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A NOTE ON IMMERSED INTERFACE METHOD FOR THREE DIMENSIONAL ELLIPTIC EQUATIONS *

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Abstract. The *Immersed Interface Method* proposed by LeVeque and Li [SIAM J. Numer. Anal. 31, No.4 (1994)] is extended to three dimensional elliptic equations of the form:

$$\nabla \cdot (\beta(x)\nabla u(x)) + \kappa(x)u(x) = f(x).$$

We study the situation in which there is an irregular interface (surface) S contained in the solution domain across which β, κ and f may be discontinuous or even singular. As a result, the solution u will usually be non-smooth or even discontinuous. A finite difference approach with a uniform Cartesian grid is used in the discretization. Local truncation error analysis is performed to estimate the accuracy of the numerical solution.

Key words. 3D elliptic equation, finite difference methods, irregular interface, discontinuous coefficients, singular source term, delta functions, Cartesian grid, immersed interface method

AMS subject classifications. 65N06, 65N50

1. Introduction. Solving elliptic equations with discontinuous coefficients is a fundamental problem in various important applications, for example at the interface between two materials with different diffusion parameters in steady state heat diffusion or electrostatic problems. Such problems also arise in multicomponent flow problems, *e.g.*, the porous media equations used to model the interface between oil and injected fluid in simulations of secondary recovery in oil reservoirs [1], [2], [10].

Consider the general three-dimensional problem

$$(1)\quad (\beta\, u_x)_x + (\beta\, u_y)_y + (\beta\, u_z)_z + \kappa(x,y,z)\, u = f(x,y,z), \qquad (x,y,z) \in \Omega,$$

in some region Ω, where all the coefficients β, κ, and f may be discontinuous across an interface, which is usually a surface S: $x = x(\mu,\nu)$, $y = y(\mu,\nu)$, $z = z(\mu,\nu)$. The interface S divides the solution domain in two parts which we denote as the $+$ side and $-$ side respectively. By convention the normal direction $\vec{n}$ points toward the $+$ side. When there is a sources or a sink on the interface, a delta function or its derivative singularity would appear in the expression of $f(x,y,z)$, for example

$$(2)\qquad f(x,y,z) = \iint_S C(\mu,\nu)\, \delta_3\left(\vec{x} - \vec{X}(\mu,\nu)\right)\, d\mu\, d\nu,$$

where $\vec{x} = (x,y,z)$, $\vec{X}(\mu,\nu) = (x(\mu,\nu), y(\mu,\nu), z(\mu,\nu))$, δ_3 is a three dimensional Dirac function and $C(\mu,\nu)$ is the source strength. Consequently there would be a jump either in the normal derivative or in the solution itself or both. To make the problem (1) well-posed, we assume we know the following jump conditions defined as the difference of the limiting values between the $+$ side and $-$ side at any point of the interface

$$(3)\qquad [u] = w(\mu,\nu),$$

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$$[\beta \frac{\partial u}{\partial n}] = q(\mu, \nu). \tag{4}$$

Such jump conditions can usually be obtained either from physical reasoning or the partial differential equation itself.

In the *immersed interface method* developed in [3], [4] and here, we are able to handle discontinuities and singularities simultaneously. The computational frame is finite difference with a uniform Cartesian grid. One obvious advantage of such a grid is that there is almost no cost for grid generation, and the conventional difference schemes can be used at most grid points (regular). Only those near the interface, which are usually much fewer than the regular grid points, need special attention.

Among other approaches in dealing with discontinuous coefficients problems are *harmonic averaging* [2], [10], [12], *the smoothing technique*, [11], [13], and *flux correction* [6] *etc.* Some of these methods work well in one dimensional problems but are hard to implement in two or three dimensions. Almost all of them are only first order accurate in two or more dimensions.

Another more complicated application with singular sources arises in using Peskin's *immersed boundary method* to solve PDEs with complicated geometry [8], [9]. In Peskin's approach the boundary is immersed in a uniform Cartesian grid and the boundary condition is converted as a singular force term which usually has the form of (2). The immersed boundary method has being widely used for many problems in recent years. In Peskin's immersed boundary method, the discretized delta function is used to deal with the singularity in the source term. However this approach would smooth the solution and hence is only first order accurate. In a different approach, Mayo [7] uses an integral equation to get the necessary information to modify the difference scheme for Poisson and biharmonic equations on irregular regions.

In our approach we make use of the jump conditions to modify the difference scheme at irregular points near the interface. The local truncation error is controlled at these points so that the solution of the difference equations maintains second order accuracy on the entire uniform grid.

Although we only consider elliptic equations here, the immersed interface method has been used for time dependent problems as well such as heat equations, the Stokes flow with a moving interface [4] and wave propagations [5] *etc.* Some other problems are currently being investigated.

This note is an extension of the work by LeVeque and Li [3] to three dimensional problems. Readers are referred to [3] and [4] for more background on the problem, and analysis in one and two dimensions.

2. Interface relations.. At a point (x^*, y^*, z^*) on the interface, we need to use local coordinates to simplify the derivation of the interface relations. The local coordinates transformation from (x, y, z) to (ξ, η, ζ) are chosen so that ξ is parallel to the normal direction of the interface pointing toward the + side. The η- and ζ-axes are in the tangent plane passing through (x^*, y^*, z^*). In the neighborhood of this point, the interface can be expressed as

$$\xi = \chi(\eta, \zeta), \qquad \text{with} \qquad \chi(0,0) = 0, \;\; \chi_\eta(0,0) = 0, \;\; \chi_\zeta(0,0) = 0. \tag{5}$$

Similar to the proof given for two dimensional case in [4], we can prove that in the local coordinates the equation (1) is unchanged, so we will use the same notation for u, w, q, β, κ and f. The jumps w and q in (3) and (4) are only defined on the interface and they are functions of η and ζ in the local coordinates.

As we did in [3] and [4], we use the jump conditions and their derivatives as well as the differential equation itself to get the interface relations between the quantities on the two sides of the interface surface. Let us first differentiate (3) with respect to η and ζ respectively to get

$$[u_\xi]\chi_\eta + [u_\eta] = w_\eta, \tag{6}$$

$$[u_\xi]\chi_\zeta + [u_\zeta] = w_\zeta. \tag{7}$$

Differentiating (6) with respect to ζ yields

$$\chi_\eta \frac{\partial}{\partial\zeta}[u_\xi] + \chi_{\eta\zeta}\,[u_\xi] + [u_{\eta\xi}]\,\chi_\zeta + [u_{\eta\zeta}] = w_{\eta\zeta}. \tag{8}$$

Differentiating (6) with respect to η and differentiating (7) with respect to ζ respectively we obtain

$$\chi_\eta \frac{\partial}{\partial\eta}[u_\xi] + \chi_{\eta\eta}\,[u_\xi] + \chi_\eta\,[u_{\eta\xi}] + [u_{\eta\eta}] = w_{\eta\eta}, \tag{9}$$

$$\chi_\zeta \frac{\partial}{\partial\zeta}[u_\xi] + \chi_{\zeta\zeta}\,[u_\xi] + \chi_\zeta\,[u_{\zeta\xi}] + [u_{\zeta\zeta}] = w_{\zeta\zeta}. \tag{10}$$

Before differentiating the jump of the normal derivative (4), we first express the unit normal vector of the interface S as

$$\vec{n} = \frac{(1,\ -\chi_\eta,\ -\chi_\zeta\ )}{\sqrt{1+{\chi_\eta}^2+{\chi_\zeta}^2}}. \tag{11}$$

So the interface condition (4) can be written as

$$[\beta\ (\,u_\xi - u_\eta\,\chi_\eta - u_\zeta\,\chi_\zeta\,)] = q(\eta,\zeta)\,\sqrt{1+{\chi_\eta}^2+{\chi_\zeta}^2}. \tag{12}$$

Differentiating this with respect to η gives

$$\begin{aligned} &[(\,\beta_\xi\,\chi_\eta + \beta_\eta\,)\ (\,u_\xi - u_\eta\,\chi_\eta - u_\zeta\,\chi_\zeta\,)] \\ &+ \left[\beta\left(\,u_{\xi\xi}\,\chi_\eta + u_{\xi\eta} - \chi_\eta\,\frac{\partial}{\partial\eta}u_\eta - \chi_\zeta\,\frac{\partial}{\partial\eta}u_\zeta - u_\eta\,\chi_{\eta\eta} - u_\zeta\,\chi_{\eta\zeta}\right)\right] \\ &= q_\eta\,\sqrt{1+{\chi_\eta}^2+{\chi_\zeta}^2} + q\,\frac{\chi_\eta\,\chi_{\eta\eta}}{\sqrt{1+{\chi_\eta}^2+{\chi_\zeta}^2}}. \end{aligned} \tag{13}$$

Similarly, differentiating (12) with respect to ζ gives

$$\begin{aligned} &[(\,\beta_\xi\,\chi_\zeta + \beta_\zeta\,)\ (\,u_\xi - u_\eta\,\chi_\eta - u_\zeta\,\chi_\zeta\,)] \\ &+ \left[\beta\left(u_{\xi\xi}\,\chi_\zeta + u_{\xi\zeta} - \chi_\eta\,\frac{\partial}{\partial\zeta}u_\eta - \chi_\zeta\,\frac{\partial}{\partial\zeta}u_\zeta - u_\eta\,\chi_{\eta\zeta} - u_\zeta\,\chi_{\zeta\zeta}\right)\right] \\ &= q_\zeta\,\sqrt{1+{\chi_\eta}^2+{\chi_\zeta}^2} + q\,\frac{\chi_\zeta\,\chi_{\zeta\zeta}}{\sqrt{1+{\chi_\eta}^2+{\chi_\zeta}^2}}. \end{aligned} \tag{14}$$

At the origin, $\chi_\eta(0,0) = \chi_\zeta(0,0) = 0$, and from (6)–(14) we can conclude that

$$
\begin{aligned}
u^+ &= u^- + w, \\
u^+_\xi &= \frac{\beta^-}{\beta^+}\, u^-_\xi + \frac{q}{\beta^+}, \\
u^+_\eta &= u^-_\eta + w_\eta, \\
u^+_\zeta &= u^-_\zeta + w_\zeta, \\
u^+_{\eta\zeta} &= u^-_{\eta\zeta} + u^-_\xi \chi_{\eta\zeta} - u^+_\xi \chi_{\eta\zeta} + w_{\eta\zeta}, \\
u^+_{\eta\eta} &= u^-_{\eta\eta} + (u^-_\xi - u^+_\xi)\chi_{\eta\eta} + w_{\eta\eta}, \\
u^+_{\zeta\zeta} &= u^-_{\zeta\zeta} + (u^-_\xi - u^+_\xi)\chi_{\zeta\zeta} + w_{\zeta\zeta}, \\
u^+_{\xi\eta} &= \frac{\beta^-}{\beta^+}\, u^-_{\xi\eta} + \left(u^+_\eta - \frac{\beta^-}{\beta^+}\, u^-_\eta\right) \chi_{\eta\eta} + \left(u^+_\zeta - \frac{\beta^-}{\beta^+}\, u^-_\zeta\right) \chi_{\eta\zeta} \\
&\quad + \frac{\beta^-_\eta}{\beta^+}\, u^-_\xi - \frac{\beta^+_\eta}{\beta^+}\, u^+_\xi + \frac{q_\eta}{\beta^+}, \\
u^+_{\xi\zeta} &= \frac{\beta^-}{\beta^+}\, u^-_{\xi\zeta} + \left(u^+_\eta - \frac{\beta^-}{\beta^+}\, u^-_\eta\right) \chi_{\eta\zeta} + \left(u^+_\zeta - \frac{\beta^-}{\beta^+}\, u^-_\zeta\right) \chi_{\zeta\zeta} \\
&\quad + \frac{\beta^-_\zeta}{\beta^+} u^-_\xi - \frac{\beta^+_\zeta}{\beta^+} u^+_\xi + \frac{q_\zeta}{\beta^+}.
\end{aligned} \tag{15}
$$

To get the relation for $u^+_{\xi\xi}$ we need to use the differential equation (1) itself from which we can write

$$
[\,\beta\,(u_{\xi\xi} + u_{\eta\eta} + u_{\zeta\zeta}) + \beta_\xi u_\xi + \beta_\eta u_\eta + \beta_\zeta u_\zeta + \kappa u\,] = [f]\,. \tag{16}
$$

Notice that

$$
\kappa^- u^- - \kappa^+ u^+ = \kappa^- u^- - \kappa^+ u^- + \kappa^+ u^- - \kappa^+ u^+ = -[\kappa] u^- - \kappa^+ [u]. \tag{17}
$$

Rearranging equation (16) and using (17), we get

$$
\begin{aligned}
&\beta^+ \left(u^+_{\xi\xi} + u^+_{\eta\eta} + u^+_{\zeta\zeta}\right) + \beta^+_\xi\, u^+_\xi + \beta^+_\eta u^+_\eta + \beta^+_\zeta u^+_\zeta = \\
&\qquad \beta^- \left(u^-_{\xi\xi} + u^-_{\eta\eta} + u^-_{\zeta\zeta}\right) + \beta^-_\xi\, u^-_\xi \\
&\qquad + \beta^-_\eta\, u^-_\eta + \beta^-_\zeta\, u^-_\zeta + [f] + \kappa^- u^- - \kappa^+ u^+.
\end{aligned} \tag{18}
$$

Plugging the sixth and seventh equations of (15) into (18) and collecting terms finally we have

$$
\begin{aligned}
u^+_{\xi\xi} &= \frac{\beta^-}{\beta^+}\, u^-_{\xi\xi} + \left(\frac{\beta^-}{\beta^+} - 1\right) u^-_{\eta\eta} + \left(\frac{\beta^-}{\beta^+} - 1\right) u^-_{\zeta\zeta} + \\
&\quad u^+_\xi \left(\chi_{\eta\eta} + \chi_{\zeta\zeta} - \frac{\beta^+_\xi}{\beta^+}\right) - u^-_\xi \left(\chi_{\eta\eta} + \chi_{\zeta\zeta} - \frac{\beta^-_\xi}{\beta^+}\right) \\
&\quad + \frac{1}{\beta^+}\left(\beta^-_\eta u^-_\eta - \beta^+_\eta u^+_\eta\right) + \frac{1}{\beta^+}\left(\beta^-_\zeta u^-_\zeta - \beta^+_\zeta u^+_\zeta\right) \\
&\quad - \frac{1}{\beta^+}\left([\kappa] u^- + \kappa^+ [u]\right) + \frac{[f]}{\beta^+} - w_{\eta\eta} - w_{\zeta\zeta}.
\end{aligned} \tag{19}
$$

3. The difference scheme. At regular grid points, we still use the classical central difference scheme which has a seven-point stencil. The local truncation errors at these grid points are $O(h^2)$. So we will concentrate below on developing difference formulas for the irregular grid points for which the interface cuts through the classical seven-point stencil. Taking a typical irregular grid point, say (x_i, y_j, z_k), we try to develop the modified difference scheme at this point. Because the interface is one dimension lower than the solution domain, the number of irregular grid points will be $O(n^2)$ compared to the total number of grid points, which is $O(n^3)$. We can require the local truncation error for the difference scheme at irregular grid points to be $O(h)$ without affecting the second order accuracy globally. Let us write the difference scheme as follows:

$$\sum_m \gamma_m \, u_{i+i_m, j+j_m, k+k_m} + \kappa_{ijk} \, u_{ijk} = f_{ijk} + C_{ijk}, \tag{20}$$

where i_m, j_m, k_m may be $0, \pm 1, \pm 2, \cdots$. Of course we want the number of grid points involved to be as few as possible. So first we need to determine the stencil, and then find the coefficients γ_m and the correction term C_{ijk} for the given stencil.

The analysis is similar to the two dimensional case as presented in [3] and [4] but more complicated in three dimensions. We take a point (x^*, y^*, z^*) on the interface surface near (x_i, y_j, z_k) and use local coordinates (ξ, η, ζ) at (x^*, y^*, z^*). For the elliptic equation the coefficients γ_m should be of order $O(1/h^2)$. So if we expand $u_{i+i_m, j+j_m, k+k_m}$ in the difference scheme about the origin of the local coordinates from each side of the surface S, we need to match up to second derivatives to guarantee that the local truncation error is $O(h)$. Using the ten interface relations (15) and (19) to eliminate quantities at the $(+)$ side of the interface, the Taylor expansion of (20) will then contain u^-, u_ξ^-, u_η^-, u_ζ^-, $u_{\xi\xi}^-$, $u_{\eta\eta}^-$, $u_{\zeta\zeta}^-$, $u_{\xi\eta}^-$, $u_{\xi\zeta}^-$, and $u_{\eta\zeta}^-$. To match them we need altogether ten grid points to get ten equations for the γ_ms. Thus we need to find three additional points besides the standard seven-point stencil. The three additional grid points can be taken from any of the twenty grid points $(i \pm 1, j \pm 1, k \pm 1)$, $(i \pm 1, j \pm 1, k)$, $(i \pm 1, j, k \pm 1)$, $(i, j \pm 1, k \pm 1)$.

Once we have determined the stencil we need to find the coefficients of the difference scheme. The local truncation error of the difference scheme is

$$T_{ijk} = \sum_m \gamma_m \, u_{i+i_m, j+j_m, k+k_m} + \kappa_{ijk} \, u_{ijk} - f_{ijk} - C_{ijk}. \tag{21}$$

We will force T_{ijk} to be $O(h)$ by choosing the coefficients γ_ms. To get the equations for those coefficients we use Taylor expansion of (20) about (x^*, y^*, z^*), the origin of the local coordinates. If the grid point (x_i, y_j, z_k) is on the $(-)$ side, we will get

$$\begin{aligned} T_{ijk} \;=\; & a_1 u^- + a_2 u^+ + a_3 u_\xi^- + a_4 u_\xi^+ + a_5 u_\eta^- + a_6 u_\eta^+ + a_7 u_\zeta^- + a_8 u_\zeta^+ \\ & + a_9 u_{\xi\xi}^- + a_{10} u_{\xi\xi}^+ + a_{11} u_{\eta\eta}^- + a_{12} u_{\eta\eta}^+ + a_{13} u_{\zeta\zeta}^- \\ & + a_{14} u_{\zeta\zeta}^+ + a_{15} u_{\xi\eta}^- + a_{16} u_{\xi\eta}^+ + a_{17} u_{\xi\zeta}^- + a_{18} u_{\xi\zeta}^+ \\ & + a_{19} u_{\eta\zeta}^- + a_{20} u_{\eta\zeta}^+ + \kappa^- u^- - f^- - C_{ijk} + O(h). \end{aligned} \tag{22}$$

The coefficients a_j depend only on the position of the stencil relative to the interface. They are independent of the functions u, κ and f. If we define the index sets K^+ and K^- by

$$K^\pm = \{k : \; (\xi_k, \eta_k, \zeta_k) \text{ is on the } \pm \text{ side of } S\},$$

then the a_j are given by

$$a_1 = \sum_{k\in K^-} \gamma_k \qquad a_2 = \sum_{k\in K+} \gamma_k$$
$$a_3 = \sum_{k\in K^-} \xi_k\gamma_k \qquad a_4 = \sum_{k\in K+} \xi_k\gamma_k$$
$$a_5 = \sum_{k\in K^-} \eta_k\gamma_k \qquad a_6 = \sum_{k\in K+} \eta_k\gamma_k$$
$$a_7 = \sum_{k\in K^-} \zeta_k\gamma_k \qquad a_6 = \sum_{k\in K+} \zeta_k\gamma_k$$
$$a_9 = \frac{1}{2}\sum_{k\in K^-} \xi_k^2\gamma_k \qquad a_{10} = \frac{1}{2}\sum_{k\in K+} \xi_k^2\gamma_k$$
$$a_{11} = \frac{1}{2}\sum_{k\in K^-} \eta_k^2\gamma_k \qquad a_{12} = \frac{1}{2}\sum_{k\in K+} \eta_k^2\gamma_k$$
$$a_{13} = \frac{1}{2}\sum_{k\in K^-} \zeta_k^2\gamma_k \qquad a_{14} = \frac{1}{2}\sum_{k\in K+} \zeta_k^2\gamma_k$$
$$a_{15} = \sum_{k\in K^-} \xi_k\eta_k\gamma_k \qquad a_{16} = \sum_{k\in K+} \xi_k\eta_k\gamma_k$$
$$a_{17} = \sum_{k\in K^-} \xi_k\zeta_k\gamma_k \qquad a_{18} = \sum_{k\in K+} \xi_k\zeta_k\gamma_k$$
$$a_{19} = \sum_{k\in K^-} \eta_k\zeta_k\gamma_k \qquad a_{20} = \sum_{k\in K+} \eta_k\zeta_k\gamma_k$$

Using the interface relations (15) and (19), and rearranging (22) we have

$$\begin{aligned}
T_{ijk} \;=\; & \left(a_1 - a_{10}\frac{[\kappa]}{\beta^+}\right)u^- + a_2\, u^+ + \left\{a_3 - a_{10}\left(\chi_{\eta\eta} + \chi_{\zeta\zeta} - \frac{\beta_\xi^-}{\beta^+}\right)\right. \\
& \left. + a_{12}\,\chi_{\eta\eta} + a_{14}\,\chi_{\zeta\zeta} + a_{16}\,\frac{\beta_\eta^-}{\beta^+} + a_{18}\frac{\beta_\zeta^-}{\beta^+} + a_{20}\,\chi_{\eta\zeta}\right\} u_\xi^- \\
& + \left\{a_4 + a_{10}\left(\chi_{\eta\eta} + \chi_{\zeta\zeta} - \frac{\beta_\xi^+}{\beta^+}\right)\right. \\
& \left. - a_{12}\,\chi_{\eta\eta} - a_{14}\,\chi_{\zeta\zeta} - a_{16}\,\frac{\beta_\eta^+}{\beta^+} - a_{18}\,\frac{\beta_\zeta^+}{\beta^+} - a_{20}\,\chi_{\eta\zeta}\right\} u_\xi^+ \\
& + \left(a_5 + a_{10}\,\frac{\beta_\eta^-}{\beta^+} - a_{16}\,\frac{\beta^-}{\beta^+}\,\chi_{\eta\eta} - a_{18}\,\frac{\beta^-}{\beta^+}\,\chi_{\eta\zeta}\right)\, u_\eta^- \\
& + \left(a_6 - a_{10}\,\frac{\beta_\eta^+}{\beta^+} + a_{16}\,\chi_{\eta\eta} + a_{18}\,\chi_{\eta\zeta}\right)\, u_\eta^+ \\
& + \left(a_7 + a_{10}\,\frac{\beta_\zeta^-}{\beta^+} - a_{16}\,\frac{\beta^-}{\beta^+}\,\chi_{\eta\zeta} - a_{18}\,\frac{\beta^-}{\beta^+}\,\chi_{\zeta\zeta}\right)\, u_\zeta^- \qquad (23)
\end{aligned}$$

$$
\begin{aligned}
&+\left(a_8 - a_{10}\,\frac{\beta^+_\zeta}{\beta^+} + a_{16}\,\chi_{\eta\zeta} + a_{18}\,\chi_{\zeta\zeta}\right)\,u^+_\zeta \\
&+\left(a_9 + a_{10}\,\frac{\beta^-}{\beta^+}\right)u^-_{\xi\,\xi} + \left(a_{11} + a_{12} + a_{10}\,(\frac{\beta^-}{\beta^+} - 1)\right)\,u^-_{\eta\,\eta} \\
&+\left(a_{13} + a_{14} + a_{10}\,\left(\frac{\beta^-}{\beta^+} - 1\right)\right)\,u^-_{\zeta\zeta} + \left(a_{15} + a_{16}\,\frac{\beta^-}{\beta^+}\right)\,u^-_{\xi\,\eta} \\
&+\left(a_{17} + a_{18}\,\frac{\beta^-}{\beta^+}\right)\,u^-_{\xi\zeta} + (a_{19} + a_{20})\,u^-_{\eta\zeta} + a_{12}\,w_{\eta\eta} + a_{14}\,w_{\zeta\zeta} \\
&+a_{10}\left(\frac{[f]}{\beta^+} - \frac{\kappa^+\,[u]}{\beta^+} - w_{\eta\eta} - w_{\zeta\zeta}\right) + a_{16}\,\frac{q_\eta}{\beta^+} \\
&+a_{18}\,\frac{q_\zeta}{\beta^+} + a_{20}\,w_{\eta\zeta} + \kappa^-\,u^- - f^- - C_{ijk}.
\end{aligned}
$$

Now it is clear that to make T_{ijk} to be $O(h)$ we should set

$$
a_1 - a_{10}\,\frac{[\kappa]}{\beta^+} + a_2 = 0, \tag{24}
$$

$$
\begin{aligned}
&a_3 - a_{10}\,\left(\chi_{\eta\eta} + \chi_{\zeta\zeta} - \frac{\beta^-_\xi}{\beta^+}\right) + a_{12}\,\chi_{\eta\eta} + a_{14}\,\chi_{\zeta\zeta} + a_{16}\,\frac{\beta^-_\eta}{\beta^+} \\
&+ a_{18}\,\frac{\beta^-_\zeta}{\beta^+} + a_{20}\,\chi_{\eta\zeta} + \frac{\beta^-}{\beta^+}\,\left\{a_4 + a_{10}\,\left(\chi_{\eta\eta} + \chi_{\zeta\zeta} - \frac{\beta^+_\xi}{\beta^+}\right)\right. \\
&\left. -a_{12}\,\chi_{\eta\eta} - a_{14}\,\chi_{\zeta\zeta} - a_{16}\,\frac{\beta^+_\eta}{\beta^+} - a_{18}\,\frac{\beta^+_\zeta}{\beta^+} - a_{20}\,\chi_{\eta\zeta}\right\} = \beta^-_\xi\,,
\end{aligned} \tag{25}
$$

$$
\begin{aligned}
&a_5 + a_{10}\frac{\beta^-_\eta}{\beta^+} - a_{16}\,\frac{\beta^-}{\beta^+}\,\chi_{\eta\eta} - a_{18}\,\frac{\beta^-}{\beta^+}\,\chi_{\eta\zeta} \\
&+ a_6 - a_{10}\,\frac{\beta^+_\eta}{\beta^+} + a_{16}\,\chi_{\eta\eta} + a_{18}\,\chi_{\eta\zeta} = \beta^-_\eta\,,
\end{aligned} \tag{26}
$$

$$
\begin{aligned}
&a_7 + a_{10}\,\frac{\beta^-_\zeta}{\beta^+} - a_{16}\,\frac{\beta^-}{\beta^+}\,\chi_{\eta\zeta} - a_{18}\,\frac{\beta^-}{\beta^+}\,\chi_{\zeta\zeta} \\
&+ a_8 - a_{10}\,\frac{\beta^+_\zeta}{\beta^+} + a_{16}\,\chi_{\eta\zeta} + a_{18}\,\chi_{\zeta\zeta} = \beta^-_\zeta\,,
\end{aligned} \tag{27}
$$

$$
a_9 + a_{10}\,\frac{\beta^-}{\beta^+} = \beta^-\,, \tag{28}
$$

$$
a_{11} + a_{12} + a_{10}\left(\frac{\beta^-}{\beta^+} - 1\right) = \beta^-, \tag{29}
$$

$$
a_{13} + a_{14} + a_{10}\left(\frac{\beta^-}{\beta^+} - 1\right) = \beta^-, \tag{30}
$$

$$
a_{15} + a_{16}\,\frac{\beta^-}{\beta^+} = 0, \tag{31}
$$

$$
a_{17} + a_{18}\,\frac{\beta^-}{\beta^+} = 0, \tag{32}
$$

$$
a_{19} + a_{20} = 0. \tag{33}
$$

This is a system of ten equations with ten variables. We can solve this system to get the coefficients γ_m of the difference scheme at this particular irregular grid point. Once we know the γ_m, we know the a_i as well, so we can calculate the correction term from the following:

$$\begin{aligned} C_{ijk} &= a_{10}\left(\frac{[f]}{\beta^+} - \frac{\kappa^+[u]}{\beta^+} - w_{\eta\eta} - w_{\zeta\zeta}\right) + a_{12}\, w_{\eta\eta} + a_{14}\, w_{\zeta\zeta} \\ &\quad + a_{16}\frac{q_\eta}{\beta^+} + a_{18}\frac{q_\zeta}{\beta^+} + a_{20}\, w_{\eta\zeta} + a_2\,[u] \\ &\quad + \frac{1}{\beta^+}\left\{a_4 + a_{10}\left(\chi_{\eta\eta} + \chi_{\zeta\zeta} - \frac{\beta^+_\xi}{\beta^+}\right) - a_{12}\,\chi_{\eta\eta}\right. \\ &\quad \left. - a_{14}\,\chi_{\zeta\zeta} - a_{16}\frac{\beta^+_\eta}{\beta^+} - a_{18}\frac{\beta^+_\zeta}{\beta^+} - a_{20}\,\chi_{\eta\zeta}\right\} q \\ &\quad + \left(a_6 - a_{10}\frac{\beta^+_\eta}{\beta^+} + a_{16}\,\chi_{\eta\eta} + a_{18}\,\chi_{\eta\zeta}\right) w_\eta \\ &\quad + \left(a_8 - a_{10}\frac{\beta^+_\zeta}{\beta^+} + a_{16}\,\chi_{\eta\zeta} + a_{18}\,\chi_{\zeta\zeta}\right) w_\zeta. \end{aligned} \tag{34}$$

If the grid point is on $(+)$ side, there are two ways to deal with it. The first one is to modify the correction term C_{ijk} and the linear system (24)–(33) slightly. Use the following relation

$$\begin{aligned} \kappa^+ u^+ &= \kappa^- u^- + \kappa^+ u^+ - \kappa^- u^- \\ &= \kappa^- u^- + \kappa^+ [u] + [\kappa]\, u^-, \end{aligned} \tag{35}$$

and let the difference scheme at this irregular (x_i, y_j, z_k) be:

$$\sum_m \hat{\gamma}_m\, u_{i+i_m, j+j_m, k+k_m} + \kappa_{ijk}\, u_{ijk} = f_{ijk} + \hat{C}_{ijk}. \tag{36}$$

Then $\hat{\gamma}_m$ still satisfy equations (25)–(33). Now the first equation becomes

$$a_1 - a_{10}\frac{[\kappa]}{\beta^+} + a_2 = -[\kappa], \tag{37}$$

and the correction term $\hat{C}_{ijk}$ is

$$\hat{C_{ijk}} = C_{ijk} + \kappa^+[u] - [f]. \tag{38}$$

The other way is simply to reverse the roles of the two sides $(+)$ and $(-)$ in the discussion above.

The immersed interface method discussed above has several nice properties. It appears to be second order accurate and can capture the sharpness if the solution is non-smooth or discontinuous. It can handle very general problems without much difficulty as we can see from an example below. Furthermore, if no interface is present then we will revert to the classical central difference scheme.

We have tested several examples. Although we can not take very fine grids to test the second order convergence due to the size limitation in three-dimensions, we do observe good numerical results. Below we give one test example.

Example 1. *We consider a problem in three dimensions with discontinuous coefficients as well as the singular sources. The equation is defined on the cube:* $-1 \le x, y, z, \le 1$ *and has the form*

$$(\beta u_x)_x + (\beta u_y)_y + (\beta u_z)_z + \kappa\, u = f,$$

where

$$\beta(x,y,z) = \begin{cases} 1 + x^2 + y^2 + z^2 & \textit{if } x^2 + y^2 + z^2 \le \frac{1}{4} \\ 1 & \textit{if } x^2 + y^2 + z^2 > \frac{1}{4}, \end{cases}$$

$$f(x,y,z) = \begin{cases} 6 + 11\left(x^2 + y^2 + z^2\right) \\ \dfrac{1}{x^2 + y^2 + z^2} - \dfrac{1}{\sqrt{x^2 + y^2 + z^2}} - \log\left(2\sqrt{x^2 + y^2 + z^2}\right), \end{cases}$$

$$\kappa(x,y,z) = \begin{cases} 1 & \textit{if } x^2 + y^2 + z^2 \le \frac{1}{4} \\ -1 & \textit{if } x^2 + y^2 + z^2 > \frac{1}{4}. \end{cases}$$

Dirichlet boundary conditions are determined from the exact solution

$$u(x,y,z) = \begin{cases} x^2 + y^2 + z^2 & \textit{if } x^2 + y^2 + z^2 \le \frac{1}{4} \\ \dfrac{1}{\sqrt{x^2 + y^2 + z^2}} + \log\left(2\sqrt{x^2 + y^2 + z^2}\right) & \textit{if } x^2 + y^2 + z^2 > \frac{1}{4}. \end{cases}$$

Table 1 lists the local truncation and global errors defined as

$$\| E_n \|_\infty = \max_{i,j,k} | u(x_i, y_j, z_k) - u_{ijk} |, \qquad \| T_n \|_\infty = \max_{i,j,k} | T_{ijk} |,$$

where n is the mesh size, $u(x_i, y_j, z_k)$ is the exact solution and u_{ijk} is the computed solution. The results show that our numerical method is about second order accurate as we refine the mesh. The ratio in column 3 approaches 4 meaning that $\| E_n \|$ is $O(h^2)$. And the ratio in column 5 approaches 2 meaning that $\| T_n \|$ is $O(h)$ as we have predicted.

TABLE 1
Numerical results for three dimensional Example 1.

n	$\| E_n \|_\infty$	ratio	$\| T_n \|_\infty$	ratio
20	9.2824×10^{-3}		1.1675	
40	2.8176×10^{-3}	3.2945	0.6587	1.7524
80	7.1043×10^{-4}	3.9656	0.3757	1.7728

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