

# PDE-Constrained Optimization for Multiscale Particle Dynamics

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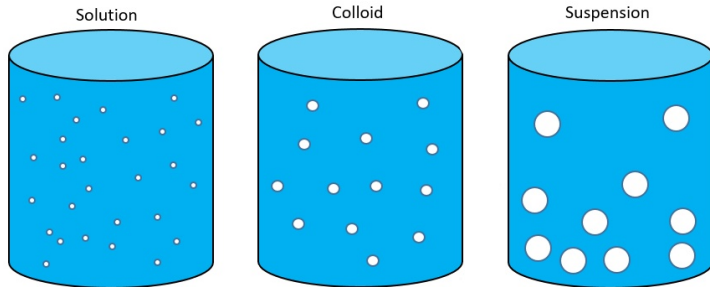
Joint work with Ben Goddard and John Pearson

12th June 2020

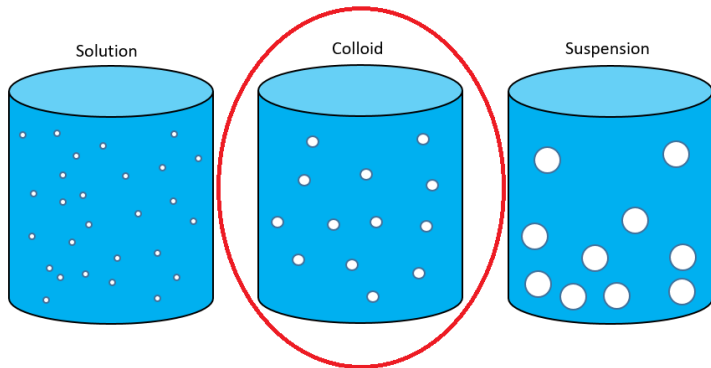
# Structure of the Talk

- ▶ 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?



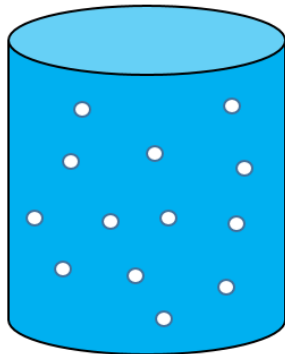
## Part 1: What is Multiscale Particle Dynamics?



# Part 1: What is Multiscale Particle Dynamics?

## Modelling on multiple scales:

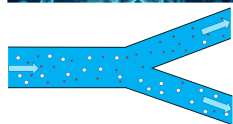
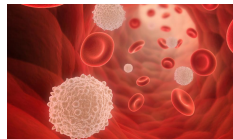
- ▶ ODEs for  $N$  particles AND  $n$  water molecules,  $n \gg N$   
(impossible computations)
- ▶ SDEs for  $N$  particles (expensive computations)
- ▶ PDEs for the  $N$  particle density (impossible computations)
- ▶ PDEs for the 1 particle density (good compromise)



# 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**

$\rho$  : particle density at  $(\vec{x}, t)$

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

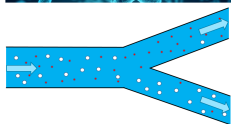
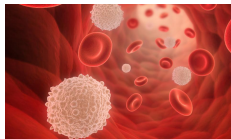
in  $\Sigma$

BC and IC:

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

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

on  $\partial \Sigma$



## Part 2: What is PDE-Constrained Optimization?

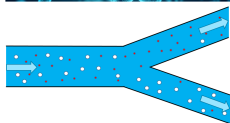
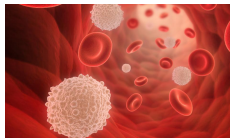
$$\min_{\rho, \vec{w}} \quad \frac{1}{2} \|\rho - \hat{\rho}\|_{L_2(\Sigma)}^2 + \frac{\beta}{2} \|\vec{w}\|_{L_2(\Sigma)}^2$$

subject to:

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

BC and IC:

$$\frac{\partial \rho}{\partial n} - \rho \vec{w} \cdot \vec{n} + \int_{\Omega} \rho(\vec{x}) \rho(\vec{x}') \frac{\partial V_2}{\partial n}(|\vec{x} - \vec{x}'|) d\vec{x}' = 0 \quad \text{on } \partial \Sigma$$
$$\rho(0, \vec{x}) = \rho_0(\vec{x})$$





## Part 2: Optimization

### Deriving (first-order) optimality conditions

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

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

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

## Part 2: Optimization

**Resulting optimality system:**

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

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

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

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

## Part 2: Optimization

**Problem:** Negative diffusion term in  $q$  causes blow-up.

**Solution:** Rewrite time for this PDE:  $\tau = T - t$ .

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

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

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

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

## 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?

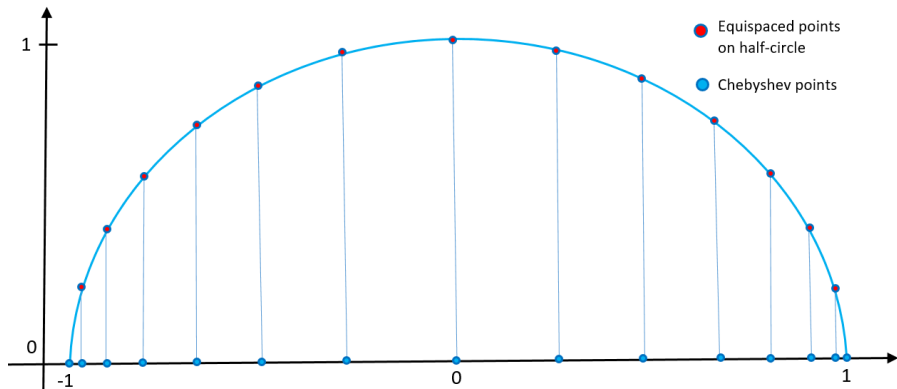
Our approach:

- ▶ Pseudospectral methods.
- ▶ Fixed point algorithm.

## Part 3: Numerical Methods

### What are pseudospectral methods?

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

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

Gradient Equation:

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

## 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  $\rho^{(i)}$ :

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

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

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

subject to:

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

### Inputs for a 2D example:

$$\rho_0 = \frac{1}{4}, \quad \vec{w}^{(1)} = 0, \quad \beta = 10^{-3}, \quad V_2(\vec{x}) = \gamma e^{-\|\vec{x}\|^2},$$

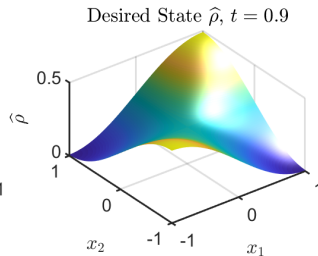
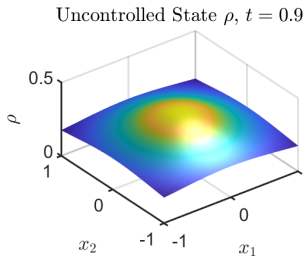
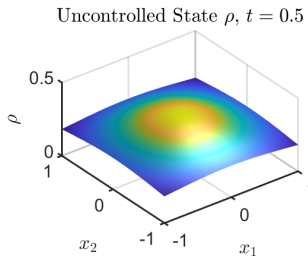
$$\hat{\rho} = (1 - t)\rho_0 + t \left( \frac{1}{4} \sin \left( \frac{\pi}{2}(x_1 - 2) \right) \sin \left( \frac{\pi}{2}(x_2 - 2) \right) + \frac{1}{4} \right),$$

$$\Sigma = \Omega \times (0, 1), \text{ where } \Omega = [-1, 1].$$

## Part 4: 2D Results

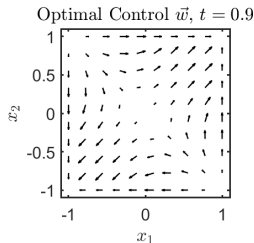
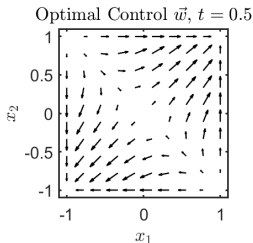
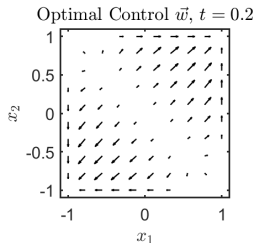
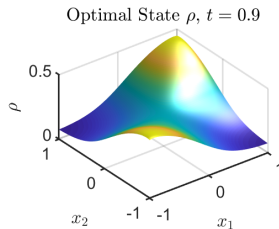
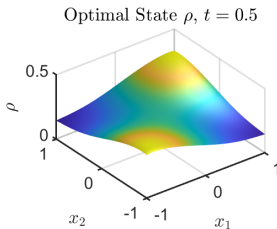
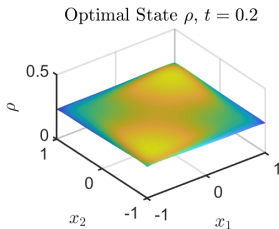
Attractive Particles:  $\gamma = -1$ .

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



## Part 4: 2D Results

Overall Cost:  $J = \frac{1}{2}\|\rho - \hat{\rho}\|_{L_2(\Sigma)}^2 + \frac{\beta}{2}\|\vec{w}\|_{L_2(\Sigma)}^2$ ,  $J_{\vec{w}=0} = 0.0130$ ,  $J_{opt} = 7.2994 \times 10^{-4}$ .



# Summary

Up to now:

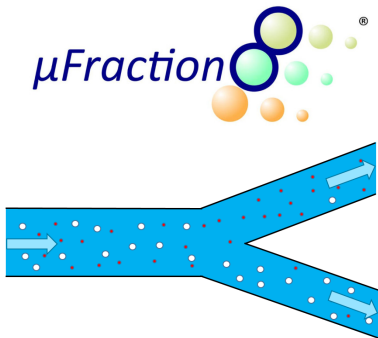
- ▶ Modelling of multiscale particle dynamics.
- ▶ Optimization with PDE constraints.
- ▶ Development of a suitable numerical method.

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:



# References

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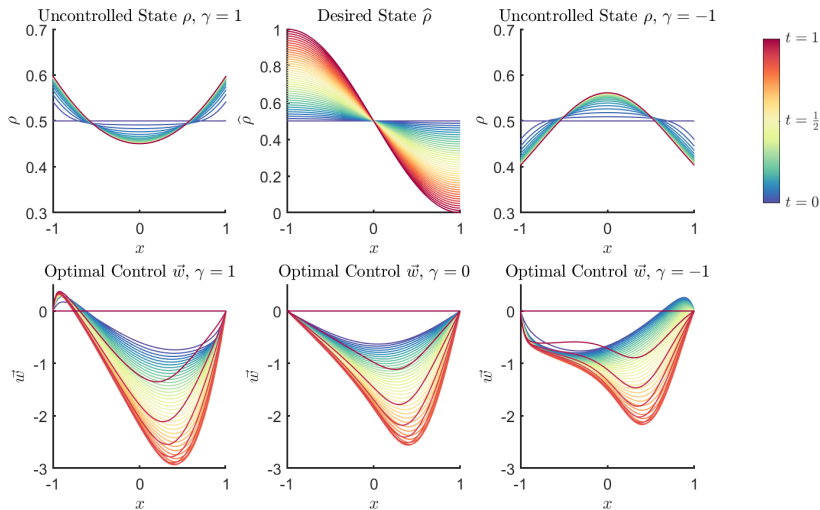
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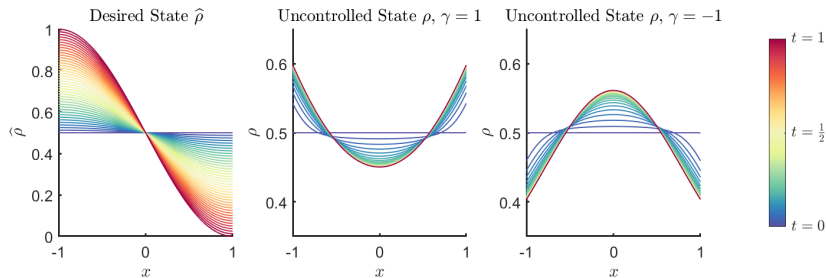
## Part 4: 1D Results

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



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