A New Mixed Stochastic-Deterministic Simulation Approach for Particle Populations in Fluid Flows

Volker John, Clemens Bartsch, Robert I.A. Patterson
Weierstrass Institute for Applied Analysis and Stochastics
john@wias-berlin.de, bartsch@wias-berlin.de, patterson@wias-berlin.de

Abstract

This talk presents a new coupled method for the solution of population balance systems (PBSs). A PBS is a system of partial (integro-)differential equations containing a population balance equation (PBE). The particular systems that will be studied come from the area of computational fluid dynamics (CFD). When modeling such systems by a PBS, the PBE describes a population of physical particles that are transported in a fluid flow and interact with each other and the surrounding fluid. This setting determines the type of the other differential equations present in the system: The Navier–Stokes equations and a set of convection-diffusion equations that describe quantities that are transported by the flow, like chemical substance concentrations or temperature.

The new approach consists in a two-way-coupling of a stochastic simulation algorithm for the particle population to a finite element simulation of the flow. For the solution of the convection-diffusion equations, special stabilized finite element methods are used Bordas et al. (2013). The particle population is tracked by a stochastic simulation algorithm in the Kinetic Monte Carlo spirit, e.g., see Patterson and Wagner (2012). A notable feature of such stochastic algorithms is their inherent capability to deal with higher-dimensional particle descriptions. The parts of the simulation are coupled to each other via a splitting scheme, exchanging coefficients, sources, and sinks. This splitting scheme enables the usage of tailored approaches for each equation. Since the particles neither have a position nor a spatial extent, the proposed approach is a so-called quasi-homogeneous method.

In this talk, we will show the successful coupling of advanced CFD techniques with a stochastic algorithm for the population of particles. Besides presenting the new algorithm and highlighting some parts of its formulation and implementation, we will present numerical results from the simulation of crystallizer devices. Such devices are used in chemical engineering to grow crystals from dissolved material to very regular shapes, exploiting the mechanisms of surface attachment growth and collision growth. We present an axisymmetric 2D simulation of tubular flow crystallizer device and a full 3D simulation of a batch crystallizer vessel. Both simulations are verified against experimental data.

References

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