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Drag Correlations for Multiphase Flows Using Artificial Neural Networks

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ABSTRACT

A novel approach for the generation of drag correlations for multiphase flows is presented. Fully resolved computational fluid dynamics simulations for multiphase flows are performed to provide ground truth data. An artificial neural network is trained to learn the accurate particle behavior based on less accurate flow data from the Lagrangian particle simulation. For the case of a settling spherical particle, this approach outperforms the existing empirical model.

1. Introduction

Due to the computational intensity of fully resolved simulations, Lagrangian point particle models are widely spread for the simulation of particle laden flow with technical relevant numbers of particles. These models rely on empirical drag correlations for the determination of particle forces. It is well known that these models are only valid for $d_p \ll \Delta x$ [1]. The goal of this work is to use artificial neural networks (ANN) instead of empirical correlations to remedy this shortcoming.

2. Methods

2.1. Resolved particle simulations

For the fully resolved particle simulation, a Lattice Boltzmann method (LBM) is combined with a rigid body solver (Fig. 1a). A detailed description of the LBM implementation can be found in [2]. The base grid has a grid size of Δx_α with additional adaptive mesh refinement around the moving particle, providing a local resolution of Δx_β. The forces acting on the particle surface $\vec{F}$ are determined by integrating the hydrodynamic forces over the particle surface using the momentum exchange method for LBM. This information is used to solve the motion equation of each particle, which is defined in a Lagrangian frame of reference

$$\frac{d^2\vec{x}_p}{dt^2} = \frac{\vec{F}_p}{m_p} + \vec{g}\left(1 - \frac{\rho_f}{\rho_b}\right) \tag{1}$$

by using a predictor-corrector scheme. At the boundary Γ_b (see Fig. 1a), the no-slip condition is enforced with $\vec{u}_\Gamma = \vec{u}_p$ where $\vec{u}_p$ refers to the particle velocity.

2.2. Lagrangian particle tracking

For the Lagrangian particle tracking simulations, the rigid body solver is replaced by a point particle approach. The particle motion is described by the Maxey-Riley equation [1]. If the added mass and history force are neglected, the motion eq. (1) is solved. Here, the momentum equation for the carrier fluid is solved on a uniformly refined grid with Δx_α. The force $\vec{F}_p$ is provided by empiric correlations C_D, such that

$$\frac{\vec{F}_p}{m_p} = \frac{C_D}{24}\frac{Re_p}{\tau_p}, \quad Re_p = \frac{\rho\|\vec{u} - \vec{u}_p\|d_p}{\mu}, \quad \tau_p = \frac{\rho_p d_p^2}{18\mu},$$

with the particle REYNOLDS number Re_p, the particle relaxation time τ_p the carrier fluid viscosity μ and particle density ρ_p. Here, the classical Schiller-Naumann equation for the drag part [1] is used, which reads as

$$C_D = \frac{24}{Re_p}(1 + \frac{1}{6}Re_p^{2/3}). \tag{2}$$

A two-way coupled approach is chosen to capture the particle motion feedback onto the flow field. The momentum equation for the carrier fluid phase is extended by the momentum source term associated with the particle reaction force, which reads as

$$\vec{F}_{f,p} = -\mathcal{G}(\|\vec{x} - \vec{x}_p\|)\vec{F}_p, \tag{3}$$

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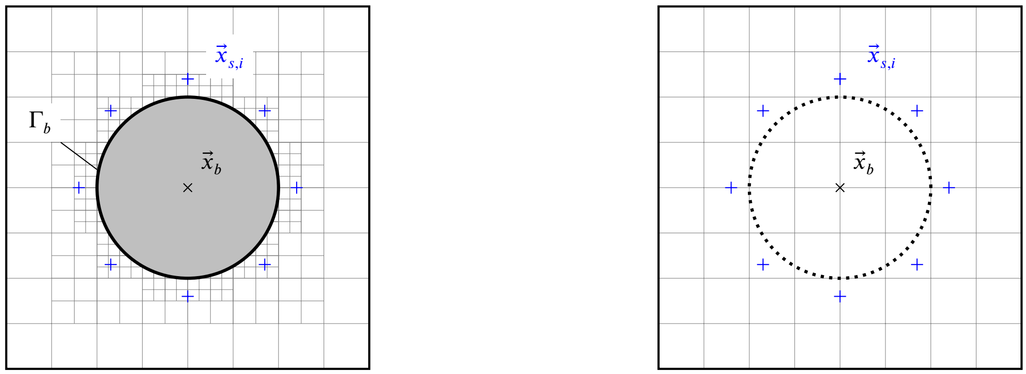

(a) (b)

Figure 1: Grid setup for fully resolved simulations (a) and Lagrange particle simulations (b). Body-relative sampling locations $\vec{x}_{s,i}$ are shown as +.

where $\mathcal{G}(\cdot)$ is a Gaussian kernel, which distributes the momentum source to the vicinity of the particle. The standard deviation is chosen as $6\sigma = 1.6d_p$. By doing so, the intrinsic drawback of the Lagrange particle tracking method becomes apparent: The velocity field is locally disturbed by the two-way coupled approach, resulting in an erroneous evaluation of the given empirical correlation defined for the undisturbed carrier fluid velocity.

2.3. ANN based correlations from fully resolved simulations

The first step is to provide an improved drag correlation by using data from fully resolved simulations. For each time step n, the hydrodynamic force $\vec{F}^n$ acting on a given particle is known. Additionally, the velocity field at N_s points $\vec{x}^{\,n}_{s,i}$ relative to the body position $\vec{x}^{\,n}_b$ is extracted (see Fig. 1a). This information forms a dataset

$$\{\vec{u}^{\,n}_{rel,i}, \vec{F}^n\} \quad \text{with} \quad \vec{u}_{rel,i} = \vec{u}_{s,i} - \vec{u}_b, \tag{4}$$

which serves as training data for an artificial neural network (ANN) to find a suitable relation in the form of $\vec{F} \approx f(\vec{u}_{s,i})$.

The ANN is a multilayer perceptron composed of an input layer with N_s neurons, three fully connected layers with 64 neurons each, and a final layer with 3 neurons, one for each force component. The relatively small network architecture is chosen to guarantee an efficient performance for parallel CFD computations on high-performance computing (HPC) systems. A larger network architecture would negatively affect the efficiency of the proposed method, since the ANN must be employed by each rank for the number of particles in the corresponding rank for every time step. The weights and biases are updated by an adaptive moments (ADAM) optimizer [3] and a mean-squared error (MSE) loss function. A leaky-Rectified linear unit (ReLU) activation function is chosen [4], a variation of the ReLU activation function [5].

The obtained ANN is used as a novel force correlation for the Lagrange particle tracking. Different to the known correlations such as eq. (2), the input data accounts for the velocity disturbance caused by the boundary condition in the fully resolved simulation. To enable the use of the obtained ANN inside the LPT simulation, the analogous velocity data at the points $x_{s,i}$ has to be obtained (see Fig. 1b).

While this approach makes use of the most accurate data, systematic deviations of the input data (i.e., the velocity field) have to be expected in Lagrangian particle simulations. This is due to the lower grid resolution and the fact, that the momentum feedback compared to the fully resolved simulation is fundamentally different.

2.4. ANN based correlations from coupled simulations

To address these drawbacks, a novel approach is proposed. Here, both the fully resolved simulation and the LPT simulation are run simultaneously. For each time step, the particle trajectory from both simulation is coupled by setting

$$\vec{u}_{p,LPT} = \vec{u}_{p,resolved}. \tag{5}$$

From this coupled simulation, a dataset similar to eq. (4) is extracted by sampling the carrier fluid velocity from the LPT. The resulting ANN can be used in LPT simulations, as described in Sec. 2.3.

3. Results

The generic case of spherical particle settling in an initially quiescent fluid is considered. The Reynolds number with respect to terminal velocity is chosen as $Re = 32$. Both

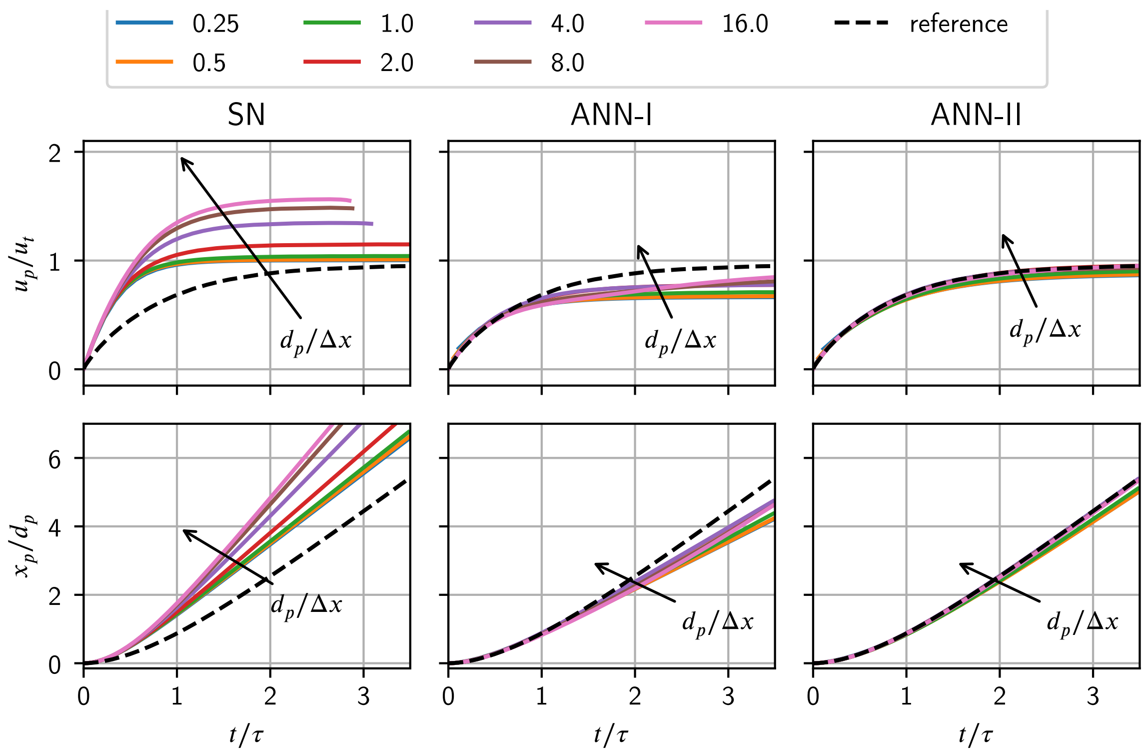

Figure 2: Particle velocity u_p/u_t and position x_p for Schiller-Naumann (SN), ANN from fully resolved simulations (ANN-I) and ANN from coupled simulations (ANN-II), with u_t as theoretical terminal velocity.

new models are only trained with data for $d_p/\Delta x = 4$. The results for all models and resolutions in the range $d_p/\Delta x = [0.25, 16.0]$ are shown in Fig. 2.

As expected, the SN model yields significant deviations from the reference values for large $d_p/\Delta x$. For smaller $d_p/\Delta x$, the solution approaches the one-way coupled case with $u_p/u_t = 1$. The variation of the result over $d_p/\Delta x$ is greatly reduced for both ANN based models. Additionally, the transient behavior is improved. Overall, the ANN-II model shows the most promising results with respect to the fully resolved reference solution.

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