DERIVATION OF PRINCIPAL JUMP CONDITIONS FOR THE IMMERSED INTERFACE METHOD IN TWO-FLUID FLOW SIMULATION

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ABSTRACT. In a flow of two immiscible incompressible viscous fluids, jump discontinuities of flow quantities appear at the two-fluid interface. The immersed interface method can accurately and efficiently simulate the flow without smearing the sharp interface by incorporating necessary jump conditions into a numerical scheme. In this paper, we systematically derive the principal jump conditions for the velocity, the pressure, and their normal derivatives.

1. Introduction. The flow of two immiscible fluids is used in many technological applications, ranging from manufacturing to lubricated transport. The direct numerical simulations of two-fluid problems have a potentially huge domain for increased understanding [3, 4]. Because of possible interface breakup/coalescence in a two-fluid flow, it is generally difficult and inefficient to simulate the dynamics of each fluid separately in its own domain using an interface-fitted grid method and couple the dynamics of the two fluids through interfacial conditions.

Following Peskin's mathematical formulation in the immersed boundary method [9, 10], the two-fluid dynamics can be formulated in a single set of conservation equations for the whole flow field [11]. In particular, interfacial effects such as surface tension are included in the equations as a force term. This force term concentrates at the interface through the Dirac $\delta$ function, so it is called a singular force. With this unified formulation, the two-fluid dynamics can be efficiently computed using a fixed grid, for example, a fixed Cartesian grid.

Following Peskin’s immersed boundary method, the Dirac $\delta$ function in the formulation can be approximated by a narrow-supported smooth function. This approximation removes the force singularity and associated discontinuities, and thus allows for standard numerical schemes, but it has the drawbacks of interface smearing and low accuracy. The immersed interface method [6, 7, 8, 13, 14, 15] can overcome these drawbacks by directly incorporating jump conditions (caused by the singular force) into numerical schemes near an interface. With necessary jump conditions known, it can achieve second-order or higher accuracy. In this paper, the principal jump conditions for the velocity, the pressure, and their normal derivatives are derived for the immersed interface method to simulate two-fluid systems.
governed by the Navier-Stokes equations. In [5, 12], similar jump conditions are derived for single-fluid systems. In [2], principal pressure jump conditions are derived for Stokes equations with discontinuous viscosity. Through the use of the vorticity, our derivation in this paper is very concise and simple.

2. **Mathematical formulation.** Considering a two-fluid system in which each fluid has constant density and viscosity, the single set of conservation equations governing the whole system read

\[
\frac{\partial u_i}{\partial t} + \frac{\partial u_j u_j}{\partial x_j} = \frac{\partial \sigma_{ij}}{\partial x_j} + F_i + \rho G_i, \quad (1)
\]

\[
\frac{\partial u_i}{\partial x_i} = 0, \quad (2)
\]

where \(\rho\) is the density of the two-fluid system, \(u_i\) is the velocity, \(t\) is time, \(x_i (i = 1, 2, 3)\) is Cartesian coordinates, \(\sigma_{ij}\) is the stress tensor, \(F_i\) is a singular force representing interfacial effects, and \(G_i\) is a finite smooth body force. The stress tensor is given by

\[
\sigma_{ij} = -p \delta_{ij} + 2\mu e_{ij} = -p \delta_{ij} + \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right), \quad (3)
\]

where \(p\) is the pressure, \(\delta_{ij}\) is the Kronecker symbol, \(e_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)\) is the strain tensor, and \(\mu\) is the dynamic viscosity of the two-fluid system. In this paper, both tensor notation and vector notion may be used for the same quantity, for example, both \(x_i\) and \(\vec{x}_i\) are used to denote Cartesian coordinates.

The system density \(\rho\) and viscosity \(\mu\) can be written as

\[
\rho = \rho_1 H(\vec{x}, t) + \rho_2 (1 - H(\vec{x}, t)), \quad (4)
\]

\[
\mu = \mu_1 H(\vec{x}, t) + \mu_2 (1 - H(\vec{x}, t)), \quad (5)
\]

where \(\rho_1\) and \(\mu_1\) are the constant density and viscosity of fluid 1, \(\rho_2\) and \(\mu_2\) are the constant density and viscosity of fluid 2, and \(H(\vec{x}, t)\) is a 3D step function (Heaviside function). The step function satisfies

\[
H(\vec{x}, t) = \begin{cases} 
1, & \vec{x} \in V_1, \\
0, & \vec{x} \notin V_1,
\end{cases} \quad (6)
\]

where \(V_1\) is the volume occupied by fluid 1 at time \(t\), as shown in Fig. 1 (a).

As shown in Fig. 1, the two-fluid interface is denoted as \(S\), and its Cartesian coordinates are denoted as \(\vec{X}\). The interface moves with the local fluid velocity

\[
\frac{d\vec{X}}{dt} = \vec{U}, \quad (7)
\]

where \(\vec{U} = \vec{u}(\vec{X}, t)\) is the fluid velocity at \(\vec{x} = \vec{X}\) and time \(t\).

In general, the singular force \(F_i\) can be expressed as

\[
F_i = \int_S f_i \delta(\vec{x} - \vec{X}) d\vec{X}, \quad (8)
\]

where \(f_i = f_i(\vec{X}, t)\) is the force density. The force density in the two-fluid system takes the following form [1]

\[
f_i = \gamma \left( \frac{1}{R_1} + \frac{1}{R_2} \right) n_i, \quad (9)
\]
3. Preparations for the derivation. The two-fluid interface is locally parametrized near an arbitrary interface point by two parameters $\alpha_1$ and $\alpha_2$ at time $t$, as shown in Fig. 1 (b). Near the point, the interface coordinates $\vec{X}$ and any jump condition can therefore be written as functions of $\alpha_1$, $\alpha_2$ and $t$. The parametrization is chosen such that at this particular point the two unit tangents $\vec{t}$ and $\vec{b}$ and the unit normal $\vec{n}$ to the interface are given by

$$
\vec{t} = \frac{\partial \vec{X}}{\partial \alpha_1}, \quad \vec{b} = \frac{\partial \vec{X}}{\partial \alpha_2}, \quad \vec{n} = \vec{t} \times \vec{b},
$$

where $\vec{n}$ points to fluid 2, as shown in Fig. 1 (a). In the following sections, jump conditions are derived for this arbitrary interface point. Although global Lagrangian parametrization was used in [13, 14, 15] for tracking solid boundaries, it is not suitable for tracking the two-fluid interface which may undergo topological change. The special local parametrization introduced here only needs local geometric information of the interface. It is convenient for both the theoretical derivation and the numerical implementation of jump conditions. The derived jump conditions can be directly used with any interface tracking/capturing techniques.

Hereafter the notation $[\cdot]$ is used to denote a jump across the interface, and it is defined as

$$
[\cdot] = (\cdot)_{\text{fluid}2} - (\cdot)_{\text{fluid}1}.
$$

Regarding the jump operator $[\cdot]$, there are two facts which will be used later without being mentioned. First, inside a jump, a piecewise constant coefficient $c$ (with
a discontinuity across the interface) can be freely moved inside or outside of a differential operator:
\[
\left\{ \frac{\partial (\cdot)}{\partial x_i} \right\} = \left\{ \frac{\partial c (\cdot)}{\partial x_i} \right\}.
\]
(12)

Second, the jump operator commutes with differentiation along the interface:
\[
\frac{\partial [\cdot]}{\partial \alpha_i} = \left\{ \frac{\partial (\cdot)}{\partial \alpha_i} \right\}, \quad l = 1, 2.
\]
(13)

Below are the formulas that will be used later for the derivation. The first one is
\[
\omega \times \vec{n} = \frac{\partial \vec{u}}{\partial \vec{n}} - (\nabla \vec{u}) \cdot \vec{n},
\]
(14)
where \(\omega\) is the vorticity. This formula comes from
\[
\epsilon_{ijk} \omega_j n_k = \epsilon_{ijp} \frac{\partial u_p}{\partial x_p} n_k = (\delta_{kp} \delta_{iq} - \delta_{kq} \delta_{ip}) \frac{\partial u_p}{\partial x_p} n_k = \frac{\partial u_p}{\partial x_p} n_k - \frac{\partial u_k}{\partial x_i} n_k,
\]
where \(\epsilon_{ijk}\) denotes the permutation symbol and \(\delta_{ij}\) the Kronecker symbol.

The second one is
\[
[(\nabla \vec{u}) \cdot \vec{n}] = 0.
\]
(15)

**Proof.** The continuity equation (2) gives
\[
\lim_{\delta n \to 0} \int \frac{\partial}{\partial x_k} \left( \frac{\partial u_k}{\partial x_i} \right) d\mathcal{V} = 0 \implies \left[ \frac{\partial u_k}{\partial x_i} \right] n_k \delta \mathcal{S} = 0 \implies \left[ \frac{\partial u_k}{\partial x_i} \right] n_k = 0,
\]
where the control volume \(\delta \mathcal{V}\) is formed by sweeping an infinitesimal area \(\delta \mathcal{S}\) on the interface \(\mathcal{S}\) in the direction of \(\vec{n}\) and \(-\vec{n}\) by \(\delta n\).

The third one is the following relation at the interface
\[
\vec{n} \cdot (\nabla \omega) = \frac{\partial (\vec{\tau} \cdot (\omega \times \vec{n}))}{\partial \alpha_1} + \frac{\partial (\vec{b} \cdot (\omega \times \vec{n}))}{\partial \alpha_2}.
\]
(16)

**Proof.** The left hand side of equation (16) is
\[
\vec{n} \cdot (\nabla \omega) = (\epsilon_{ijk} \tau_j b_k) \left( \epsilon_{imn} \frac{\partial \omega_n}{\partial x_m} \right) = (\delta_{jm} \delta_{kn} - \delta_{jn} \delta_{km}) \tau_j b_k \frac{\partial \omega_n}{\partial x_m} = \tau_j b_k \frac{\partial \omega_k}{\partial x_j} - \tau_j b_k \frac{\partial \omega_j}{\partial x_k} = \frac{\partial \vec{\omega}}{\partial \tau} \cdot \vec{b} - \frac{\partial \vec{\omega}}{\partial \vec{b}} \cdot \vec{\tau}.
\]
Using the equality
\[
\omega \times \vec{n} = \vec{\omega} \times (\vec{\tau} \times \vec{b}) = (\vec{\omega} \cdot \vec{b}) \vec{\tau} - (\vec{\omega} \cdot \vec{\tau}) \vec{b},
\]
the right hand side of equation (16) is
\[
\frac{\partial (\vec{\tau} \cdot (\omega \times \vec{n}))}{\partial \alpha_1} + \frac{\partial (\vec{b} \cdot (\omega \times \vec{n}))}{\partial \alpha_2} = \frac{\partial (\vec{\omega} \cdot \vec{b})}{\partial \alpha_1} \frac{\partial \vec{\tau}}{\partial \alpha_2} + \frac{\partial (\vec{\omega} \cdot \vec{\tau})}{\partial \alpha_1} \frac{\partial \vec{b}}{\partial \alpha_2} = \frac{\partial \vec{\omega}}{\partial \alpha_1} \cdot \vec{b} - \frac{\partial \vec{\omega}}{\partial \alpha_2} \cdot \vec{\tau} + \vec{\omega} \cdot \left( \frac{\partial \vec{b}}{\partial \alpha_1} - \frac{\partial \vec{\tau}}{\partial \alpha_2} \right).
\]
The particular local parametrization introduced above implies
\[
\frac{\partial \tilde{\omega}}{\partial \alpha_1} = \frac{\partial \tilde{\omega}}{\partial \tau}, \quad \frac{\partial \tilde{\omega}}{\partial \alpha_2} = \frac{\partial \tilde{\omega}}{\partial b}, \quad \frac{\partial \tilde{b}}{\partial \alpha_1} - \frac{\partial \tilde{\tau}}{\partial \alpha_2} = 0.
\]
So the right hand side of equation (16) also equals to
\[
\frac{\partial \tilde{\omega}}{\partial \tau} \cdot \tilde{b} - \frac{\partial \tilde{\omega}}{\partial b} \cdot \tilde{\tau},
\]
and equation (16) is proved. \(\square\)

4. Principal jump conditions. First, jump conditions for the velocity, the pressure, and their normal derivatives are derived. These jump conditions are called the principal jump conditions since they are the starting point for the derivation of jump conditions of Cartesian derivatives.

Continuity equation (2) implies the continuity of the normal component of the velocity across the interface, and the continuity of the tangential component is a physical requirement of the viscous flow, so the velocity is continuous.

**Proposition 1.** The velocity is continuous at the two-fluid interface,
\[
[u_i] = 0. \tag{17}
\]
Equation (7) in Section 2, which indicates that the interface moves with the local fluid velocity, has already assumed the continuity of the velocity. Define
\[
u_i = \frac{\nu_i}{\rho} = \nu u_i, \tag{18}
\]
where \(\nu = \frac{\mu}{\rho}\) denotes the kinematic viscosity. Proposition 1 gives
\[
[u_i^*] = [\nu] U_i, \tag{19}
\]
where \(U_i\) is the interface velocity (as defined before for equation (7)). Using Proposition 1, it can be proved that the acceleration is also continuous [12].

**Corollary 1.**
\[
\frac{d[u_i]}{dt} = \left[\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j}\right] = 0. \tag{20}
\]
Equations (1), (3) and (20) (with the application of the continuity equation (2)) therefore imply
\[
\left[\frac{1}{\rho} \frac{\partial p}{\partial x_i}\right] = \left[\nu \frac{\partial^2 u_i}{\partial x_j \partial x_j}\right]. \tag{21}
\]

**Theorem 4.1.** The jump condition of the pressure satisfy
\[
[p] = f_n - 2[\mu] \left(\frac{\partial \tilde{U}}{\partial \tau} \cdot \tilde{\tau} + \frac{\partial \tilde{U}}{\partial b} \cdot \tilde{b}\right). \tag{22}
\]
where \(f_n = \tilde{f} \cdot \tilde{n}\) is the normal component of the force density.

**Proof.** As \(\delta n \to 0\), the momentum balance based on the momentum equation (1) in the control volume \(\delta V\) (\(\delta n\) and \(\delta V\) are defined in the proof of equation (14)) gives
\[
[\sigma_{ij}] n_j + f_i = 0,
\]
which can be written out as
\[
- [p] n_i + \left[\mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)\right] n_j + f_i = 0. \tag{23}
\]
Multiplying $n_i$ above and then using the equality
$$\tau_i \tau_j + b_i b_j + n_i n_j = \delta_{ij},$$
and applying the continuity equation (2) and equation (17), the result follows.  

**Theorem 4.2.** The normal derivative of the velocity satisfies the jump condition

$$-|\mu| \left( \begin{array}{c} \frac{\partial U}{\partial r} \cdot \hat{n} \\ \frac{\partial U}{\partial b} \cdot \hat{n} \end{array} \right) \tau_i + \left( \frac{\partial U}{\partial n} \right) \cdot \hat{b} = -f_\tau \tau_i - f_b b_i,$$

where $f_\tau = \hat{f} \cdot \hat{\tau}$ and $f_b = \hat{f} \cdot \hat{b}$ (For the two-fluid system with $\hat{f}$ given by equation (9), $f_\tau$ and $f_b$ equal to zero).

**Proof.** Equations (22) and (23) indicate

$$\mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) n_j = -f_i + f_n n_i - 2|\mu| \left( \frac{\partial U}{\partial r} \cdot \hat{\tau} + \frac{\partial U}{\partial b} \cdot \hat{b} \right) n_i.$$

Multiplying $\tau_i, b_i, \text{and} n_i$ above gives

$$\left[ \mu \left( \frac{\partial u_i}{\partial n} \right) \tau_i + \frac{\partial u_i}{\partial \hat{n}} \right] n_j = -f_i \Rightarrow \hat{n} \cdot \left[ \mu \left( \frac{\partial u_i}{\partial n} \right) \right] = \frac{\partial U}{\partial n} \cdot \hat{b},$$

which forms a linear system for $\left[ \mu \frac{\partial u_i}{\partial n} \right]$ as

$$C_1 \left[ \begin{array}{c} \mu \frac{\partial u_1}{\partial n} \\ \mu \frac{\partial u_2}{\partial n} \\ \mu \frac{\partial u_3}{\partial n} \end{array} \right] = \begin{pmatrix} -f_\tau - |\mu| \left( \frac{\partial U}{\partial r} \cdot \hat{n} \right) \\ -f_b - |\mu| \left( \frac{\partial U}{\partial b} \cdot \hat{n} \right) \\ -|\mu| \left( \frac{\partial U}{\partial r} \cdot \hat{\tau} + \frac{\partial U}{\partial b} \cdot \hat{b} \right) \end{pmatrix}, \quad (25)$$

where $[\cdot]$ denotes a jump for a column vector, and the non-singular coefficient matrix $C_1$ and its inverse $C_1^{-1}$ are

$$C_1 = \begin{pmatrix} \tau_1 & \tau_2 & \tau_3 \\ b_1 & b_2 & b_3 \\ n_1 & n_2 & n_3 \end{pmatrix}, \quad C_1^{-1} = \begin{pmatrix} \tau_1 & b_1 & n_1 \\ \tau_2 & b_2 & n_2 \\ \tau_3 & b_3 & n_3 \end{pmatrix}. \quad (26)$$

Solving this linear system gives equation (24).
The jump condition \( \frac{\partial u_i^*}{\partial n} \) (where \( u_i^* = \nu u_i \)) is related with the jump condition \( \left[ \frac{\partial u_i}{\partial n} \right] \) by

\[
\left[ \frac{\partial u_i^*}{\partial n} \right] = \frac{1}{\rho_2} \left[ \frac{\partial u_i}{\partial n} \right] - \frac{\rho_1}{\rho_1 \rho_2} \mu_1 \frac{\partial u_i}{\partial n}_{\text{fluid 1}}.
\] (27)

or

\[
\left[ \frac{\partial u_i^*}{\partial n} \right] = \frac{1}{\rho_1} \left[ \frac{\partial u_i}{\partial n} \right] - \frac{\rho_2}{\rho_1 \rho_2} \mu_2 \frac{\partial u_i}{\partial n}_{\text{fluid 2}}.
\] (28)

**Proof.** The first equality comes from

\[
\left[ \frac{\partial u_i^*}{\partial n} \right] = \left[ \nu \frac{\partial u_i}{\partial n} \right] - \frac{\mu_2}{\rho_2} \left[ \frac{\partial u_i}{\partial n}_{\text{fluid 2}} \right] - \frac{\mu_1}{\rho_1} \frac{\partial u_i}{\partial n}_{\text{fluid 1}} = \frac{1}{\rho_2} \left( \left[ \frac{\partial u_i}{\partial n}_{\text{fluid 2}} \right] + \mu_1 \frac{\partial u_i}{\partial n}_{\text{fluid 1}} \right) - \frac{\mu_1}{\rho_1} \frac{\partial u_i}{\partial n}_{\text{fluid 1}}.
\]

The second one can be shown similarly. \( \square \)

**Theorem 4.3.** The normal derivative of the pressure satisfies the jump condition

\[
\left[ \frac{1}{\rho} \frac{\partial p}{\partial n} \right] = \frac{\partial \tilde{f}_1}{\partial \alpha_1} + \frac{\partial \tilde{f}_2}{\partial \alpha_2}.
\] (29)

where \( \tilde{f}_1 \) and \( \tilde{f}_2 \) are

\[
\tilde{f}_1 = \bar{\tau} \cdot \left[ \nu \frac{\partial \bar{u}^*}{\partial n} \right] - \left[ \nu \right] \left( \frac{\partial \bar{U}}{\partial \tau} \cdot \bar{n} \right), \quad \tilde{f}_2 = \bar{b} \cdot \left[ \nu \frac{\partial \bar{u}^*}{\partial b} \right] - \left[ \nu \right] \left( \frac{\partial \bar{U}}{\partial b} \cdot \bar{n} \right).
\]

**Proof.** With the identity \( \Delta \bar{u} = -\nabla \times \bar{\omega} + \nabla (\nabla \cdot \bar{u}) \), Equations (21) and (16) indicate

\[
\left[ \frac{1}{\rho} \frac{\partial p}{\partial n} \right] = -\left[ \nu \bar{n} \cdot (\nabla \times \bar{\omega}) \right] = \frac{\partial}{\partial \alpha_1} (\bar{\tau} \cdot [\nu \bar{\omega} \times \bar{n}]) + \frac{\partial}{\partial \alpha_2} (\bar{b} \cdot [\nu \bar{\omega} \times \bar{n}]).
\]

Equations (14) and (15) indicate

\[
\bar{\tau} \cdot [\nu \bar{\omega} \times \bar{n}] = \bar{\tau} \cdot \left[ \nu \frac{\partial \bar{u}}{\partial n} \right] - \left[ \nu \right] \left( \frac{\partial \bar{U}}{\partial \tau} \cdot \bar{n} \right),
\]

\[
\bar{b} \cdot [\nu \bar{\omega} \times \bar{n}] = \bar{b} \cdot \left[ \nu \frac{\partial \bar{u}}{\partial b} \right] - \left[ \nu \right] \left( \frac{\partial \bar{U}}{\partial b} \cdot \bar{n} \right).
\]

So equation (29) follows. \( \square \)

Define

\[
p^* = \frac{p}{\rho}.
\] (30)

There are no local expressions for the jump conditions \( [\rho^*] \) and \( \left[ \frac{\partial \bar{u}}{\partial n} \right] \). These jump conditions depend on the global flow field, and they can be computed numerically.

Note that jump conditions for a uniform-fluid system are recovered with \( [\mu] = 0 \), \( [\rho] = 0 \) and \( [\nu] = 0 \).
REFERENCES


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