

# PDE-Constrained Optimization for Multiscale Particle Dynamics

Jonna Roden

University of Edinburgh/MIGSAA

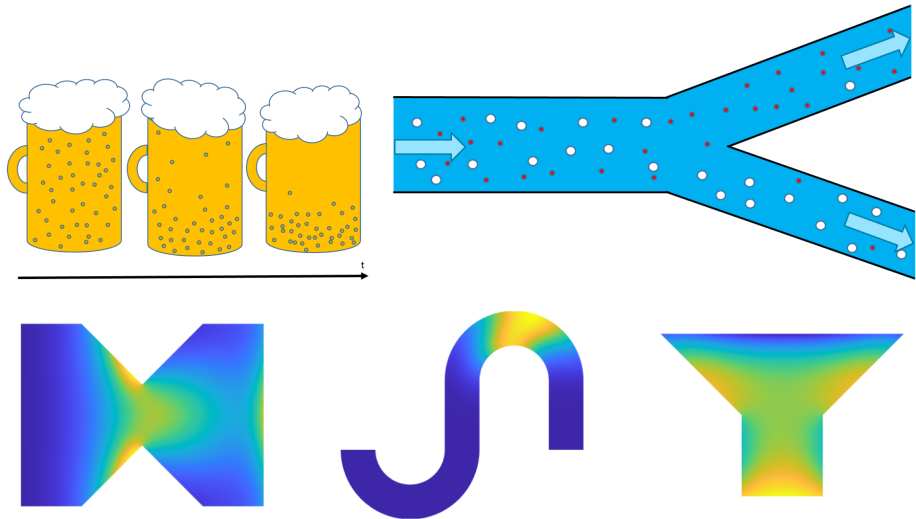
Joint work with Ben Goddard and John Pearson

06/05/2021

# Structure of the Talk

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

# Motivation



# PDE-Constrained Optimization

A simple model

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

subject to:

$$\partial_t \rho = \nabla^2 \rho + f \quad \text{in } \Sigma := (0, T) \times \Omega$$

BC and IC:

$$\frac{\partial \rho}{\partial n} = 0 \quad \text{on } \partial \Sigma := (0, T) \times \partial \Omega$$

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

# PDE-Constrained Optimization

Deriving (first-order) optimality conditions

Define the Lagrangian  $\mathcal{L}$ :

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

Compute directional derivatives and set equal to zero:

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

# PDE-Constrained Optimization

Deriving (first-order) optimality conditions

Define the Lagrangian  $\mathcal{L}$ :

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

Computing  $\mathcal{L}_q(\rho^*, f^*, q)h = 0$  results in the forward problem:

$$\begin{aligned}\partial_t \rho &= \nabla^2 \rho + f && \text{in } \Sigma \\ \frac{\partial \rho}{\partial n} &= 0 && \text{on } \partial \Sigma \\ \rho(0, \vec{x}) &= \rho_0(\vec{x})\end{aligned}$$

# PDE-Constrained Optimization

Deriving (first-order) optimality conditions

Define the Lagrangian  $\mathcal{L}$ :

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

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

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

# PDE-Constrained Optimization

Deriving (first-order) optimality conditions

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

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

Adjoint equation:

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



# PDE-Constrained Optimization

Deriving (first-order) optimality conditions

Define the Lagrangian  $\mathcal{L}$ :

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

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

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

Gradient equation:

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

# PDE-Constrained Optimization

The (first-order) optimality system

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

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

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

$$\frac{\partial \rho}{\partial n} = 0, \quad \rho(0, \vec{x}) = \rho_0(\vec{x}),$$

$$\frac{\partial q}{\partial n} = 0, \quad q(T, \vec{x}) = 0.$$

# PDE-Constrained Optimization

A simple model

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

subject to:

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

BC and IC:

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

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

# Optimization for DDFT

A (simple) DDFT model

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

subject to:

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

BC and IC:

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

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

# Optimization for DDFT

A (simple) DDFT model

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

subject to:

$$\partial_t \rho = \nabla^2 \rho - \nabla \cdot (\rho \vec{w}) + \nabla \cdot (\rho \nabla V_{\text{ext}}) \quad \text{in } \Sigma$$

BC and IC:

$$\frac{\partial \rho}{\partial n} - \rho \vec{w} \cdot \vec{n} + \rho \frac{\partial V_{\text{ext}}}{\partial n} = 0 \quad \text{on } \partial \Sigma$$

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

# Optimization for DDFT

A (simple) DDFT model

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

subject to:

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

BC and IC:

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

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

# Optimization for DDFT

The (first-order) optimality system

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

$$\begin{aligned} \partial_t q = & -\nabla^2 q - \nabla q \cdot \vec{w} + \nabla q \cdot \nabla V_{\text{ext}} - \rho + \hat{\rho} \\ & + \int_{\Omega} \rho(\vec{x}') \left( \nabla_{\vec{x}} q(\vec{x}) - \nabla_{\vec{x}'} q(\vec{x}') \right) \cdot \nabla V_2(|\vec{x} - \vec{x}'|) d\vec{x}' \end{aligned}$$

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

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

# Optimization for DDFT

**Problem:** Negative diffusion term in  $q$  causes numerical instability.

**Solution:** Change of time variable for this PDE:  $\tau = T - t$ .

$$\begin{aligned}\partial_t \rho(t, \vec{x}) = & \nabla^2 \rho(t, \vec{x}) - \nabla \cdot (\rho(t, \vec{x}) \vec{w}(t, \vec{x})) + \nabla \cdot (\rho(t, \vec{x}) \nabla V_{\text{ext}}(t, \vec{x})) \\ & + \nabla \cdot \int_{\Omega} \rho(t, \vec{x}) \rho(t, \vec{x}') \nabla V_2(|\vec{x} - \vec{x}'|) d\vec{x}'\end{aligned}$$

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

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

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



# Numerical Methods

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

⇒ **Pseudospectral methods**

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

⇒ **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

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

2. Solve  $\partial_{\tau} q = \nabla^2 q + \nabla q \cdot \vec{w}^{(i)} - \nabla q \cdot \nabla V_{\text{ext}} + \rho^{(i)} - \hat{\rho}$

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

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  $\mathcal{E} < TOL$ .

# Optimization for DDFT

Reminder: (Simple) DDFT model

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

subject to:

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

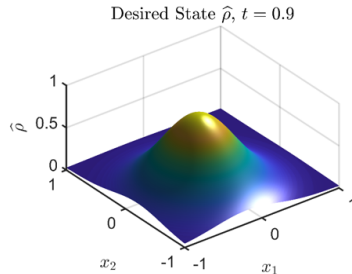
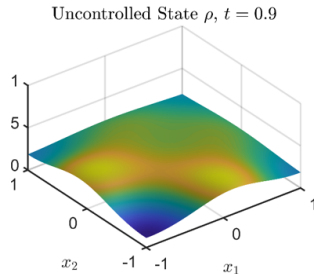
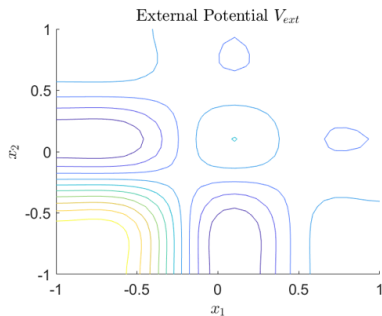
BC and IC:

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

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

## Results - Example 1

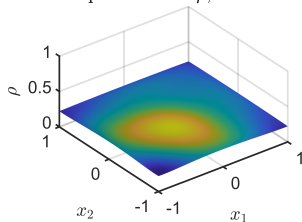
Overall Cost:  $\mathcal{J} = \frac{1}{2}\|\rho - \hat{\rho}\|_{L_2(\Sigma)}^2 + \frac{\beta}{2}\|\vec{w}\|_{L_2(\Sigma)}^2$ ,  $\mathcal{J}_{\vec{w}=\vec{0}} = 0.0400$ .



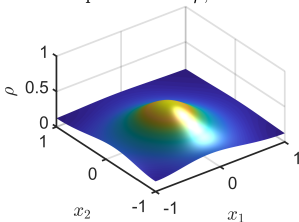
# Results - Example 1

Overall Cost:  $\mathcal{J} = \frac{1}{2}\|\rho - \hat{\rho}\|_{L_2(\Sigma)}^2 + \frac{\beta}{2}\|\vec{w}\|_{L_2(\Sigma)}^2$ ,  $\mathcal{J}_{\vec{w}=\vec{0}} = 0.0400$ ,  $\mathcal{J}_{opt} = 0.0046$ .

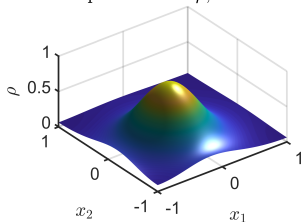
Optimal State  $\rho$ ,  $t = 0.1$



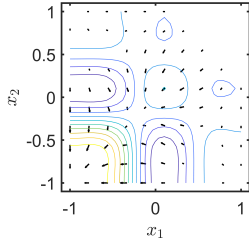
Optimal State  $\rho$ ,  $t = 0.5$



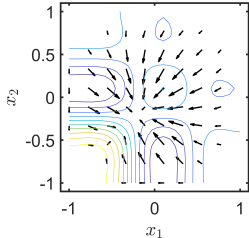
Optimal State  $\rho$ ,  $t = 0.9$



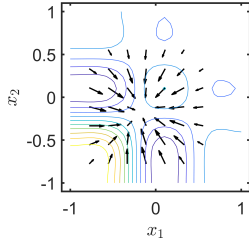
Optimal Control  $\vec{w}$ ,  $t = 0.1$



Optimal Control  $\vec{w}$ ,  $t = 0.5$



Optimal Control  $\vec{w}$ ,  $t = 0.9$



# Optimization for DDFT

A more general DDFT model

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

subject to:

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

$$\mathcal{F}[\rho] = \mathcal{F}_{id}[\rho] + \mathcal{F}_{ext}[\rho] + \mathcal{F}_{int}[\rho] + \int_{\Omega} \rho \left( -1 - \ln(1 - a\rho) + \frac{1}{1 - a\rho} \right) d\vec{x}$$

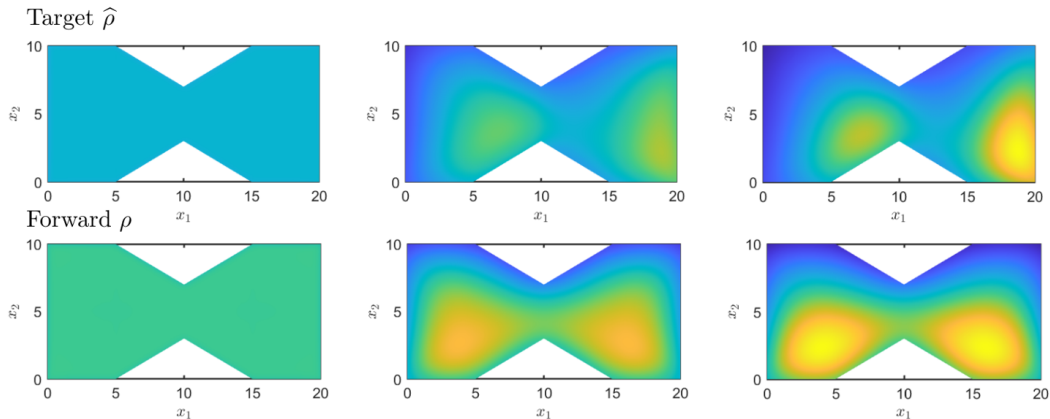
BC and IC:

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

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

## Results - Example 2

Overall Cost:  $\mathcal{J} = \frac{1}{2}\|\rho - \hat{\rho}\|_{L_2(\Sigma)}^2 + \frac{\beta}{2}\|\vec{w}\|_{L_2(\Sigma)}^2$ ,  $\mathcal{J}_{\vec{w}=\vec{0}} = 0.0484$ .

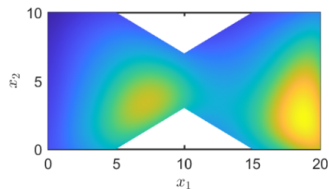
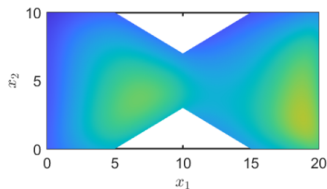
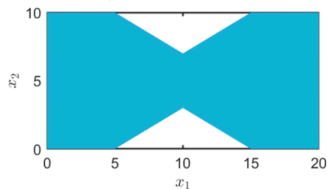




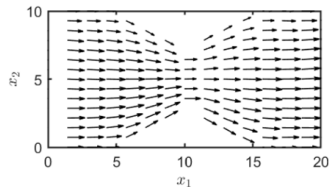
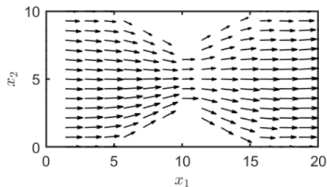
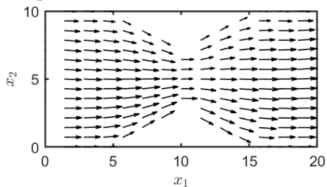
## Results - Example 2

Overall Cost:  $\mathcal{J} = \frac{1}{2}\|\rho - \hat{\rho}\|_{L_2(\Sigma)}^2 + \frac{\beta}{2}\|\vec{w}\|_{L_2(\Sigma)}^2$ ,  $\mathcal{J}_{\vec{w}=\vec{0}} = 0.0484$ ,  $\mathcal{J}_{opt} = 0.0258$ .

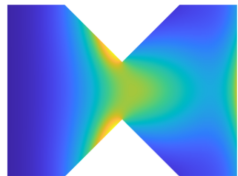
Optimal  $\rho$



Optimal control  $w$



# Summary



Up to now:

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

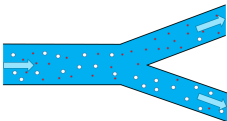
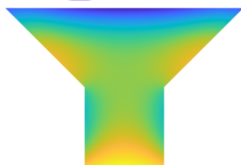


Current:




- ▶ Complex domains.
- ▶ Extended PDE models.
- ▶ Different boundary conditions.

Up next:

- ▶ More extended models.
- ▶ Application 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



ufraction8 Logo. Digital Image.  
*www.ufraction8.ufraction8.com*



WEST Logo. Digital Image.  
*WEST Brewery* *www.westbeer.com*

# Data for Example 1

		$\beta = 10^{-3}$	$\beta = 10^{-1}$	$\beta = 10^1$	$\beta = 10^3$
$\kappa = -1$	$\mathcal{J}_{\vec{w}=\vec{0}}$	0.0400	0.0400	0.0400	0.0400
	$\mathcal{J}_{opt}$	0.0046	0.0370	0.0400	0.0400
	Iter	717	778	347	1
$\kappa = 0$	$\mathcal{J}_{\vec{w}=\vec{0}}$	0.0478	0.0478	0.0478	0.0478
	$\mathcal{J}_{opt}$	0.0064	0.0450	0.0478	0.0478
	Iter	718	784	343	1
$\kappa = 1$	$\mathcal{J}_{\vec{w}=\vec{0}}$	0.0556	0.0556	0.0556	0.0556
	$\mathcal{J}_{opt}$	0.0085	0.0530	0.0556	0.0556
	Iter	720	787	339	1

Table: Cost when  $\vec{w} = \vec{0}$ , optimal control cost, and iterations required, for a range of values for interaction strength  $\kappa$  and regularization parameter  $\beta$ .