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A fast method to compute triply-periodic Brinkman flows

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ABSTRACT

A fast method is developed to efficiently compute three-dimensional Brinkman flows induced by triply-periodic arrays of points forces and regularized forces. For point forces, we decompose the periodic Brinkman velocity into the sum of two series: one in real space and one in Fourier space. To do the splitting, we create a regularized solution with special decay properties so that both summands will decay in a Gaussian manner. For regularized forces, the same methodology is used to split the regularized velocity, and again, Gaussian decay of the summands is achieved. When there are N forces (N periodic arrays), the overall complexity is $\mathcal{O}(N^2)$. We discuss different ways to reduce the complexity to $\mathcal{O}(N^{3/2})$ and to $\mathcal{O}(N\log N)$. Finally, we present two sets of numerical results. The first validates the computational complexity of the algorithm and the second illustrates how this method can be used to study microscopic flows of organisms in a porous medium. A simple dumbbell model of swimmers is implemented that exhibits a large scale flow that varies based on the number of swimmers and the resistance within the porous medium.

1. Introduction

The Brinkman equation is a linear model of fluid flow through porous media. The model describes a viscous fluid flowing through random, sparse arrays of obstructions such as fibers or dissolved polymer chains [1–3]. There have been numerous biological applications for which the Brinkman model has been utilized. For example, multiple studies have explored flow through the endothelial surface layer [4–10], while some others are focused on flow through basement membranes [11], biofilms [12,13], and blood vessels with blockages or blood clots [7,14–19]. In addition, the Brinkman model has recently been used to study a swimming organism in 2D and 3D [20–26].

In dimensionless form, the incompressible Brinkman equations are given by

$$-\nabla p + \left(\Delta - \alpha^2\right)\mathbf{u} + \mathbf{F} = \mathbf{0}, \tag{1a}$$

$$\nabla \cdot \mathbf{u} = 0, \tag{1b}$$

where $\mathbf{u}$ is the fluid velocity, p is the pressure, and $\mathbf{F}$ is the body force. Letting $\mathcal{L}$ be a characteristic length scale and K the Darcy permeability of the medium, the parameter $\alpha = \mathcal{L}/\sqrt{K}$ represents the dimensionless permeability factor. This factor can be thought of as a measure of extra resistance in the fluid due to obstacles that comprise the porous medium. The velocity is scaled by a characteristic velocity, $\mathcal{U}$, and the pressure and force are scaled by $\mu\mathcal{U}/\mathcal{L}$ and $\mu\mathcal{U}/\mathcal{L}^2$, respectively. When $\mathbf{F}$ is a point force, the solution to (1a)–(1b) is called a Brinkmanlet (see Section 2.1). When $\mathbf{F}$ is a regularized force, the solution to (1a)–(1b) is called a regularized Brinkmanlet (see Section 2.2). In the limit as $\alpha \to 0$, the Brinkman equations become Stokes equations, and the (regularized) Brinkmanlet becomes a (regularized) Stokeslet [20].

In this paper, we are interested in developing methods to study microscopic Brinkman flows generated by active matter in a triply-periodic domain. Examples of active matter include biofilaments and molecular motors, collective motion of microorganisms such as sperm or bacteria, and active colloids [27,28]. Collective motion can lead to self organization into arrangements much larger than the individual organism or structure. For example, sperm at a high density have been observed to line up and form 'sperm trains' [29], as well as self organize into arrays of sperm vortices [30]. Bacteria also self organize into dynamic clusters and can form veils, vortices, and jets [31–33]. Comprehensive computational models and analysis has been completed to understand the role of hydrodynamic, steric, and chemical interactions on collective motion of a large number of structures [34–42]. In models where the domain was not confined by a wall, periodic boundary conditions were implemented. Many studies have assumed the fluid is governed by

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the Stokes equations, although the natural environments of many swimmers can be much more complex. The addition of obstacles in the fluid, such as fibers or polymer chains, may lead to other interesting dynamics not observed in the Stokes regime. A fast summation method has not been developed previously for a Brinkman model of a porous medium and this is the focus here.

Formally, due to the linearity of the Brinkman equation, Brinkman flows due to triply-periodic arrays of point forces and regularized forces can be computed as the periodic summations of Brinkmanlets and regularized Brinkmanlets, respectively. However, due to the $1/r^3$ decay of (regularized) Brinkmanlets, these triply-periodic sums are not absolutely convergent and thus, the direct summation is divergent. One common approach to circumvent this type of difficulty is to use Ewald or Ewald-like summation methods [43–47]. In this paper, we follow Beenakker's approach [43,47,48], and first decompose the (regularized) Brinkmanlet into the sum of a 'local' term and a 'global' term. Here, we point out that the 'global' term is, in fact, chosen to be a regularized Brinkmanlet. However, it is a regularized Brinkmanlet related to efficiency and the splitting of the 'local' and 'global' domain, not necessarily the regularized Brinkmanlet associated with the regularized force in the physical model. This will become more clear when we describe the details of the method. The periodic summation of the 'local' term is performed in real space and the periodic summation of the 'global' term is performed in Fourier space using the Poisson summation formula. For appropriate choices of regularization, both the real space sum and the Fourier space sum will converge very fast. However, the computational complexity of the direct Ewald summation in the case of N triply-periodic arrays of (regularized) forces is $\mathcal{O}(N^2)$. There have been many proposed fast methods to reduce the complexity to $\mathcal{O}(N^{3/2})$ and $\mathcal{O}(N\log N)$ for periodic electric potentials and periodic Stokes flows [49–53]. We incorporate one of these methods [53] to reduce the complexity of our formulation to $\mathcal{O}(N\log N)$.

The outline of our paper is as follows. In Section 2, we present known results about the Brinkmanlet and the regularized Brinkmanlet in three dimensions and provide new insight about the decay rate of their difference. This result is then used in Section 3 to develop an Ewald-like summation formula for triply-periodic (regularized) Brinkman flows. In Section 3, we also discuss ways to reduce the complexity of our formulation to $\mathcal{O}(N^{3/2})$ and $\mathcal{O}(N\log N)$. In Section 4, we demonstrate the computation time and accuracy of the $\mathcal{O}(N\log N)$ method, and present initial results for a simplified dumbbell model of an active suspension.

2. Background

In this section, we review known results about the Brinkmanlet and the regularized Brinkmanlet in three dimensions (see, for example, [20]), and state the problem for triply-periodic Brinkman flows. We also provide new insight into the decay rate of the difference between the Brinkmanlet and the regularized Brinkmanlet. This decay rate plays an important role in constructing the fast summation method for triply-periodic flows in Section 3.

2.1. Brinkmanlet

The Brinkmanlet, or the fundamental solution of the Brinkman equation, is the solution to (1a)–(1b) when the body force is a point force $\mathbf{F}(\mathbf{x}) = \mathbf{f}\delta(\mathbf{x}-\mathbf{x}_0)$. Here $\delta(\ \cdot\ )$ is the Dirac delta function, $\mathbf{f}$ is the force strength, and $\mathbf{x}_0$ is the force location. To find the Brinkmanlet in three dimensions, we proceed as follows.

Taking the divergence of the momentum Eq. (1a) and using the continuity Eq. (1b), we have

$$\Delta p(\mathbf{x}) = \nabla\cdot\Big(\mathbf{f}\delta(\mathbf{x}-\mathbf{x}_0)\Big). \tag{2}$$

With $G(\mathbf{x})$ as the fundamental solution of the Laplace equation, $\Delta G(\mathbf{x}) = \delta(\mathbf{x})$, the solution to (2) is

$$p(\mathbf{x}) = \mathbf{f}\cdot\nabla G(\mathbf{x}-\mathbf{x}_0). \tag{3}$$

Plugging this expression for pressure back into the momentum equation, we have

$$\begin{aligned}(\Delta-\alpha^2)\mathbf{u}(\mathbf{x}) &= \nabla p(\mathbf{x}) - \mathbf{f}\delta(\mathbf{x}-\mathbf{x}_0)\\ &= \mathbf{f}\cdot\nabla\nabla G(\mathbf{x}-\mathbf{x}_0) - \mathbf{f}\Delta G(\mathbf{x}-\mathbf{x}_0)\\ &= \mathbf{f}\cdot\Big(\nabla\nabla - \mathbf{I}\Delta\Big)G(\mathbf{x}-\mathbf{x}_0),\end{aligned} \tag{4}$$

where $\mathbf{I}$ is the identity matrix. Now implicitly define $B(\mathbf{x})$ as the solution to the non-homogeneous modified Helmholtz equation $\Big(\Delta-\alpha^2\Big)B(\mathbf{x}) = G(\mathbf{x})$ so that the solution to (4) is

$$\mathbf{u}(\mathbf{x}) = \mathbf{u}(\mathbf{x},\mathbf{x}_0)[\mathbf{f}] = \mathbf{f}\cdot\Big(\nabla\nabla - \mathbf{I}\Delta\Big)B(\mathbf{x}-\mathbf{x}_0). \tag{5}$$

This is the Brinkman velocity (Brinkmanlet) observed at the point $\mathbf{x}$ due to a point force of strength $\mathbf{f}$ located at $\mathbf{x}_0$. Further, with $r = \|\mathbf{x}\|_2$ for $\mathbf{x}\in\mathbb{R}^3$, we have

$$G(\mathbf{x}) = G(r) = -\frac{1}{4\pi r}, \qquad \text{and} \qquad B(\mathbf{x}) = B(r) = \frac{1-e^{-\alpha r}}{4\pi\alpha^2 r}.$$

After some manipulations, the Brinkmanlet (5) can be written as

$$\mathbf{u}(\mathbf{x},\mathbf{x}_0)[\mathbf{f}] = \mathbf{f}H_1(r) + \Big(\mathbf{f}\cdot(\mathbf{x}-\mathbf{x}_0)\Big)(\mathbf{x}-\mathbf{x}_0)H_2(r), \tag{6}$$

where $r = \|\mathbf{x}-\mathbf{x}_0\|_2$ and

$$\begin{aligned}H_1(r) &= -\frac{1}{4\pi\alpha^2 r^3} + \frac{e^{-\alpha r}}{4\pi r}\Big(1+\frac{1}{\alpha r}+\frac{1}{\alpha^2 r^2}\Big),\\ H_2(r) &= \frac{3}{4\pi\alpha^2 r^5} - \frac{e^{-\alpha r}}{4\pi r^3}\Big(1+\frac{3}{\alpha r}+\frac{3}{\alpha^2 r^2}\Big).\end{aligned} \tag{7}$$

In the limit as $\alpha\to 0$, $H_1(r)\to 1/(8\pi r)$ and $H_2(r)\to 1/(8\pi r^3)$, and, thus, the Brinkmanlet approaches the Stokeslet.

2.2. Regularized Brinkmanlet

The regularized Brinkmanlet is the solution to the Brinkman Eqs. (1a)–(1b) when the Dirac delta function in the above section is replaced by a smooth approximation. Usually, this approximation, called a blob, is chosen to be a radially symmetric function $\varphi^\varepsilon(\mathbf{x}) = \varphi^\varepsilon(\|\mathbf{x}\|_2)$. The blob parameter ε controls the concentration of the blob $\varphi^\varepsilon(\mathbf{x})$ near the origin, and, as ε goes to zero, $\varphi^\varepsilon(\mathbf{x})$ approaches the Dirac delta function centered at the origin. Similar to the regularized Stokeslet [54,55], we can think of the regularized Brinkmanlet approximately as the Brinkman flow due to a solid ball of radius ε centered at $\mathbf{x}_0$. Below, we review the derivation of the regularized Brinkmanlet, as detailed in [20].

Given an arbitrary radially symmetric blob $\varphi^\varepsilon(\mathbf{x}) = \varphi^\varepsilon(\|\mathbf{x}\|_2)$, following the same steps as in Section 2.1, we can write the regularized Brinkmanlet due to the regularized force $\mathbf{F}(\mathbf{x}) = \mathbf{f}\varphi^\varepsilon(\mathbf{x}-\mathbf{x}_0)$ of strength $\mathbf{f}$ located at $\mathbf{x}_0$ in the following form

$$\mathbf{u}^{\varphi^\varepsilon}(\mathbf{x},\mathbf{x}_0)[\mathbf{f}] = \mathbf{f}\cdot(\nabla\nabla - \mathbf{I}\Delta)B^{\varphi^\varepsilon}(\mathbf{x}-\mathbf{x}_0), \tag{8}$$

where $\Delta G^{\varphi^\varepsilon}(\mathbf{x}) = \varphi^\varepsilon(\mathbf{x})$, and $(\Delta-\alpha^2)B^{\varphi^\varepsilon}(\mathbf{x}) = G^{\varphi^\varepsilon}(\mathbf{x})$. Since $\varphi^\varepsilon(\mathbf{x})$ is a radially symmetric function, both $G^{\varphi^\varepsilon}(\mathbf{x})$ and $B^{\varphi^\varepsilon}(\mathbf{x})$ are also radially symmetric. Thus, by defining $r = \|\mathbf{x}-\mathbf{x}_0\|_2$, after some manipulations, we have

$$\mathbf{u}^{\varphi^\varepsilon}(\mathbf{x},\mathbf{x}_0)[\mathbf{f}] = \mathbf{f}H_1^{\varphi^\varepsilon}(r) + (\mathbf{f}\cdot(\mathbf{x}-\mathbf{x}_0))(\mathbf{x}-\mathbf{x}_0)H_2^{\varphi^\varepsilon}(r), \tag{9}$$

where

$$\begin{aligned}H_1^{\varphi^\varepsilon}(r) &= -\frac{r\Big(B^{\varphi^\varepsilon}(r)\Big)'' + \Big(B^{\varphi^\varepsilon}(r)\Big)'}{r}, \qquad \text{and}\\ H_2^{\varphi^\varepsilon}(r) &= \frac{r\Big(B^{\varphi^\varepsilon}(r)\Big)'' - \Big(B^{\varphi^\varepsilon}(r)\Big)'}{r^3}.\end{aligned} \tag{10}$$

In the limit as $\alpha\to 0$, this regularized Brinkmanlet approaches a regularized Stokeslet. Note that the Brinkmanlet is singular at the force location $\mathbf{x} = \mathbf{x}_0$, while the regularized Brinkmanlets are finite everywhere.