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Adjoint-based optimization of particle trajectories in laminar flows

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ABSTRACT

We present a performant numerical algorithm for the optimal control of particle controls in low Reynolds number flows. In particular, circular particles with mass are considered. An optimal control problem for the particle trajectories is presented, which is solved by means of a steepest descent algorithm. Here, the derivative information is obtained using adjoint calculus. Finally, numerical results are presented underlining the feasibility of our approach.

1. Introduction

The numerical simulation and optimization of particle dispersions in all kind of Reynolds number flows is of great interest in a wide range of industrial applications (filtering, sorting, mixing and production processes). For example, during the production process of efficient solar cells the control of dispersion of inorganic nanocrystals or nanorods in a polymer is important for the creation of a large interfacial area for the transfer of charges between the two active materials [1]. In the manufacturing of technical textiles (e.g. nonwoven materials, glass wool) small filaments are spun, stretched and distributed by turbulent air flows to form a specific kind of web [2]. The quality assessment of these products requires the control of the dynamics and/or the distribution of particles that might vary from tiny spherical light to large elongated heavy ones depending on the application. Therefore, it is necessary to investigate and develop efficient techniques for optimizing particle dispersions in laminar and turbulent flows.

In order to control the particle trajectories in the fluid one should be able to influence the fluid either by regulating some mechanical or fluid force at the boundary (boundary control) or by the modification of the distributed body force (distributed control) defined in the entire flow domain, for example by means of magnetic fields. Boundary control can be closer to real situations, however the effects of the controlling force over the controlled flow will be weaker than the effects of the controlling force determined by distributed control [3]. In this work, we consider a distributed optimal control problem of tracking-type, where the target particle path is given in advance. This can be seen as feasibility study and a benchmark for the industrial application.

Different techniques have been proposed to solve tracking-type problems for flow problems (see, e.g., [3–6]). A comprehensive treatment of distributed optimal control of NSE, comparing instantaneous and optimal control as well as first and second order methods can be found in [7].

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Regarding the modeling of particles dispersed in fluids, part of the literature (see, e.g., [8–24]) is dedicated to the development of accurate models to simulate the interaction between particles and fluid. In this direction the existing methods in the literature can be classified at least in two types: approximate methods and direct simulations. A good discussion on approximate methods can be found for example in the papers by Hu [25] and Esmaeeli [26]. The second kind of methods, i.e., direct simulations started with the paper of Hu et al. [13]. Schemes like the ones described in [25,27] use unstructured grid and require a remeshing technique to deal with the time-dependent domain determined by the moving particle boundaries. In order to prevent the expensive remeshing procedure the so called fictitious domain or domain embedding methods have been used in the simulation of particulate flows. These methods were first introduced by Hyman [28] and discussed later by Saul'eV [29] and Buzbee et al. [30]. The main idea of these methods is to extend a problem given in a complex domain to a larger but simpler domain which could admit more regular meshes (for details see [31,11,32,33]).

Here, we are going to combine for the first time these ideas to provide an optimal control technique for particle trajectories in fluids. We are going to study optimal control techniques for optimizing particle dispersions in a fluid which is contained in small channel. The main goal is to find the optimal force distribution over the flow domain such that the dispersed fibers reach a desired position, after some given time. The models and techniques discussed in this work can be applied in two and three dimensions. For simplicity, we restrict ourselves to the two dimensional case for the numerical experiments.

The paper is organized as follows: the combined fluid-particle modeling is described in detail in the next section, the corresponding optimal control problem is formally posed in Section 3 followed by the introduction of the corresponding adjoint equations in Section 4. The numerical results are discussed in Section 5 and conclusions are given in last section.

2. Mathematical modeling

Next, we describe the mathematical model which will be used in order to simulate the fluid flow, as well as the equations describing the particles dynamics. In particular, we consider a two-way coupling for particles with mass.

2.1. Navier–Stokes equations

Consider a fluid of viscosity μ and density ρ contained in a given domain $\Omega \subset \mathbb{R}^3$. The fluid velocity field is described by $\mathbf{y}(t,\mathbf{x}) : [0,T] \times \bar{\Omega} \to \mathbb{R}^3$ and its pressure by $p(t,\mathbf{x}) : [0,T] \times \bar{\Omega} \to \mathbb{R}$, with $\mathbf{x} \in \Omega$. The fluid flow is modeled as an incompressible flow using the time-dependent Navier–Stokes equations (NSE) equipped with suitable initial and boundary conditions. The conservation of momentum reads

$$\rho\mathbf{y}_t + \rho(\mathbf{y}\cdot\nabla)\mathbf{y} = \text{div}\,\mathbf{T}, \quad \text{in } \Omega \times (0,T) \tag{1}$$

and the conservation of mass

$$\text{div}\,\mathbf{y} = 0, \quad \text{in } \Omega \times (0,T), \tag{2}$$

where

$$\mathbf{T} := -p\mathbf{I} + 2\mu\mathbf{S} \tag{3}$$

expresses the normal and viscous stresses with $\mathbf{I}$ denoting the unit tensor and

$$\mathbf{S} := \frac{1}{2}\left(\nabla\mathbf{y} + (\nabla\mathbf{y})^T\right) \tag{4}$$

the strain-rate velocity tensor of the fluid. The derivation of (1) and (2) can be found for example in [34,35].

Remark 1. In the incompressible case, (1) simplifies to

$$\rho\mathbf{y}_t - \mu\triangle\mathbf{y} + \rho(\mathbf{y}\cdot\nabla)\mathbf{y} + \nabla p = 0. \tag{5}$$

2.1.1. Non-dimensionalization

In order to work with non-dimensional variables typical characteristic scales L and y for the length and flow velocity, respectively, are chosen which at the same time imply $\tau = \mathrm{L}/\mathrm{y}$ as a characteristic time scale. By introducing the new dimensionless variables

$$\tilde{\mathbf{x}} = \frac{\mathbf{x}}{\mathrm{l}}, \quad \tilde{t} = \frac{t}{\tau}, \quad \tilde{\mathbf{y}} = \frac{\mathbf{y}}{\mathrm{y}}, \quad \tilde{p} = \frac{p}{\Sigma} \tag{6}$$

where $\Sigma = \frac{\rho v \mathrm{y}}{\mathrm{L}}$, and applying the chain rule in (1) one obtains the following non-dimensional form of the NSE

$$\mathbf{y}_t + (\mathbf{y}\cdot\nabla)\mathbf{y} = \frac{1}{\mathrm{Re}}\text{div}\,\mathbf{T}, \tag{7}$$

where

$$\mathrm{Re} = \frac{\mathrm{Ly}}{v} \quad \text{and} \quad \mathbf{T} = -p\mathbf{I} + 2\mathbf{S} \tag{8}$$