PDE-Constrained Optimization for Multiscale Particle Dynamics

Jonna Roden

Joint work with Ben Goddard and John Pearson

May 28, 2020

Structure of the Talk

- Part 1: Multiscale Particle Dynamics
- Part 2: PDE-Constrained Optimization
- Part 3: Numerical Methods
- Part 4: Results

Part 1: What is Multiscale Particle Dynamics?

What do these pictures have in common?

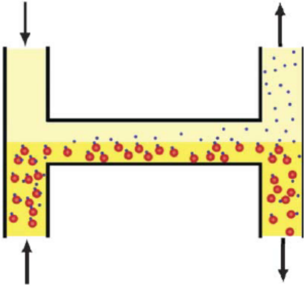


Figure: Nanofiltration Device

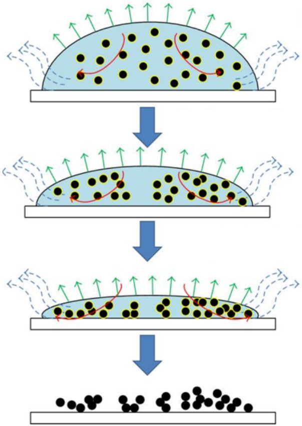


Figure: Ink Droplet Drying Process

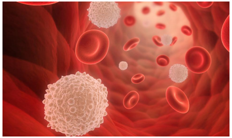
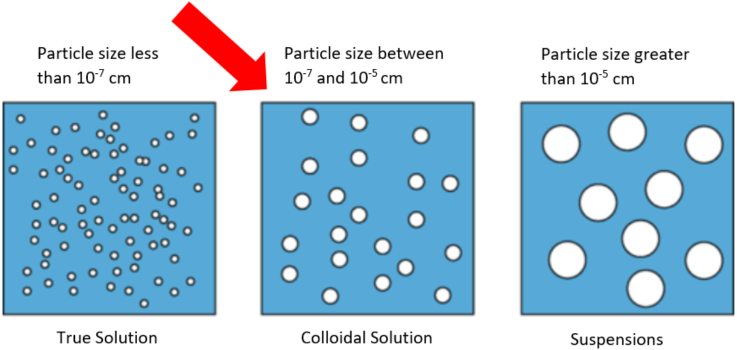


Figure: Blood Cells in Blood Vessels

Figure: Yeast Sedimentation in Beer

Part 1: What is Multiscale Particle Dynamics?

Mathematically, they are like this picture!



Modelling

Diffusion and Advection

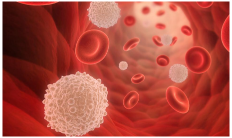
ρ : particle density at (x, t)

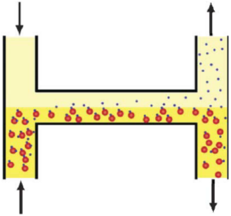
$$\partial_t \rho = \nabla^2 \rho - \nabla \cdot (\rho \mathbf{w}) \qquad \text{in } \Sigma = \Omega \times (0, T)$$

BC and IC:

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

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

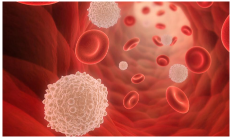




Modelling

Diffusion, Advection and Particle Interactions

ρ : particle density at (x, t)

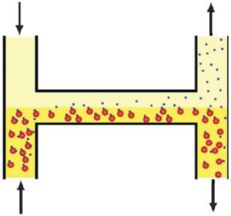


$$\partial_t \rho = \nabla^2 \rho - \nabla \cdot (\rho \mathbf{w}) + \nabla \cdot \int_\Omega \rho(x)\rho(x')\nabla V_2(|x - x'|)dx' \qquad \text{in } \Sigma$$

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:

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

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

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

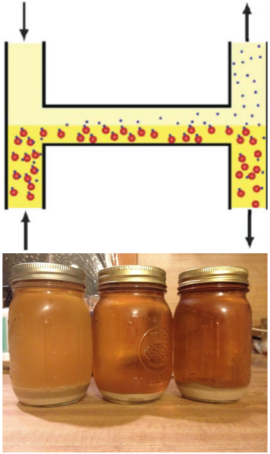


Figure: Top: Nano-Filtration Device
Bottom: Yeast Sedimentation in Beer

Optimization

Deriving (first-order) optimality conditions

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

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

Optimization

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

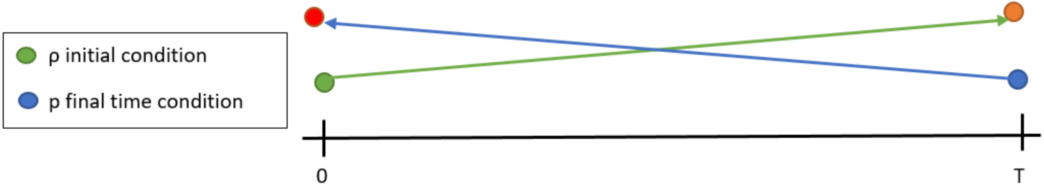
Problem: Negative diffusion term in q causes blowup.
Solution: Rewrite time for this PDE: $\tau = T - t$.

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

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

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

++ add gradient equation ++



Part 3: 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.
- Fixed Point algorithm.

Numerics

What are pseudospectral methods?

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

Numerics: The Algorithm

The fixed point algorithm:

- Reduce PDE to ODEs using pseudospectral methods.

Numerics: The Algorithm

The fixed point algorithm:

- Same thing for q, but backwards.

Numerics: The Algorithm

The fixed point algorithm:

- next step

Results

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

$J_{FW} =$

$J_{Opt} =$

Results

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

$J_{FW} =$ $J_{Opt} =$

Summary

We have:

- Modelled multiscale particle dynamics.
- Solved PDE-constrained optimization problems.
- Used pseudospectral methods and a fixed point algorithm for numerical solutions.

We will:

- Apply this method to industrial processes...

What's next?

Two industrial partners of the PhD:

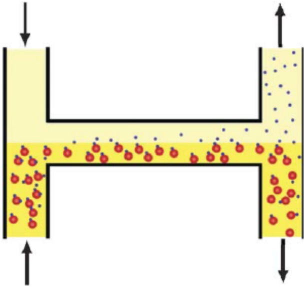


Figure: Nanofiltration Device

Figure: Yeast Sedimentation in Beer

References

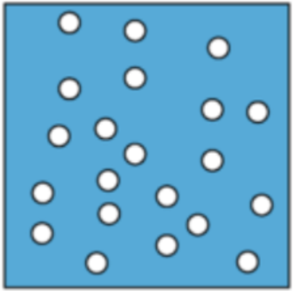
T. Carraro, M. Geiger and R. Rannacher.
Indirect Multiple Shooting for Nonlinear Parabolic Optimal Control Problems with Control Constraints.
SIAM Journal on Scientific Computing, 36(2), 452-481, 2015.

J.C. De los Reyes.
Numerical PDE-Constrained Optimization.
Springer, 2015.

A. Nold, B.D. Goddard, P. Yatsyshin, N. Savva and S. Kalliadasis.
Pseudospectral Methods for Density Functional Theory in Bounded and Unbounded Domains.
Journal of Computational Physics, 334, 639-664, 2017.
`https://datashare.is.ed.ac.uk/handle/10283/2647` (2DChebClass)

Part 1: What is Multiscale Particle Dynamics?

How can we describe this picture mathematically?



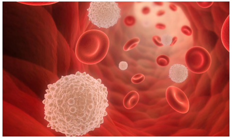
On Multiple Scales:

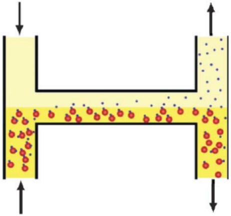
- Experimentally (expensive in cost and time!)
- ODEs for N particles AND n water molecules (expensive computations!)
- SDEs for N particles (expensive computations!)
- PDEs for the N particle density (impossible computations!)
- PDEs for the 1 particle density (good compromise)
- PDEs for the bulk fluid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





Numerical Methods

Numerics: What are pseudospectral methods?

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