

Dancing with the flow: Numerical modelling of non-ideal micro-particles in fluids

by Dr.-Ing. Jana Wedel (📍 UM, 📍 FAU)

📍 University of Maribor, Slovenia 📍 Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany

Supervisors: Prof. Paul Steinmann (📍 FAU), Prof. Jure Ravník (📍 UM), Prof. Matjaž Hriberšek (📍 UM)

From Idealized Spheres to Real Particles in Flows

Micron-sized particles are ubiquitous in natural, biomedical, and engineering flows. They determine how pollutants and aerosols spread, how inhaled drug carriers deposit in the respiratory tract, how bacteria and sludge flocs move in water treatment systems, and how particulate materials behave in industrial processes. Reliable prediction of their motion is therefore essential for environmental risk assessment, biomedical design, and process optimisation. Despite this relevance, most computational particle models still rely on strong idealisations: particles are commonly treated as rigid, spherical, homogeneous, and isolated objects. Real particles, however, are rarely ideal. They may have complex non-spherical shapes (volcanic ash, dust, microplastics), internal mass distributions (micro-organisms, sludge flocs), deform under fluid-flow-induced tractions (cells, bacteria) and collide with other particles or domain boundaries. These idealisations can therefore lead to inaccurate predictions of particle dynamics, compromising both the reliability of simulations and the conclusions drawn from them. This thesis targets these shortcomings by developing a new generation of computational particle models within the Lagrangian point-particle framework. Specifically, I developed methods to represent complex non-spherical particle shapes using superellipsoids, model particle-particle/particle-wall collisions for non-spherical particles, account for internal mass distributions, and simulate for the first time soft particles without costly surface or volume discretisation. Together, these developments provide both a novel modelling framework and new physical insights into how shape, internal structure, interactions, and deformability affect particle motion in fluid flows, while systematically extending classical particle tracking towards realistic non-ideal particles without sacrificing the computational efficiency required for engineering-scale simulations. The developed methods are implemented in the open-source software OpenFOAM and validated against analytical solutions and benchmark cases. Applications range from aerosol transport in realistic human airways to collision dynamics, soft-particle transport, and environmental particulate flows. Overall, the thesis establishes a scalable modelling framework for realistic particle-laden flows that was previously unavailable, providing new tools for both fundamental fluid mechanics and engineering practice.

Scientific Summary

The Fundamental Challenge Lagrangian point-particle tracking is the method of choice for large populations of dilute particles in fluid flows. However, classical particle-tracking approaches are usually built on multiple idealizations: particles are assumed to be spherical, homogeneous, rigid, and isolated. Real particles violate these assumptions simultaneously (see Fig. 1). Examples include volcanic ash, mineral dust, pollen, microplastics, asbestos fibres, bacteria, algae, biological cells, vesicles, and hydrogel particles. Moreover, statistically meaningful predictions often require particle populations on the order of 10^4 – 10^5 particles, making fully resolved approaches based on particle surface or volume discretisation computationally infeasible.

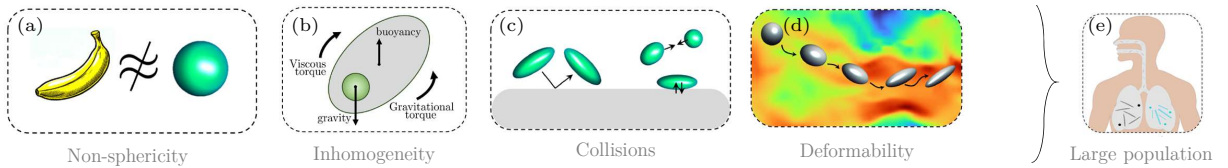


Figure 1. Sketch of selected key challenges in modelling particles in fluid flows, including (a) non-spherical shapes, (b) internal heterogeneity, (c) particle interactions, (d) deformability and (e) the need for statistically relevant particle numbers.

Central Research Question: How can realistic particles be represented within Lagrangian point-particle tracking while preserving the computational efficiency required for engineering-scale simulations?

Scientific Advancement I: Shape Matters As a first step during my doctoral research, I addressed the question: *How can non-spherical particles, such as pollen, dust, fibres, or other irregular micro-particles be modelled efficiently and how does shape affect their motion in fluid flows?*

To answer this question, I developed a novel superellipsoidal particle framework that enables an unprecedented range of realistic particle shapes to be represented within the Lagrangian point-particle approach [4]. In contrast to conventional methods, which often rely on spherical particle approximation supplemented by empirical shape correction factors (an assumption intentionally exaggerated in Fig. 1(a)) the proposed framework directly incorporates particle shape into the governing equations of motion. This was achieved by deriving numerical resistance tensor models for superellipsoidal particles in Stokes flow from dedicated direct numerical simulations. These models allow shape-dependent hydrodynamic forces and torques to be incorporated without resorting to costly particle surface or volume discretisation.

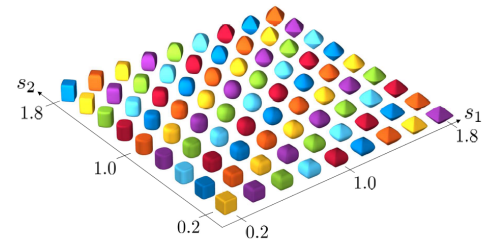


Figure 2. Examples of superellipsoids for aspect ratios $\lambda_1 = \lambda_2 = 1$ and varying shape factors s_1, s_2 .

The novel model allows an unprecedented range of particle shapes to be tracked in arbitrary flow fields, enabling the representation of shapes ranging from spheres and ellipsoids to cubes, diamond-like particles, and fibres (see Fig. 2). Extensive validation against benchmark cases demonstrated that particle shape has a profound influence on translational and orientational dynamics, and ultimately transport and deposition characteristics. In particular, the results revealed that commonly employed spherical approximations, simplified ellipsoidal descriptions, and shape-factor-based correction approaches can lead to substantial errors in the prediction of particle motion. The developed framework therefore established that **shape matters**: particle shape is not a secondary correction, but a governing parameter in particle-laden flows, significantly improving the predictive capabilities of Lagrangian particle-tracking methods for realistic particulate systems.

Scientific Advancement II: Superellipsoid Particle Collisions After establishing superellipsoid tracking, the next question naturally arose: *How can we model the deposition and interaction of these non-spherical particles efficiently?*

To address this research gap, I developed a novel collision model for superellipsoidal particles [5]. The method combines a Newton–Raphson-based Lagrangian multiplier technique for collision detection with the compact superellipsoidal shape representation, enabling particle–particle and particle–wall collision modelling without surface discretisation. The model was validated against analytical solutions for well-defined collision configurations and tested extensively in increasingly complex systems. These tests demonstrated reliable performance in dilute systems of arbitrary geometry, where collisions arise from clustering or wall interactions, as well as in more densely populated particle configurations (see Fig. 3 (a,b)).

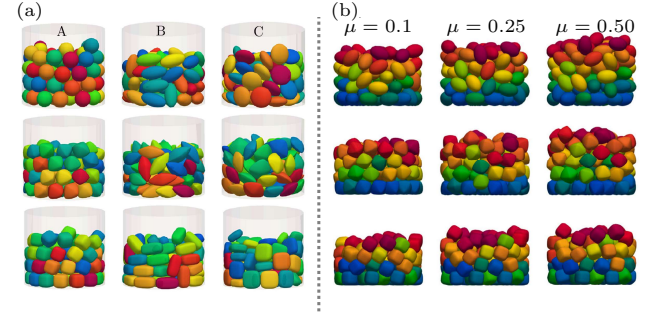


Figure 3. Collision example: (a) cylinder filling with different superellipsoids and (b) influence of friction coefficient μ .

In addition, a novel frictional collision model was developed, including a generalized tangential coefficient of restitution for arbitrarily shaped particles (see Fig. 3(b)). The model captures for the first time the influence of relative normal and tangential collision velocities and particle shape, while remaining consistent with established spherical-particle results.

Scientific Advancement III: Internal Structure Matters During my doctoral research, the next question arose: *How can particles such as algae, micro-organisms, or composite particles with non-homogeneous mass distributions be modelled efficiently, and how does internal inhomogeneity affect their motion in fluid flows?*

To tackle this research gap, I developed a novel inhomogeneous particle model within the Lagrangian point-particle framework [2]. In this model, internal inhomogeneity is represented by a mass inclusion embedded in the particle matrix (see Fig. 4(a)). I derived the (coupled) equations of translational and rotational motion in both barycentric and geometric-centre formulations, allowing the effects of non-uniform mass distributions on particle dynamics to be captured efficiently. The formulation provides a general description of particle kinematics and dynamics and is not restricted to a specific inclusion or matrix geometry.

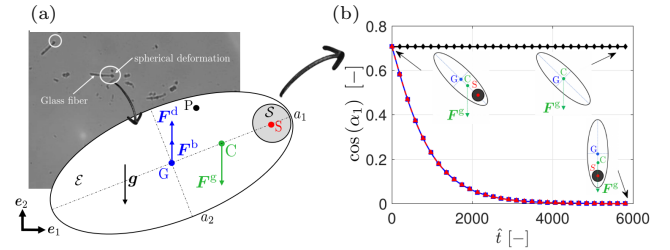


Figure 4. (a) Inhomogeneous particle model (b) Settling of a prolate spheroid ($\lambda = 6$, $d_{eq} = 1 \mu m$) in air.

The model was validated and tested in settling simulations (see Fig. 4 (b)) and laminar shear-flow configurations. The results demonstrated clearly that **internal structure matters**: internal mass distributions can significantly alter translational and rotational dynamics and must therefore be explicitly considered when modelling realistic particles in flows.

Scientific Advancement IV: Soft Particles After the various extensions (complex shapes, internal mass distributions, and particle interactions), one major question remained: *How can the vast class of soft particles in flows (cells, bacteria, hydrogel particles) be modelled efficiently?* (Note that existing approaches rely almost exclusively on surface or volume discretisation methods, which become prohibitively expensive when large particle populations are considered.)

This led to my most significant contribution: **an utmost efficient pseudo-rigid-body approach** for soft particles, combining, for the first time, affine deformations (see Fig. 5) with Lagrangian point-particle tracking and reducing soft-particle tracking to a minimum of 12 DOF [1,3]. The method is not restricted to a specific constitutive law and can easily be extended to different material models. The approach enables simulations of both soft initially spherical and ellipsoidal particles in dilute viscous flow, including particle populations on the order of 10^5 . It was validated against benchmark cases and applied to soft-particle transport in complex geometries, including inhalation of soft particles in a realistic human nasal cavity, demonstrating both robustness and engineering-scale applicability.

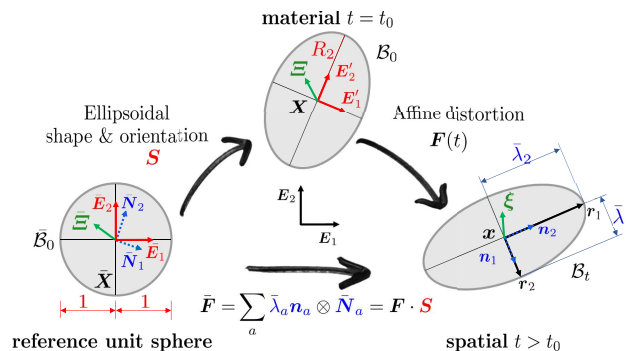


Figure 5. Initial ellipsoid (material conf.) with half axes R_a deforming affinely into an ellipsoid with half axes r_a , $a = 1, 2, 3$.

Novelty, Originality, Scientific Impact, and Engineering Relevance

The principal contribution of this work is a unified modelling framework that systematically extends state-of-the-art Lagrangian point-particle tracking towards realistic particles. By enabling the efficient simulation of non-spherical, interacting, inhomogeneous and soft particles, this work closes several long-standing gaps between idealized particle models and real-world particulate systems.

The work provides several scientific advancements:

- a novel superellipsoidal Lagrangian frameworks for non-spherical micro-particles [4];
- a novel efficient collision for superellipsoids (+ the first tangential restitution model for arbitrary particle shapes) [5];
- a novel and general inclusion-based formulation for inhomogeneous particles with non-uniform mass distributions [2];
- the first scalable Lagrangian point-particle framework for large populations of soft initially spherical and ellipsoidal particles in dilute flow [1,3].

Due to these advancements, our developed framework significantly expands the applicability of state-of-the-art Lagrangian point-particle tracking to realistic particulate systems. It enables the investigation of particle transport, deposition, collision, and deformation phenomena that were previously computationally infeasible or poorly understood.

The engineering relevance is broad because all developed models are formulated independently of a specific application and can be coupled to arbitrary macroscopic flow fields. Potential applications include aerosol transport and respiratory drug delivery, environmental particle dispersion and microplastic transport, water and wastewater treatment, bioreactors, industrial particle processing, micro- and nano-particle technologies, and biological cell transport. The resulting framework therefore provides not only fundamental scientific advances in particle-laden flows but also practical tools for addressing important engineering challenges across multiple disciplines.

All methods have been implemented within the open-source CFD platform *OpenFOAM*, ensuring broad accessibility, reproducibility, and transferability to future academic and industrial applications. Beyond the software implementation, I actively contribute to the PiFlow community on Zenodo, where codes and datasets are made freely available to the research community.

Selected Publications and Research Output

The doctoral thesis was completed with distinction. The research output comprises 19 published journal articles, 7 published conference articles, and 3 additional accepted conference articles, with an h-index of 6 excluding self-citations. The candidate has personally presented this work at 16 conferences. The publications appeared in leading international journals, including *Journal of Computational Physics*, *Computer Methods in Applied Mechanics and Engineering*, *International Journal of Multiphase Flow*, *Powder Technology*, and *Physics of Fluids*. Furthermore, the work has been recognized by the ECCOMAS Award for the Best PhD Theses 2026, the GACM Best PhD Award 2026, and the WCCM Best Presentation Award 2022.

- [1] **Wedel J.**, Hriberšek M., Ravnik J., Steinmann P.: *Ellipsoidal soft micro-particles suspended in dilute viscous flow*. Computer Methods in Applied Mechanics and Engineering, 2025.
- [2] **Wedel J.**, Steinmann P., Prinz F., Lízal F., Hriberšek M., Ravnik J.: *Mass distribution impacts on particle translation and orientation dynamics in dilute flows*. Powder Technology, 2025.
- [3] **Wedel J.**, Hriberšek M., Ravnik J., Steinmann P.: *A novel pseudo-rigid body approach to the non-linear dynamics of soft micro-particles in dilute viscous flow*. Journal of Computational Physics, 2024.
- [4] **Wedel J.**, Steinmann P., Štrákl M., Hriberšek M., Ravnik J.: *Shape matters: Lagrangian tracking of complex nonspherical microparticles in superellipsoidal approximation*. International Journal of Multiphase Flow, 2023.
- [5] **Wedel J.**, Štrákl M., Hriberšek M., Steinmann P., Ravnik J.: *A novel particle-particle and particle-wall collision model for superellipsoidal particles*. Computational Particle Mechanics, 2023.

Beyond the scientific contributions, my work was embedded in a strong international research environment. Since 2021, I have maintained frequent scientific exchange and collaboration with the University of Maribor, Slovenia, resulting in joint research activities, publications, and co-supervision. The doctoral work further involved collaborations with international partners including Prof. Yan Cui (Huazhong University of Science and Technology, Wuhan, China), Prof. František Lízal (Brno University of Technology, Czech Republic), and Prof. Jordi Pallarès (Universitat Rovira i Virgili, Tarragona, Spain), leading to joint publications in areas ranging from aerosol transport to particle inhomogeneity and deposition phenomena.

In addition, I actively contributed to large-scale international Computational Fluid Dynamics (CFD) benchmark initiatives on aerosol dispersion, involving research teams from up to 18 countries worldwide, resulting in the publications “*Numerical simulations of the flow and aerosol dispersion in a violent expiratory event: Outcomes of the 2022 International Computational Fluid Dynamics Challenge on violent expiratory events*” (*Physics of Fluids*, 2023) and “*Computational fluid dynamics challenge on indoor dispersion of pathogen-laden aerosols*” (*Physics of Fluids*, 2025). These activities strengthened the international visibility of the research and fostered scientific exchange within the global CFD community.

During my doctoral research, I have also shown strong commitment to teaching and knowledge transfer. Since September 2020, I have taught the practical component of the Master’s course *Computational Fluid Dynamics* at TH Nürnberg Georg Simon Ohm, where I instruct students in the use of OpenFOAM and have successfully supervised one master’s thesis. Since 2025, I have also been part of the teaching team for the course *OpenFOAM Essentials* at the University of Maribor, targeting industry professionals and researchers and thereby actively contributing to knowledge transfer between academia and industry.