PDE-Constrained Optimization for Multiscale Particle Dynamics

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Joint work with Ben Goddard and John Pearson

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Structure of the Talk

- Part 1: What is Multiscale Particle Dynamics?
- Part 2: What is PDE-Constrained Optimization?
- Part 3: Numerical Methods and Results

What do these pictures have in common?

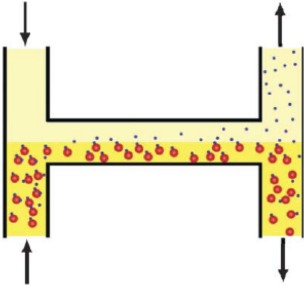


Figure: Nanofiltration Device

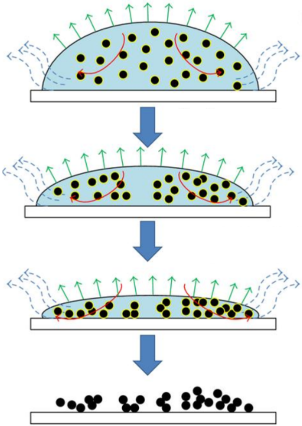


Figure: Ink Droplet Drying Process

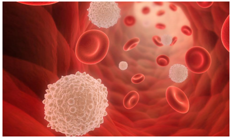
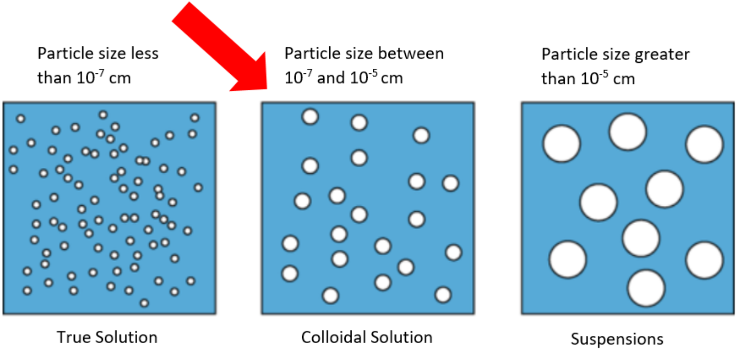


Figure: Blood Cells in Blood Vessels

Figure: Yeast Sedimentation in Beer

Part 1: What is Multiscale Particle Dynamics?

Mathematically, they are like this picture!



Modelling of the (Industrial) Process

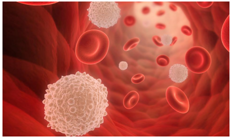
Modelling: Diffusion and Flow

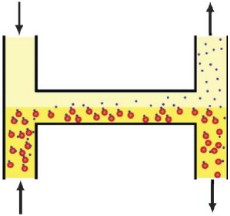
$$\partial_t \rho = \nabla^2 \rho - \nabla \cdot (\rho \mathbf{w}) \qquad \text{in } \Sigma = \Omega \times (0, T)$$

BC and IC:

$$\frac{\partial \rho}{\partial n} - \rho \mathbf{w} \cdot \mathbf{n} = 0 \qquad \text{on } \partial\Sigma = \partial\Omega \times (0, T)$$

$$\rho(0, x) = \rho_0(x)$$





Modelling of the (Industrial) Process

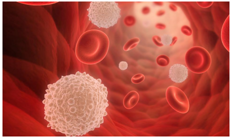
Modelling: Diffusion, Flow and Particle Interactions

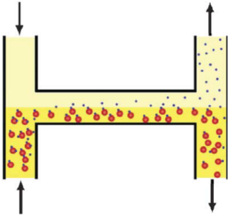
$$\partial_t \rho = \nabla^2 \rho - \nabla \cdot (\rho \mathbf{w}) + \nabla \cdot \int_\Omega \rho(x)\rho(x')\nabla V_2(|x - x'|)dx' \qquad \text{in } \Sigma$$

BC and IC:

$$\frac{\partial \rho}{\partial n} - \rho \mathbf{w} \cdot \mathbf{n} + \int_\Omega \rho(x)\rho(x')\frac{\partial V_2}{\partial n}(|x - x'|)dx' = 0 \qquad \text{on } \partial\Sigma$$

$$\rho(0, x) = \rho_0(x)$$





Part 2: What is PDE-Constrained Optimization?

$$\min_{\rho, u} \quad \frac{1}{2}\|\rho - \hat{\rho}\|^2_{L_2(\Sigma)} + \frac{\beta}{2}\|\mathbf{w}\|^2_{L_2(\Sigma)},$$

subject to:

$$\partial_t \rho = \nabla^2 \rho - \nabla \cdot (\rho \mathbf{w})$$

$$+ \nabla \cdot \int_\Omega \rho(x)\rho(x')\nabla V_2(|x - x'|)dx' \qquad \text{in } \Sigma$$

$$+ \text{BC} + \text{IC}$$

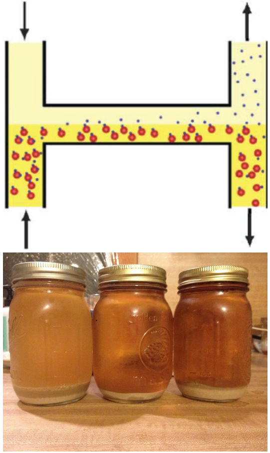


Figure: Top: Nano-Filtration Device
Bottom: Yeast Sedimentation in Beer

Deriving (first-order) optimality conditions

Idea: Define the Lagrangian $\mathcal{L}(\rho, \mathbf{w}, q)$:

$$\begin{aligned}\mathcal{L}(\rho, \mathbf{w}, q) &= \frac{1}{2}\|\rho - \hat{\rho}\|^2_{L_2(\Sigma)} + \frac{\beta}{2}\|\mathbf{w}\|^2_{L_2(\Sigma)} \\ &+ \int_\Sigma q\left(\partial_t \rho - \nabla^2\rho + \nabla\cdot(\rho\mathbf{w}) - \nabla\cdot\int_\Omega \rho(x)\rho(x')\nabla V_2(|x-x'|)dx'\right)drdt \\ &+ \int_{\partial\Sigma} q\ (\mathrm{BC})\ drdt\end{aligned}$$

Deriving (first-order) optimality conditions

1. Take derivatives of $\mathcal{L}(\rho, \mathbf{w}, q)$ with respect to ρ, $\mathbf{w}$ and q.
2. Set derivatives to zero to find stationary points.

$$\partial_t \rho = \nabla^2 \rho - \nabla \cdot (\rho \mathbf{w}) + \nabla \cdot \int_\Omega \rho(x)\rho(x')\nabla V_2(|x - x'|)dx'$$

$$\partial_t q = -\nabla^2 q - \nabla q \cdot \mathbf{w} + \int_\Omega \rho(x')\Big(\nabla q(x) + \nabla q(x')\Big) \cdot \nabla V_2(|x - x'|)dx'$$

$$\mathbf{w} = -\frac{1}{\beta}\rho\nabla q$$

$$\rho(0, x) = \rho_0(x), \qquad q(T, x) = 0$$

$$+ BC$$

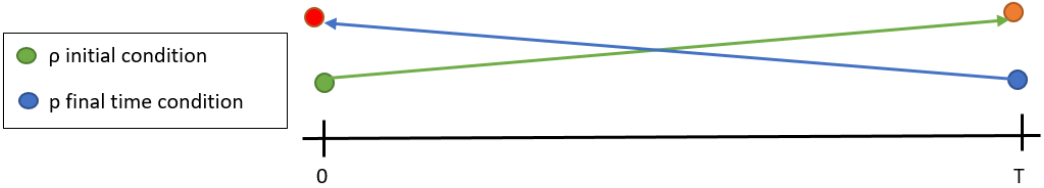
Optimization of the (Industrial) Process

Problem: Negative diffusion term in q causes blowup.
Solution: Rewrite time for this PDE: $\tau = T - t$.

$$\partial_t \rho(t,x) = \nabla^2 \rho(t,x) - \nabla \cdot (\rho(t,x)\mathbf{w}(t,x)) + \nabla \cdot \int_\Omega \rho(t,x)\rho(t,x')\nabla V_2(|x-x'|)dx'$$

$$\partial_\tau q(\tau,x) = \nabla^2 q(\tau,x) + \nabla q(\tau,x) \cdot \mathbf{w}(\tau,x) - \int_\Omega \rho(\tau,x')\Big(\nabla q(\tau,x) + \nabla q(\tau,x')\Big) \cdot \nabla V_2(|x-x'|)dx'$$

$$\rho(0,x) = \rho_0(x), \qquad q(0,x) = 0$$



Numerical Methods

Numerics:
Optimization = Solving the system of PDEs

- Challenge 1: One PDE is forward in time, the other backward.
  How to do time stepping?
- Challenge 2: Particle interaction term is nonlinear and nonlocal (+ nonlocal BCs).
- Standard methods (FEM/FDM) are not easily applicable.

We use:

- Pseudospectral methods.
- Multiple shooting method.

Numerics: What are pseudospectral methods?

- Polynomial interpolation using e.g. Chebyshev nodes.
- Discretize space: $\Delta\rho \to D\rho$ (PDE $\to$ ODEs).

Numerical Methods

Numerics: What is the multiple shooting method?

- Reduce PDE to ODEs using pseudospectral methods.
- Discretize the time interval, guess solution for ρ (and q) on each t_i.
- Interpolate q between t_i and t_{i+1}.
- Solve ODE on each time interval, match endpoints.

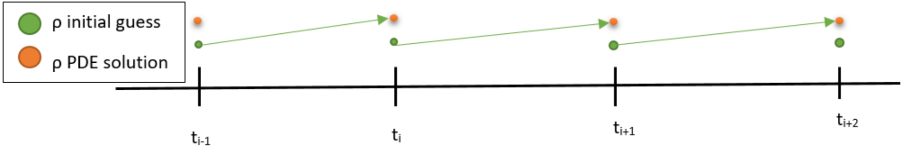


Figure: Multiple Shooting

Numerics: What is the multiple shooting method?

- Same thing for q, but backwards.

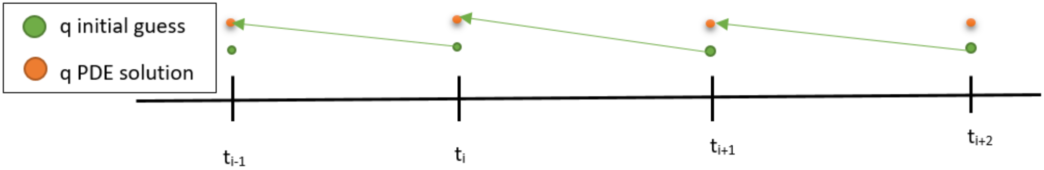
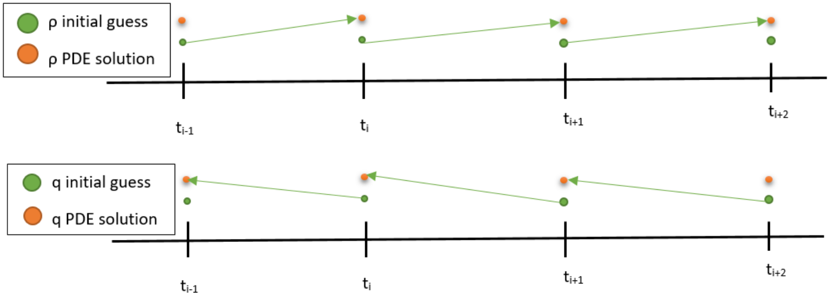


Figure: Multiple Shooting

The Numerical Algorithm

Numerics: What is the multiple shooting method?

- Create an initial guess for all ρ, q on t_i.
- Solve both PDEs on subintervals.
- If endpoints don't match, refine initial guess on t_i.
- Iterate until endpoints match (within a tolerance) on all t_i.



A Demonstration of the Numerical Method

Overall Cost: $J = \frac{1}{2}\|\rho - \hat{\rho}\|^2 + \frac{\beta}{2}\|\mathbf{w}\|^2$

$J_{FW} = 1.1930$

$J_{Opt} = 0.8414$

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Summary

We have:

- Modelled multiscale particle dynamics.
- Solved PDE-constrained optimization problems.
- Used pseudospectral methods and multiple shooting for numerical solutions.

We will:

- Apply this method to industrial processes...

Two industrial partners of the PhD:

µFraction®

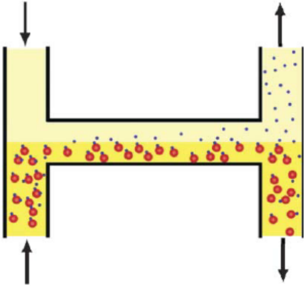

Figure: Nanofiltration Device

WEST

Figure: Yeast Sedimentation in Beer

References

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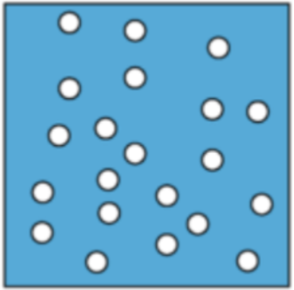
How can we describe this picture mathematically?



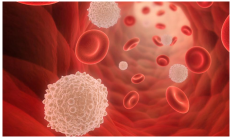
On Multiple Scales:

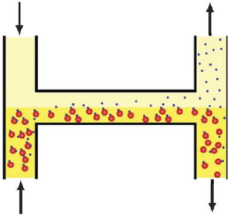
- Experimentally (expensive in cost and time!)
- ODEs for N particles AND n water molecules (expensive computations!)
- SDEs for N particles (expensive computations!)
- PDEs for the N particle density (impossible computations!)
- PDEs for the 1 particle density (good compromise)
- PDEs for the bulk fluid (inaccurate for many processes!)

Modelling of the (Industrial) Process

Modelling: What can we describe with our PDEs?

- Forces
- Particle Interactions
- Multiple Species
- Self-Propelled Particles
- Different Geometries
- ...





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