)$$

We can easily compute the matrix vector product d using the following algorithm

```

Initialize vector d = 0
for each triangular panel ABC
    dA = dA+qA+qB/2+qC/2
    dB = dB+qB+qA/2+qC/2
    dC = dC+qC+qA/2+qB/2
end for

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The division by 2 above comes from the fact that any two adjacent panels share a common edge.

2.2. $O(h)$ computation of $\left[\frac{\partial^2 p}{\partial x_i \partial x_j}\right]$

To compute $\left[\frac{\partial^2 p}{\partial x_i \partial x_j}\right]$ with $O(h)$ accuracy, we use $\left[\frac{\partial p}{\partial x_i}\right]$ computed at each vertex with $O(h^2)$ accuracy in Section 2.1 and the principal jump condition $[\Delta p]$ supposed to be known at each vertex with at least $O(h)$ accuracy.

For an arbitrary triangular panel $\triangle ABC$ illustrated in Fig. 2 (a), below we present how to compute $\left[\frac{\partial^2 p}{\partial x_i \partial x_j}\right]$ with $O(h)$ accuracy at an arbitrary vertex of the panel, say the vertex A . In Fig. 2 (a), s_τ and s_b are the axes along AB and AC with unit vectors τ and $\mathbf{b}$. We approximate the following derivatives along s_τ and s_b at the vertex A using one-sided finite difference approximations

$$\frac{\partial[\nabla p]}{\partial s_\tau} = \tau_1 \frac{\partial[\nabla p]}{\partial x_1} + \tau_2 \frac{\partial[\nabla p]}{\partial x_2} + \tau_3 \frac{\partial[\nabla p]}{\partial x_3} = \frac{[\nabla p]_B - [\nabla p]_A}{|AB|} + O(h), \quad (10)$$

$$\frac{\partial[\nabla p]}{\partial s_b} = b_1 \frac{\partial[\nabla p]}{\partial x_1} + b_2 \frac{\partial[\nabla p]}{\partial x_2} + b_3 \frac{\partial[\nabla p]}{\partial x_3} = \frac{[\nabla p]_C - [\nabla p]_A}{|AC|} + O(h). \quad (11)$$

Combining Eqs. (10,11) with the following given principal jump condition at the vertex A

$$\left[\frac{\partial^2 p}{\partial x_1^2}\right] + \left[\frac{\partial^2 p}{\partial x_2^2}\right] + \left[\frac{\partial^2 p}{\partial x_3^2}\right] = [\Delta p], \quad (12)$$

we obtain the following over-determined linear system for $\left[\frac{\partial^2 p}{\partial x_i \partial x_j}\right]$ at the ver-

tex A

$$\begin{pmatrix} 1 & 0 & 0 & 1 & 0 & 1 \\ \tau_1 & \tau_2 & \tau_3 & 0 & 0 & 0 \\ 0 & \tau_1 & 0 & \tau_2 & \tau_3 & 0 \\ 0 & 0 & \tau_1 & 0 & \tau_2 & \tau_3 \\ b_1 & b_2 & b_3 & 0 & 0 & 0 \\ 0 & b_1 & 0 & b_2 & b_3 & 0 \\ 0 & 0 & b_1 & 0 & b_2 & b_3 \end{pmatrix} \begin{pmatrix} \left[\frac{\partial^2 p}{\partial x_1^2} \right] \\ \left[\frac{\partial^2 p}{\partial x_1 \partial x_2} \right] \\ \left[\frac{\partial^2 p}{\partial x_1 \partial x_3} \right] \\ \left[\frac{\partial^2 p}{\partial x_2^2} \right] \\ \left[\frac{\partial^2 p}{\partial x_2 \partial x_3} \right] \\ \left[\frac{\partial^2 p}{\partial x_3^2} \right] \end{pmatrix} = \begin{pmatrix} [\Delta p] \\ \frac{\partial}{\partial s_\tau} \left[\frac{\partial p}{\partial x_1} \right] \\ \frac{\partial}{\partial s_\tau} \left[\frac{\partial p}{\partial x_2} \right] \\ \frac{\partial}{\partial s_\tau} \left[\frac{\partial p}{\partial x_3} \right] \\ \frac{\partial}{\partial s_b} \left[\frac{\partial p}{\partial x_1} \right] \\ \frac{\partial}{\partial s_b} \left[\frac{\partial p}{\partial x_2} \right] \\ \frac{\partial}{\partial s_b} \left[\frac{\partial p}{\partial x_3} \right] \end{pmatrix}, \quad (13)$$

which has a unique solution and can be solved analytically by Gaussian elimination [6, 7].

Using this process, We can solve $\left[\frac{\partial^2 p}{\partial x_i \partial x_j} \right]$ at the vertex A from all the n_A panels surrounding the vertex A as shown in Fig. 2 (b). We use a weighted average to obtain the final $\left[\frac{\partial^2 p}{\partial x_i \partial x_j} \right]$ at the vertex A as the following

$$\left[\frac{\partial^2 p}{\partial x_i \partial x_j} \right] = \frac{\sum_{k=1}^{n_A} \left(w_k \left[\frac{\partial^2 p}{\partial x_i \partial x_j} \right]_k \right)}{\sum_{k=1}^{n_A} w_k}, \quad (14)$$

where w_k is a weight and $\left[\frac{\partial^2 p}{\partial x_i \partial x_j} \right]_k$ denotes $\left[\frac{\partial^2 p}{\partial x_i \partial x_j} \right]$ computed from the panel k surrounding the vertex A . The weight w_k is chosen to be $w_k = A_k^{-1}$, where A_k is the area of the panel k , such that a smaller panel has a larger weight. Since the vertices of a smaller panel are closer in general, the weighted average improves the accuracy in computing $\left[\frac{\partial^2 p}{\partial x_i \partial x_j} \right]$.

3. Interpolation at Panel-Grid Intersections

We now present how to use the computed Cartesian jump conditions in the IIM to solve an interface problem in 3D. An interface is represented by a triangular mesh with mesh size of order $O(h)$.

We need to distinguish grid points inside and outside the interface. This can be done by the ray casting scheme. As indicated in Section 1, we need to identify finite difference stencils which are cut by the interface. This can be done by finding all the intersections (without omission or repetition) between Cartesian grid lines and all the triangular panels of the triangular mesh [7]. In order to determine the jump contributions to those finite difference stencils using Eqn. (1), we need to know the necessary Cartesian jump conditions at all these intersections. Below we present how to interpolate a Cartesian jump condition at an intersections from the surrounding vertices with required accuracy.

Let the point Q in Fig. 2 (a) be an intersection between a Cartesian grid line and the triangular panel $\triangle ABC$ of the interface. We use f to denote a Cartesian jump condition $\left[\frac{\partial p}{\partial x_i}\right]$ or $\left[\frac{\partial^2 p}{\partial x_i \partial x_j}\right]$. We denote the known values of f at the vertices A, B and C of the panel as f_A, f_B and f_C , respectively. We can interpolate the value of f at Q , denoted as f_Q , using the following formula

$$f_Q = \frac{\|\vec{QB} \times \vec{QC}\|f_A + \|\vec{AQ} \times \vec{AC}\|f_B + \|\vec{AB} \times \vec{AQ}\|f_C}{\|\vec{AB} \times \vec{AC}\|} + O(h^2) \quad (15)$$

The interpolation is of second order accuracy, so it keeps the desired accuracy in $\left[\frac{\partial p}{\partial x_i}\right]$ or $\left[\frac{\partial^2 p}{\partial x_i \partial x_j}\right]$.

We now show how to interpolate $[p]$ at the intersection Q , denoted as $[p]_Q$. According to Eqn. (1), we need $[p]_Q$ with $O(h^3)$ accuracy so that the local truncation error of the seven-point discrete Laplacian is $O(h)$. For an arbitrary triangular panel $\triangle ABC$ shown in Fig. 2 (a), suppose we are given the principal jump condition $[p]$ at the vertices A, B and C and the edge middle points D, E and F with at least $O(h^3)$ accuracy. We can interpolate $[p]_Q$ with $O(h^3)$ accuracy using the following third order quadratic interpolation scheme

$$[p] = c_0 + c_1\xi + c_2\eta + c_3\xi^2 + c_4\eta^2 + c_5\xi\eta + O(h^3), \quad (16)$$

where $\xi = s_\alpha/\ell_\alpha$ and $\eta = s_\beta/\ell_\beta$ are nondimensional coordinates along the s_α and s_β axes in Fig. 2 (a), and c' s are coefficients. The points A, B, C, D, E and F are represented by the nondimensional coordinates as $A(-1, 0)$, $B(1, -2)$, $C(1, 2)$, $D(0, -1)$, $E(1, 0)$ and $F(0, 1)$, and $[p]$ at these points are given as $[p]_A$, $[p]_B$, $[p]_C$, $[p]_D$, $[p]_E$ and $[p]_F$. So we have the following linear system to

determine the coefficients $c's$

$$\begin{pmatrix} 1 & -1 & 0 & 1 & 0 & 0 \\ 1 & 1 & -2 & 1 & 4 & -2 \\ 1 & 1 & 2 & 1 & 4 & 2 \\ 1 & 0 & -1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} c_0 \\ c_1 \\ c_2 \\ c_3 \\ c_4 \\ c_5 \end{pmatrix} = \begin{pmatrix} [p]_A \\ [p]_B \\ [p]_C \\ [p]_D \\ [p]_E \\ [p]_F \end{pmatrix}, \quad (17)$$

which has the solution

$$\begin{aligned} c_0 &= \frac{[p]_D + [p]_F}{2} - \frac{[p]_B + [p]_C - 2[p]_E}{8}, \\ c_1 &= \frac{[p]_E - [p]_A}{2}, \quad c_2 = \frac{[p]_F - [p]_D}{2} \\ c_3 &= \frac{[p]_A - [p]_D - [p]_F}{2} + \frac{[p]_B + [p]_C + 2[p]_E}{8}, \\ c_4 &= \frac{[p]_B + [p]_C - 2[p]_E}{8}, \quad c_5 = \frac{[p]_C - [p]_B}{4} - \frac{[p]_F - [p]_D}{2}. \end{aligned}$$

To use the interpolation scheme in Eqn. (16) to interpolate $[p]_Q$, we need to know the nondimensional coordinates (ξ_Q, η_Q) of the point Q . From $\vec{MQ} = \xi_Q \ell_\alpha \boldsymbol{\alpha} + \eta_Q \ell_\beta \boldsymbol{\beta}$, we obtain

$$\xi_Q = \frac{(\vec{MQ} \times \boldsymbol{\beta}) \cdot \mathbf{n}}{\ell_\alpha (\boldsymbol{\alpha} \times \boldsymbol{\beta}) \cdot \mathbf{n}}, \quad \eta_Q = \frac{(\vec{MQ} \times \boldsymbol{\alpha}) \cdot \mathbf{n}}{\ell_\beta (\boldsymbol{\beta} \times \boldsymbol{\alpha}) \cdot \mathbf{n}}. \quad (18)$$

4. Numerical Tests

To test our computation of the Cartesian jump conditions, we construct the function p analytically such that it is discontinuous across a closed interface Γ as

$$p(x_1, x_2, x_3) = \begin{cases} \sin(x_1) \sin(x_2) \sin(x_3), & \text{outside } \Gamma, \\ e^{-x_1} e^{-x_2} e^{-x_3}, & \text{inside } \Gamma. \end{cases} \quad (19)$$

We represent the interface using a triangular mesh with mesh size of $O(h)$. We compute the Cartesian jump conditions from the analytical principal jump conditions using the processes presented in Sections 2.1 and 2.2. We then compare the computed results with the analytical Cartesian jump conditions. Fig. 3 shows that we obtain the desired second order accuracy for

Figure 3: The scaled infinity norms of the errors versus the scaled mesh sizes for (a) $\left[\frac{\partial p}{\partial x_1}\right]$ and (b) $\left[\frac{\partial p^2}{\partial x_1^2}\right]$.

$\left[\frac{\partial p}{\partial x_1}\right]$ and first order accuracy for $\left[\frac{\partial p^2}{\partial x_1^2}\right]$. We also obtain the desired accuracy for the other Cartesian jump conditions (not shown here).

The number of CG iterations required in computing $\left[\frac{\partial p}{\partial x_i}\right]$ (Section 2.1) remains relatively constant when the triangular meshes are refined for an interface, as indicated by Table 1. Note that as the meshes for a cone or a cylinder are refined, some of the triangular panels become very thin, but the relatively constant iteration numbers in the CG method suggests that the method is not sensitive to the distortion of the meshes. This is expected because the coefficient matrix of the linear system in Eqn. (8) depends on the connectivity but not the geometry of a mesh. Only drastic changes in mesh topology may change the condition number of the coefficient matrix.

Lastly, we use the computed Cartesian jump conditions to solve a Poisson equation subject to given principal jump conditions across a closed interface in 3D. The mathematical description of the test problem is

$$\begin{aligned} \Delta p &= f \quad \text{in } \Omega, \\ [p] &= J_p, \quad \left[\frac{\partial p}{\partial \mathbf{n}}\right] = J_n \quad \text{and} \quad [\Delta p] = [f] \quad \text{on } \Gamma, \\ \frac{\partial p}{\partial \mathbf{n}} &= b \quad \text{on } \partial\Omega, \end{aligned}$$

cube		cylinder		cone	
vertices/panels	iter	vertices/panels	iter	vertices/panels	iter
1352/2700	23	5762/11520	22	4322/8640	22
5768/11532	23	23810/47616	22	17858/35712	22
23816/47628	23	96770/193536	23	72578/145152	22
96776/193548	23	390146/780288	24	292610/585216	24
390152/780300	23	1566722/3133440	25	1175042/2350080	25

Table 1: The number of CG iterations vs the number of vertices/panels for a cube, a cylinder and a cone.

where Ω is a rectangular domain with the boundary $\partial\Omega$, and Γ is the interface in the domain. The right-hand side of the Poisson equation is

$$f(x_1, x_2, x_3) = \begin{cases} -3 \sin(x_1) \sin(x_2) \sin(x_3), & \text{outside } \Gamma, \\ 3e^{-x_1}e^{-x_2}e^{-x_3}, & \text{inside } \Gamma. \end{cases} \quad (20)$$

which is constructed using the analytical solution p given in Eqn. (19).

With the computed Cartesian jump conditions, the Poisson problem can be discretized on a uniform Cartesian grid of the spatial step h according to Eqn. (1), as described in Section 1. We use FFT from *fftpack* in serial computing (or MG from *hypre* in parallel computing) to solve the discretized Poisson problem and obtain the numerical solution. Fig. 4 shows the contours of the numerical solution at two slices of the computational domain for an interface of cone shape. As expected, we observe sharp jumps in the solution contours. Fig. 5 demonstrates that we achieve the desired second order accuracy of our solution in the infinity norm for an interface of sphere, cube, cylinder or cone shape. In the grid refinement study for Fig. 5, the Cartesian grid and the triangular mesh are refined together to keep the same order of sizes.

5. Conclusions

In this paper, we present and test a method to compute the necessary Cartesian jump conditions from the given principal jump conditions for a function that is discontinuous across an interface in 3D using triangular mesh representation of the interface. All the necessary Cartesian jump conditions are computed very efficiently with desired accuracy.

Figure 4: Contours of the solution at two slices for a Poisson equation subject to an interface with the shape of a cone: (a) an x_1x_3 slice, (b) an x_1x_2 slice.

Figure 5: The scaled infinity norms of the errors versus the scaled sizes of triangular meshes and Cartesian grids for the computed solution p of a Poisson equation.

We first establish a small 3×3 linear system for the Cartesian jump conditions of the first-order derivatives of the function at the middle point (the point M in Fig. 2 (a)) inside each triangular panel of the triangular mesh by differentiating the jump condition of the function itself on the panel. The Cartesian jump conditions of the first-order derivatives at the vertices of the mesh are related through interpolation with those at the middle points as a SPD system. The SPD system is solved using CG, which needs only a small number of iterations regardless of the interface shape, the mesh size and the mesh distortion. By differentiating the Cartesian jump conditions of the first-order derivatives along the edges of the mesh, we then establish a small over-determined 7×6 linear system for the Cartesian jump conditions of the second-order derivatives at each vertex. This linear system has a unique solution and can be solved analytically. We also present how to interpolate from the vertices the necessary Cartesian jump conditions at the intersections of the interface and Cartesian grid lines. The jump corrections for finite difference stencils along the grid lines can then be obtained. Finally, we test our method by using the computed Cartesian jump conditions in the IIM to solve a Poisson equation subject to an interface with the shape of a sphere, cube, cylinder or cone. The results demonstrate the expected second-order accuracy of the solution in the infinity norm.

The triangular mesh representation is simple and robust to represent a complex or non-smooth interface. Our contributions in this paper therefore enhance the robustness of the IMM to handle complex or non-smooth interfaces in applications, including fluid-solid interaction.

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