A single oblate spheroid settling in unbounded ambient fluid: 
a benchmark for simulations in steady 
and unsteady wake regimes

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Abstract

We have performed spectral/spectral-element simulations of a single oblate spheroid with small 
geometrical aspect ratio settling in an unbounded ambient fluid, for a range of Galileo numbers 
covering the various regimes of motion (steady vertical, steady oblique, vertical periodic and 
chaotic). The high-fidelity data provided includes particle quantities (statistics in the chaotic 
case), as well as flow profiles and pressure maps. The reference data can be used as an additional 
benchmark for other numerical approaches, where a careful grid convergence study for a specific 
target parameter point is often useful. We further describe an extension of a specific immersed 
boundary method (Uhlmann, J. Comput. Phys, 209(2):448–476, 2005) to enable the tracking of 
non-spherical particles. Finally, the reference cases are computed with this immersed boundary 
method at various spatial and temporal resolutions, and grid convergence is discussed over the 
various regimes of spheroidal particle motion. The cross-validation results can serve as a guideline 
for the design of simulations with the aid of similar non-conforming methods, involving spheroidal 
particles with Galileo numbers of $O(100)$.

1 Introduction

The flow around a single particle settling/rising in an otherwise quiescent fluid has received the attention from the scientific community for many years (Ern et al., 2012). The non-trivial particle paths which result in these flows play a significant role in a variety of fields such as meteorology, sedimentology or bio-inspired aerodynamics. The complex dynamics that govern particle-fluid interactions are influenced by fluid properties, particle shape, inertia, and gravity. As a consequence, the size of the parameter space of the problem is quite large, and, despite the progress made in the last decades, it has still not been fully explored in all detail. When the Reynolds number of the flow around the particle exceeds values of $O(10)$, wake effects become significant. In this scenario, analytical solutions are not available, and in engineering problems one needs to resort to empirical correlations in order to predict the hydrodynamic forces acting on particles (Balachandar and Eaton, 2010). Therefore, experiments

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and/or numerical simulations in which the flow and the particle motion are fully resolved are one way to drive further model development.

When a single sphere is fixed in a uniform flow, different flow regimes appear as a function of the Reynolds number based on the free stream velocity and the sphere’s diameter \( \text{Re} \) (Natarajan and Acrivos 1993; Tomboulides and Orszag 2000). For freely-mobile particles the Reynolds number is not a predetermined parameter any more, but the result of the balance of hydrodynamic and gravitational forces. In this situation, the resultant flow regime is uniquely defined by the density ratio of the two phases, \( \rho = \rho_p/\rho_f \), and the Galileo number \( Ga = U_g d/\nu \) (where \( U_g = \sqrt{(\rho - 1)gd} \) is a characteristic gravitational velocity, \( g \) is the gravitational acceleration, \( d \) the sphere’s diameter, and \( \nu \) the kinematic viscosity of the fluid). Spheres have been widely studied in the literature (Jenny et al., 2004; Veldhuis and Biesheuvel, 2007; Uhlmann and Dušek, 2014) mainly because the simplicity of their shape allows to reduce the complexity of the problem. However, particles found in real flows are often non-spherical.

One possible single-parameter deviation from a spherical shape is a spheroid, also called ellipsoid of revolution. A spheroid is non-isotropic, but axi-symmetric, and is uniquely defined by its equatorial diameter \( d \) and its aspect ratio \( \chi = d/a \), where \( a \) is the length of the symmetry axis of the spheroid. In a very simple way one can obtain flat, disk-like particles by setting \( \chi > 1 \) (oblate spheroid), elongated, rod-like particles with \( \chi < 1 \) (prolate spheroid) or recover a sphere with \( \chi = 1 \). This implies that the flow regimes appearing when a fixed spheroid is placed in a free stream are defined by the Reynolds number \( \text{Re} \) and \( \chi \) (Chrust et al., 2010); when the spheroid is released the problem is defined by the triplet \( Ga, \rho \) and \( \chi \). The case of fixed oblate spheroids has been investigated by Christ et al. (2010) who provided a detailed analysis of the flow transition as a function of the geometrical aspect ratio. The dynamics of free falling oblate spheroids have recently been analyzed by Zhou et al. (2017). They found that the two parameter \( Ga, \rho \) state diagram for a given aspect ratio \( \chi \) features a higher degree of complexity than that of a sphere. Furthermore, they found strong quantitative and qualitative differences for different \( \chi \). Overall, the state diagram for \( \chi = 1.1 \) resembles some features of spheres and the state diagram for \( \chi = 10 \) resembles that of a flat disk (Chrust et al., 2013). For intermediate values, there are strong differences between \( \chi = 1.1 \) and \( \chi = 2 \), whereas the transition in the behavior from \( \chi = 2 \) to 10 is somehow progressive. We will discuss these various flow states in more detail in § 2.1 below.

Understanding the underlying physics of the settling/rising of a single suspended particle also serves as a basis for understanding collective effects which arise in corresponding multi-particle systems. For example, Uhlmann and Doychev (2014) related the onset of clustering of a dilute set of settling spheres in unbounded fluid with the transition of wake regimes in the case of an isolated sphere.

The cost of simulating the flow around freely moving particles by means of particle resolved direct numerical simulations (DNS) is very high, but thanks to the efficiency of non-conforming algorithms like the immersed boundary method (IBM) (Mittal and Iaccarino, 2003) or the Lattice-Boltzmann method (Chen and Doolen, 1998), simulations of the flow around \( O(10^6) \) particles can be found in the literature (Kidanemariam and Uhlmann, 2017). However, these algorithms based on non-conforming meshes require careful validation and grid-convergence analysis, which is a difficult undertaking when systems featuring significant particle wakes are to be simulated. A discussion of how the validation process of the flow around spheres could benefit from detailed reference data at higher particle Reynolds numbers can be found in Uhlmann and Dušek (2014). Regarding particles with spheroidal shape, many numerical studies found in the literature resort to the analytical solution describing the rotational motion of a particle placed in shear flow under creeping flow conditions (obtained by Jeffery, 1922) for the purpose of validation (Aidun et al., 1998; Huang et al., 2012; Eshghinejadfard et al., 2016; Ardekani et al., 2016). On the other hand, the studies of Chrust et al. (2013) and Zhou et al. (2017) have demonstrated that high-fidelity data for settling rigid bodies with an axi-symmetric shape can be
generated with the aid of a body-conforming spectral element method (SEM). Previously, [Tschisgale et al. 2018] have performed a validation study of a (non-grid-conforming) immersed boundary method with the aid of spectral-element data for the case of a light oblate spheroid and for a heavy thin disc, while [Arranz et al. 2018] used spectral-element data for a settling oblate spheroid for the same purpose. In the present work we provide additional benchmark data for settling spheroids at several parameter points, including detailed information on the particle motion as well as on the hydrodynamic fields. Our goal is to complement the existing set of reference data in order to further facilitate the development of efficient numerical methods.

The present work focuses on settling spheroids with two different geometrical aspect ratios: $\chi = 1.1$ with an almost spherical shape, and a moderate value $\chi = 1.5$. For these two geometries the respective Ga-$\rho$ state diagrams still maintain similarities with the one of the sphere, since qualitative differences are observed for $\chi \geq 2$. Beyond the immediate use as validation data, this choice allows future studies on the settling of non-spherical particles to relate their results with the widely studied problem of settling spheres.

Furthermore, in the present work we discuss an extension of one specific immersed-boundary method for the simulation of particulate flow (Uhlmann, 2005) such that the motion of non-spherical particles can be tackled. The modifications with respect to the original algorithm concern two aspects: the tracking of rotational motion (involving a quaternion description, as well as its temporal discretization), and the distribution of Lagrangian force points per particle. It should be noted that a number of authors have previously proposed immersed-boundary methods valid for the flow around mobile, non-spherical particles (e.g. Yang and Stern 2015; Eshghinejadfard et al. 2016; Ardekani et al. 2016; Tschisgale et al. 2018 and others). Generally speaking, the present method is kept as simple as possible, and algorithmic differences compared to alternative techniques are provided where appropriate in the technical description below.

The overall purpose of the present work is, therefore, threefold: (a) provide high-fidelity data of settling spheroids of low and moderate aspect ratio at particle Reynolds numbers $O(100)$; (b) extend the existing IBM algorithm of Uhlmann (2005) such that non-spherical particle motion can be handled efficiently; (c) present an extensive validation process that can in principle be used in the context of a wide range of numerical methods for the simulation of submerged, mobile, rigid bodies.

The manuscript is organized as follows. In §2 the setup of the problem under investigation is presented together with an overview of the flow regimes that a free-falling spheroid can encounter. In §3 the spectral/spectral-element approach is described together with the reference solutions obtained. In §4 the extension of the immersed boundary method of Uhlmann (2005) is described and validated in §5 against the spectral-element reference data.

### 2 Problem description

We consider the settling of a single particle under the action of gravity in an incompressible Newtonian fluid. The particle is a rigid oblate spheroid with equatorial diameter $d$, aspect ratio $\chi = d/a$, where $a$ is the length of the symmetry axis, and uniform density $\rho_p$. Two Cartesian coordinate systems are used in this work. The first one is an inertial reference frame $O_{xyz}^{\text{fix}}$, in which the fluid velocity is zero in the absence of the particle. The vertical axis of this coordinate system $z_{\text{fix}}$ is represented by the unit vector $\mathbf{e}_z = -\mathbf{g}/g$, where $g = |\mathbf{g}|$ is the magnitude of the gravitational acceleration vector $\mathbf{g}$. Second, a non-inertial reference frame $O_{xyz}$ is aligned with $O_{xyz}^{\text{fix}}$, and it has an origin which is attached to the particle’s center of gravity.

The governing equations for the flow field are the Navier-Stokes equations for an incompressible
Figure 1: a) View along the symmetry axis and perpendicular to it of the spheroid with equatorial diameter $d$ and length of symmetry axis $a$ and b) sketch of the spheroid in the unbounded domain.

The fluid equations are:

\[
\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} + \nabla p = \nu \nabla^2 \mathbf{u},
\]

(1a)

\[
\nabla \cdot \mathbf{u} = 0,
\]

(1b)

where $p$ is the pressure normalized by the fluid density, $\mathbf{u} = (u, v, w)$ is the fluid velocity expressed in the inertial reference frame $O_{xyz}$ and $\nu$ is the fluid’s kinematic viscosity. The no slip and no penetration condition is imposed at the boundary of the particle. The position and velocity of the particle are obtained by integration of the Newton-Euler equations of rigid body motion over the surface of the particle $S$

\[
V_p \rho_p \frac{d\mathbf{u}_p}{dt} = \rho_f \int_S \mathbf{r} \times (\mathbf{n} \cdot \mathbf{r}) d\sigma,
\]

(2a)

\[
\frac{d(I_p \mathbf{\omega}_p)}{dt} = \rho_f \int_S \mathbf{r} \times (\mathbf{n} \mathbf{r}) d\sigma,
\]

(2b)

where $\mathbf{u}_p = (u_p, v_p, w_p)$ and $\mathbf{\omega}_p = (\omega_{px}, \omega_{py}, \omega_{pz})$ are the linear and angular velocity of the particle expressed in the inertial reference frame $O_{xyz}^g$, respectively, $\mathbf{r} = -p I + \nu (\nabla \mathbf{u} + (\nabla \mathbf{u})^T)$ is the hydrodynamic stress tensor ($I$ is the identity matrix), $V_p = \pi d^3/(6 \chi)$ is the volume of the particle, $I_p$ is the inertia tensor, $\mathbf{n}$ is a unit vector normal to the surface of the particle pointing towards the fluid, and $\mathbf{r}$ is the position vector of a point on the surface of the particle with respect to its center.

Dimensional analysis shows that the problem is governed by three non-dimensional parameters, namely the aspect ratio $\chi$, the density ratio between the particle and the fluid $\tilde{\rho} = \rho_p/\rho_f$ and the Galileo number $Ga = U_g d/\nu$, where $U_g$ is a gravitational velocity scale defined for heavy particles ($\tilde{\rho} > 1$) as $U_g = \sqrt{(\tilde{\rho} - 1) g V_p / d^2}$. The definition of $U_g$ and hence $Ga$ is the same as in Chrust et al. (2013) and Zhou et al. (2017). In the case of spheres, previous authors have typically rather used $Ga^* = U_g^* d/\nu$, where $U_g^* = \sqrt{(\tilde{\rho} - 1)gd}$, which differ by factors $\sqrt{\pi/6}$ and $\chi^{2/3} \sqrt{\pi/6}$, respectively, from the above counterparts. We also introduce the non-dimensional mass $m^* = \tilde{\rho} \pi / (6 \chi)$, which has been used in previous work in the literature since it provides a somewhat more straightforward scaling of the path regime boundaries than the density ratio itself. Note that as shown by Chrust et al. (2013) the steady and non-rotating regimes (steady vertical and steady oblique) are independent of the non-dimensionalized mass or, equivalently, the density ratio.
2.1 Overview of flow regimes and dynamics of oblate spheroids

In this section we present a brief description of the flow regimes that appear when an oblate spheroid settles in an unbounded fluid under the action of gravity. This presents a summary of the relevant results of Zhou et al. (2017).

For each aspect ratio $\chi$ the main characteristics of the two parameter $(Ga, \tilde{\rho})$ state diagram are presented, focusing on the appearance of the sphere-like scenario, flutter and tumbling modes. The sphere-like scenario corresponds to a successive transition from the steady axisymmetric regime to a steady oblique regime and, eventually, to unsteady regimes. This transition scenario is found for all density ratios in the case of spheres (Jenny et al., 2004). Flutter is characterized by a periodic swinging motion with significant amplitude but with deviations from the vertical of less than 90 degrees. Tumbling is a rotating motion during which the angular velocity varies periodically without changing sign.

Figure 2 shows an outline of the main features of the $(Ga, \tilde{\rho})$ state diagrams discussed here. For spheroids with aspect ratio as low as $\chi = 1.1$ the sphere-like scenario is present for all values of $\tilde{\rho} > 1$. Flutter is observed for light particles and for small excess particle densities if $Ga \gtrsim 200$, while tumbling is not observed. For $\chi = 1.5$ the sphere-like scenario is still observed for heavy particles and for light particles if $\tilde{\rho} \gtrsim 0.3$. The region in which flutter is observed is shrunk compared to $\chi = 1.1$, and there is no tumbling. When the aspect ratio is increased to $\chi = 2$ and $3$, the lower bound of $\tilde{\rho}$ for the sphere-like scenario increases, therefore reducing the region in which it is observed. Flutter is observed neither for $\chi = 2$ nor $3$, while tumbling starts to appear for heavy particles with large density ratios. It should be noted that for $\chi = 3$ the first bifurcation leading to the sphere-like scenario is subcritical, allowing the coexistence of steady vertical and tumbling modes. For $\chi = 4$ and $5$ there is no sphere-like scenario. Flutter is recovered for particles with intermediate non-dimensionalized mass. Regarding tumbling modes, the subcritical behavior at large density ratios is progressively increased. Finally, if the aspect ratio is increased to $\chi = 6$ or $10$ the sphere-like scenario is recovered for $\tilde{\rho} \lessgtr 3$ or $5$, respectively, which correspond in both cases to $m^* \lesssim 0.25$. For these aspect ratios the regions in which flutter and tumbling are observed continue to increase, showing stronger subcriticality in their first bifurcation. It should be noted that although the increase in the region where flutter is observed includes light particles, tumbling is restricted to heavy particles. It should also be mentioned that for large aspect ratios $\chi \geq 5$, intermittent modes can be found between the flutter and tumbling regions, especially (but not exclusively) in the non-overlapping space between these two.

2.2 Geometric definitions and notation

In this section we introduce the notation used to present the subsequent results. When the regime under study is axisymmetric with respect to the axis $z^{\text{fix}}$ (regime A), no additional definitions are needed. However, when the axisymmetry is broken, we define the following local coordinate system as in Uhlmann and Dusek (2014).

First, we define a reference system that maintains one coordinate along the vertical direction $e_z$, while the horizontal directions are given by the projection of the particle velocity and the direction perpendicular to it, viz.:

\[
\begin{align*}
\mathbf{e}_{pH} &= \left( u_p, v_p, 0 \right) / \sqrt{u_p^2 + v_p^2}, \\
\mathbf{e}_{pHz\perp} &= \mathbf{e}_z \times \mathbf{e}_{pH}.
\end{align*}
\]

Note that the temporal dependence in cases with unsteady particle motion will be made precise below. With these definitions the following linear and angular velocity projections, made dimensionless with
Figure 2: Outline of the state diagrams for different aspect ratios. The horizontal magenta line corresponds to $\hat{\rho}=1$, and the coloured regions indicate the occurrence of sphere-like, flutter or tumbling motion (see legend). The first bifurcation from the steady vertical regime is also indicated by a dashed gray line. The represented sphere-like domain includes the steady oblique and oblique oscillating regimes. The range of values shown in all the panels is $45 < Ga < 300$ and $0 < m^* < 5$. $Ga$ is represented in logarithmic scale whereas the represented values of $m^*$ are linear in $\log m^* + 0.1$. The complete diagrams for all aspect ratios except $\chi = 1.5$ can be found in Zhou et al. (2017). For a more detailed view of the case with $\chi = 1.5$ see the present figure 6.

the gravitational velocity $U_g$, can be defined:

\[ u_{pH} = \frac{(u_p/U_g)}{e_{pH}}, \]  
\[ u_{pH\perp} = \frac{(u_p/U_g)}{e_{pH\perp}}, \]  
\[ u_{pV} = \frac{(u_p/U_g)}{e_z}, \]  
\[ \omega_{pH} = \frac{(\omega_p/d/U_g)}{e_{pH}}, \]  
\[ \omega_{pH\perp} = \frac{(\omega_p/d/U_g)}{e_{pH\perp}}, \]  
\[ \omega_{pV} = \frac{(\omega_p/d/U_g)}{e_z}. \]  

The particle Reynolds is defined as follows

\[ Re_\parallel = \frac{|u_p|}{\nu} = \frac{|u_p|}{U_g}Ga. \]  

Please note that $u_p$ is defined with respect to the fixed coordinate system $O_{xyz}$ (see figure 1), such that it automatically constitutes a relative velocity with respect to the ambient fluid (this is different from the definition used in Uhlmann and Dušek, 2014).

Second, we define a reference system that shares the horizontal component $e_{pH\perp}$, which is normal to the trajectory plane. The unit vector aligned with the particle’s trajectory is

\[ e_{p\parallel} = u_p/|u_p|, \]  
and the unit vector perpendicular to $e_{pH\perp}$ and $e_{p\parallel}$ (see figure 3a) is obtained from:

\[ e_{p\perp} = e_{pH\perp} \times e_{p\parallel}. \]
With this, we can define the following components of the relative fluid velocity \( \mathbf{u}_r(x, t) = (u_r, v_r, w_r) = \mathbf{u} - \mathbf{u}_p \)

\[
\begin{align*}
  u_{r\|} &= (\mathbf{u}_r / U_g) \cdot (-\mathbf{e}_{p\|}), \\
  u_{r\perp} &= (\mathbf{u}_r / U_g) \cdot \mathbf{e}_{p\perp}, \\
  u_{rHz\perp} &= (\mathbf{u}_r / U_g) \cdot \mathbf{e}_{pHz\perp}.
\end{align*}
\] (8a, 8b, 8c)

Note that in the case of axi-symmetric solutions the axial component of the relative velocity is simply \( u_{r\|} \) and the radial component is denoted as \( u_{\text{rad}} = \sqrt{u_r^2 + v_r^2} / U_g \).

Finally, we define the direction \( y_{p\perp} \) along the unitary vector \( \mathbf{n}_{\perp} \), which is perpendicular to the symmetry axis and contained in the trajectory plane

\[
\mathbf{n}_{\perp} = \mathbf{n}_z \times \mathbf{e}_{pHz\perp},
\] (9)

where \( \mathbf{n}_z \) is a unitary vector parallel to the symmetry axis of the spheroid pointing towards positive values of \( z \).

3 Spectral/spectral–element computations

3.1 Numerical method

The reference data has been generated with the aid of the spectral/spectral-element method proposed by [Chrust et al. 2013]. It solves the Navier-Stokes equations in a cylindrical domain of length \( L_c = 15d \) and radius \( R_c = 2.67d \), with the cylinder axis along the gravity vector (cf. figure). The
Figure 4: a) Cylindrical domain used in the SEM computations. The length of the domain is $L_c = 15d$ and its radius $R_c = 2.67d$. The spherical sub-domain of radius $R_s = d$ is also represented. c) Top and side view of the particles used in the simulation ($\chi = 1.1, 1.5$) together with a sphere ($\chi = 1$) to appreciate the differences.
particle’s centroid is located on the cylinder axis at a distance $L_u = 5d$ from the lower (upstream) domain boundary. A spherical sub-domain with a radius equal to $R_s = d$ is fitted around the spheroidal particle. The sub-domain is rotating with the angular particle motion, while the outer computational domain is linearly translating with the particle motion. As a consequence, the mesh remains body-conforming, while the outer computational domain maintains its vertical orientation.

At the inflow (bottom) cylinder basis the velocity is set equal to zero to simulate an asymptotically quiescent fluid. At the outflow (top) cylinder basis and at its side a no stress Neumann boundary condition is imposed on the velocity field and a zero pressure is set.

The Navier-Stokes equations are spatially discretized in the axial/radial plane with the aid of the spectral-element method, while a truncated Fourier expansion is employed in the azimuthal direction. In the present work the Fourier expansion is truncated at the 15-th mode, and the spectral-element meshes shown in figure 5 are used with a polynomial order of 6. The solutions of the inner sub-domain and the outer domain are coupled at the common spherical interface through spherical harmonics (please refer to Chrust, 2012 for more details and validation). Grid convergence for this choice as well as the location of the interface between the two subdomains has been demonstrated previously both for spheres and thin disks in § 3.12 of the PhD thesis by Chrust (2012) and in Tables I and II of Chrust et al. (2013). The temporal discretization is performed with a third-order Adams-Bashforth scheme.

The present numerical method has been used in the past for the simulation of the sedimentation of spheres (Jenny et al., 2004; Uhlmann and Dušek, 2014), disks (Chrust et al., 2013) as well as spheroids (Zhou et al., 2017). Note that, in order to reduce the computational cost of these simulations for further use for validation purposes, the domain used in this work is smaller than the one presented in Chrust (2012); Chrust et al. (2013); Zhou et al. (2017). In Uhlmann and Dušek (2014) the difference in the results using both of these domain sizes was shown to be small for the case of spheres at comparable Galilean numbers.
Fig. 6: Flow regime maps for a) $\chi = 1.1$ (Zhou et al. 2017) and b) $\chi = 1.5$ (unpublished).

Table 1: Set of cases indicating the flow regime and the parameter point ($\chi, Ga, \tilde{\rho}$). The non-dimensional mass $m^* = \tilde{\rho}\pi/(6\chi)$ is also included for completeness.

| Case identifier | Flow regime       | $\chi$ | $Ga$ | $m^*$ | $\tilde{\rho}$ |
|-----------------|-------------------|--------|------|-------|----------------|
| A11-M100        | Steady vertical   | 1.1    | 100  | 1     | 2.1           |
| B11-M100        | Steady oblique    | 1.1    | 115  | 1     | 2.1           |
| B15-M075        | Vertical periodic | 1.5    | 110  | 0.75  | 2.14          |
| C15-M075        | Vertical periodic | 1.5    | 150  | 0.75  | 2.14          |
| D11-M100        | Chaotic           | 1.1    | 200  | 1     | 2.1           |
| D15-M500        | Chaotic           | 1.5    | 220  | 5     | 14.32         |

3.2 Results

In this section we present detailed results of selected cases for low ($\chi = 1.1$) and moderate ($\chi = 1.5$) aspect ratio oblate spheroids.

We have selected four different regimes to analyze in detail and provide benchmark data to use for validation purposes. These regimes are the steady axisymmetric (labelled A), the steady oblique (labelled B), the periodic oscillating vertical in the mean (labelled C) and the chaotic regime (labelled D). The complete set of cases can be found in table 1 and the representation of these cases in the $Ga, \tilde{\rho}$ diagram in figure 6. Both the zig-zag and vertical periodic regimes refer to periodically oscillating trajectories, vertical in the mean. The zig-zag regime is part of the sphere-like scenario and has about four times longer period than the vertical periodic regimes in figure 6.

3.2.1 Steady vertical regime

For Galileo number $Ga = 100$ an oblate spheroid of aspect ratio $\chi = 1.1$ reaches a steady axisymmetric state. The symmetry axis of the solution coincides with the symmetry axis of the spheroid, which in turn is aligned with the gravitational acceleration vector. No particle rotation is observed; therefore,
Figure 7: Flow visualization for a spheroid with $\chi = 1.1$ at $Ga = 100$, $\tilde{\rho} = 2.1$ ($m^* = 1$) which results in a steady vertical regime. Isosurface of a) relative velocity $\vec{u}_{r||} = 1.5$ and b) $\lambda_2 = -0.015d^2/U_g^2$ (Jeong and Hussain 1995). c) Isocontours of relative velocity $\vec{u}_{r||} = (-0.4 : 0.2 : 1.4)$ in a vertical plane passing through the center of the particle. The red line in c) corresponds to $\vec{u}_{r||} = 0$. The cyan and purple dashed lines indicate the location of the velocity profiles used for benchmarking purposes in §5.2.1 and given in the supplementary material. The cross stream profiles (cyan lines) are located at $z/d = 1, 3, 5, 7$.

the particle kinematics are uniquely defined by the vertical component of the velocity $u_{pV}$ (see table 2).

Figure 7 shows different flow visualizations of spectral-element data interpolated to a Cartesian grid for later comparison. As expected by the axi-symmetry found in this case, the wake is aligned with the trajectory of the particle (panel a). Following Jeong and Hussain (1995), vortical structures are identified by regions where the second largest eigenvalue of the tensor $\lambda_2 = S^2 + \Omega^2$ is negative (where $S$ and $\Omega$ are the symmetrical and anti-symmetrical parts of the fluid velocity gradient tensor), showing a clear toroidal vortex around the particle (panel b). The flow is also characterized by a recirculation region attached to the downstream face of the particle and an abrupt deceleration close to the stagnation point in the upstream face of the particle (panel c). Figure 7 also shows the recirculation length $L_r$, which is defined as the largest distance between any point on the boundary of the recirculation region ($\vec{u}_{r||} = 0$) and the center of the particle. The value of $L_r$ for the steady vertical case is presented in table 2.

The pressure field is obviously also axisymmetric in this case. Pressure profiles along the great circles will be discussed below in section 5.2.1 cf. figure 18.
Table 2: SEM reference results for steady vertical regime of spheroid with $\chi = 1.1$.

| Case      | $u_pV$   | $L_r/d$ | $Re_{||}$ |
|-----------|----------|---------|-----------|
| A11-M100  | -1.6863  | 1.818   | 168.63    |

Table 3: SEM reference results for steady oblique regime of spheroid with $\chi = 1.1$ and $\chi = 1.5$.

| Case      | $\chi$ | $u_pV$ | $u_pH$ | $\alpha(\degree)$ | $\varphi(\degree)$ | $L_r/d$ | $Re_{||}$ |
|-----------|--------|--------|--------|---------------------|---------------------|---------|-----------|
| B11-M100  | 1.1    | -1.76  | 0.057  | 1.858               | 2.755               | 1.966   | 202.46    |
| B15-M075  | 1.5    | -1.682 | 0.113  | 3.842               | 5.318               | 2.039   | 185.43    |

3.2.2 Steady oblique regime

The second regime under study is still steady, but instead of axisymmetric, the solution is planar symmetric. Both aspect ratios are evaluated ($\chi = 1.1, 1.5$) with Galileo 100 and 110, respectively. In this regime the kinematics of the particle are defined by its vertical ($u_pV$) and horizontal ($u_pH$) velocity, and by the angle $\varphi$ between the symmetry axis of the spheroid and the vertical (cf. the sketch in figure 3). We also include the angle of the particle’s gravity center trajectory with respect to the vertical

$$\tan(\alpha) = \frac{u_pH}{|u_pV|}. \quad (10)$$

Differently than for spheres, the angular velocity of the converged state is zero (Jenny et al., 2004; Uhlmann and Dusek, 2014). Note that the orientation of the vector $e_{ph}$ is arbitrarily selected by the solution. The resulting values obtained for both aspect ratios can be seen in table 3.

Figure 8 shows side and front views of the isocontours of relative velocity ($u_r|| = 1.5$) and of $\lambda_2$ for the spheroid with $\chi = 1.1(1.5)$ and $Ga = 100(110)$. The wake shows a similar structure to that found in the steady regime A, but it is here aligned with the particle’s oblique trajectory. It can also be seen that the angle of the trajectory followed by the particle with $\chi = 1.1$ (8a) is smaller than that of the particle with $\chi = 1.5$ (8g). Regarding the vortical structure, the strong toroidal vortex is still present and, additionally, two counter rotating streamwise vortices appear a few diameters downstream of the particle. Note that these double-threaded vortices are very weak compared to the toroidal vortex, especially for the spheroid with $\chi = 1.1$. Therefore, different thresholds of $\lambda_2$ are used in these visualizations.

Figure 8 also shows isolines of constant streamwise relative velocity $u_{r||}$. The side view of the contours of $u_{r||}$ show that the furthest point of the recirculation bubble, which is used to measure the recirculation length $L_r$, is not located on the trajectory of the center of the particle, but slightly deviated in the direction $e_{p\perp}$. The planar symmetry of this regime can be seen in the frontal view. Also indicated in the figure are the downstream locations where cross-stream profiles of the velocity components are reported in the supplementary material; these are also used in the benchmarking of the IBM results in section 5.2.2.

Figure 9 shows isocontours of constant pressure on the surface of both spheroids with $\chi = 1.1$ and 1.5 for the steady oblique regime. The contours on the surface are projected to a plane perpendicular to the symmetry axis of the spheroid which is not, in general, parallel to the trajectory of the particle. Therefore, the projection plane is spanned by $n_{\perp}$ and $e_{ph\perp}$ (see figure 3). We identify as upper (lower)
the surface that predominatly faces downstream or upwards (upstream or downwards). Interestingly
the distribution of the contours in the upstream-facing side of the spheroid (panels a and b) is almost
concentrical, as it would be in the case of an axi-symmetric solution. Only the small displacement of
the pressure maxima in the direction $e_p$ breaks the axi-symmetry of the contours. Conversely, the
contours in the downstream face of the particle (panels a and c) are clearly not axi-symmetric, with
a more pronounced deviation in the case with higher aspect ratio (panel d). In the future it will be
of interest to investigate in more detail the trends (with the aspect ratio $\chi$) of the flow pattern in the
wake, and of the resulting surface stress distribution.

### 3.2.3 Vertical periodic regime

In this section we evaluate the periodic oscillations that appear for a spheroid of aspect ratio $\chi = 1.5,$
$Ga = 150$ and $\tilde{\nu} = 2.14$ ($m^* = 0.75)$ (see figure 6). The motion in this regime is vertical in the
mean and it is restricted to a plane. Therefore, the kinematics can be reduced to vertical ($u_{pV}$) and
horizontal ($u_{pH}$) velocity components and to the angular velocity around the axis perpendicular to
the plane in which the motion takes place ($\omega_{pHz}$). It should be noted that the definition of $e_{pH}$
(3a) involves quantities evaluated at the reference time $t^*$, which is defined as the time instant of the
oscillation cycle in which $\sqrt{u_p^2 + v_p^2}$ is maximum. Therefore, equation (3a) is rewritten as

$$e_{pH} = (u_p(t^*), v_p(t^*), 0) / \sqrt{u_p^2(t^*) + v_p^2(t^*)}. \quad (11)$$

The remaining definitions presented in § 2.2 prevail.

Table 4 shows the results of the vertical periodic case. These cases are time periodic with frequency
of oscillation $f$ and period $T$, from which we can define the Strouhal number $St = fd/U_g$. The
amplitude and mean values of any function $\phi$ can be obtained from the fully developed data as follows:

$$\phi' = \max_t (\phi(t)) - \min_t (\phi(t)), \quad t^* < t < t^* + T,$$

$$\overline{\phi} = \frac{1}{T} \int_{t^*}^{t^* + T} \phi(t) dt. \quad (12b)$$

The time history of the kinematic variables follows a sinusoidal shape (figure omitted). The amplitude
of the oscillation in the vertical direction ($u_{pV}'$) is very small compared to the horizontal one ($u_{pH}'$),
which in turn is small compared to the mean vertical velocity of the particle ($\overline{u_{pV}}$) (see figure 10).
Regarding the orientation of the particle, the axis of the spheroid is tilted so that the drag is maximized
by aligning the axis of the spheroid with the trajectory, similarly to the steady oblique regime (see
figure 10). This regime is referred in the literature as a fluid mode (Zhou et al., 2017), in which the
unsteady motion is governed by the fluid behavior: this corresponds to a planar symmetric wake with
alternate shedding of hairpin-like vortices.
Figure 8: Flow visualization of cases B11-M075 (top row) and B15-M075 (bottom row). Panels a, d, g and j show isosurface of $u_r = 1.5U_g$, panels b and e, show isosurfaces of $\lambda_2 = -10^{-4}d^2/U_g^2$ and panels h and k, $\lambda_2 = -0.015d^2/U_g^2$. Panels c, f, i and l show isocontours of $u_r = -0.4 : 0.2 : 1.2$, highlighting with a thick, red line the isocontour $u_r = 0$. The cyan and purple dashed lines in panels c,f,i,l indicate the location of the velocity profiles provided for benchmarking purposes in the supplementary material. The cross stream profiles (cyan lines) are located at $x_{p||}/d = -1, -3, -5, -7$. 
Figure 9: Isocontours of pressure on the surface of a,b) B11-M075 and c,d) B15-M075. Left (right) panels correspond to the projection of the contours of the lower (upper) surface on a plane perpendicular to the symmetry axis. Positive contours are represented in black ($0.1:0.1:1.5$) and zero and negative contours are represented in red ($-1.5:0.1:0$). The red circle (cross) marker in panels a and c (b and d) indicates the position of the minimum (maximum) pressure. The intersecting point of the particle’s center trajectory with the surface of the spheroid is represented with a square in every panel.
Figure 10: a) Sketch of the kinematics in the vertical periodic regime. Note that the inclination and path deviations are exaggerated for clarity. b) Phase-space trajectory in the plane defined by the horizontal and vertical velocities \( u_{pH} \) and \( u_{pV} \) for the periodic oscillating case of the spheroid with \( \chi = 1.5, \, Ga = 150 \) and \( m^* = 0.75 \, (\tilde{\rho} = 2.14) \) computed with the SEM.

Figure 11: Chaotic regime of spheroid with \( \chi = 1.1 \) at \( Ga = 200 \) and \( m^* = 1 \, (\tilde{\rho} = 2.1) \) computed with the SEM. a) Time history of vertical velocity and b) the phase-space trajectory in the plane defined by the two horizontal velocity components.
Table 5: Averaged quantities of linear and angular velocities for chaotic cases of spheroids with $\chi = 1.1$ and $\chi = 1.5$ at $Ga = 200$ and $Ga = 220$ and $\tilde{\rho} = 2.1$ and 14.32, respectively. These data were computed with the SEM.

| cases     | $\chi$ | $\langle w_p \rangle / U_g$ | $\langle \omega^{\prime \prime}_p w_p^{\prime \prime} \rangle / U_g$ | $\langle \omega^{\prime \prime}_p w_p^{\prime \prime} \rangle / \bar{c}_g$ | $\langle \omega^{\prime \prime}_p \omega^{\prime \prime}_p \rangle / U_g/d$ | $\langle \omega^{\prime \prime}_p \omega^{\prime \prime}_p \rangle / U_g/d$ | $Re_{||}$ | $T_{obs} U_g/d$ |
|-----------|--------|-----------------------------|-------------------------------------------------|-------------------------------------------------|-------------------------------------------------|-------------------------------------------------|-----------|---------------|
| D11-M100  | 1.1    | -1.9533                     | 0.0220                                           | 0.1153                                           | 0.0025                                           | 0.0403                                           | 391       | 2.536         |
| D15-M500  | 1.5    | -1.8681                     | 0.0124                                           | 0.0464                                           | 0.0005                                           | 0.0144                                           | 411       | 2.830         |

3.2.4 Chaotic regime

Here, we discuss the data obtained in the regime of chaotic particle motion, for $\chi = 1.1$ (1.5), $Ga = 200$ (220), and $\tilde{\rho} = 2.1$ (14.32). Figure 11 shows the time history of the vertical velocity as well as the phase-space plot spanned by the horizontal components of the velocity for the case with $\chi = 1.5$. Because of the chaotic behavior of the particle’s motion, the results are described using statistical analysis. Let the mean of any time dependant variable $\phi(t)$ be defined as

$$\langle \phi \rangle = \frac{1}{T_{obs}} \int_{T_{obs}} \phi(t) dt,$$

where $T_{obs}$ is the observation time as stated in table 5. Then, the fluctuation of this quantity $\phi''(t)$ is defined as

$$\phi''(t) = \phi(t) - \langle \phi \rangle.$$

Table 5 shows results of mean and fluctuating part of the linear and angular velocities of both cases. It can be seen that the amplitude of the vertical velocity fluctuations is very small compared to the mean value (< 1%) and that the fluctuations in the horizontal direction are approximately 5 times more intense than in the vertical direction. There is no mean angular velocity in any of its components. Regarding the fluctuating part of $\omega_p$, the intensity of the horizontal component is likewise greater than the vertical one, but now by a factor of approximately 20. These results are consistent with previous observations in the case of spheres (Uhlmann and Dušek 2014).

Additional information on the kinematics of the particle can be found in the representation of the probability density function (pdf) for both linear and angular velocities in figure 12. For the lower aspect ratio ($\chi = 1.1$) the pdf of the horizontal component is very similar to a normal distribution, but the vertical exhibits some positive skewness. The angular velocities of this case show no skewness but moderate excess kurtosis as compared to a Gaussian. Interestingly, for $\chi = 1.5$ the pdf of the horizontal component of the velocity shows positive kurtosis, whereas the vertical component shows negative skewness. Regarding the angular velocities, for $\chi = 1.5$ the horizontal component pdf resembles that of a normal distribution whereas the vertical component exhibits excess kurtosis. These results are different from those found for spheres in which the angular velocities and the vertical velocity approximately follow a normal distribution, and where the horizontal component of the velocity showed negative excess kurtosis (Uhlmann and Dušek 2014).

The behavior in time of the signals can be evaluated through the auto-correlation functions of velocity and angular velocity components. The auto-correlation function (cf. figure 13) of a time dependent variable $\phi(t)$ is defined as

$$R_{\phi \phi}(\tau) = \frac{\int_a^b \phi''(t)\phi''(t + \tau)dt}{\int_a^b \phi''(t)\phi''(t)dt}.$$
Figure 12: SEM results in the chaotic regime: pdf of linear (left panels) and angular (right panels) velocities of the spheroid with $\chi = 1.1$ and $\tilde{\rho} = 2.1$ at $Ga = 200$ (top row) and $\chi = 1.5$ and $\tilde{\rho} = 14.32$ at $Ga = 220$ (bottom row). The normal distribution is included as a blue line to support the graphical interpretation of the data.
It can be seen that the auto-correlation of both vertical and horizontal velocities of the spheroid with $\chi = 1.1$ decay rapidly on a time scale of $O(10)$ gravitational units, and then maintain a periodic behavior with small amplitude. Similar behavior is found for the vertical component of the angular velocity, whereas the horizontal component exhibits a more intense oscillation periodic correlation correlated over longer times. For the larger aspect ratio ($\chi = 1.5$) the auto-correlation functions for the linear velocities show a clear decay and lack of periodicity. Both angular velocity components of the case with $\chi = 1.5$ show a damped periodic behavior similar to the horizontal angular velocity of the case with $\chi = 1.1$.

4 Extension of the immersed boundary approach for non-spherical particles

Here we present an extension of the direct forcing IBM proposed by Uhlmann (2005) in order to simulate the presence of non-spherical particles in an incompressible flow. In this formulation the non-conforming feature of the grid with respect to the particle is treated with a direct-forcing approach, in which a forcing term $f^{ibm}$ is included on the right hand side of the momentum equation (1a) to model the presence of the particle. Time marching is performed with a three-step Runge-Kutta scheme for the advective term and a Crank-Nicholson scheme for the viscous term. Continuity is enforced by using a fractional-step method, and spatial discretization is done by finite-differences of second order on a uniform, staggered grid. The interpolation/spreading steps between the Eulerian (fluid) and
Lagrangian (particle) grids make use of a regularized Dirac delta function (Peskin, 1972); in particular we use the variant with a support of three grid points as proposed by Roma et al. (1999).

In its original description (Uhlmann, 2005), the algorithm takes advantage of the isotropic shape of spherical particles in two different aspects:

- Rotations need not to be tracked due to the isotropy of a spherical particle.
- The angular momentum \( I_p \omega_p \) is parallel to the angular velocity \( \omega_p \), so the integration of the angular momentum equation (2b) is simplified.

Both assumptions become invalid when dealing with non-spherical particles; therefore, here we propose an extension of the algorithm. Since the treatment of the fluid part (equation 1) as well as the linear momentum equation for the particles (equation 2a) are unchanged compared to the original description, they are not included here. However, the entire algorithm is reproduced in the present A for completeness.

Please note that we have previously used essentially the same extension in a different context and in a different code (Arranz et al., 2018), where, however, little numerical details and only limited evidence of validation were given.

The first modification of the original algorithm concerns the integration of the angular momentum equation 2b in a body-fixed reference frame, in which the moment of inertia tensor \( I_{p,b} \) is constant in time such that we can write:

\[
I_{p,b} \frac{d\omega_{p,b}}{dt} + \omega_{p,b} \times I_{p,b} \omega_{p,b} = R \left( \rho_f \int r \times (\tau \cdot n - pn) \, dA \right),
\]

where \( R \) is the rotation matrix (cf. A for more details) and the subscript \( b \) is used to identify quantities expressed in the body-fixed reference frame. Assuming full rigid motion of the fluid inside the particle, the discretized equation for the \( k \)th substep of the Runge-Kutta scheme used to update the angular velocity reads:

\[
\frac{\omega_{p,b}^{k+1} - \omega_{p,b}^{k-1}}{\Delta t} = -\frac{\rho_f}{\rho_p - \rho_f} \rho_p (I_{p,b})^{-1} T_0^k - \gamma_k (I_{p,b})^{-1} (\omega_{p,b}^{k-1} \times I_{p,b} \omega_{p,b}^{k-1}) - \zeta_k (I_{p,b})^{-1} (\omega_{p,b}^{k-2} \times I_{p,b} \omega_{p,b}^{k-2})
\]

where \( \Delta t \) is the time step, \( T_0 \) is the contribution to the torque due to the forcing \( f^{(ibm)} \) expressed in the body-fixed coordinate system (cf. A for precise definitions). The coefficients \( \gamma_k \) and \( \zeta_k \) are coefficients of the Runge-Kutta scheme used in Uhlmann (2005), originally taken from Rai and Moin (1991). It should be mentioned that if one chooses the orientation of the body-fixed reference frame so that it is aligned with the principal axes of the body, the inertia tensor and its inverse become diagonal, and the implementation of (17) is accordingly simplified: the inertia tensor \( I_{p,b} \) and its inverse \( (I_{p,b})^{-1} \) can be stored in a buffer of only three positions, the components of \( (I_{p,b})^{-1} \) are simply computed as \( (I_{p,b})^{-1}(i,i) = 1/I_{p,b}(i,i) \) (note that \( (I_{p,b})^{-1}(i,j) = I_{p,b}(i,j) = 0 \) for \( i \neq j \) when the orientation of the body-fixed reference frame is aligned with the principal axes of the body). Furthermore, every operation involving any of \( I_{p,b} \) or \( (I_{p,b})^{-1} \) and a vector is computed as the component by component multiplication of two vectors. Also note that the choice of a fully explicit discretization in (17) does not lead to any adverse numerical stability properties.

The next modification of the algorithm is the tracking of the particle rotations. Here we use a formulation based on quaternions, \( q = (q_1, q_2, q_3, q_4) \), whose components are defined in terms of the...
vector defining the rotating axis, \( \mathbf{e} \), and the rotated angle, \( \varphi \), as \( q_i = e_i \sin (\varphi/2) \) for \( i = 1, 2, 3 \) and \( q_4 = \cos (\varphi/2) \). The evolution equation for the quaternion reads (Tewari, 2007)

\[
\frac{dq}{dt} = \frac{1}{2} Q q,
\]

where the matrix \( Q \) is defined in terms of the angular velocity as

\[
Q = \begin{pmatrix}
0 & \omega_{pz,b} & -\omega_{py,b} & \omega_{px,b} \\
-\omega_{pz,b} & 0 & \omega_{px,b} & -\omega_{py,b} \\
\omega_{py,b} & -\omega_{px,b} & 0 & \omega_{pz,b} \\
-\omega_{px,b} & \omega_{py,b} & -\omega_{pz,b} & 0
\end{pmatrix}.
\]

Using the same temporal discretization as in (17), the \( k \)th substage of the Runge-Kutta scheme for the quaternion reads

\[
\frac{q^k - q^{k-1}}{\Delta t} = \gamma_k \frac{1}{2} Q^{k-1} q^{k-1} + \zeta_k \frac{1}{2} Q^{k-2} q^{k-2}.
\]

Finally, the distribution of points on the surface of the spheroid has to be done considering that the non-spherical particles are not isotropic. In the case of spheroids one can use a similar approach as the method (2) described in appendix A.2.1 of Uhlmann (2005), but considering geodesic distances (along the shortest path restricted to the spheroid’s surface) to calculate the mutual repulsive energy instead of Euclidean distances; this is the approach which we have chosen herein. Details of the procedure can be found in the present B.1.

Additionally, for one of the cases discussed below (cf. §5.2.2) we employ a distribution of points on the surface of the spheroid as well as throughout its interior (cf. B.2) in order to impose the constraint of rigid body motion more strongly, and thereby to reduce residual flow inside the particle. It should be mentioned that by using this approach the number of Lagrangian force points per particle varies as \((d/\Delta x)^3\), as compared to a power-2 increase for the standard surface-only forcing. As a consequence, forcing the entire volume occupied by the particles becomes computationally expensive when high solid volume fractions are to be simulated. Therefore, it would be worthwhile to explore alternatives in a future study. One possibility is to analyze the effectiveness of multi-stage immersed boundary algorithms (such as Luo et al., 2007) on the residual currents in the configuration of §5.2.2 below.

It should be mentioned that the choice of integrating the angular equation of motion in a body-fixed reference frame as well as using a formulation based on quaternions can also be found in the work of Eshghinejadfard et al. (2016) and of Tschisgale et al. (2018) who employ immersed boundary algorithms based on discrete delta functions for the description of non-spherical particles in lattice Boltzmann and finite-difference frameworks, respectively. Yang and Stern (2015) have likewise used a combination of body-fixed and inertial reference frames as well as quaternions in an immersed boundary method; the latter, however, uses a reconstruction technique instead of a discrete delta function. A substantially different choice for the integration of the angular momentum equation can be found in the direct forcing IBM by Ardekani et al. (2016), where the rotation matrix (instead of quaternions) is advanced in time in an inertial reference frame in which the inertia tensor of the particle is computed at each time step by an iterative process.

5 Immersed boundary computations

In this section the results presented in §3.2 are reproduced with the direct forcing IBM originally proposed by Uhlmann (2005) and modified according to section 4. Each case will be computed with
increasing spatial resolutions in order to perform a grid convergence study for the case of settling spheroidal particles.

5.1 Computational set-up

The domain is a cuboid of side-lengths $L_x = L_y = 5.33d$ and $L_z = 16d$ as shown in figure 14. The size of the domain has been selected based on Uhlmann and Dušek (2014). Regarding the boundary conditions, a uniform vertical velocity $U_\infty$ is imposed at the lower boundary and an advective boundary condition at the top boundary of the domain. Periodic boundary conditions are set in the lateral directions ($x$ and $y$) in order to allow the particle to freely move in the horizontal directions.

Each of the cases presented in section 3.2 is reproduced using uniform and isotropic spatial resolutions up to $d/\Delta x = 48$. This results in a grid size of [96 x 96 x 288] points for the lowest resolution and a grid of [256 x 256 x 768] points for the highest resolution. Except where stated otherwise, the time step is set to $\Delta t U_\infty/d = 1.78 \times 10^{-2}, 1.33 \times 10^{-2}, 0.89 \times 10^{-2}$ and $0.67 \times 10^{-2}$ for the cases with resolution $d/\Delta x = 18, 24, 36$ and 48, respectively, which leads to CFL $\lesssim 0.5$.

In order for the particle to remain inside of the computational domain for a sufficiently long time, the values of $g$ and $\nu$ must be adjusted to match a given $Ga$ and, on average, balance the hydrodynamic force with gravity. A brief description of the steps taken to fulfill these two conditions is:

1. Run a simulation in which the particle is fixed and set $\nu$ to match an (estimated) target $Re$.

2. From the hydrodynamic force obtained in the previous step, compute the value of $g$ needed to
compensate it as if the particle were free to move. Use this value of \( g \) to set \( \nu \) to match the desired \( Ga \) and run a second simulation (particle is still fixed).

3. Again, compute the value of \( g \) from the hydrodynamic force obtained in the previous step and adjust \( \nu \) to match the desired \( Ga \). Run a simulation in which the particle is free to move. Repeat this step updating the value of gravity depending on the mean drift of the particle with respect to the computational domain: Reduce (increase) \( g \) if the particle drifts towards the inlet (outlet).

In this work, a simple bisection method with a relaxation factor of 0.5 was successfully employed.

5.2 Results

In the following, errors of converged values are computed for any quantity \( \phi \)

\[
\varepsilon(\phi) = \frac{|\phi - \phi_{\text{ref}}|}{\phi^*_{\text{ref}}}, \tag{21}
\]

where the subscript “ref” indicates a value taken from the spectral-element computations presented in section 3 and the superscript * is used to indicate that we use \( \phi^*_{\text{ref}} = u^*_p V \) for vanishing reference values (e.g. those velocities \( v \) for which \( v \ll U_g \)) and \( \phi^*_{\text{ref}} = \phi_{\text{ref}} \) otherwise. This procedure guarantees that the values obtained for the errors are meaningful and not amplified. Therefore, we use the vertical reference velocity component \( u^*_p \) in the denominator of (21) for the normalization of \( u_p H \) and \( u_p H z \), and similarly for \( \omega_{pHz} \) (cf. Uhlmann and Dušek, 2014, p. 234, for an extended discussion).

5.2.1 Steady vertical regime

Table 6 shows the terminal falling velocity \( u_p V \) and the recirculation length \( L_r \) obtained using different spatial resolutions and CFL. It can be seen that the error in the terminal velocity \( u_p V \) is consistently reduced towards the reference value, except for the case with the highest spatial and temporal resolution \( (d/\Delta x = 48, \text{ CFL} = 0.06) \), in which the value of \( u_p V \) is slightly overestimated. Please note that the error for such refined simulations is already well below one percent, and that minor differences in the two setups (e.g. the slight variation in the blockage ratio due to different cross-sections of the computational domain) might become relevant. On the contrary, the recirculation length \( L_r \) seems to converge to a slightly different value than that of the spectral-element solution. We will return to
this point shortly. Figure 15a shows isocontours of relative velocity $u_r$ for the case with $d/\Delta x = 24$, highlighting the extent of the recirculation bubble ($u_r = 0$). Figures 15b and c show the extent of the recirculation bubble for all the spatial resolutions. Note that, in the same fashion as in figures 7 and 8, the dashed lines in figure 15 represent the location at which the velocities supplied in the additional material are sampled.

It can be seen in figure 15(c) that under spatial grid refinement (while keeping the CFL number fixed) the IBM computations converge to a solution which exhibits a slight discrepancy as compared to the spectral-element reference solution. When decreasing the CFL number, however, the solution for a fixed spatial resolution (figure 15) can be seen to successively approach the reference solution. The convergence is quantified in table 6, where both errors in $u_p V$ and $L_r$ are seen to decrease with decreasing time step. Note that although the solution is steady in the frame of reference moving with the particle, it is still unsteady in the frame attached to the grid in the IBM method. The present observation of a necessity to refine the time step in order to obtain convergence for very fine grids has already been made previously in the context of settling spheres by [Uhlmann and Dušek, 2014], cf. their § 3.2.2. More recently, [Zhou and Balachandar, 2021] have analyzed the spatio-temporal convergence of the direct forcing immersed boundary method in more detail. They have confirmed theoretically and in terms of numerical experiments that satisfying the CFL condition alone does not guarantee the solution to converge under spatial grid refinement. Rather, one needs to make sure that the time step is sufficiently small with respect to the characteristic time scales of the problem at the fluid-solid interface.

Despite the previous remarks on convergence in the immediate vicinity of the immersed solid object, the solution does indeed get in general much better with increasing spatial resolution, even while keeping the value of the CFL number constant. This can be seen e.g. when considering the relative velocity $u_{r\parallel}$ along the vertical axis passing through the particle center, as shown in figure 16. In particular the error plotted in panel 16 clearly decreases with increasing spatial resolution. More specifically, it can be observed that the error changes from overpredicting the value of $u_{r\parallel}$ for $z/d < 1$ to underpredicting it for $z/d > 2$. The r.m.s. error $\langle \epsilon(u_{r\parallel}) \rangle^{1/2}$ (evaluated for the intervals $-2 \leq z/d \leq -0.5/\chi$ and $0.5/\chi \leq z/d \leq 10$) is included in table 6: it shows first order convergence with $\Delta x$.

Velocity profiles of $u_{r\parallel}$ and $u_{r\text{rad}}$ along lines perpendicular to the vertical direction at different positions of $z$ (as indicated in figure 15) are shown in figure 17 for two different resolutions. In both cases the qualitative features of the flow are captured and the small quantitative discrepancies found when $d/\Delta x = 18$ are significantly reduced by increasing the resolution.

Finally, the non-dimensional pressure coefficient $C_p = (p - p_{\infty})/(0.5 \rho_f U_\infty^2)$ along the great circle is represented in figure 18. Similarly as in the case of spheres (Uhlmann and Dušek, 2014), the larger differences of the case with low resolution ($d/\Delta x = 18$) are found in the vicinity of the stagnation point ($\theta = \pm \pi$). With double resolution ($d/\Delta x = 36$), the profile obtained from the IBM computation is in excellent agreement with the reference solution.

### 5.2.2 Steady oblique regime

Table 7 shows the IBM results of the steady oblique regime cases. In addition to $u_{pV}$ and $L_r$, the values of $u_{pH}$ and $\varphi$ are included in the table to characterize the lateral drift of the particle as well as the tilting of its symmetry axis. For the spheroid with $\chi = 1.1$ the values of $u_{pH}$ and $\varphi$ obtained with spatial resolutions $d/\Delta x = 18$ or 24 are one order of magnitude smaller than the reference value. When the spatial resolution is increased to $d/\Delta x = 36$ and 48, the agreement with the spectral-element solution is remarkable. This means that the regime is only marginally captured by the IBM.
Figure 15: a) Iso contours of relative velocity $u_r ||$ for the steady vertical case A11-M100 ($Ga = 100$, $\chi = 1.1$ and $m^* = 1$) using the IBM with a resolution of $d/\Delta x = 24$. The contour $u_r || = 0$ is highlighted in red. b) Recirculation region ($u_r || = 0$) for different spatial resolutions of the same case and CFL = 0.52 (zoom inset shown in c). d) Recirculation region for different time steps with $d/\Delta x = 24$ (zoom inset shown in e).
Figure 16: a) Profiles of $u_{r||}$ for steady vertical regime ($Ga = 100$, $\chi = 1.1$, $m^* = 1$) on the vertical axis through the particle center. b) Zoom on the wake next to the particle shown in a). c) Difference of IBM computations with respect to the reference solution $\epsilon(u_{r||}) = u_{r||}^{IBM} - u_{r||}^{SEM}$. The inset in c) contains the additional cases with resolution $d/\Delta x = 24$ and smaller time step (CFL = 0.26, 0.13) together with the case with CFL = 0.52. d) Convergence of the error shown in panel c averaged over the vertical direction. The legend in d) indicates the value of CFL.
Figure 17: Cross profiles of vertical and horizontal components of the relative velocity for steady vertical regime case A11-M100 ($Ga = 100$, $\chi = 1.1$, $m^* = 1$) at different positions of $z$ (see legend) obtained with the IBM with a resolution of $d/\Delta x = 18$ (a and b) and $d/\Delta x = 36$ (c and d), both with CFL = 0.52. The reference solution is represented with dashed lines.

Figure 18: Pressure coefficient along the great circle for the steady vertical regime case A11-M100 ($\chi = 1.1$, $Ga = 100$ and $m^* = 1$) obtained from the IBM computations with resolutions $d/\Delta x = 18$ (black circles) and 36 (green circles). Reference solution obtained with SEM is represented with a solid red line.
using spatial resolutions $d/\Delta x = 18, 24$. For the spheroid with $\chi = 1.5$, the error in $u_{\rho V}$, $u_{\rho H}$ and $\varphi$ is systematically reduced with increasing spatial resolution. We observe a similar trend in the value of $L_r$ as in the steady vertical cases (discussed in § 5.2.1).

Figure [19] shows isolines of constant velocity $u_{\rho r}$ for the steady oblique regime cases of the spheroid with $\chi = 1.5$. Panels [19]-b show contours for the case with spatial resolution $d/\Delta x = 24$ highlighting the recirculation bubble ($u_{\rho r} = 0$). Panels [19]-f show the recirculation bubble obtained for different spatial resolutions and an additional case in which forcing points are distributed also in the interior of the particle (cf. [3]). The motivation to carry out this additional case is that we observe a small amplitude path oscillation for the case with the highest spatial resolution ($d/\Delta x = 48$), which can be appreciated in the small lateral deviation of the recirculation bubble shown in figure [19]. Inspection of the volume occupied by the particle (cf. figures [20]a and c) reveals that some parasitic flow develops therein. We have therefore recomputed this case while applying the rigid-body forcing throughout the volume occupied by the particle. As can be seen from figures [20]h, c), the parasitic flow is effectively suppressed. As a consequence it can be seen in figure [19] how the shape of the recirculation bubble is notably better captured when forcing inside. Cases with forcing in the interior of the particle with spatial resolutions $d/\Delta x = 24, 36$ are further discussed.

Figure [21] shows the relative velocity $u_{\rho r}$ on a line parallel to the trajectory of the particle ($e_{\rho r}$) passing through the center of the particle for all spatial resolutions employed in the steady oblique case with $\chi = 1.5$. The error $\varepsilon(u_{\rho r})$ is represented in figure [21] where, again, we confirm that $\langle \varepsilon(u_{\rho r})\rangle_{x}^{1/2}$ systematically decreases with increasing spatial resolution (at constant CFL). Figure [21] shows that the convergence of $\langle \varepsilon(u_{\rho r})\rangle_{x}^{1/2}$ with the spatial resolution is of first order. The figure also includes the additional cases in which forcing points are distributed also in the interior of the particle for spatial resolutions $d/\Delta x = 24, 36, 48$. The above mentioned oscillations for the highest spatial resolution can be observed in figure [21] as well as their absence by forcing in the interior of the particle. Furthermore, figure [21] shows how the convergence of the error with the spatial resolution approaches second order when forcing also inside the particle’s volume.

Based on the results obtained for the steady vertical regime and on analogous work for spheres (Uhlmann and Dusek 2014), the higher resolution needed in the case of the spheroid with lower aspect ratio ($\chi = 1.1$) compared to the higher aspect ratio ($\chi = 1.5$) is somehow unexpected. However, a look at the two-parameter state diagram in figure [5] reveals that the width of the region in which the

| Case            | $d/\Delta x$ | $u_{\rho V}$ | $\varepsilon$ | $u_{\rho H}$ | $\varepsilon$ | $\varphi^{(\circ)}$ | $\varepsilon$ | $L_r/d$ | $\varepsilon$ |
|-----------------|--------------|--------------|---------------|--------------|---------------|---------------------|---------------|---------|---------------|
| B11-M100        | 18           | $-1.7193$    | 0.0229        | 0.0041       | 0.0301        | 0.357               | 0.8706        | 1.9878  | 0.0110        |
| B15-M075        | 18           | $-1.6514$    | 0.0182        | 0.0832       | 0.0177        | 4.090               | 0.2399        | 2.0739  | 0.0171        |
| B15-M075 Forc. in. | 24           | $-1.6614$    | 0.0122        | 0.1164       | 0.0020        | 5.710               | 0.0737        | 2.0757  | 0.0180        |
|                 | 36           | $-1.6773$    | 0.0028        | 0.1188       | 0.0035        | 5.628               | 0.0583        | 2.0814  | 0.0207        |
|                 | 48           | $-1.6843$    | 0.0014        | 0.1198       | 0.0041        | 5.600               | 0.0532        | 2.0832  | 0.0216        |
Figure 19: a-b) Iso contours of relative velocity $u_r^\parallel$ for the steady oblique regime case B15-M075 ($\chi = 1.5$, $Ga = 110$ and $\tilde{\rho} = 2.14$) with a spatial resolution of $d/\Delta x = 24$. The contour $u_r^\parallel = 0$ is highlighted in red. c,e) Recirculation region ($u_r^\parallel = 0$) for different spatial resolutions of the same case (zoom inset shown in d,f).
Figure 20: a) Unmasked contours of relative velocity \( u_{r\parallel} \) of steady oblique case with \( Ga = 110, \chi = 1.5, \tilde{\rho} = 2.14 \) with spatial resolution \( d/\Delta x = 36 \) distributing Lagrangian force points on the particle surface only, and b) forcing throughout the volume occupied by the solid particle. c) Profile of relative velocity \( u_{r\parallel} \) along a line parallel to the trajectory passing through the center of the particle \( (x_{p\perp} = x_{pHz\perp} = 0) \) for both cases, represented with a dashed line in a,b. The black contours shown in a,b correspond to \( u_{r\parallel} = -0.4, -0.2, 0.2 : 0.2 : 1.2 \) and the blue and red contours to \( u_{r\parallel} = -0.02 \) and 0.02, respectively. The green line in the three panels represents the surface of the spheroid.

steady-oblique regime occurs for a spheroid of \( \chi = 1.1 \) and \( \tilde{\rho} = 2.1 \) is of the order of a few units of \( Ga \), which is narrower than that of the spheroid with \( \chi = 1.5 \) and \( \tilde{\rho} = 2.14 \). Furthermore, the selected value of \( Ga = 115 \) for the spheroid with \( \chi = 1.1 \) is clearly closer to the critical \( Ga \) leading to the first bifurcation (boundary between white and gray regions in figure 6a) than the corresponding case with \( \chi = 1.5 \). Please recall that small numerical inaccuracies can induce an upward shift of the threshold leading to the first bifurcation by several Galileo number units (Uhlmann and Dušek 2014). Therefore, the higher spatial resolution needed in this case seems reasonable.

5.2.3 Vertical periodic regime

Here we evaluate the convergence with spatial resolution of the solution obtained by means of the IBM for the vertical periodic cases that appear for a spheroid of aspect ratio \( \chi = 1.5 \), \( Ga = 150 \) and \( \tilde{\rho} = 2.14 \). Table 8 shows the statistical moments, as well as errors which are computed with respect to the SEM reference data presented in §3.2.3 (cf. statistics in table 4). Note that \( u_{pHz\perp} \) was not included in the reference results presented in table 4 because it is zero (the flow maintains planar symmetry).

It can be seen that the results generally converge under grid refinement while keeping the CFL number constant. However, concerning the average settling velocity \( u_{pV} \), we observe once more a convergence to a value which is approximately 1.5% off the reference value (for \( d/\Delta x = 48 \)) under purely spatial refinement. Again, when further reducing the time step (i.e. for \( d/\Delta x = 24 \) and reducing CFL from 0.56 to 0.28) the solution does approach the reference value, as already discussed above (cf. §5.2.1). Figure 22 shows the time-evolution of the horizontal particle velocity \( u_{pH} \), which is dominated by a single harmonic. It can be seen how both the amplitude as well as the period improve under spatial and temporal refinement.
Figure 21: a) Profiles of $u_{rl}$ for steady oblique regime ($Ga = 110$, $\chi = 1.5$, $\bar{\rho} = 2.14$) along a line parallel to the trajectory passing through the center of the particle ($x_{p\perp} = x_{pHz\perp} = 0$). b) Zoom of the wake shown in panel a. c) Difference of IBM computations with respect to the reference solution $\varepsilon(u_{rl}) = u_{rl}^{IBM} - u_{rl}^{SEM}$. d) Convergence of the error shown in panel (c) averaged over the line parallel to the trajectory passing through the particle’s center. The legend in (d) indicates the forcing point distribution are distributed on the surface (“surf”) or in the entire volume of the spheroid (“f.i.”).

Table 8: Results and corresponding error measures of particle-related quantities for the vertical periodic cases computed by means of the IBM with $\chi = 1.5$, $Ga = 150$ and $m^* = 0.75$ ($\bar{\rho} = 2.14$).

| $\frac{dx}{\Delta x}$ | CFL | $St$ | $\varepsilon$ | $\pi_{pV}$ | $\varepsilon$ | $u'_{p\perp}$ | $\varepsilon$ | $u'_{pHz\perp}$ | $\varepsilon$ | $\omega'_{pHz\perp}$ | $\varepsilon$ | $\varphi_{\max}$ | $\varepsilon$ |
|------------------------|-----|-----|---------------|-------------|---------------|----------------|---------------|----------------|---------------|----------------|---------------|----------------|-------------|
| 18                     | 0.56| 0.1829 | 0.0782      | $-1.7454$   | 0.0030       | 0.0076        | 0.0022       | 0.1434        | 0.0290       | 0.0091        | 0.0053        | 0.2736        | 0.0771       |
| 24                     | 0.56| 0.1857 | 0.0639      | $-1.7307$   | 0.0054       | 0.0027        | 0.0006       | 0.1635        | 0.0174       | 0.0004        | 0.0003        | 0.3176        | 0.0518       |
| 36                     | 0.56| 0.1888 | 0.0485      | $-1.7170$   | 0.0133       | 0.0039        | 0.0000       | 0.1858        | 0.0046       | 0.0014        | 0.0008        | 0.3479        | 0.0344       |
| 48                     | 0.56| 0.1904 | 0.0405      | $-1.7126$   | 0.0158       | 0.0041        | 0.0002       | 0.1919        | 0.0011       | 0.0007        | 0.0004        | 0.3531        | 0.0315       |
| 24                     | 0.28| 0.1869 | 0.0581      | $-1.7493$   | 0.0053       | 0.0026        | 0.0007       | 0.1626        | 0.0180       | 0.0005        | 0.0003        | 0.3117        | 0.0552       |
5.2.4 Chaotic regime

The chaotic regime cases presented in §3.2.4 are reproduced here with a resolution of \( d/\Delta x = 36 \). Table 9 shows the statistics of the linear and angular particle velocities of the cases with \( \chi = 1.1 \) (\( Ga = 200, m^* = 1 \)) and \( \chi = 1.5 \) (\( Ga = 220, m^* = 5 \)). For the case with \( \chi = 1.1 \) the error in the mean vertical velocity is 1\% and for the case with \( \chi = 1.5 \) as low as 0.2\%.

Figure 23 shows the pdf for both linear and angular velocities of the chaotic regime cases computed with the IBM together with the spectral-element reference solutions. For the lower aspect ratio (\( \chi = 1.1 \)) the IBM computation captures the almost normal distribution found for the horizontal component of the velocity as well as the long positive tail in the vertical component and its positive skewness, whereas the decay of the negative tail is clearly slower compared to the SEM solution. The moderate excess kurtosis observed in the horizontal and vertical components of the angular velocity is also captured. For the higher aspect ratio (\( \chi = 1.5 \)) the slow decay of the negative tail in the pdf of the vertical velocity is captured, but not the fast decay of the positive tail of the curve. Regarding the horizontal component of the velocity, the positive kurtosis is only partially captured by the IBM solution. The horizontal component of the angular velocities of the case with \( \chi = 1.5 \) shows good agreement with the reference data, whereas the moderate excess kurtosis found in the vertical component is not captured.

Finally, the auto-correlations presented in figure 24 show a very good agreement for the case with \( \chi = 1.1 \), where both the decay and the frequency of oscillation are well captured. For the case with \( \chi = 1.5 \) the decay observed in the vertical velocity is faster for the IBM computation compared to the SEM solution. This behavior is switched for the horizontal component. Also, the slow decay of the vertical component found for separations of \( \tau U_g/d \gtrsim 15 \) is captured by the IBM solution as an oscillatory behavior. Regarding the angular velocity of the case with \( \chi = 1.5 \), the IBM solution features a slower decay than the reference solution in the vertical component, although the observed frequency of oscillation is well represented. The agreement between IBM and SEM in the horizontal component of the angular velocity of this case is very good; in particular the frequency of the oscillation is very well captured.
Table 9: Statistics of linear and angular particle velocities for chaotic cases of spheroids with $\chi = 1.1$ and $\chi = 1.5$ at $Ga = 200$ and $Ga = 220$, respectively, obtained from immersed-boundary computations with $d/\Delta x = 36$. The reference value used to compute the errors is taken from the spectral-element solution presented in table 5.

| $\chi$ | $(u_p)_{\tau_{uu}}$ | $\varepsilon$ | $\frac{\langle u_p' w_p'' \rangle^{1/2}}{U_g}$ | $\varepsilon$ | $\frac{\langle u_p' w_p'' \rangle^{1/2}}{U_g}$ | $\varepsilon$ | $\frac{\langle u_p' u_p'' \rangle^{1/2}}{U_g}$ | $\varepsilon$ | $\frac{\langle u_p' u_p'' \rangle^{1/2}}{U_g/d}$ | $\varepsilon$ | $\frac{\langle \omega p_z' \omega_p'' \rangle^{1/2}}{U_g}$ | $\varepsilon$ | $\frac{\langle \omega p_z' \omega_p'' \rangle^{1/2}}{U_g/d}$ | $\varepsilon$ | $\frac{T_{obs}}{d}$ |
|-------|-------------------|--------------|---------------------------------|--------------|---------------------------------|--------------|---------------------------------|--------------|---------------------------------|--------------|---------------------------------|--------------|---------------------------------|--------------|--------------|
| 1.1   | -1.9302           | 0.0118       | 0.0153                          | 0.0034       | 0.1009                          | 0.0074       | 0.0030                          | 0.0002       | 0.0272                          | 0.0067       | 1.430                           | 1.43          |
| 1.5   | -1.8656           | 0.0014       | 0.0098                          | 0.0014       | 0.0456                          | 0.0004       | 0.0014                          | 0.0005       | 0.0146                          | 0.0001       | 1.761                           | 1.76          |

Figure 23: IBM results of chaotic regime for cases D11-M100 (top row) and D15-M500 (bottom row). Pdf of vertical and horizontal components of the linear (left panels) and angular (right panels) velocity are represented together with a Gaussian distribution (see legend).
Figure 24: IBM results of chaotic regime for cases D11-M100 (top row) and D15-M500 (bottom row). Temporal auto-correlations of vertical and horizontal components of the linear (left panels) and angular (right panels) velocity are represented together with the spectral-element reference data (see legend).
6 Conclusions

We have presented accurate spectral-element data on low and moderate aspect ratio oblate spheroids settling under gravity in an unbounded fluid computed in a comparatively small domain in order to facilitate its use in benchmarking studies. The data-set which is freely available for download includes all aspects of the particle motion, as well as fluid velocity profiles and pressure maps. In this context, we present an extension to the immersed boundary method proposed by Uhlmann (2005) in order to handle non-spherical particles, which is validated against the spectral-element solutions.

The cases analyzed in this work have been carefully selected to cover the most relevant features encountered by finite-size heavy spheroids in wake dominated flows. First, the regime of steady vertical motion is considered in which the flow field is axi-symmetric. Then, we analyze the flow after the first regular bifurcation in which the axial symmetry of the solution is broken, leading to a steady regime with planar symmetry. We also analyze a vertical periodic regime which is not present in the case of spheres. The last regime presented is chaotic, requiring a statistical data analysis.

The extension of the IBM originally proposed by Uhlmann (2005) presented here makes use of quaternions and a combination of inertial and body-fixed reference systems to track rotations efficiently without presenting numerical instabilities. Please recall that, although in this work we have only presented results for spheroidal particles, the validity of the present algorithm is not restricted to any particular geometric shape. Furthermore, we have explored the possibility to apply the immersed boundary forcing throughout the volume occupied by the solid particles (instead of only at the surface) which was found to noticeably improve the results for a given spatial resolution.

In the last part of the manuscript we evaluate the accuracy of the enhanced immersed boundary algorithm. For upper end of the steady vertical regime (Ga = 100) the error in the particle settling velocity is systematically reduced from approximately 3% using \( d/\Delta x = 18 \) to approximately 1% when \( d/\Delta x = 48 \). We also demonstrate a convergence of \( O(\Delta x) \) of the error in the fluid velocity field when keeping the CFL number constant and, additionally, how the reduction of the time step for a given spatial resolution further reduces the error. Please note that, despite the simplicity of the kinematics obtained in this case, the flow is characterized by a wake whose recirculation bubble extends approximately two diameters downstream from the rear stagnation point, implying that non-trivial phenomena of flow separation must be accurately captured. Similar accuracy is achieved for the steady oblique regime, except for the spheroid with \( \chi = 1.1 \) and spatial resolutions \( d/\Delta x = 18, 24 \), where comparatively low horizontal velocity and particle tilting are obtained. Here the narrowness of the Ga interval in which this regime appears is making it hard to be captured with a non-conforming method. Nevertheless, the loss of axial symmetry and the orientation of the particle indicates that, despite the quantitative differences, the results are qualitatively in agreement with the reference solution. This highlights the fact that capturing the steady oblique regime (or any regime that takes place in a narrow region of the two parameter state diagram shown in figure 6) is already a hard test for a non-conforming-grid algorithm. We have also found that IBM forcing on the surface of the particle leads to an unphysical unsteadiness of the particle motion when using a very fine grid \( (d/\Delta x = 48) \) in a nominally steady case with relatively small excess particle density \((\chi = 1.5, Ga = 110, \hat{\rho} = 2.14)\). In this case, forcing throughout the volume occupied by the particle eliminates the unphysical coupling between the (parasitic) internal flow and the exterior; it also improves the prediction for a given spatial resolution. The results obtained for the vertical periodic regime show a systematic reduction of the error under spatial refinement, except for the mean settling velocity, which exhibits an error of approximately 1.5% when \( d/\Delta x = 24 \) is used. The latter error, however, can be substantially decreased by reducing the time step at a fixed spatial resolution. Finally, statistical errors obtained in the chaotic regime using a resolution of \( \Delta x/d = 36 \) are shown to be very small (first and second
moment of the particle velocity are predicted with errors below 1%) and probability density functions as well as auto-correlation functions are reasonably captured.

It is expected that the present study serves as an additional benchmark for numerical tools aimed to simulate flows involving non-spherical particles at Reynolds numbers of $\mathcal{O}(100)$. New algorithms can include the reference cases presented here in their benchmarking process in order to gauge their resolving efficiency, and hence their performance. The data-set further allows to precisely determine the required resolution depending on the tolerance and on the parameter regime of interest. Last but not least the data-set includes additional parameter points and additional physical quantities which have not been published up to this point. It can therefore be of interest in future work on the collective dynamics of settling oblate spheroids. Additional potential lies in the analysis of the present simulation results with respect to hydrodynamic force and torque. A number of previous authors have performed parametric studies for fixed spheroids placed in uniform inflow, using the simulation data to derive empirical force/torque correlation formulas as a function of aspect ratio, Reynolds number and relative orientation of the body [Zastawny et al. 2012; Ouchene et al. 2016; Sanjeevi et al. 2018; Andersson and Jiang 2019]. These correlations can then be utilized in Eulerian-Lagrangian point-particle simulations beyond the Stokes flow limit (e.g. van Wachem et al. 2015). Based on the data for the regime of steady particle motion in the present set, it will be possible to enlarge the available parameter space. This perspective, as well as further developments applicable to the modelling of forces and torque acting on spheroids undergoing unsteady motion, should be investigated in future studies.

The present reference data is available for download under the following persistent DOI: https://dx.doi.org/10.4121/13042793

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A Algorithm of the immersed boundary method

Each $k$th Runge-Kutta substep of the algorithm ($k = 1, 2, 3$) starts with the computation of the volume forcing $f^{(ibm)}$ from an explicit estimation of the velocity field ($\tilde{u}$), in which the presence of the particle is not considered. Then, the velocity field without considering the continuity constraint ($u^*$) is obtained (from a Helmholtz solve) by making use of the forcing $f^{(ibm)}$ to model the presence of the particle. After that, a Poisson problem is solved in order to obtain the pseudo-pressure $\phi$, with which the velocity field $u^*$ is corrected to obtain a divergence-free velocity field $u$ and, which serves to update the pressure field. Finally, the linear and angular position and velocity of the particle are updated. The complete algorithm reads
\[
\begin{align*}
\hat{u} &= u^{k-1} + \Delta t \left( 2\alpha \nu \nabla^2 u^{k-1} - 2\alpha \nu p^{k-1} - \gamma_k \left((u \cdot \nabla)u\right)^{k-1} - \zeta_k \left((u \cdot \nabla)u\right)^{k-2} \right), \\
\tilde{U}_l^{\beta,(m)} &= \sum_{ijk} \tilde{u}_\beta(x_{ij}^\beta) \delta_h \left(x_{ij}^\beta - x_i^{k-1,(m)}\right) \Delta x^3, \quad \forall l; m; \beta \\
F_l^{(m)} &= \frac{U_l^{d,k-1,(m)} - \tilde{U}_l^{(m)}}{\Delta t}, \quad \forall l; m \\
f_{\beta}^{(ibm),k}(x_{ij}^\beta) &= \sum_{m=1}^{N_p} \sum_{l=1}^{N_b} F_l^{\beta,(m)} \delta_h \left(x_{ij}^\beta - x_i^{k-1,(m)}\right) \Delta V_l^{(m)}, \quad \forall m; \beta; i; j; k \\
\nabla^2 u^* &= \frac{-1}{\alpha_k \nu \Delta t} \left( \frac{\nabla \cdot u^*}{\Delta t} + f^{(ibm),k} \right) + \nabla^2 u^{k-1} \\
\nabla^2 \phi &= \frac{\nabla \cdot u^*}{2\alpha_k \Delta t} \\
u^k &= u^* - 2\alpha_k \Delta t \nabla \phi, \\
p^k &= p^{k-1} + \phi - \alpha_k \Delta t \nu \nabla^2 \phi, \\
\mathcal{F}^{k,(m)} &= \sum_l F_l^{(m)} \Delta V_l^{(m)}, \quad \forall m, \\
\mathcal{T}_b^{k,(m)} &= R^{l-1,(m)} \sum_l (x_l^{k-1,(m)} - x_p^{k-1,(m)}) F_l^{(m)} \Delta V_l^{(m)}, \quad \forall m, \\
\frac{u_p^{k,(m)} - u_p^{k-1,(m)}}{\Delta t} &= -\frac{\rho_f}{V_p(\rho_p - \rho_f)} \mathcal{F}_b^{k,(m)} + 2\alpha_k g, \quad \forall m \\
\frac{x_p^{k,(m)} - x_p^{k-1,(m)}}{\Delta t} &= \alpha_k \left(u_p^{k,(m)} + u_p^{k-1,(m)}\right), \quad \forall m \\
\frac{\omega_p^{k,(m)} - \omega_p^{k-1,(m)}}{\Delta t} &= -\frac{\rho_f}{\rho_p - \rho_f} \rho_p \left(I_{p,b}\right)^{-1} \mathcal{T}_b^{k,(m)} - \gamma_k \left(I_{p,b}\right)^{-1} \left(\omega_p^{k-1,(m)} \times I_{p,b} \omega_p^{k-1,(m)}\right) \\
&\hspace{1cm} - \zeta_k \left(I_{p,b}\right)^{-1} \left(\omega_p^{k-2,(m)} \times I_{p,b} \omega_p^{k-2,(m)}\right), \\
\frac{\tilde{q}^{k,(m)} - q^{k-1,(m)}}{\Delta t} &= \gamma_k \frac{1}{2} Q^{k-1,(m)} q^{k-1,(m)} + \zeta_k \frac{1}{2} Q^{k-2,(m)} q^{k-2,(m)}, \\
q^{k,(m)} &= \begin{cases} \tilde{q}^{k,(m)} \bigg|_{\tilde{q}^{k,(m)}} \\
(22a) \end{cases} \\
U_l^{d,k,(m)} &= \frac{u_p^{k,(m)} + (R_l^{k,(m)})^T \left(\omega_p^{k,(m)} \times (x_I^{\beta,(m)} - x_p^{\beta,(m)})\right)}{2}, \\
\end{align*}
\]

where \(m\) is the index of a given particle (1 \(\leq m \leq N_p\)), \(\beta\) denotes a spatial direction (1 \(\leq \beta \leq 3\)), \(X_I^{\beta}\) is the position of a Lagrangian force point with index \(l\) (where 1 \(\leq l \leq N_l\)) attached to the \(n\)th particle, \(\delta_h\) is the discrete delta function of Roma et al. (1999), \(x_{ij}^{\beta}\) is the position vector of a node of the staggered Cartesian fluid grid of the velocity component in the \(x_{ij}\) direction with index triplet \("ij\)". \(\tilde{U}_l^{\beta}\) is the velocity in the \(x_{ij}\)-direction interpolated to a Lagrangian position, \(U_l^{(d)}(X_I)\) is the solid body velocity of the Lagrangian force point, \(F(X_I^{\beta})\) is the immersed boundary force at a Lagrangian force point, \(\Delta V_l^{(m)}\) is the forcing volume associated to the \(l\)th Lagrangian forcing point.
of the $m$th particle, $x_p \cdot m$ is the centroid position of the $m$th particle, $F \cdot m$ is the hydrodynamic force computed from the sum of the immersed boundary contributions of the $m$th particle, $T \cdot m$ is the analogous hydrodynamic torque contribution expressed in the body-fixed coordinate system, $\hat{q}$, $q$ and $Q$ are the quaternion before and after normalization and the evolution matrix defined in § 4, $R$ is the rotation matrix (defined below), and $I_{p,b}$ is the inertia tensor in the body-fixed reference system. The set of coefficients $\alpha_k$, $\gamma_k$, $\xi_k$ for a low-storage scheme leading to second-order temporal accuracy has been given in Rai and Moin (1991). Please refer to the original publication Uhlmann (2005) for more details on the algorithm.

It is important to note that the both $T_b$ and $\omega_{p,b}$ are expressed in the body-fixed reference system. Therefore, proper transformations through the rotation matrix $R$ and its transpose $R^T$ must be applied in steps (22j) and (22p). Following Tewari (2007) (equation 2.48), the rotation matrix to express global (or inertial) coordinates in the body-fixed reference frame is given from the quaternion $q$ by

$$R = \begin{pmatrix}
q_1^2 - q_2^2 - q_3^2 + q_4^2 & 2(q_1q_2 + q_3q_4) & 2(q_1q_3 - q_2q_4) \\
2(q_1q_2 - q_3q_4) & -q_1^2 + q_2^2 - q_3^2 + q_4^2 & 2(q_2q_3 + q_1q_4) \\
2(q_1q_3 + q_2q_4) & 2(q_2q_3 - q_1q_4) & -q_1^2 + q_2^2 + q_3^2 - q_4^2
\end{pmatrix}. \tag{23}$$

Note that the same algorithm (22) applies to the case when we distribute Lagrangian force points throughout the volume occupied by the solid particles. The distribution of force points itself in both cases (surface forcing and volume forcing) is described in B. Let us also note that we have performed extensive tests of the stability and convergence of the numerical integration scheme chosen for the rotational rigid body motion, including the evaluation of various alternative formulations. Although more sophisticated approaches with favorable properties exist (e.g. based on Lie group methods, Sveier et al. (2019), which circumvent the quaternion re-normalization step), the present approach was found to be sufficiently accurate and robust.

## B Forcing points distribution

### B.1 Distributing points on the surface of the spheroid

Here we briefly describe the procedure to distribute the forcing points on the surface of spheroidal particles. These forcing points are the points in which the explicit estimation of the velocity is interpolated (see equation 22b) and where the forcing term that models the no-slip boundary condition is computed (equation 22c). For more details the reader is referred to the original description of the algorithm Uhlmann (2005).

In the case of a sphere Uhlmann (2005) defined as an “even” distribution of points the final state of a simulation in which the total repulsive force between all the forcing points, considered as point-particles with a finite and equal charge, is minimized (method 2 of their appendix A.2.1). The repulsive force considered was quadratic with the Euclidean distance between each pair of points. This methodology cannot be directly applied to spheroids because of the lack of isotropy in the particle shape. In the case of oblate spheroids this anisotropy will result in a higher concentration of points in the poles of the spheroid. As expected, the nonuniformity of the points distribution increases as the aspect ratio is increased with respect to unity. In this work we use a similar approach to the one proposed by Uhlmann (2005), but modifying the definition of the repulsive force. Here, we define the modulus of the repulsive force between two points to be proportional to the $N$-th power of the geodesic distance, where $N$ is adjusted to minimize the nonuniformity of the final distribution. The direction of the repulsive force between two points is given at each point by the tangent to the geodesic line that
Figure 25: a) View along the symmetry axis and b) perpendicular to it of the spheroid with aspect ratio $\chi = 1.5$ with the distribution of Lagrangian markers on its surface. c) Surface of the spheroid (green) together with the inner (white) and outer (red) surfaces that define the shell of thickness $\Delta x$. d) Lagrangian markers distribution (red points) and the 3D Voronoï tessellation used to distribute the points in the interior of the particle and assign the Lagrangian markers volume $\Delta V$ for the spheroid (green surface).
connects both points. We found that using exponents \( N = 2 \) and 3 for the definition of the modulus of the repulsive force results in “even” distributions for the spheroids with aspect ratio \( \chi = 1.1 \) and 1.5, respectively. In the same fashion as in Uhlmann (2005), several runs with different initial conditions are computed in order to minimize the possibility of finding local minima. Figures 25a and b show the distribution of 1450 points on the surface of the spheroid with aspect ratio \( \chi = 1.5 \), which corresponds to the Lagrangian markers distribution used for the simulations with spatial resolution \( d/\Delta x = 24 \).

The number of points for a given spheroid at a given resolution is obtained as

\[
N \approx \frac{V_{\text{shell}}}{\Delta x^3},
\]

(24)

where \( V_{\text{shell}} \) represents the volume contained between the inner and outer surfaces, which are defined as the surfaces separated by a distance of \( -\Delta x/2 \) and \( +\Delta x/2 \) (in the normal direction) from the surface of the spheroid (see figure 25). For small aspect ratios the inner and outer surfaces in figure 25 can be approximated by two spheroids of diameter and symmetry axis length of \((d - \Delta x, a - \Delta x)\) and \((d + \Delta x, a + \Delta x)\), respectively, resulting in

\[
V_{\text{shell}} = \frac{\pi d^3 \left( \chi + \chi r^2 + 2 r^2 \right)}{3 r^3 \chi},
\]

(25)

where \( r = d/\Delta x \) is the spatial resolution. In order to assign the Lagrangian volume \( \Delta V \) to each forcing point, we generate a Voronoï tessellation on the surface of the spheroid based, again, on geodesic distances. The result is that the surface of the spheroid is divided into cells of fairly even distributed area. The ratio between the area of each cell and the total area of the surface of the spheroid is used as a factor to assign the volume \( \Delta V \) from the volume of the shell \( V_{\text{shell}} \).

### B.2 Distributing points throughout the volume of the spheroid

To distribute points inside the spheroid we use the distribution of points on the surface of the spheroid from the above mentioned procedure (appendix B.1), and consider these points as fixed. Then, we randomly fill the interior of the inner surface with \( N_i \) points

\[
N_i \approx \frac{V_{\text{in}}}{\Delta x^3},
\]

(26)

where \( V_{\text{in}} \) is the volume enclosed by the inner surface. The position of the \( N_i \) interior points is iteratively updated following Lloyd’s method to obtain a centroidal Voronoï tessellation (Lloyd 1982; Liu et al. 2009). Figure 25c shows the distribution of points in the volume occupied by a spheroid of \( \chi = 1.5 \) using a spatial resolution of \( d/\Delta x = 24 \). This procedure is very attractive because of its simplicity and it can be summarized in the following steps:

1. Generate a 3D Voronoï tessellation of all the forcing points.
2. Clip the Voronoï cells of the points located at the surface of the spheroid with the outer surface.
3. Move each interior point to the centroid of its associated Voronoï cell.
4. Repeat the procedure from step 1 until some convergence criteria is met. In practice we use the maximum displacement in the most recent step which is required to be below \( 10^{-8} d \).

\[\text{Note that the resultant edges of each cell are nor a straight line, nor a geodesic line, therefore they are generated numerically to be equidistant (under a threshold and in geodesic context) between the two adjacent points.}\]
5. Set the Lagrangian volume $\Delta V$ equal to the volume of its Voronoï cell.

The implementation to distribute the points on the surface of the spheroid is heavily based on the library GeodesicLib [Karney, 2013]. Similarly, the 3D Voronoï tessellations to carry out Lloyd’s method to distribute points in the interior of the spheroid uses the library voro++ [Rycroft, 2009] with a custom implementation of spheroidal walls.

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