**Workshop:**

**PDE-Constrained Optimization for Multiscale Particle Dynamics**

There are many industrial and biological processes, such as beer brewing, nano-separation and bird flocking, which can be described by integro-PDEs. These PDEs can be regarded as DDFTs and define the dynamics of a particle density within a fluid bath, under the influence of diffusion, external forces and particle interactions. They often include complex, nonlocal boundary conditions.

A key challenge is to optimize these types of processes. For example, in nano-separation, it is of interest to determine the optimal inflow rate of particles (the control), which leads to high separation of the particles (the target), at a minimal financial cost.

Mathematically, this requires tools from PDE-constrained optimization. A standard technique is to derive a system of optimality conditions and solve it numerically. Due to the nonlinear, nonlocal nature of the governing PDE and boundary conditions, the optimization of multiscale particle dynamics problems requires the development of new theoretical and numerical methods.

I will present the system of nonlinear, nonlocal 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 sweeping algorithm. This provides a tool for the fast and accurate solution of these optimality systems. Finally, some examples of current work and future industrial applications will be given. This is joint work with Ben Goddard and John Pearson.^

Correction:

There are many industrial and biological processes, such as beer brewing, nano-separation and bird flocking, which can be described by integro-PDEs. These PDEs describe the dynamics of a particle density within a fluid bath, under the influence of diffusion, external forces and particle interactions, and can be regarded as DDFTs. They often include nonlinear, nonlocal boundary conditions.

A key challenge is to optimize these types of processes. For example, in nano-separation, it is of interest to determine the optimal inflow rate of particles (the control), which leads to high separation of the particles (the target), at a minimal financial cost.

Mathematically, this requires tools from PDE-constrained optimization. A standard technique is to derive a system of optimality conditions and solve it numerically, but the nonlocal nature of the PDE and boundary conditions presents additional theoretical and numerical challenges.

I will present the integro-PDEs that describe the optimality conditions for such a DDFT optimization problem. Furthermore, I will introduce a numerical method, which combines pseudospectral methods with a sweeping algorithm. This provides a tool for the fast and accurate solution of these optimality systems. Finally, some examples of current work and future industrial applications will be given. This is joint work with Ben Goddard and John Pearson.