Numerical Methods for PDE-Constrained Optimization of Particle Dynamics

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Structure of the Talk

- The Optimization Problem
- Numerical Methods
  - Pseudospectral and Spectral Element Methods
  - Fixed Point Algorithm
  - Newton-Krylov Algorithm
- Results

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:

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

BC and IC:

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

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

The Optimization Problem

The (first-order) optimality system

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

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

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

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

Numerical Methods

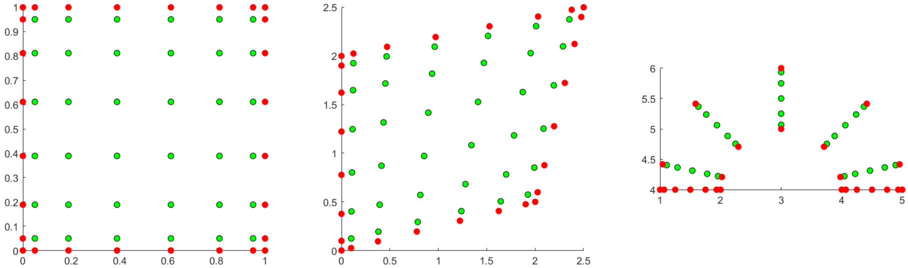
- Challenge 1: Particle interaction term is nonlinear and nonlocal ($+$ nonlocal BCs). How to avoid shortcomings of standard methods (FEM/FDM)?

  $\Rightarrow$ **Pseudospectral Method**
  AND
  $\Rightarrow$ **Spectral Element Method**

- Challenge 2: One PDE has an initial, the other a final time condition. The Laplacians have opposite signs.
  How to do time stepping?

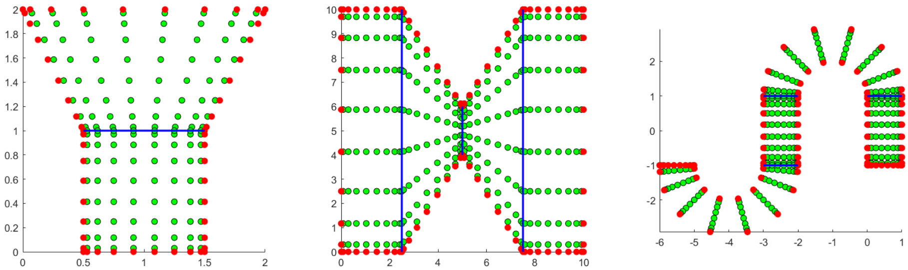
  $\Rightarrow$ **Fixed Point Algorithm**
  OR
  $\Rightarrow$ **Newton-Krylov Algorithm**

Pseudospectral Method



- Reduce both PDEs to systems of ODEs.
- Discretize time (accurate interpolation).
- Equations can now be solved using the Fixed Point Algorithm (with DAE solvers) or the Newton-Krylov Algorithm.

Spectral Element Method



- Discretize PDE on each element using pseudospectral methods.
- Match solution and flux between elements.

Fixed Point Algorithm

The (first-order) optimality system

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

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

Fixed Point Algorithm

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

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

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:

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

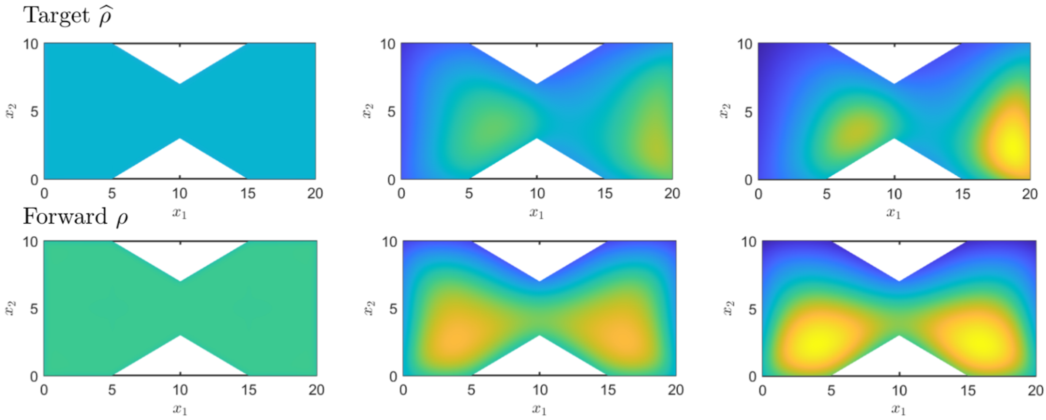
BC and IC:

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

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

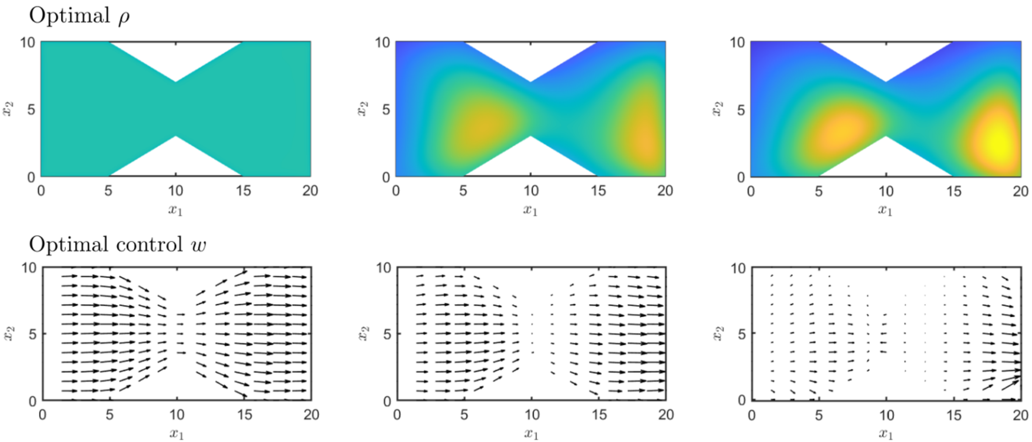
Fixed Point Algorithm Results

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



Fixed Point Algorithm Results

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



Newton-Krylov Algorithm

The (first-order) optimality system

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

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

Newton-Krylov Algorithm

$$\partial_t \rho = \nabla^2 \rho + \frac{1}{\beta}\nabla \cdot (\rho\rho\nabla q) + \nabla \cdot (\rho \nabla V_{ext}) + \nabla \cdot \int_\Omega \rho(\vec{x})\rho(\vec{x}\,')\nabla V_2(|\vec{x} - \vec{x}\,'|)d\vec{x}\,'$$

$$\partial_t q = -\nabla^2 q + \frac{1}{\beta}\nabla q \cdot \rho \nabla q + \nabla q \cdot \nabla V_{ext}$$
$$+ \int_\Omega \rho(\vec{x}\,')\Big(\nabla q(\vec{x}) + \nabla q(\vec{x}\,')\Big) \cdot \nabla V_2(|\vec{x} - \vec{x}\,'|)d\vec{x}\,'$$

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

Newton-Krylov Algorithm

$$r_\rho(t) = \int_0^t \left(\nabla^2 \rho + \frac{1}{\beta} \nabla \cdot (\rho^2 \nabla q) + \nabla \cdot (\rho \nabla V_{ext}) + \nabla \cdot \int_\Omega \rho(\vec{x}) \rho(\vec{x}\,') \nabla V_2(|\vec{x} - \vec{x}\,'|) d\vec{x}\,' \right.$$
$$\left. - \partial_\tau \rho \right) d\tau$$

$$r_q(t) = \int_0^t \left(-\nabla^2 q + \frac{1}{\beta} \rho \nabla q \cdot \nabla q + \nabla q \cdot \nabla V_{ext} \right.$$
$$\left. + \int_\Omega \rho(\vec{x}\,') \Big(\nabla q(\vec{x}) + \nabla q(\vec{x}\,') \Big) \cdot \nabla V_2(|\vec{x} - \vec{x}\,'|) d\vec{x}\,' - \partial_\tau q \right) d\tau$$

Newton-Krylov Algorithm

$$
\begin{aligned}
r_\rho(t) &= \int_0^t \Big(\nabla^2 \rho + \frac{1}{\beta} \nabla \cdot (\rho^2 \nabla q) + \nabla \cdot (\rho \nabla V_{ext}) + \nabla \cdot \int_\Omega \rho(\vec{x}) \rho(\vec{x}\,') \nabla V_2(|\vec{x} - \vec{x}\,'|) d\vec{x}\,' \\
&\qquad - \partial_\tau \rho \Big)\, d\tau \\
r_q(t) &= \int_0^t \Big(-\nabla^2 q + \frac{1}{\beta} \rho \nabla q \cdot \nabla q + \nabla q \cdot \nabla V_{ext} \\
&\qquad + \int_\Omega \rho(\vec{x}\,') \Big(\nabla q(\vec{x}) + \nabla q(\vec{x}\,') \Big) \cdot \nabla V_2(|\vec{x} - \vec{x}\,'|) d\vec{x}\,' - \partial_\tau q \Big)\, d\tau
\end{aligned}
$$

Newton-Krylov Algorithm

$$
\begin{aligned}
r_\rho(t) = \int_0^t \left(\nabla^2 \rho + \frac{1}{\beta} \nabla \cdot (\rho^2 \nabla q) + \nabla \cdot (\rho \nabla V_{ext}) + \nabla \cdot \int_\Omega \rho(\vec{x}) \rho(\vec{x}\,') \nabla V_2(|\vec{x} - \vec{x}\,'|) d\vec{x}\,' \right) d\tau \\
-\rho(t) + \rho(0)
\end{aligned}
$$

$$
\begin{aligned}
r_q(t) = \int_0^t \Bigg(-\nabla^2 q + \frac{1}{\beta} \rho \nabla q \cdot \nabla q + \nabla q \cdot \nabla V_{ext} \\
+ \int_\Omega \rho(\vec{x}\,') \left(\nabla q(\vec{x}) + \nabla q(\vec{x}\,') \right) \cdot \nabla V_2(|\vec{x} - \vec{x}\,'|) d\vec{x}\,' \Bigg) d\tau - q(t) + q(0)
\end{aligned}
$$

Newton-Krylov Algorithm

$$r_\rho(t) = \int_0^t \left(\nabla^2 \rho + \frac{1}{\beta} \nabla \cdot (\rho^2 \nabla q) + \nabla \cdot (\rho \nabla V_{ext}) + \nabla \cdot \int_\Omega \rho(\vec{x}) \rho(\vec{x}\,') \nabla V_2(|\vec{x} - \vec{x}\,'|) d\vec{x}\,' \right) d\tau$$
$$-\rho(t) + \rho(0)$$

$$r_q(t) = \int_0^t \left(-\nabla^2 q + \frac{1}{\beta} \rho \nabla q \cdot \nabla q + \nabla q \cdot \nabla V_{ext} \right.$$
$$\left. + \int_\Omega \rho(\vec{x}\,') \Big(\nabla q(\vec{x}) + \nabla q(\vec{x}\,') \Big) \cdot \nabla V_2(|\vec{x} - \vec{x}\,'|) d\vec{x}\,' \right) d\tau - q(t) + q(0)$$

Discretizing in space:

$$\begin{pmatrix} r_\rho(t) \\ r_q(t) \end{pmatrix} = \begin{pmatrix} \int_0^t F(\rho, q, \tau) d\tau \\ \int_0^t G(\rho, q, \tau) d\tau \end{pmatrix} + \begin{pmatrix} -\rho(t) + \rho(0) \\ -q(t) + q(0) \end{pmatrix}$$

Newton-Krylov Algorithm

$$\begin{pmatrix} r_\rho(t) \\ r_q(t) \end{pmatrix} = \begin{pmatrix} \int_0^t F(\rho, q, \tau) d\tau \\ \int_0^t G(\rho, q, \tau) d\tau \end{pmatrix} + \begin{pmatrix} -\rho(t) + \rho(0) \\ -q(t) + q(0) \end{pmatrix}$$

Numerical quadrature:

$$R([\rho, q], t) = \begin{pmatrix} Q(t) F(\rho, q) \\ Q(t) G(\rho, q) \end{pmatrix} + \begin{pmatrix} -\rho(t) + \rho(0) \\ -q(t) + q(0) \end{pmatrix}$$

Define $\mathbf{y} := [\rho, q]$. Full residual vector:

$$\mathbf{R}(\mathbf{y}) = \left[R(\mathbf{y}, t_0), R(\mathbf{y}, t_1), \ldots, R(\mathbf{y}, t_n) \right] .$$

Newton-Krylov Algorithm

Aim: Approximate $\mathbf{R}(\mathbf{y}) = \mathbf{0}$, with $\mathbf{y} := [\rho, q]$.

- Update $\mathbf{y}$ using a Newton step

$$\mathbf{y}^{(i+1)} = \mathbf{y}^{(i)} + \left[D\mathbf{R}\left(\mathbf{y}^{(i)}\right) \right]^{-1} \mathbf{R}\left(\mathbf{y}^{(i)}\right).$$

- Approximate $D\mathbf{R}\left(\mathbf{y}^{(i)}\right)$.
- Approximate

$$D\mathbf{R}\left(\mathbf{y}^{(i)}\right)\mathbf{x} = \mathbf{R}\left(\mathbf{y}^{(i)}\right),$$

using GMRES and the preconditioner in Güttel and Pearson[1].

[1] S. Güttel and J. W. Pearson. "A spectral-in-time Newton–Krylov method for nonlinear PDE-constrained optimization". In: *IMA Journal of Numerical Analysis* (2021).

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:

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

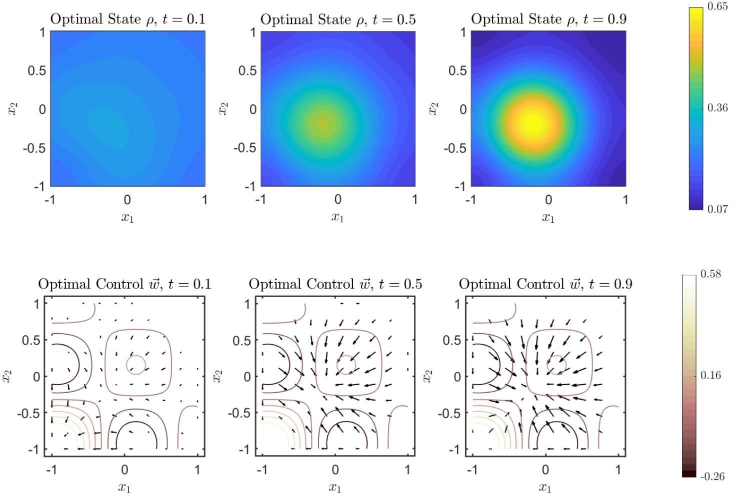
BC and IC:

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

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

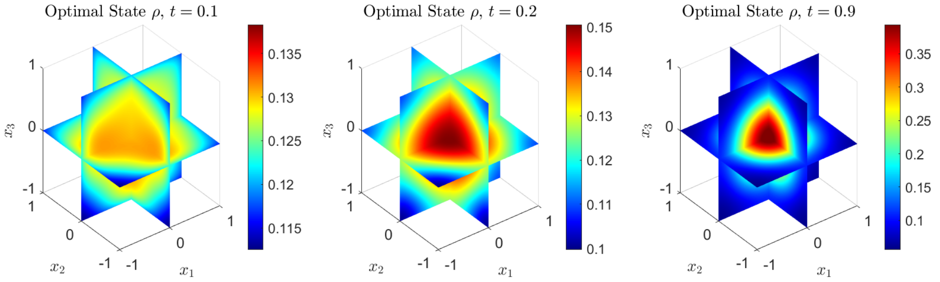
Newton Krylov Result 2D

Overall Cost: $\mathcal{J} = \frac{1}{2}\|\rho - \widehat{\rho}\|^2_{L_2(\Sigma)} + \frac{\beta}{2}\|\vec{w}\|^2_{L_2(\Sigma)}$, $\mathcal{J}_{\vec{w}=\vec{0}} = 0.0209$, $\mathcal{J}_{opt} = 0.0026$.



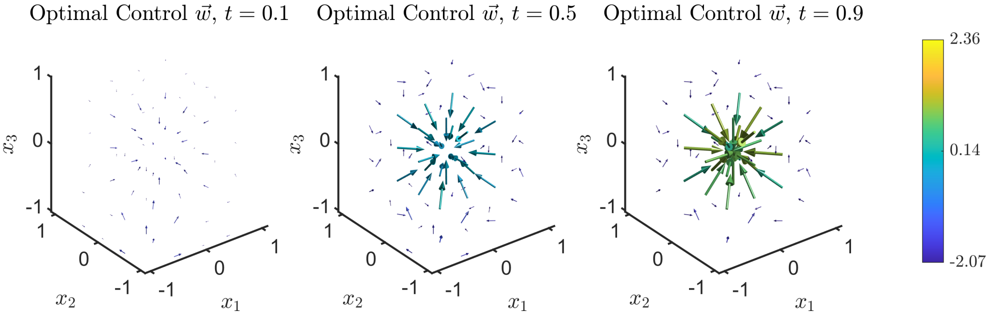
Newton Krylov Result 3D

Overall Cost: $\mathcal{J} = \frac{1}{2}\|\rho - \widehat{\rho}\|^2_{L_2(\Sigma)} + \frac{\beta}{2}\|\vec{w}\|^2_{L_2(\Sigma)}$, $\mathcal{J}_{\vec{w}=\vec{0}} = 0.0477$, $\mathcal{J}_{opt} = 0.0059$.



Newton Krylov Result 3D

Overall Cost: $\mathcal{J} = \frac{1}{2}\|\rho - \widehat{\rho}\|^2_{L_2(\Sigma)} + \frac{\beta}{2}\|\vec{w}\|^2_{L_2(\Sigma)}$, $\mathcal{J}_{\vec{w}=\vec{0}} = 0.0477$, $\mathcal{J}_{opt} = 0.0059$.



Next steps

Industrial partners of the PhD

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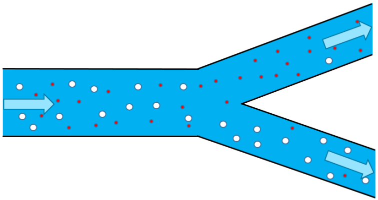

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Summary

Up to now:

- Developed a numerical framework for solving PDE-constrained optimization problems.

Current:

- More complex domains.
- Extended models.
- Different boundary conditions.

Up next:

- Application of the Newton-Krylov Algorithm to more complex domains.
- Application of the method to other extended models.
- Application of the numerical framework to industrial processes.

Aduamoah, M. et al. “PDE-constrained optimization models and pseudospectral methods for multiscale particle dynamics”. In: *Preprint* (2020).

Güttel, S. and J. W. Pearson. “A spectral-in-time Newton–Krylov method for nonlinear PDE-constrained optimization”. In: *IMA Journal of Numerical Analysis* (2021).

Nold, A. et al. “Pseudospectral methods for density functional theory in bounded and unbounded domains”. In: *Journal of Computational Physics* 334 (2017), pp. 639–664. URL: https://datashare.is.ed.ac.uk/handle/10283/2647(2DChebClass).

2D Results Table

		$\beta = 10^{-5}$	$\beta = 10^{-3}$	$\beta = 10^{-1}$	$\beta = 10^{1}$	$\beta = 10^{3}$
$\kappa = 0$	$\mathcal{J}_{uc}$	$2{,}67 \cdot 10^{-2}$	$2{,}67 \cdot 10^{-2}$	$2{,}67 \cdot 10^{-2}$	$2{,}67 \cdot 10^{-2}$	$2{,}67 \cdot 10^{-2}$
	$\mathcal{J}_{c}$	$8{,}23 \cdot 10^{-5}$	$3{,}87 \cdot 10^{-3}$	$2{,}50 \cdot 10^{-2}$	$2{,}67 \cdot 10^{-2}$	$2{,}67 \cdot 10^{-2}$
$\kappa = 1$	$\mathcal{J}_{uc}$	$3{,}29 \cdot 10^{-2}$	$3{,}29 \cdot 10^{-2}$	$3{,}29 \cdot 10^{-2}$	$3{,}29 \cdot 10^{-2}$	$3{,}29 \cdot 10^{-2}$
	$\mathcal{J}_{c}$	$1{,}16 \cdot 10^{-4}$	$5{,}44 \cdot 10^{-3}$	$3{,}13 \cdot 10^{-2}$	$3{,}29 \cdot 10^{-2}$	$3{,}29 \cdot 10^{-2}$
$\kappa = -1$	$\mathcal{J}_{uc}$	$2{,}09 \cdot 10^{-2}$	$2{,}09 \cdot 10^{-2}$	$2{,}09 \cdot 10^{-2}$	$2{,}09 \cdot 10^{-2}$	$2{,}09 \cdot 10^{-2}$
	$\mathcal{J}_{c}$	$5{,}71 \cdot 10^{-5}$	$2{,}63 \cdot 10^{-3}$	$1{,}92 \cdot 10^{-2}$	$2{,}09 \cdot 10^{-2}$	$2{,}09 \cdot 10^{-2}$

Table: Flow Control No-Flux Problem: Cost when $\vec{w} = \vec{0}$ and optimal control cost for a range of κ, β.

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:

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

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

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.

Figure References

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

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

Some References

M. Aduamoah et al. "PDE-constrained optimization models and pseudospectral methods for multiscale particle dynamics". In: *Preprint* (2020) and A. Nold et al. "Pseudospectral methods for density functional theory in bounded and unbounded domains". In: *Journal of Computational Physics* 334 (2017), pp. 639–664. URL: https://datashare.is.ed.ac.uk/handle/10283/2647(2DChebClass)