PDE-Constrained Optimization for Multiscale Particle Dynamics

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Joint work with Ben Goddard and John Pearson

April 21, 2021

Structure of the Talk

- PDE-Constrained Optimization
- Optimization for DDFT
- Numerical Methods
- Results


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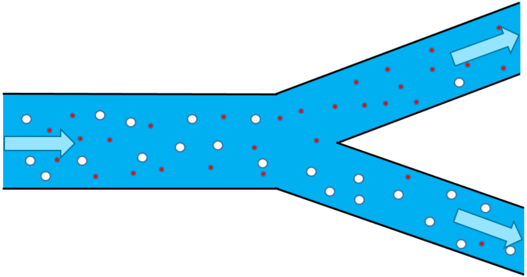
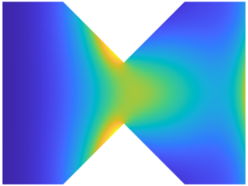
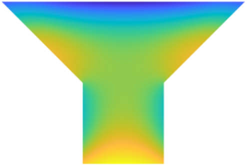






PDE-Constrained Optimization

A simple model

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

subject to:

$$\partial_t \rho = \nabla^2 \rho + f \qquad \text{in } \Sigma$$

BC and IC:

$$\frac{\partial \rho}{\partial n} = 0 \qquad \text{on } \partial\Sigma$$

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

PDE-Constrained Optimization

Deriving (first-order) optimality conditions

Define the Lagrangian $\mathcal{L}$:

$$\mathcal{L}(\rho, f, q) = \frac{1}{2}\|\rho - \widehat{\rho}\|^2_{L_2(\Sigma)} + \frac{\beta}{2}\|f\|^2_{L_2(\Sigma)} - \int_{\Sigma} q\Big(\partial_t \rho - \nabla^2 \rho - f\Big) d\vec{x} dt - \int_{\partial\Sigma} q \frac{\partial \rho}{\partial n} d\vec{x} dt$$

Compute the directional derivatives:

$$\mathcal{L}_q(\rho^*, f^*, q)h = 0, \quad \mathcal{L}_\rho(\rho^*, f^*, q)h = 0, \quad \mathcal{L}_f(\rho^*, f^*, q)h = 0.$$

PDE-Constrained Optimization

Deriving (first-order) optimality conditions

Computing $\mathcal{L}_\rho(\rho^*, f^*, q)h$:

$$\begin{aligned}\mathcal{L}(\rho, f, q) =& \frac{1}{2}\int_\Sigma (\rho - \widehat{\rho})^2\, d\vec{x}dt + \frac{\beta}{2}\int_\Sigma f^2 d\vec{x}dt - \int_\Sigma q\Big(\partial_t \rho - \nabla^2\rho - f\Big) d\vec{x}dt \\ & - \int_{\partial\Sigma} q\frac{\partial \rho}{\partial n} d\vec{x}dt\end{aligned}$$

$$\begin{aligned}\mathcal{L}_\rho(\rho^*, f^*, q)h =& \int_\Omega \big(q(T)h(T) - q(0)h(0)\big)\, d\vec{x} - \int_\Sigma \Big(h(-\rho + \widehat{\rho}) - h\partial_t q - h\nabla^2 q\Big)\, d\vec{x}dt \\ & - \int_{\partial\Sigma} q\frac{\partial h}{\partial n} - q\frac{\partial h}{\partial n} + h\frac{\partial q}{\partial n} d\vec{x}dt\end{aligned}$$

PDE-Constrained Optimization

Deriving (first-order) optimality conditions

Computing $\mathcal{L}_\rho(\rho^*, f^*, q)h = 0$:

$$\mathcal{L}_\rho(\rho^*, f^*, q)h = \int_\Omega q(T)h(T)d\vec{x} - \int_\Sigma h\left(-\rho + \widehat{\rho} - \partial_t q - \nabla^2 q\right) d\vec{x}dt - \int_{\partial\Sigma} h\frac{\partial q}{\partial n}d\vec{x}dt = 0$$

Adjoint equation:

$$\begin{aligned} \partial_t q &= -\nabla^2 q - \rho + \widehat{\rho} && \text{in} \quad \Sigma \\ \frac{\partial q}{\partial n} &= 0 && \text{on} \quad \partial\Sigma \\ q(T) &= 0 \end{aligned}$$

PDE-Constrained Optimization

Deriving (first-order) optimality conditions

Computing $\mathcal{L}_f(\rho^*, f^*, q)h = 0$:

$$\mathcal{L}(\rho, f, q) = \frac{1}{2}\int_{\Sigma} (\rho - \widehat{\rho})^2 \, d\vec{x}dt + \frac{\beta}{2}\int_{\Sigma} f^2 d\vec{x}dt - \int_{\Sigma} q\Big(\partial_t \rho - \nabla^2 \rho - f\Big) d\vec{x}dt - \int_{\partial\Sigma} q\frac{\partial \rho}{\partial n} d\vec{x}dt$$

$$\mathcal{L}_f(\rho^*, f^*, q)h = \int_{\Sigma} h\left(\beta f + q\right) d\vec{x}dt = 0$$

Gradient equation:

$$f = -\frac{1}{\beta} q$$

PDE-Constrained Optimization

The (first-order) optimality system

$$\partial_t \rho = \nabla^2 \rho + f$$

$$\partial_t q = -\nabla^2 q - \rho + \widehat{\rho}$$

$$f = -\frac{1}{\beta} q$$

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

PDE-Constrained Optimization

A simple model

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

subject to:

$$\partial_t \rho = \nabla^2 \rho + f \qquad \text{in } \Sigma$$

BC and IC:

$$\frac{\partial \rho}{\partial n} = 0 \qquad \text{on } \partial\Sigma$$

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

Optimization for DDFT

A (simple) DDFT model

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

subject to:

$$\partial_t \rho = \nabla^2 \rho - \nabla \cdot (\rho \vec{w}) \qquad \text{in } \Sigma$$

BC and IC:

$$\frac{\partial \rho}{\partial n} - \rho \vec{w} \cdot \vec{n} = 0 \qquad \text{on } \partial\Sigma$$

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

Optimization for DDFT

A (simple) DDFT model

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

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:

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

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

Optimization for DDFT

The (first-order) optimality system

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

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

Optimization for DDFT

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

$$
\begin{aligned}
\partial_t \rho(t,\vec{x}) =& \nabla^2 \rho(t,\vec{x}) - \nabla \cdot (\rho(t,\vec{x})\vec{w}(t,\vec{x})) + \nabla \cdot \int_\Omega \rho(t,\vec{x})\rho(t,\vec{x}\,')\nabla V_2(|\vec{x}-\vec{x}\,'|)d\vec{x}\,' \\
\partial_\tau q(\tau,\vec{x}) =& \nabla^2 q(\tau,\vec{x}) + \nabla q(\tau,\vec{x}) \cdot \vec{w}(\tau,\vec{x}) + \rho(\tau,\vec{x}) - \widehat{\rho}(\tau,\vec{x}) \\
& - \int_\Omega \rho(\tau,\vec{x}\,')\Big(\nabla_{\vec{x}} q(\tau,\vec{x}) - \nabla_{\vec{x}\,'} q(\tau,\vec{x}\,')\Big) \cdot \nabla V_2(|\vec{x}-\vec{x}\,'|)d\vec{x}\,' \\
\vec{w}(t,\vec{x}) =& -\frac{1}{\beta}\rho(t,\vec{x})\nabla q(t,\vec{x})
\end{aligned}
$$

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

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**

Numerical Methods

Pseudospectral 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).

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
$\partial_\tau q = \nabla^2 q + \nabla q \cdot \vec{w}^{(i)} + \rho^{(i)} - \widehat{\rho} - \int_\Omega \rho^{(i)}(\vec{x}\,')\Big(\nabla q(\vec{x}) - \nabla q(\vec{x}\,')\Big) \cdot \nabla V_2(|\vec{x} - \vec{x}\,'|)d\vec{x}\,'$.
3. Solve $\vec{w}_g^{(i)} = -\frac{1}{\beta}\rho^{(i)}\nabla q^{(i)}$.
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 $\mathcal{E} < TOL$.

Optimization for DDFT

A more general DDFT model

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

subject to:

$$\partial_t \rho = \nabla \cdot \left(\rho \nabla \frac{\delta \mathcal{F}[\rho]}{\delta \rho} - \rho \vec{w} \right) := \nabla \cdot \vec{j} \qquad \text{in } \Sigma$$

BC and IC:

$$\vec{j} \cdot \vec{n} = 0 \qquad \text{on } \partial\Sigma$$

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

Optimization for DDFT

Reminder: (Simple) DDFT model

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

subject to:

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

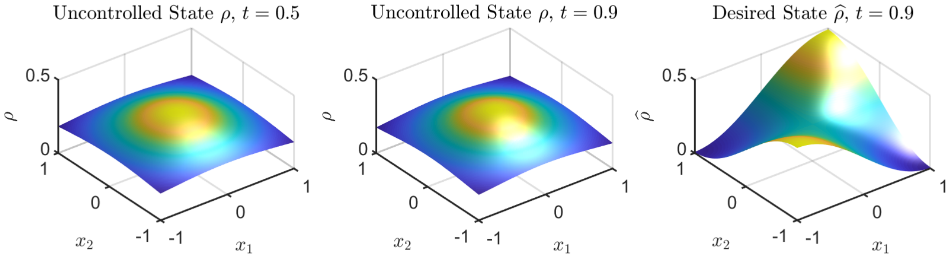
BC and IC:

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

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

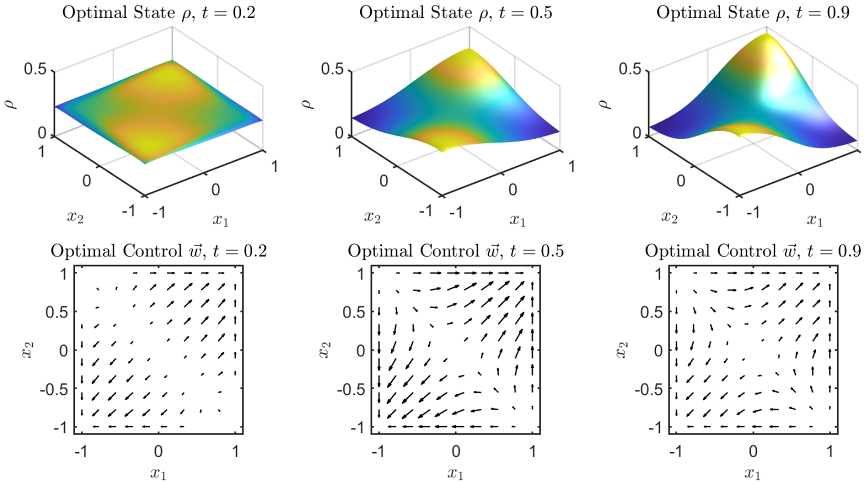
Results

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



Results

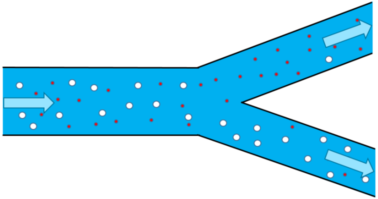
Overall Cost: $\mathcal{J} = \frac{1}{2}\|\rho - \widehat{\rho}\|^2_{L_2(\Sigma)} + \frac{\beta}{2}\|\vec{w}\|^2_{L_2(\Sigma)}$, $\mathcal{J}_{\vec{w}=\vec{0}} = 0.0130$, $\mathcal{J}_{opt} = 7.2994 \times 10^{-4}$.



Current work

Next steps

Industrial partners of the PhD



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