PDE-Constrained Optimization for Multiscale Particle Dynamics

Jonna Roden

University of Edinburgh/MIGSAA

Joint work with Ben Goddard and John Pearson

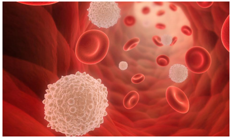
7th April 2021

Structure of the Talk

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

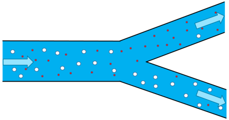
Part 1: Modelling

Consider a particle density ρ on $\Sigma = (0, T) \times \Omega$, where $\partial\Sigma := (0, T) \times \partial\Omega$.



Diffusion, advection and particle interactions

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



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

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

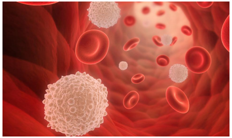
subject to:

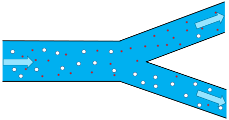
$$\partial_t\rho=\nabla^2\rho-\nabla\cdot(\rho\vec{w})+\nabla\cdot\int_\Omega\rho(\vec{x})\rho(\vec{x}\,')\nabla V_2(|\vec{x}-\vec{x}\,'|)d\vec{x}\,' \qquad \text{in } \Sigma$$

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

The (first-order) optimality system

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

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

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

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

Part 2: Optimization

Problem: Negative diffusion term in q causes numerical instability.
Solution: Change of time variable for this PDE: $\tau = T - t$.

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

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

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

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

Part 3: Numerical Methods

- Challenge 1: Particle interaction term is nonlinear and nonlocal (+ nonlocal BCs).
  How to avoid shortcomings of standard methods (FEM/FDM)?

  $\Rightarrow$ **Pseudospectral methods**

- Challenge 2: One PDE is forward in time, the other backward.
  How to do time stepping?

  $\Rightarrow$ **Fixed point algorithm**

Part 3: Numerical Methods

Pseudospecral Methods

- Reduce both PDEs to systems of ODEs.
- Discretize time (accurate interpolation).
- Equations can now be solved using a DAE solver (when given all necessary inputs).

Part 3: Numerical Methods

Fixed point algorithm

Initialize with guess $\vec{w}^{(0)}$.

1. Solve $\partial_t \rho = \nabla^2 \rho - \nabla \cdot (\rho \vec{w}^{(i)}) + \nabla \cdot \int_\Omega \rho(\vec{x})\rho(\vec{x}\,')\nabla V_2(|\vec{x} - \vec{x}\,'|)d\vec{x}\,'$.
2. Solve $\partial_\tau q = \nabla^2 q + \nabla q \cdot \vec{w}^{(i)} - \int_\Omega \rho^{(i)}(\vec{x}\,')\left(\nabla q(\vec{x}) + \nabla q(\vec{x}\,')\right) \cdot \nabla V_2(|\vec{x} - \vec{x}\,'|)d\vec{x}\,'$.
3. Solve $\vec{w}_g^{(i)} = -\frac{1}{\beta}\rho^{(i)}\nabla q^{(i)}$.
4. Measure the error: $\mathcal{E} = ||\vec{w}^{(i)} - \vec{w}_g^{(i)}||$.
5. Update control, with $\lambda \in [0, 1]$: $\vec{w}^{(i+1)} = (1-\lambda)\vec{w}^{(i)} + \lambda \vec{w}_g^{(i)}$.

Iterate until $\mathcal{E} < TOL$.

Part 4: Results

Reminder: The Optimization Problem

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

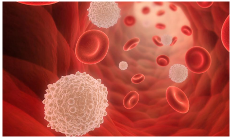
subject to:

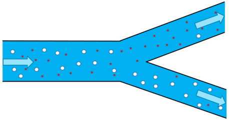
$$\partial_t \rho = \nabla^2 \rho - \nabla \cdot (\rho \vec{w}) + \nabla \cdot \int_\Omega \rho(\vec{x})\rho(\vec{x}\,')\nabla V_2(|\vec{x} - \vec{x}\,'|)d\vec{x}\,' \qquad \text{in } \Sigma$$

BC and IC:

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

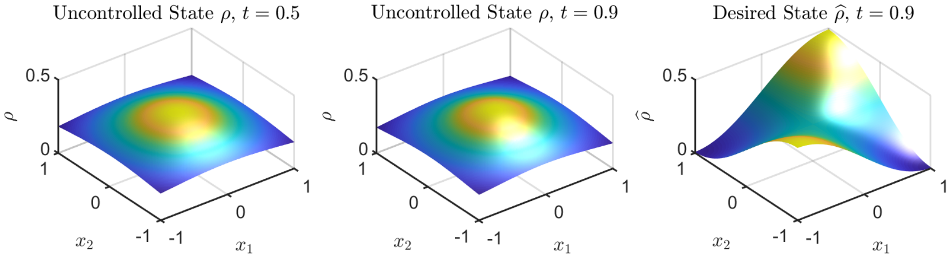
$$\rho(0, \vec{x}) = \rho_0(\vec{x})$$





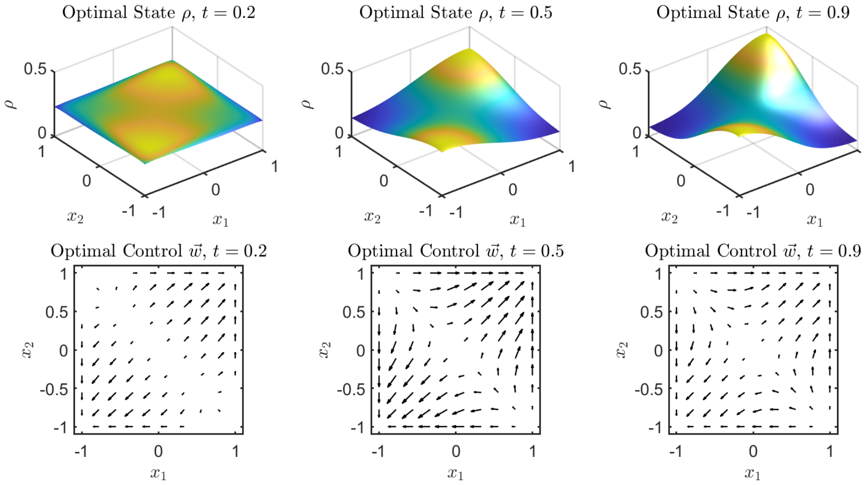
Part 4: Results

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



Part 4: Results

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

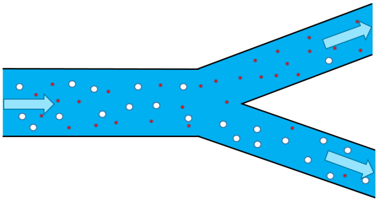


Current work

Next steps

Industrial partners of the PhD

µFraction®



WEST

Summary

Up to now:

- Deriving PDE-constrained optimization models.
- Developing a suitable numerical method to solve them.

Current:

- Complex domains.
- Extended models (e.g. sedimentation, multiple species).
- Different boundary conditions.

Up next:

- Application of the method to other extended models.
- Application of the numerical framework to industrial processes.

References

M. Aduamoah, B. D. Goddard, J. W. Pearson and J. C. Roden.
PDE-constrained optimization models and pseudospectral methods for multiscale particle dynamics.
Preprint, 2020.

M. Burger, M. Di Francesco, P.A. Markowich and M.-T. Wolfram.
Mean field games with nonlinear mobilities in pedestrian dynamics.
Discrete and Continuous Dynamical Systems - Series B, 19(5), 1311-1333, 2014.

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)

References: Figures

- Bacteria. Digital Image. *USCNews.* 12 February 2008, https://news.usc.edu/135660/how-bacteria-adapt-to-hostile-environments/
- Red and White Bloodcells. Digital Image. *The Franklin Institute.* https://www.fi.edu/heart/white-blood-cells
- ufraction8 Logo. Digital Image. *www.ufraction8.* ufraction8.com
- WEST Logo. Digital Image. *WEST Brewery* www.westbeer.com

Part 4: Results

		$\beta = 10^{-3}$	$\beta = 10^{-1}$	$\beta = 10^{1}$	$\beta = 10^{3}$
	$\mathcal{J}_{\vec{w}=\vec{0}}$	0.0113	0.0113	0.0113	0.0113
$\kappa = -1$	$\mathcal{J}_{Opt}$	0.0013	0.0104	0.0113	0.0113
	Iterations	676	700	290	1

Table: Results for the test problem, with different β

Part 2: Optimization

Deriving (first-order) optimality conditions

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.