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Approximating the Basset force by optimizing the method of van Hinsberg et al.

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ABSTRACT

In this work we put the method proposed by van Hinsberg et al. [29] to the test, highlighting its accuracy and efficiency in a sequence of benchmarks of increasing complexity. Furthermore, we explore the possibility of systematizing the way in which the method's free parameters are determined by generalizing the optimization problem that was considered originally. Finally, we provide a list of worked-out values, ready for implementation in large-scale particle-laden flow simulations.

1. Introduction

The equation of motion of an isolated, small, spherical particle submerged in a Newtonian fluid is well described by the equation proposed by Maxey and Riley [47], often referred to as the Maxey–Riley Equation, or, MRE. It reads

$$\begin{aligned} m_p \frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} = m_f \frac{\mathrm{D}\mathbf{u}}{\mathrm{D}t} + \frac{1}{2} m_f \left(\frac{\mathrm{D}}{\mathrm{D}t} \left(\mathbf{u} + \frac{1}{10} a^2 \nabla^2 \mathbf{u} \right) - \frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} \right) + C_D \left(\mathbf{u} - \mathbf{v} + \frac{1}{6} a^2 \nabla^2 \mathbf{u} \right) \\ + C_B \frac{\mathrm{d}}{\mathrm{d}t} \int_{t_0}^{t} \frac{1}{\sqrt{t-s}} \left(\mathbf{u} - \mathbf{v} + \frac{1}{6} a^2 \nabla^2 \mathbf{u} \right) \mathrm{d}s + (m_f - m_p)\mathbf{g} \end{aligned} \tag{1}$$

where $C_D = 6\pi a\mu$, $C_B = 6a^2\sqrt{\pi \rho_f \mu}$, m_p is the mass of the particle, m_f is the mass of the displaced fluid volume, a is the particle radius, ρ_f and μ are the density and dynamic viscosity of the fluid; and $\boldsymbol{g}$ is the acceleration due to gravity. The vector $\boldsymbol{v}$ is the velocity of the (point-)particle and $\boldsymbol{u}$ that of the surrounding fluid field, evaluated at the particle's centre. $\mathrm{D}/\mathrm{D}t$ denotes the material derivative of the fluid. Equation (1), together with $\boldsymbol{v} = \mathrm{d}\boldsymbol{r}/\mathrm{d}t$ and the initial conditions $\boldsymbol{r}(t_0) = \boldsymbol{r}_0$ and $\boldsymbol{v}(t_0) = \boldsymbol{v}_0$ form an initial value problem that must be solved to obtain the trajectory of the particle (where $\boldsymbol{r}$ is the particle's position vector).

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The different terms on the right-hand side of (1) have distinct physical interpretations and can be identified as: (from left to right) the force applied to the volume displaced by the particle in the undisturbed flow ($\boldsymbol{F}_U$), the added mass or virtual mass force ($\boldsymbol{F}_A$),[1] the Stokes drag ($\boldsymbol{F}_D$), the Basset–Boussinesq history force ($\boldsymbol{F}_H$) and the force due to the weight of the particle minus its buoyancy ($\boldsymbol{F}_W$).

Equation (1) can be used to simulate the dynamics of a number of particles suspended in fluid, provided that the particles are small enough, so that the flow around each of them can be accurately modelled by the instationary Stokes equations; and that they spend most of the time far enough from each other to justify applying this single-particle theory [47]. Under these conditions, (1) accurately describes how the motion of the submerged particles is determined by the background flow field, $\boldsymbol{u}$.

Typically, $\boldsymbol{u}$ is calculated with a suitable numerical method, such as the finite element method, on a static mesh. Hence the relevant flow variables need to be somehow interpolated in order to have $\boldsymbol{u}$ and its needed derivatives defined exactly at the particles' centres. The motion of each particle can then be calculated by solving the MRE numerically, in a stepwise fashion, alternating advances in time with updates of the fluid flow at the particles' locations. A detailed review of this kind of methods, among others, is given by Loth [39]. A discussion of alternative interpolation methods can be found in [30]. Some relevant examples of applications of these simulation techniques are the study of turbulent dispersion of suspended particles, [56]; contaminants convection in cracks, [52]; liquid crystal growth, [12]; and transport in biological vessels, [51].

In this work, we focus on the solution of the MRE itself, avoiding any discussion about either the fluid calculation or the interpolation process. Instead, we make use of analytical fluid fields, which we directly impose at the particle locations. This simplifies the arguments, eliminating any influences from interpolation errors and from errors in the numerical solution of the Navier–Stokes Equations.

Several studies have recently stressed its importance, particularly in liquid particulate flows [61,14]. However, the inclusion of the history term in the numerical implementation of the Maxey–Riley equation is still widely regarded as impractical due to the large memory requirements and the corresponding overheads involved in the calculation of the associated integral. Indeed, the following two issues arise:

A: The integral is defined over the totality of the particles' past trajectories. It is therefore necessary to keep track of an ever-increasing number of historical flow values (per particle) to perform the quadrature. Such number grows in proportion to the simulated duration.
B: Standard quadrature methods perform poorly due to the singularity at the upper integration limit, requiring a large number of quadrature points per time unit to sufficiently reduce the quadrature error.

An attempt to alleviate the severity of A was put forward by Dorgan and Loth [20], with the so-called *window method*. This approach takes advantage of the decreasing influence of past flow conditions on the advancing present to avoid having to store the complete history of the particles. Unfortunately, the decay associated with the Basset kernel (the $1/\sqrt{t-s}$ prefactor of the integrand) is too slow at the very low particle Reynolds numbers[2] that concern us, going as the inverse of the square root of time [40]. This implies that the number of points to be recorded still has to be large, and in fact radically limiting the performance of the method if accuracy is to be preserved [21].

The recent developments by Daitche [13] and van Hinsberg et al. [29] have certainly improved the situation. The first of these works addressed B through the construction of higher order schemes. The other work addressed A with a kind of window model that approximates, rather than neglects, the tail contribution to the Basset integral. In this work, we build upon these two methods, combining them and further adding to the result. The focus is placed on the optimization problem that leads to the determination of the free parameters of the model of van Hinsberg et al. We analyse the performance of the resulting algorithm in a succession of steps, each adding a layer of complexity toward real-world applications. Consistently, we show its remarkable efficiency and accuracy. We are also concerned with the validity ranges and robustness of the method, about which we draw some generic recommendations. Finally, a worked out list of optimal parameters is included (Appendix E), ready to be used in numerical implementations for particle-laden flow simulations.

2. Window models and the Hinsberg method

2.1. Preliminaries

Once discretized in time, the Basset–Boussinesq history term, $\boldsymbol{F}_H$ will have been replaced by its finite difference counterpart. That is, a linear combination of the integral itself evaluated at different times. Therefore, the problem of how to

[1] The form of the added mass force used here, with the material derivative applied to the field $\boldsymbol{u}$ corresponds to the more commonly applied form of this term, derived by Auton et al. [2] for inviscid flow. This form turns out to be also accurate for low and intermediate Reynolds numbers, as has been shown in several studies; see [48,44,66]. However, the difference with its alternative, involving $\frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t}$, is negligible in the range of validity of the MRE; see [47].

[2] The particle Reynolds number is defined as $Re_p = aw/\nu$, where w is the modulus of the slip velocity. The MRE is derived under the assumption that $Re_p \ll 1$.