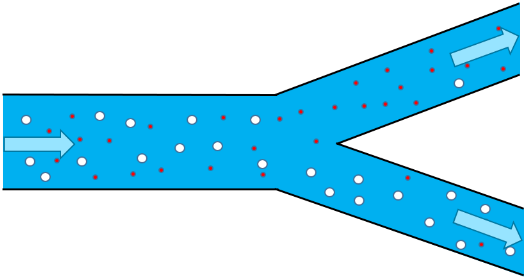
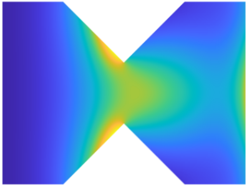
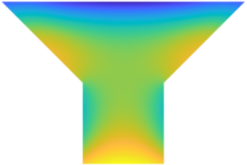

t







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:

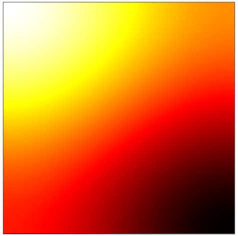
$$\partial_t \rho = \nabla^2 \rho + f \qquad \text{in} \quad \Sigma := (0, T) \times \Omega$$

BC and IC:

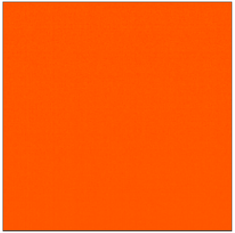
$$\frac{\partial \rho}{\partial n} = 0 \qquad \text{on } \partial\Sigma := (0, T) \times \partial\Omega$$

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

Forward ρ



Target $\widehat{\rho}$



PDE-Constrained Optimization

Deriving (first-order) optimality conditions

Define the Lagrangian $\mathcal{L}$:

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

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 $\mathcal{L}$:

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

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

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

PDE-Constrained Optimization

Deriving (first-order) optimality conditions

Define the Lagrangian $\mathcal{L}$:

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

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

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

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:

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

PDE-Constrained Optimization

Deriving (first-order) optimality conditions

Define the Lagrangian $\mathcal{L}$:

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

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

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

Gradient equation:

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

PDE-Constrained Optimization

The (first-order) optimality system

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

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

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

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

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

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:

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

BC and IC:

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

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

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:

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

BC and IC:

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

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

Optimization for DDFT

The (first-order) optimality system

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

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

Optimization for DDFT

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

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

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

Numerical Methods

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

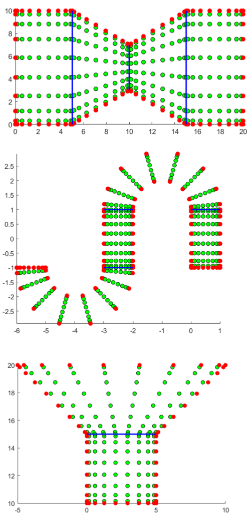
  $\Rightarrow$ **Pseudospectral methods**

- 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).
- For more 'complex' domains, pseudospectral methods are extended to spectral element methods.

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 $\partial_\tau q = \nabla^2 q + \nabla q \cdot \vec{w}^{(i)} - \nabla q \cdot \nabla V_{\text{ext}} + \rho^{(i)} - \widehat{\rho}$
$$- \int_\Omega \rho^{(i)}(\vec{x}\,')\Big(\nabla q(\vec{x}) - \nabla q(\vec{x}\,')\Big) \cdot \nabla V_2(|\vec{x} - \vec{x}\,'|)d\vec{x}\,'.$$
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 $\lambda \in [0,1]$: $\quad \vec{w}^{(i+1)} = (1-\lambda)\vec{w}^{(i)} + \lambda \vec{w}_g^{(i)}$.

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

Optimization for DDFT

Reminder: (Simple) DDFT model

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

subject to:

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

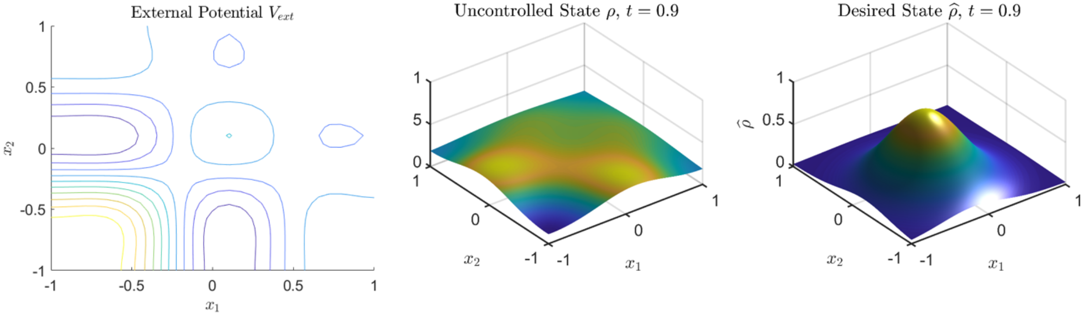
BC and IC:

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

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

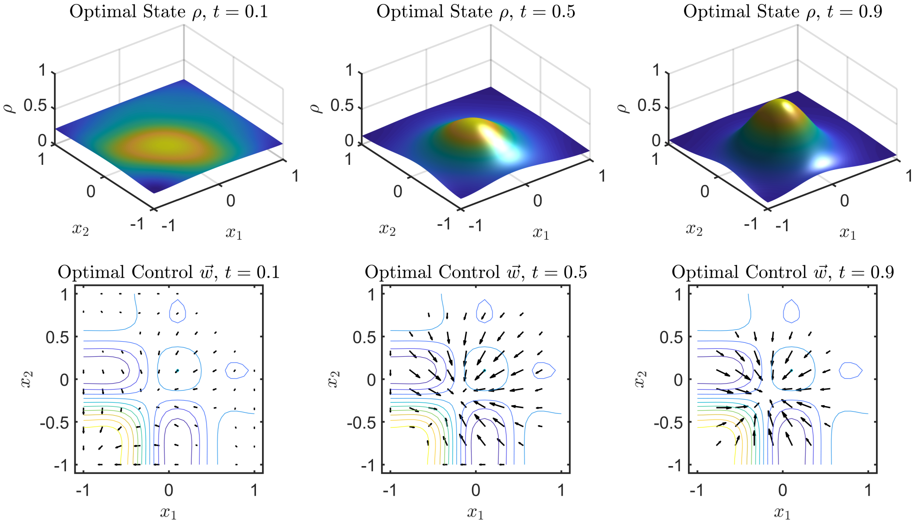
Results - Example 1

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



Results - Example 1

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



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:

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

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

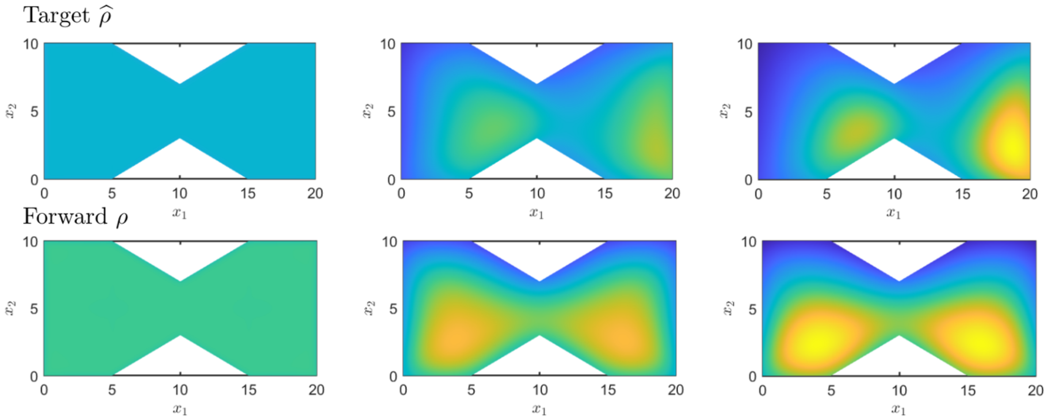
BC and IC:

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

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

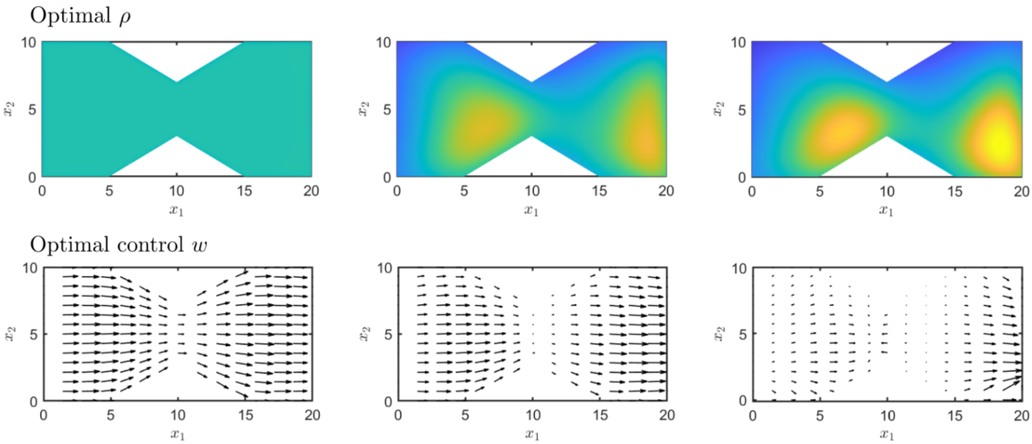
Results - Example 2

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

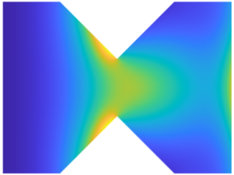


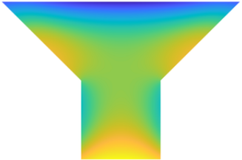
Results - Example 2

Overall Cost: $\mathcal{J} = \frac{1}{2}\|\rho - \widehat{\rho}\|^2_{L_2(\Sigma)} + \frac{\beta}{2}\|\vec{w}\|^2_{L_2(\Sigma)}$, $\mathcal{J}_{\vec{w}=\vec{0}} = 0.0484$, $\mathcal{J}_{\text{opt}} = 0.0146$.



Summary





Up to now:

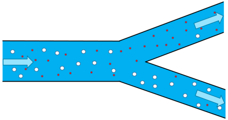
- Deriving PDE-constrained optimization models.
- Developing a suitable numerical method to solve them.

Current:

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

Up next:

- More extended models.
- Different controls.
- Application to industrial processes.



Some References

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Some More References

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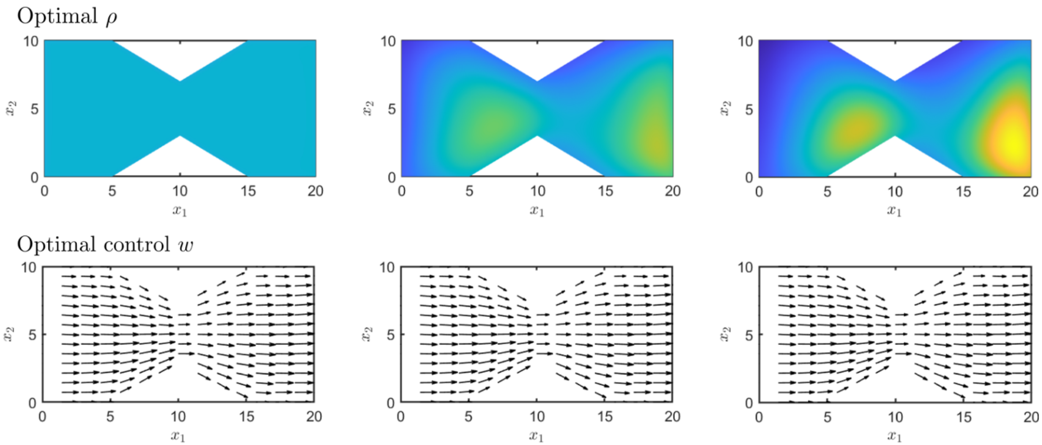
Results - Example 2, with Time-Independent Control

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



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
	$\mathcal{J}_{\text{opt}}$	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
	$\mathcal{J}_{\text{opt}}$	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
	$\mathcal{J}_{\text{opt}}$	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 κ and regularization parameter β.

References: Figures

ufraction8 Logo. Digital Image.
www.ufraction8. `ufraction8.com`

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WEST Brewery `www.westbeer.com`