**PDE-constrained Optimization for Multiscale Particle Dynamics – Numerics and Industrial Applications**

There are many industrial and biological processes, such as beer brewing, cell separation and nano-filtration, which can be described by integro-PDEs. These PDEs define the dynamics of a particle density within a fluid, under the influence of diffusion, forces and particle interactions, and often include complex, non-local boundary conditions. It is of great interest to industry and academia to optimize this type of process. PDE-constrained optimization is an area of research concerned with finding the optimal state and cost of a system. This aim is constrained by the physics of the problem, which is often described by a PDE. A standard solution technique is to derive a system of optimality conditions and solve it numerically. Treating optimization problems, which involve multiscale particle dynamics, requires the development of new theoretical and numerical methods. Standard results in optimal control cannot readily be applied, due to the nonlinear, non-local nature of the PDE-constraint, as well as the complexity of the boundary conditions.

In this talk, I will present the system of integro-PDEs that describe the optimality conditions for such an optimization problem. Furthermore, I will introduce a numerical method, which combines pseudospectral methods with a multiple shooting approach. This provides a tool for the fast and accurate solution of these optimality systems. Finally, some examples of future industrial applications will be given.