PDE-Constrained Optimization for Multiscale Particle Dynamics

With Industrial Applications

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$$\min_{y,u} \quad \frac{1}{2}||y(x,t) - \hat{y}(x,t)||^2_{L_2(\Omega\times(0,T))} + \frac{\beta}{2}||u(x,t)||^2_{L_2(\Omega\times(0,T))}$$

subject to:

$$\partial_t y(x,t) = \nabla^2 y(x,t) + u(x,t) + \alpha\nabla\cdot\int_\Omega y(x,t)y(x',t)\nabla V_2(|x-x'|)dx'$$

$$y(x,0) = y_0$$

$+$ Boundary Conditions for y.

A non-standard solution strategy is needed because of the non-local term in the PDE:

Pseudospectral Methods and Multiple Shooting

- Pseudospectral Methods lead to systems with small, dense matrices.
- Boundary Conditions easily applied within existing framework (2DChebClass).
- IVP solver & Interpolation.
- Spectral Accuracy.

Industrial Applications

- Brewing.
- Nano-filtration.
- ...

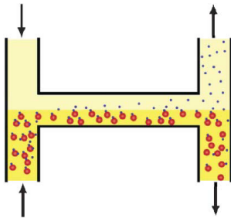

Figure: Brewing and Nano-filtration