This Is What We Do: PDE-Constrained Optimization for Multiscale Particle Dynamics

Jonna Roden

With Dr Ben Goddard (UoE), Dr John Pearson (UoE)
and Mildred Aduamoah (MIGSAA, 3rd Year)

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Structure of the Talk

- Part 1: What is Multiscale Particle Dynamics?
- Part 2: What is PDE-Constrained Optimization?
- Part 3: This Is What We Do (Modelling, Numerics, Analysis)

Part 1: What is Multiscale Particle Dynamics?

What do these pictures have in common?

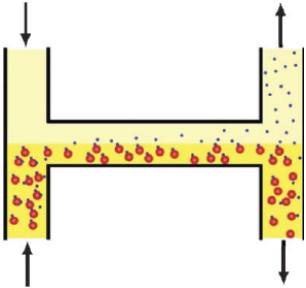


Figure: Nanofiltration Device

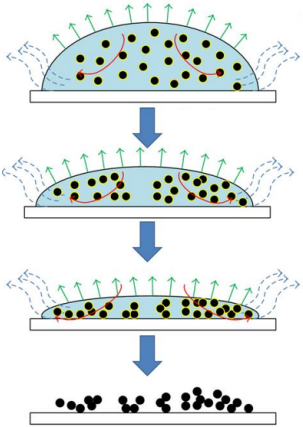


Figure: Ink Droplet Drying Process

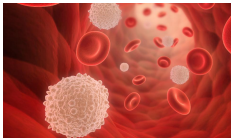
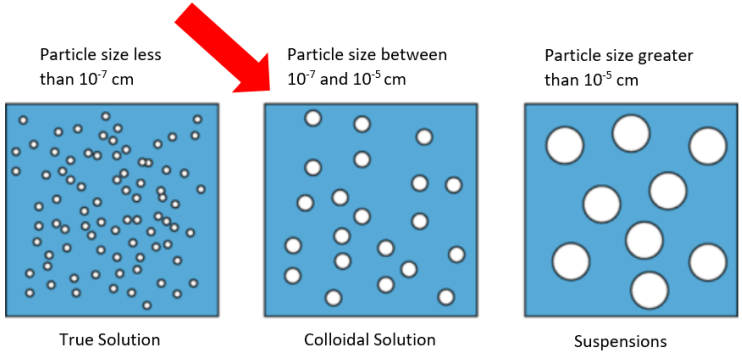


Figure: Blood Cells in Blood Vessles

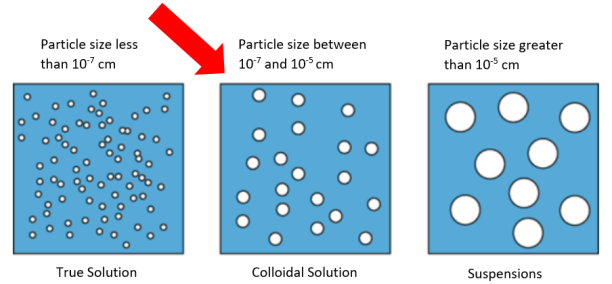
Figure: Yeast Sedimentation in Beer

Part 1: What is Multiscale Particle Dynamics?

Mathematically, they are like this picture!



Part 1: What is Multiscale Particle Dynamics?



Part 1: What is Multiscale Particle Dynamics?

How can we describe this picture mathematically?

On Multiple Scales:

- Experimentally
- ODEs for N particles AND n water molecule
- SDEs for N particles
- PDEs for the N particle density
- PDEs for the 1 particle density
- PDEs for the bulk fluid

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 molecule (impossible computations!)
- SDEs for N particles (expensive computations!)
- PDEs for the N particle density (expensive computations!)
- PDEs for the 1 particle density (good compromise)
- PDEs for the bulk fluid (inaccurate for many processes!)

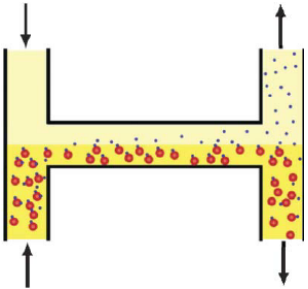
Part 1: What is Multiscale Particle Dynamics?

Why do we want to describe this mathematically?

Many processes can be described by this type of fluid model!...

Part 1: What is Multiscale Particle Dynamics?

....Such as these ones!



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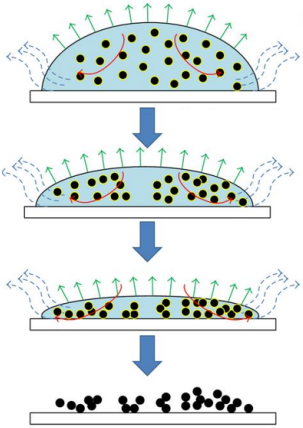

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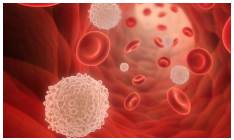

Figure: Blood Cells in Blood Vessles

Figure: Yeast Sedimentation in Beer

Part 1: What is Multiscale Particle Dynamics?

Two industrial partners of the PhD:

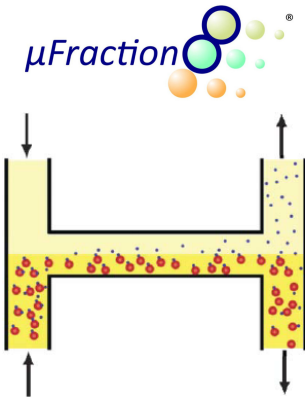

Figure: Nanofiltration Device

Figure: Yeast Sedimentation in Beer

Part 2: What is PDE-Constrained Optimization?

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

subject to:

$$\frac{\partial \rho}{\partial t} = \Delta \rho + u$$

Example:

- ρ: Current temperature.
- $\hat{\rho}$: Desired temperature.
- u: Cost of reaching $\hat{\rho}$.
- PDE: Heat equation.

Part 2: What is PDE-Constrained Optimization?

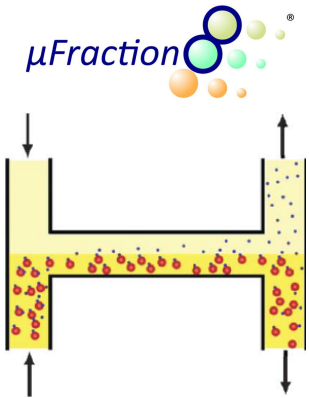

Figure: Nanofiltration Device

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subject to:

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Figure: Yeast Sedimentation in Beer

Part 3: What is it that we do?

- Modelling
- Numerics
- (Analysis)

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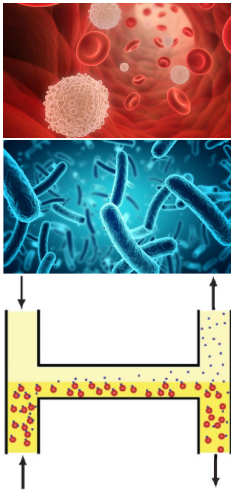
Modelling: What can we describe with our PDEs?

- Forces
- Particle Interactions
- Multiple Species
- Self-propelled particles
- Different Geometries
- ...



Part 3: What is it that we do?

Modelling: How do we approach the modelling process?

- Choose the most basic (but meaningful) model.
- Add on one effect.
- Develop numerics for this model (next slide!).
- Add on more effects, step by step.
- Get final model.

$$\frac{\partial \rho}{\partial t} = \Delta \rho + u + \alpha \int_{\Omega} \rho(x)\rho(x')\nabla V_2(|x - x'|)dx'$$

Part 3: What is it that we do?

Numerics: Optimization = Solving systems of PDEs

- Challenge: Particle interaction term is nonlinear and non-local.
- Standard methods (FEM/FDM) are not enough.

We use:

- Pseudospectral methods.
- Multiple shooting method.

Part 3: What is it that we do?

Numerics: What are pseudospectral methods?

- Polynomial interpolation using Chebyshev points.
- Discretize space: $\Delta\rho \to D\rho$ (PDE $\to$ ODE)

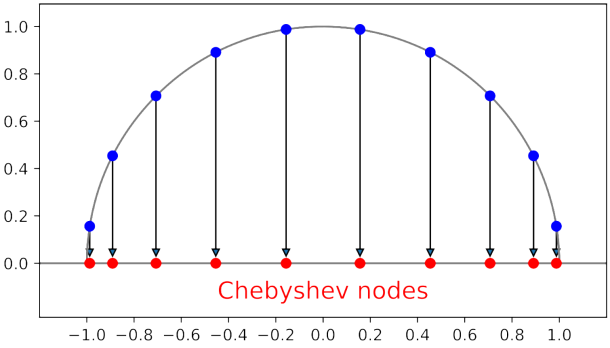


Figure: Chebyshev Points

Part 3: What is it that we do?

Numerics: What is the multiple shooting method?

- Reduce PDEs to ODEs using pseudospectral methods.
- Discretize the time interval, guess solution on t_i.
- Solve ODEs on each time interval, match endpoints.

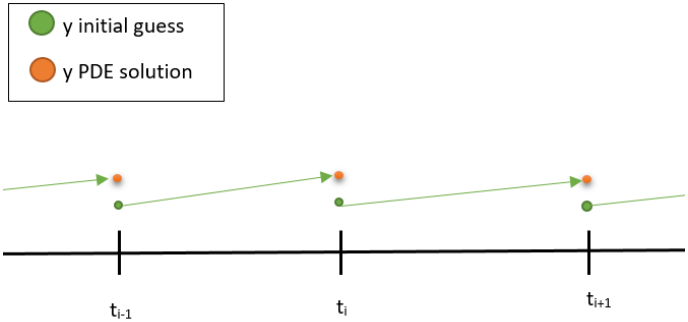


Figure: Multiple Shooting

Summary: What We Do

- Modelling multiscale particle dynamics.
- Solving PDE-constrained optimization problems.
- Using pseudospectral methods and multiple shooting for numerical solutions.
- Application to industrial processes.

References

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