PDE-Constrained Optimization for Multiscale Particle Dynamics

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Joint work with Ben Goddard and John Pearson

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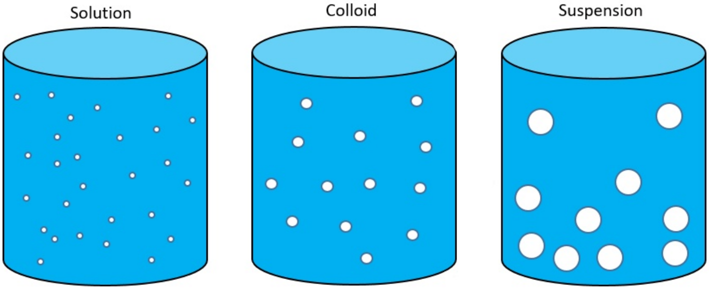
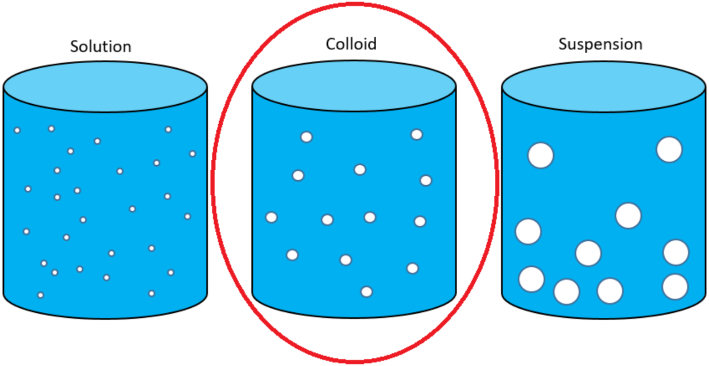
Structure of the Talk

- Part 1: Modelling (Multiscale Particle Dynamics)
- Part 2: Optimization (with PDE constraints)
- Part 3: Numerical Methods
- Part 4: Results

Part 1: What is Multiscale Particle Dynamics?



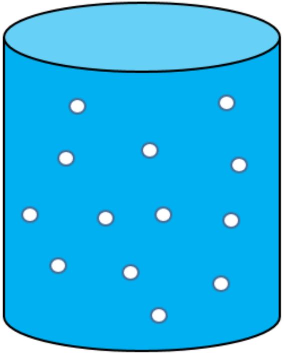
Part 1: What is Multiscale Particle Dynamics?



Part 1: What is Multiscale Particle Dynamics?

Modelling on multiple scales:

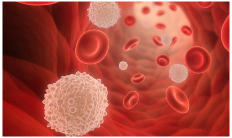
- ODEs for N particles AND n water molecules, $n \gg N$ (impossible computations)
- SDEs for N particles (expensive computations)
- PDEs for the N particle density (impossible computations)
- PDEs for the 1 particle density (good compromise)

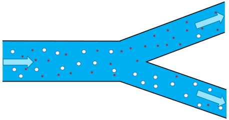


Part 1: Modelling

What effects can be described with a (non-local) PDE model?

- Forces
- Particle interactions
- Multiple species
- Self-propelled particles
- Anisotropic particles
- Different geometries
- ...





Part 1: Modelling

Diffusion, advection and particle interactions

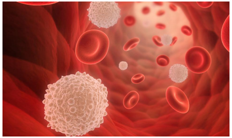
ρ : particle density at $(\vec{x}, t)$, $\quad \Sigma = (0, T) \times \Omega$

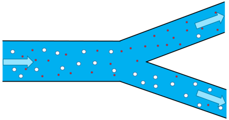
$$\partial_t \rho = \nabla^2 \rho - \nabla \cdot (\rho \vec{w}) + \nabla \cdot \int_\Omega \rho(\vec{x}) \rho(\vec{x}\,') \nabla V_2(|\vec{x} - \vec{x}\,'|) d\vec{x}\,' \qquad \text{in } \Sigma$$

BC and IC:

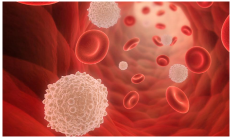
$$\frac{\partial \rho}{\partial n} - \rho \vec{w} \cdot \vec{n} + \int_\Omega \rho(\vec{x}) \rho(\vec{x}\,') \frac{\partial V_2}{\partial n}(|\vec{x} - \vec{x}\,'|) d\vec{x}\,' = 0 \qquad \text{on } \partial\Sigma$$

$$\rho(0, \vec{x}) = \rho_0(\vec{x})$$





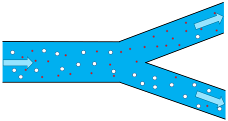
Part 2: What is PDE-Constrained Optimization?



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

subject to:

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



BC and IC:

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

$$\rho(0,\vec{x})=\rho_0(\vec{x})$$

Part 2: Optimization

Deriving (first-order) optimality conditions

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

$$\begin{aligned}
\mathcal{L}(\rho, \vec{w}, q) = {} & \frac{1}{2}\|\rho - \widehat{\rho}\|^2_{L_2(\Sigma)} + \frac{\beta}{2}\|\vec{w}\|^2_{L_2(\Sigma)} \\
& + \int_{\Sigma} q\left(\partial_t \rho - \nabla^2 \rho + \nabla \cdot (\rho \vec{w}) - \nabla \cdot \int_{\Omega} \rho(\vec{x})\rho(\vec{x}\,')\nabla V_2(|\vec{x} - \vec{x}\,'|)d\vec{x}\,'\right) d\vec{x}dt \\
& + \int_{\partial\Sigma} q\left(\frac{\partial \rho}{\partial n} - \rho \vec{w} \cdot \vec{n} + \int_{\Omega} \rho(\vec{x})\rho(\vec{x}\,')\frac{\partial V_2}{\partial n}(|\vec{x} - \vec{x}\,'|)d\vec{x}\,'\right) d\vec{x}dt
\end{aligned}$$

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

Part 2: Optimization

Resulting optimality system:

$$
\begin{aligned}
\partial_t \rho &= \nabla^2 \rho - \nabla \cdot (\rho \vec{w}) + \nabla \cdot \int_\Omega \rho(\vec{x})\rho(\vec{x}\,')\nabla V_2(|\vec{x} - \vec{x}\,'|)d\vec{x}\,' \\
\partial_t q &= -\nabla^2 q - \nabla q \cdot \vec{w} + \int_\Omega \rho(\vec{x}\,')\Big(\nabla q(\vec{x}) + \nabla q(\vec{x}\,')\Big) \cdot \nabla V_2(|\vec{x} - \vec{x}\,'|)d\vec{x}\,' \\
\vec{w} &= -\frac{1}{\beta}\rho \nabla q
\end{aligned}
$$

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

Part 2: Optimization

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

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

$$\begin{aligned}\partial_\tau q(\tau,\vec{x}) &= \nabla^2 q(\tau,\vec{x}) + \nabla q(\tau,\vec{x}) \cdot \vec{w}(\tau,\vec{x}) \\ &\quad - \int_\Omega \rho(\tau,\vec{x}\,')\Big(\nabla q(\tau,\vec{x}) + \nabla q(\tau,\vec{x}\,')\Big) \cdot \nabla V_2(|\vec{x}-\vec{x}\,'|)d\vec{x}\,'\end{aligned}$$

$$\vec{w}(t,\vec{x}) = -\frac{1}{\beta}\rho(t,\vec{x})\nabla q(t,\vec{x})$$

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

Part 3: Numerical Methods

Optimization $\rightarrow$ Solving the system of PDEs

- Challenge 1: Particle interaction term is nonlinear and nonlocal ($+$ nonlocal BCs). How to avoid shortcomings of standard methods (FEM/FDM)?
- Challenge 2: One PDE is forward in time, the other backward. How to do time stepping?

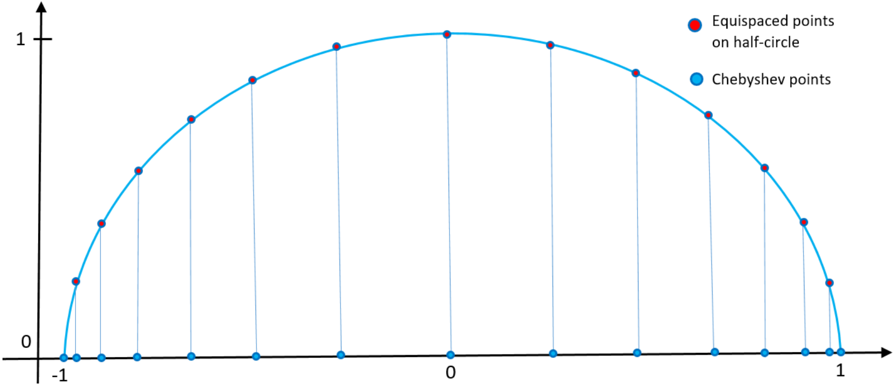
Our approach:

- Pseudospectral methods.
- Fixed point algorithm.

Part 3: Numerical Methods

What are pseudospectral methods?

- Polynomial interpolation using e.g. Chebyshev points.
- Space discretization: $\Delta\rho \to D\rho$ (PDE $\to$ ODEs).



Part 3: Numerical Methods

Initialization of optimization algorithm:

- Reduce both PDEs to systems of ODEs using pseudospectral methods.
- Discretize time using Chebyshev points.
- Given the required input variables, each equation can now be solved using a standard ODE solver.

Part 3: Numerical Methods

Reminder: The optimality system

State Equation:

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

Adjoint Equation:

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

Gradient Equation:

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

Part 3: Numerical Methods

The fixed point algorithm

Start optimization algorithm with an initial guess $\vec{w}^{(1)}$.

At each iteration i:

1. Solve the state equation; input $\vec{w}^{(i)}$:
$$\partial_t \rho = \nabla^2 \rho - \nabla \cdot (\rho \vec{w}^{(i)}) + \nabla \cdot \int_\Omega \rho(\vec{x})\rho(\vec{x}\,')\nabla V_2(|\vec{x} - \vec{x}\,'|) d\vec{x}\,'.$$
2. Solve the adjoint equation; input $\vec{w}^{(i)}$ and $\rho^{(i)}$:
$$\partial_\tau q = \nabla^2 q + \nabla q \cdot \vec{w}^{(i)} - \int_\Omega \rho^{(i)}(\vec{x}\,')\Big(\nabla q(\vec{x}) + \nabla q(\vec{x}\,')\Big) \cdot \nabla V_2(|\vec{x} - \vec{x}\,'|) d\vec{x}\,'.$$
3. Solve the gradient equation; input $\rho^{(i)}$ and $q^{(i)}$:
$$\vec{w}_g^{(i)} = -\frac{1}{\beta}\rho^{(i)}\nabla q^{(i)}.$$

Part 3: Numerical Methods

The fixed point algorithm, continued:

4. Measure the error: $\mathcal{E} = ||\vec{w}^{(i)} - \vec{w}_g^{(i)}||$.
5. Update control to $\vec{w}^{(i+1)}$, with $\lambda \in [0, 1]$:

$$\vec{w}^{(i+1)} = (1 - \lambda)\vec{w}^{(i)} + \lambda \vec{w}_g^{(i)}.$$

Convergence:

- If $\mathcal{E} < TOL$: Algorithm converged.
- If $\mathcal{E} > TOL$: Increase i to $i + 1$.

Part 4: Results

Reminder: The optimization problem

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

subject to:

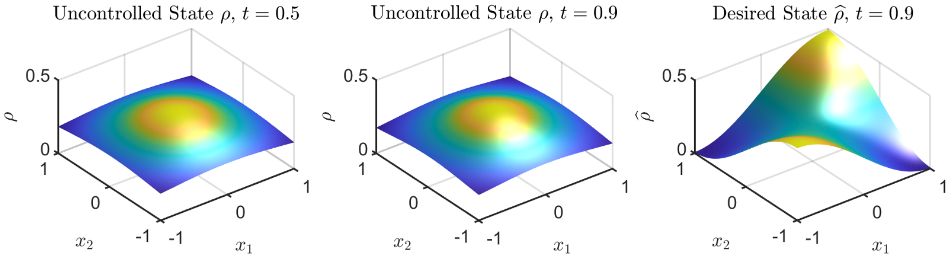
$$\partial_t \rho = \nabla^2 \rho - \nabla \cdot (\rho \vec{w}) + \nabla \cdot \int_\Omega \rho(\vec{x})\rho(\vec{x}\,')\nabla V_2(|\vec{x} - \vec{x}\,'|) d\vec{x}\,' \qquad \text{in } \Sigma$$

Inputs for a 2D example:

$\rho_0 = \frac{1}{4}$, $\vec{w}^{(1)} = 0$, $\beta = 10^{-3}$, $V_2(\vec{x}) = -\gamma e^{-\|\vec{x}\|^2}$,
$\widehat{\rho} = (1-t)\rho_0 + t\left(\frac{1}{4}\sin\left(\frac{\pi}{2}(x_1 - 2)\right)\sin\left(\frac{\pi}{2}(x_2 - 2)\right) + \frac{1}{4}\right)$,
$\Sigma = \Omega \times (0, 1)$, where $\Omega = [-1, 1]$.

Part 4: 2D Results

Attractive Particles: $\gamma = -1$.
Overall Cost: $J = \frac{1}{2}\|\rho - \widehat{\rho}\|^2_{L_2(\Sigma)} + \frac{\beta}{2}\|\vec{w}\|^2_{L_2(\Sigma)}$, $J_{\vec{w}=0} = 0.0130$.



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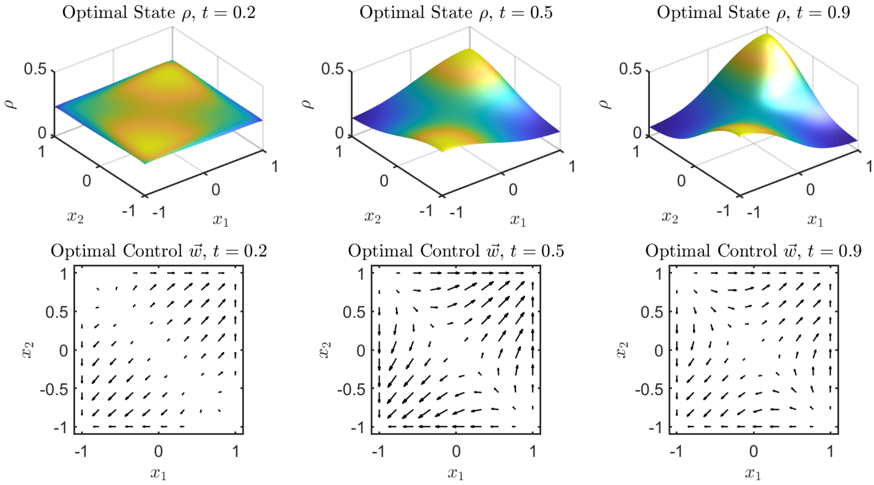


Summary

Up to now:

- Modelling of multiscale particle dynamics.
- Optimization with PDE constraints.
- Development of a suitable numerical method.

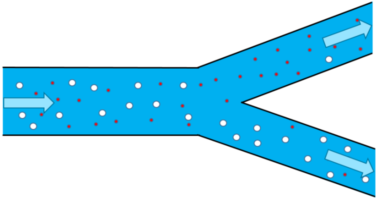
Up next:

- Improvement of the algorithm's efficiency.
- Application of the method to extended models.
- Application of the numerical framework to industrial processes.

What's next?

Industrial partners of the PhD:

μFraction



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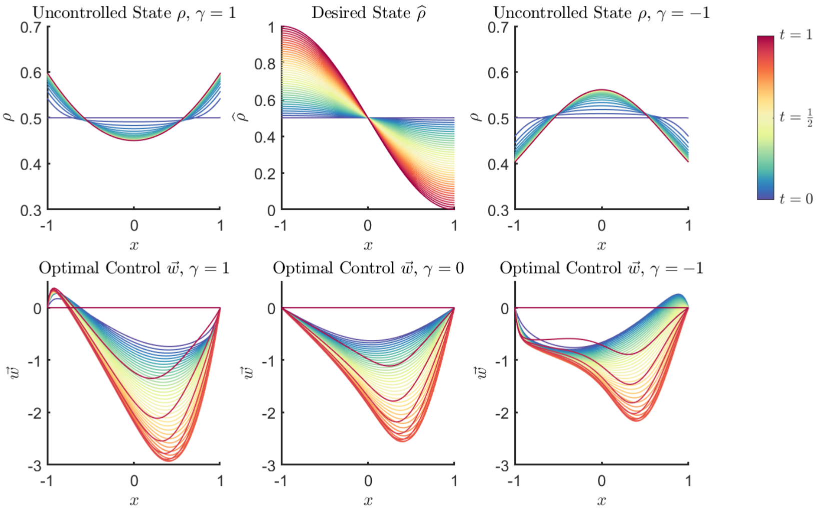
Part 4: 1D Results

Repulsive particles: $\gamma = 1$, Attractive particles: $\gamma = -1$, No interaction: $\gamma = 0$.



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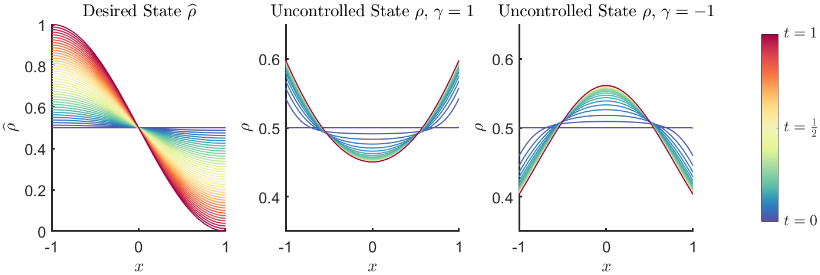

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