METHOD OF MULTIPLE COORDINATES FOR MOTIONS OF PARAMAGNETIC PARTICLES

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ABSTRACT

Method of multiple coordinates is used to investigate the motion of paramagnetic particles under a uniform magnetic field. The equation for the magnetic field decoupled from the equation for the flow field is solved with a series; the total magnetic field is considered as the sum of the locally defined fields written in terms of the local coordinates attached to each of the particles. The equation for the fluid flow is also solved with a series form in a similar fashion but some of the leading terms must be treated implicitly to avoid the numerical instability. The translational and rotational motions of the particles are determined from the balance between the magnetic and fluid’s viscous forces. We validated our methodology by comparing the numerical solutions with those given from the asymptotic analysis for a pair of particles in a very close proximity. The numerical solutions are also compared with those given from the solutions obtained with the use of the bi-polar coordinates. The motions of the paramagnetic particles are then investigated for various parameter sets.

INTRODUCTION

Understanding the motions of micro- and nano-particles in a viscous fluid is important in their applications, such as magnetic tweezers[1], biological assays[2-3], drug targeting[4], and mixing of fluid[5-10]. Very recently even a prototype of magnetic lab-on-a-chip for point-of-care sepsis diagnosis was reported [11]. Various applications of magnetism in microfluidic areas have been introduced by Pamme[12].

Most of the previous theoretical and numerical investigation of the motions of paramagnetic particles submerged in a viscous fluid has been performed with simple models, i.e. dipole models[13-17]. In this model the particle is considered as a dipole point which responding to an external magnetic field moves toward the field direction. Therefore interaction between neighboring particles has been considered through the dipole-dipole interaction only. Obviously this simple model cannot precisely capture the real dynamics of paramagnetic particles when the domain size is decreased or equivalently the particle size is increased, as is usual for the micro- and nano-fluidics.

Alternative approach to the investigation of the particle motions is performing the direct numerical simulation for the particles in suspension. Kang et al.[18] recently reported the simulation results for the two-dimensional case where particles in the cylindrical shape are scattered within a circular container under a uniform magnetic field. Their numerical results for a pair of particles however are open to validation because no solutions, numerical or analytical, have been reported to date for comparison.

Thus, this study has been motivated by the need to present accurate data for the motions of scattered paramagnetic particles subjected to a uniform magnetic field, to be used in verification of any new simulation method for investigating the particle motions. In this study
we propose the method of multiple coordinates in constructing semi-analytic solutions for the motions of multiple particles under a uniform magnetic field. The method will be validated by comparing the numerical results with those obtained from an asymptotic analysis for a pair of particles in a very close proximity. We also verify our method by comparing the numerical data with those calculated from the solutions treated in terms of the bi-polar coordinates.

FORMULATION AND NUMERICAL METHODS

Consider multiple paramagnetic particles with radius $a$ suspended within a circular cylinder of radius $aR$ containing a viscous fluid subject to a uniform magnetic field as shown in Fig. 1. We study the motion of particles as well as the induced fluid flow by using a semi-analytic method, i.e. a series-solution method, at low-Reynolds-number regime. Hereafter, all the variables are made dimensionless except for those having * as the superscript and those separately indicated. The lengths and spatial coordinates are scaled by $a$.

For two-dimensional problems, we can introduce magnetic scalar field $A$ (scaled by $aB_0^*$, where $B_0^*$ is the external magnetic field intensity) satisfying the Laplace equation, $\nabla^2 A = 0$. This equation must be solved both for the fluid and particle regions. We apply a constant flux density on the surrounding boundary $\partial \Omega_0$, corresponding to

$$A = y \quad \text{on } \partial \Omega_0. \quad (1)$$

Boundary conditions (in short BC hereafter) on the interface between the fluid and a particle $\Omega_i$ are

$$A_f = A_p \quad \text{on } \partial \Omega_i \quad (2)$$

$$\left( \frac{\partial A}{\partial n} \right)_f = \frac{1}{\mu_r} \left( \frac{\partial A}{\partial n} \right)_p \quad \text{on } \partial \Omega_i \quad (3)$$

where the subscripts “f” and “p” denote evaluation at the fluid and particle, respectively, and $n$ the local coordinate normal to the surface. The parameter $\mu_r$ is defined as $\mu_r = \mu_p / \mu_f$, where $\mu_f$ and $\mu_p$ denote the magnetic permeability of the fluid and solid, respectively. The fluid flow is solely driven by the motion of particles caused by the magnetic force. It can be shown that the magnetic force (in this paper, forces are scaled by $a^2 B_0^{*2} / \mu_f$) of the particle exerting on the fluid in contact reads

$$\mathbf{F}_m = \frac{1}{2} (1 - 1/\mu_r) \int_{\partial \Omega_i} \left[ \left( \frac{\partial A}{\partial s} \right)_p + \frac{1}{\mu_r} \left( \frac{\partial A}{\partial n} \right)_p \right] \mathbf{n}(s) \, ds \quad (4)$$

where the coordinate $s$ is along the tangential direction on the surface of the particle.

To solve the Laplace equation for the domain $\Omega_0$, we decompose $A$ into three parts as follows.

$$A = y + A^{(0)}(\xi_0, \eta_0) + \sum_{i=1}^N A^{(i)}(\xi_i, \eta_i) \quad \text{for } \Omega_0 \quad (5)$$

where $N$ is the number of particles. Each coordinate system $(\xi_i, \eta_i)$ is transformed from the Cartesian coordinates $(x_i, y_i)$ their origin being at the center of the particle with the mapping,
$x_i = \exp(\xi_i) \cos \eta_i$ and $y_i = \exp(\xi_i) \sin \eta_i$. The first term on the RHS of (5) corresponds to the external uniform magnetic field applied to the system. The second term represents the contribution from the outer boundary $\partial \Omega_0$ whereas the third reflects the disturbance caused by the presence of all the particles. As the solutions of the Laplace equation for the domain $\Omega_0$ each of these terms can be expanded in Fourier series as follows.

\begin{align*}
A^{(0)}(\xi, \eta) &= \sum_{k=0}^{\infty} \left[ T_{1,k}^{(0)}(\xi, \eta) \cos k\eta + T_{2,k}^{(0)}(\xi, \eta) \sin k\eta \right] \\
A^{(i)}(\xi, \eta) &= \sum_{k=0}^{\infty} \left[ T_{1,k}^{(i)}(\xi, \eta) \cos k\eta + T_{2,k}^{(i)}(\xi, \eta) \sin k\eta \right] 
\end{align*}

(6) \quad (7)

For the domain inside the particle $i$, we assume the following form as the solution.

\begin{align*}
A &= \vec{A}^{(i)} = \sum_{k=0}^{\infty} \left[ \vec{T}_{1,k}^{(i)}(\xi, \eta) \cos k\eta + \vec{T}_{2,k}^{(i)}(\xi, \eta) \sin k\eta \right]
\end{align*}

(8)

The coefficients $T_{1,k}^{(i)}$, $T_{2,k}^{(i)}$, $\vec{T}_{1,k}^{(i)}$ and $\vec{T}_{2,k}^{(i)}$ are obtained by applying the BC’s (1)-(3). For instance, when we apply the BC (1) to the particle 1, we first evaluate all the other functions $A^{(i)}$ for $i \neq 1$ on the surface of the particle 1. Then sum of these is expanded in a Fourier series in terms of the local coordinate $\eta_i$. Then collecting coefficients for each mode of $\cos k\eta$ and $\sin k\eta$ provide linear equations to be solved. In this way we also apply the other BC’s (2)-(3) to obtain the remaining equations. The resulting system of equations is then solved by using the Gauss elimination method. For $k = 0$, the solution is indeterminate. In fact we can impose an arbitrary value to either $T_{1,k}^{(i)}$ or $\vec{T}_{1,k}^{(i)}$ and either $T_{2,k}^{(i)}$ or $\vec{T}_{2,k}^{(i)}$. We take $T_{1,k}^{(i)} = \vec{T}_{2,k}^{(i)} = 0$ in this study.

For the Stokes-flow regime, the fluid flow is governed by the bi-harmonic equation $\nabla^4 \psi = 0$, where $\psi$ is the stream function. We seek the solution of this equation for the case having $N$ circular particles inside the cylinder in the following form.

\begin{align*}
\psi &= C_{00} + \sum_{i=0}^{N} \psi^{(i)}(\xi_i, \eta_i) \\
\end{align*}

(9)

where $C_{00}$ is a constant and $\psi^{(i)}(\xi_i, \eta_i)$ represents the local stream function for the particle $i$ satisfying $\nabla^2 \left( \psi^{(i)} \right) = 0$. The function $\psi^{(i)}(\xi_i, \eta_i)$ can be written in the following form.

\begin{align*}
\psi^{(i)} &= \sum_{m=0}^{K} C_{m}^{(i)} q^{(i)}(\xi_i, \eta_i) + Q^{(i)}(\xi_i, \eta_i) \\
\end{align*}

(10)

where the function $Q^{(i)}$ is defined as follows.

\begin{align*}
Q^{(i)} &= \sum_{k=2}^{\infty} \left[ D_{1,k}^{(i)} g_{1,k}^{(i)}(\xi_i) + D_{2,k}^{(i)} g_{2,k}^{(i)}(\xi_i) \right] \cos k\eta_i + \left[ E_{1,k}^{(i)} g_{1,k}^{(i)}(\xi_i) + E_{2,k}^{(i)} g_{2,k}^{(i)}(\xi_i) \right] \sin k\eta_i \\
\end{align*}

(11)
The modal functions \( q_\mu^i(\xi), g_{1,k}^i(\xi) \) and \( g_{2,k}^i(\xi) \) are multiplication of the exponential and power functions. The modal functions \( p_m(\eta) \) are defined as; \( p_1 = 1, p_2 = p_3 = \cos \eta \), \( p_4 = p_5 = \sin \eta \). Our target for the analysis is to obtain the unknown coefficients \( C_{00}, C_{11}, D_{1,k}, D_{2,k}, E_{1,k}^1 \) and \( E_{2,k}^2 \) from the BC’s to be specified on each of the walls of the cylinder and particles;

\[
\begin{align*}
\frac{\partial \psi}{\partial \eta} &= u_{p_1}^{(i)} \cos \eta_i + u_{p_2}^{(i)} \sin \eta_i \quad \text{on } \partial \Omega_i \\
\frac{\partial \psi}{\partial \xi} &= -u_{p_3}^{(i)} \cos \eta_i + u_{p_4}^{(i)} \sin \eta_i - \omega_p^{(i)} \quad \text{on } \partial \Omega_i
\end{align*}
\]

where \( u_{p_1}^{(i)} \) and \( u_{p_2}^{(i)} \) are velocity components of the particle’s translational motion and \( \omega_p^{(i)} \) indicates its angular velocity. Note that BC’s on the walls must be satisfied for the total stream function \( \psi \) not for the local function \( \psi^{(i)} \). When \( u_{p_1}^{(i)}, u_{p_2}^{(i)} \) and \( \omega_p^{(i)} \) are specified, we do not need any further constraints. In general, however, these are not given a priori and knowing them is a part of the solution. For these, we employ the balance between the magnetic force \( F_m \) and hydrodynamic force \( F_f \); \( F_m + F_f = 0 \). The magnetic force is calculated from (4), while \( F_f \) is given from the following formula.

\[
F_{js} = \int_0^{2 \pi} \left( \frac{\partial \zeta}{\partial \xi} - \zeta \right) \sin \eta \, d\eta, \quad F_{J\eta} = \int_0^{2 \pi} \left( \frac{\partial \zeta}{\partial \eta} + \zeta \right) \cos \eta \, d\eta
\]

where \( \zeta \) is the vorticity, \( \zeta = -\exp(-2\xi) \nabla \psi \). Further we need the torque-free condition on each of the particle walls reading

\[
\int_0^{2 \pi} \left( \zeta + 2 \frac{\partial \psi}{\partial \xi} \right) \, d\eta = 0
\]

Using the method similar to the one used for the magnetic field, we can obtain the unknown coefficients by solving the relevant equations using the Gauss elimination method. The number of unknowns is \( 8N + 9 \) including the translational and rotational velocities.

Motion of particles are simply obtained from the time integration of the equation of motion \( d\mathbf{x}_p / dt = \mathbf{u}_p \). We employed the Euler explicit method for the time integration.

**NUMERICAL RESULTS AND DISCUSSION**

The semi-analytic multiple-coordinate method proposed in this study was applied to the problem of calculating the interactive force between a pair of circular particles arranged in line with the external magnetic field. When the two particles are very close to each other, the circles can be approximated by parabola and we can apply the lubrication approximation to obtain the flow solution in the gap between the particles. Figure 1(a) shows the comparison between the approximated, asymptotic solutions and the ones given from the present method. It reveals very good agreement between the two data. The present method was also verified by comparing the numerical results with the ones obtained by the solutions obtained by using the bi-polar coordinates as shown in Fig. 1(b).
Figure 1. Validation of the present method; (a) comparison between the asymptotic solutions (solid line) and the present calculation (symbols) for the ratio of the approaching velocity and the inline force; (b) comparison between the numerical solutions with the bi-polar coordinates (solid line) and the present calculation (symbols) for the magnetic force.

Various parameter set has been imposed to study the motions of particles under a uniform external magnetic field, including the number of particles $N$, the permeability ratio $\mu_r$, the domain size $R$, and the initial configuration of the particle positions. Figure 2 shows that a slight difference in the initial position for three particle set-up was found to result in a dramatic difference in the final state.

Figure 2. Dramatic difference in the particle path as well as the final sequence of the arrangement for three-particle configuration.

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