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Advection of inertial particles in the presence of the history force: Higher order numerical schemes

Anton Daitche

Institute for Theoretical Physics, Westfälische Wilhelms-Universität, Wilhelm-Klemm-Str. 9, D-48149 Münster, Germany

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ABSTRACT

The equations describing the motion of finite-size particles (inertial particles) contain in their full form the history force. This force is represented by an integral whose accurate numerical evaluation is rather difficult. Here, a systematic way is presented to derive numerical integration schemes of arbitrary order for the advection of inertial particles with the history force. This involves the numerical evaluation of integrals with singular, but integrable, integrands. Explicit specifications of first, second and third order schemes are given and the accuracy and order of the schemes are verified using known analytical solutions.

The advection of finite-size particles (often called inertial particles) plays an important role in engineering [1] and in many environment-related phenomena ranging from meteorology to oceanography, e.g. cloud microphysics [2]. Particle-based modeling has been applied to the formation of planetesimals in the early solar system [3] and the aggregation and fragmentation processes in fluid flows [4]. Example applications are pollutant-transport forecasting for homeland defense [5], and the location of a toxin or biological pathogen spill (e.g. anthrax) from outbreaks in a street canyon [6]. Other recent results indicate that inertial particles might play a role in hurricane dynamics [7] and in the feeding dynamics of certain marine animals [8].

The basic equation of motion for a small spherical particle of radius a and mass m_p in a viscous fluid is given by the Maxey–Riley equation [9,10]:

$$m_p \frac{\mathrm{d}\boldsymbol{v}}{\mathrm{d}t} = m_f \frac{\mathrm{D}\boldsymbol{u}}{\mathrm{D}t} - \frac{m_f}{2}\left(\frac{\mathrm{d}\boldsymbol{v}}{\mathrm{d}t} - \frac{\mathrm{D}\boldsymbol{u}}{\mathrm{D}t}\right) - 6\pi a \varrho_f \nu(\boldsymbol{v}-\boldsymbol{u}) - 6a^2\varrho_f\sqrt{\pi\nu}\int_{t_0}^{t} \frac{1}{\sqrt{t-\tau}}\left(\frac{\mathrm{d}\boldsymbol{v}}{\mathrm{d}\tau} - \frac{\mathrm{d}\boldsymbol{u}}{\mathrm{d}\tau}\right)\mathrm{d}\tau. \tag{1}$$

Here, $\boldsymbol{v} = \mathrm{d}\boldsymbol{r}/\mathrm{d}t$ is the particle velocity, $\boldsymbol{u}(\boldsymbol{r}, t)$ the fluid velocity, m_f the mass of the fluid excluded by the particle, ν the kinematic viscosity of the fluid and ϱ_f the density of the fluid. The two appearing derivatives

$$\frac{\mathrm{d}\boldsymbol{u}}{\mathrm{d}t} = \frac{\partial \boldsymbol{u}}{\partial t} + \boldsymbol{v}\cdot\nabla\boldsymbol{u} \quad \text{and} \quad \frac{\mathrm{D}\boldsymbol{u}}{\mathrm{D}t} = \frac{\partial \boldsymbol{u}}{\partial t} + \boldsymbol{u}\cdot\nabla\boldsymbol{u}$$

denote the full derivative along the trajectory of the particle and of the corresponding fluid element, respectively. The terms on the right-hand side of (1) are: the force exerted by the fluid on a fluid element at the location of the particle, the added mass term describing the impulsive pressure response of the fluid, the Stokes drag, and the history force. In this form of the

E-mail address: anton.d@wwu.de.

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equation, gravity and the so-called Faxén corrections are not included. The history force accounts for the viscous diffusion of vorticity from the surface of the particle along its trajectory [9] and renders the advection equation to be an integro-differential equation whose solution is much more demanding than that of an ordinary differential equation. Because of this difficulty, this integral term is neglected in nearly all the applications mentioned above. However, experimental and analytic efforts [11,12] indicate that the history force might have significant effects for non-neutrally-buoyant particles in simple flows. Recent studies have also shown that the history force is relevant in turbulent flows [13,14] and chaotic advection [15]. The present paper will detail the derivation and analysis of the numerical schemes developed for the investigations in the latter study.

An important condition for the validity of Eq. (1) is that the particle Reynolds number $Re_p = |\boldsymbol{v} - \boldsymbol{u}|a/\nu$ remains small during the entire dynamics [9]. Furthermore the particle's size a and its diffusive time scale $\tau_\nu = a^2/\nu$ have to be (much) smaller then the smallest length and time scales of the flow, respectively. For particles of comparable size as the smallest length scale so-called Faxén corrections will become important [9]. Several attempts [16–18] have been made to extend (1) to the case of finite particle Reynolds numbers by modifying the particular form of the forces. Part of all of these approaches is a different form of the history force. The numerical schemes presented here can be applied to these forms as well (with some minor modifications) as will be discussed in Section 5. Note also that besides the history force, further modifications of (1) can be necessary for finite particle Reynolds numbers, e.g. non-linear drag and the so-called lift force (see [19] for a review).

The history force poses the main difficulty for a numerical integration of (1). There are basically three problems: (i) the singularity of the kernel $1/\sqrt{t-\tau}$, (ii) the fact that (1) is an implicit integro-differential equation due to the appearance of $\mathrm{d}\boldsymbol{v}/\mathrm{d}t$ on the right-hand side and (iii) the high computational costs for a numerical integration. The first point (i) is the most involved one and will be addressed by a special quadrature[1] scheme. The implicitness (ii) is not a major issue and can be addressed rather easily as we will see. The last point (iii) stems from the necessity to recompute the history force — an integral over all previous time-steps — for every new time-step. Therefore the computational costs grow with the square of the number of time-steps and can become quite substantial for long integration periods. This difficulty is inherent to the dynamics governed by the history force and cannot be addressed without further approximations. Note however that a higher order scheme reduces the number of necessary time-steps and therefore diminishes the problem of high computational costs indirectly. Furthermore the final form of the numerical scheme will be formulated as a weighed sum, which is well suited for a numerical evaluation on modern CPU architectures.

The correct numerical treatment of the full Maxey–Riley equation and in particular of the history force has received little interest in the past, in spite of an increasing number of studies supporting its importance. Michaelides [20] transformed the Maxey–Riley equation to a second order equation in which the history integral contains only the fluid velocity, but not the particle velocity. This makes the evolution equation explicit. Furthermore, according to Michaelides, this form of the equation allows a sparser sampling of the particle's history, which leads to savings in computational time and computer memory. However, the history integral still has a similar form as in (1) and the difficulties of an accurate numerical evaluation remain. Two previously proposed schemes addressing the history integral have been tested by Bombardelli et al. [21]. They found the accuracy of the schemes to be $\mathcal{O}(\sqrt{h})$ and $\mathcal{O}(h)$, where h is the time-step. In a recent work Hinsberg et al. [22] have proposed a first order[2] scheme for the computation of the history force, i.e. the error is $\mathcal{O}(h^2)$, which represents a significant advancement over previously known schemes. Furthermore Hinsberg et al. developed a method to decrease the needed amount of history for the computation of the history force, by approximating the tail of the history kernel with exponential functions. This leads to significant savings of computational time and computer memory. This method can be viewed as a major improvement over the method of a window kernel where the kernel is set to zero for time lags larger then a certain window time [18,21].

The present paper will describe the construction of arbitrary high order methods for the integration of particle trajectories with the history force and will give explicit specification of the first, second and third order methods with an accuracy of $\mathcal{O}(h^2)$, $\mathcal{O}(h^3)$ and $\mathcal{O}(h^4)$, respectively. Approximate forms of the history kernel as mentioned above will not be considered. However, the developed schemes can be easily adapted to the window kernel or the more advanced approach proposed by Hinsberg et al.

The rest of the paper is structured as follows: First some general notes about the history force and the Maxey–Riley equation will given. Afterwords a numerical quadrature scheme for the history force and its derivation will be presented. In the following section this quadrature scheme will be incorporated into an integration scheme for the numerical solution of the full Maxey–Riley equation. The full integration scheme will then be tested against known analytical solutions. This is followed by a section on the stability properties of the algorithm, and by a discussion and conclusion.

[1] In this article the term "quadrature scheme" refers to a numerical scheme for the approximation of an integral whereas the term "integration scheme" refers to a scheme for the approximation of the solution of the whole integro-differential equation.

[2] In the paper by Hinsberg et al. the scheme is said to be of second order. This is due to a different definition of the meaning of "order". Here, a scheme with an error term proportional to the square of the time-step is considered to be of first order as it is accurate up to the first order; in the same sense as the Euler-method is a first order scheme.