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Simulation of Transient Channel Flow with Multi-Particle Collision Dynamics

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Multi-Particle Collision Dynamics (MPC) is a particle-based simulation method that mimics a fluid in a stochastically coarse-grained manner [1,2]. It incorporates fluid point particles that alternately undergo a streaming and a collision time step. During the streaming time step, the fluid particles move according to their velocity. During the collision step, the particles are sorted into collision cells and their relative velocities are stochastically redistributed, e.g., by random rotations also known as Stochastic Rotation Dynamics.

The MPC method offers an extremely parallelized numerical framework for modelling of flow on the micro and on the nano scale. It incorporates hydrodynamic interactions as well as thermal fluctuations. Recent studies utilizing the MPC method however focused on stationary flows and large time scales to guarantee convergence [2]. Pulsating pressure signals in biological and industrial applications nevertheless span time scales of several orders. The present study thus reviews the capabilities of the MPC framework to simulate transient channel flow. This work covers the entire range from slow, viscosity-dominated Hagen-Poiseuille flow to inertia-dominated flow under fast pressure perturbations. The time scale is quantified using the Womersley number, relating the stimulation frequency to the ratio of kinematic viscosity over the squared channel height [3].

The MPC simulations yield flow profiles that perfectly match the analytical solutions at low, intermediate and large time scales. We can thus prove the feasibility of highly parallelized MPC simulations not only for stationary but also for transient flow problems. The numerical parameters are adjusted to achieve a compromise between accuracy and efficiency. An optimal numerical setting is discussed based on the dimensionless numbers of the mechanical problem and simulations on 512 cores. An outlook is given on how the numerical setting can be coupled to self-propelled nano particles of biological and artificial origins.

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