

An Accurate and Scalable Direction-Splitting Solver for Flows Laden with Non-Spherical Rigid Bodies – Part 1: Fixed Rigid Bodies

Aashish Goyal¹ and Anthony Wachs^{2,*}

¹ Department of Chemical and Biological Engineering, University of British Columbia, 2360 East Mall, V6T 1Z3, Vancouver, British Columbia, Canada.

² Department of Mathematics, University of British Columbia, 1984 Mathematics Road, V6T 1Z4, Vancouver, British Columbia, Canada.

Received 30 June 2023; Accepted (in revised version) 6 October 2023

Abstract. Particle-resolved direct numerical flow solvers predominantly use a projection method to decouple the non-linear mass and momentum conservation equations. The computing performance of such solvers often decays beyond $\mathcal{O}(1000)$ cores due to the cost of solving at least one large three-dimensional pressure Poisson problem per time step. The parallelization may perform moderately well only or even poorly sometimes despite using an efficient algebraic multigrid preconditioner [38]. We present an accurate and scalable solver using a direction splitting algorithm [12] to transform all three-dimensional parabolic/elliptic problems (and in particular the elliptic pressure Poisson problem) into a sequence of three one-dimensional parabolic sub-problems, thus improving its scalability up to multiple thousands of cores. We employ this algorithm to solve mass and momentum conservation equations in flows laden with fixed non-spherical rigid bodies. We consider the presence of rigid bodies on the (uniform or non-uniform) fixed Cartesian fluid grid by modifying the diffusion and divergence stencils on the impacted grid node near the rigid body boundary. Compared to [12], we use a higher-order interpolation scheme for the velocity field to maintain a second-order stress estimation on the particle boundary, resulting in more accurate dimensionless coefficients such as drag C_d and lift C_l . We also correct the interpolation scheme due to the presence of any nearby particle to maintain an acceptable accuracy, making the solver robust even when particles are densely packed in a sub-region of the computational domain. We present classical validation tests involving a single or multiple (up to $\mathcal{O}(1000)$) rigid bodies and assess the robustness, accuracy and computing speed of the solver. We further show that the Direction Splitting solver is ~ 5 times faster on 5120 cores than our solver [38] based on a classical projection method [5].

AMS subject classifications: 76D05, 76T20, 74F10, 65M55, 65Y05

*Corresponding author. *Email addresses:* wachs@math.ubc.ca (A. Wachs), goyal001@mail.ubc.ca (A. Goyal)

Key words: Highly scalable solver, particle-laden flow, particle resolved direct numerical simulation, incompressible flow, non-spherical rigid bodies.

1 Introduction

Particle-laden flows pervade broad industrial applications such as packed-bed reactors, fluidized beds, and particle-based solar receivers [26]. A detailed understanding of hydrodynamics, mass, and heat transfer in these processes can provide significant opportunities for productivity enhancement and cost savings. The critical difficulties in particle-laden flows are the influence of particles on the fluid flow, the potential high particle loading, and the multiple degrees of freedom of the particles, such as shape, size, polydispersity, and orientation. Computational studies of particle-laden systems have successfully provided valuable information on the flow characteristics, whether computations are performed on a uniform or a non-uniform distribution of grid nodes. However, a large flow configuration consists of numerous points ($\mathcal{O}(10^9)$), resulting in high computing time and hence requires massive parallel platforms. Various numerical methods are present in the literature to solve particle-laden flows, which can feature either fast computational speed or high accuracy depending on how the rigid bodies are resolved. These methods are broadly characterized into microscale and mesoscale models. In mesoscale models, the particle surface is not treated as a boundary, and the fluid-particle interactions are captured by adding the factor of a local void fraction to the mass and momentum conservation equations. As a result, the computational cost is less, and closure models for C_d and C_l are required to approximate the fluid-particle interaction. Additionally, using the local void fraction as the only variable may not correctly capture the particle degrees of freedom. On the other hand, a microscale model assumes the particle size of at least an order of magnitude larger than the largest fluid grid step size resulting in a fully-resolved fluid-particle interface, also known as Particle Resolved-Direct Numerical Simulation (PR-DNS). Resolving particle boundaries and considering all particle degrees of freedom make the microscale method computationally expensive but exhibit high accuracy without any approximation of closure relations.

The Lattice Boltzmann method and classical methods such as Finite Volume (FV) or Finite Difference (FD) are becoming the primary computational techniques in PR-DNS. The former computes the fluid flow using a particle collision approach over fixed lattice points, and the latter discretizes the coupled non-linear partial differential equations over a uniform or non-uniform spatial grid. Space and time discretization in both methods uses a first or second-order scheme to get an approximate solution. A second-order scheme in space and time computes the solution more accurately for a time-varying particle-laden flow. For example, a numerically estimated drag coefficient converges quickly to a grid-independent value in a second-order scheme, requiring fewer spatial and temporal variables in computing. However, even with the second-order scheme,