Paper Examples 2D

All the below examples are run with Newton-Krylov. They all converged within 10 outer iterations. The baseline for the cost functional is the problem computed with $\beta = 10^3$. I changed the colormap to fewer colors, so that the differences between the different κ are visible in the initial times, while also scaling the colormap for the overall maximum of ρ over all times and κ. The controls are also scaled for all times and κ (for flow control we use the largest value over all times and κ as the scaling for the arrow).

1 Neumann Source Control

We choose

$$\begin{aligned}
\rho_0 &= \frac{1}{4} \\
V_{ext} &= \frac{3}{2}\cos\left(\frac{\pi x_1}{5} - \frac{\pi}{5}\right)\sin\left(\frac{\pi x_2}{5}\right) \\
\widehat{\rho} &= \frac{1}{4}(1-t) + t\left(\frac{1}{4}\sin\left(\frac{\pi\,(x_1-2)}{2}\right)\sin\left(\frac{\pi(x_2-2)}{2}\right) + \frac{1}{4}\right)
\end{aligned}$$

We choose the domain $[-1,1]^2$ with a time horizon $(0,1)$ and $N = 20$, $n = 11$. For $\beta = 10^{-3}$, for $\kappa = -1$ we have $\mathcal{J}_c = 0.0018$, for $\kappa = 0$ (compared to $\mathcal{J}_{uc} = 0.0274$ from $\beta = 10^3$), $\mathcal{J}_c = 0.0017$ and for $\kappa = 1$, $\mathcal{J}_c = 0.0018$. Each of these computations takes around 200 seconds for 10 outer iterations. The results can be seen in Figures 1, 2 and 3.
We run the same example with $\beta = 10^{-5}$. This gives for $\kappa = -1$, $\mathcal{J}_c = 8.0673 \times 10^{-4}$, for $\kappa = 0$, $\mathcal{J}_c = 8.1989 \times 10^{-4}$, and for $\kappa = 1$, $\mathcal{J}_c = 8.4241 \times 10^{-4}$. Notably, these calculations only take around 20 seconds.

2 Dirichlet Source Control

We choose

$$\begin{aligned}
\rho_0 &= \frac{1}{4}\cos\left(\frac{\pi x_1}{2}\right)\cos\left(\frac{\pi x_2}{2}\right) + \frac{1}{4} \\
V_{ext} &= 2(1-t)\left(-\cos\left(\frac{\pi x_1}{2}\right)\sin\left(\frac{\pi x_2}{2}\right) + 1\right) \\
\widehat{\rho} &= (1-t)\left(\frac{1}{4}\cos\left(\frac{\pi x_1}{2}\right)\cos\left(\frac{\pi x_2}{2}\right) + \frac{1}{4}\right) - t\left(\frac{1}{4}\sin\left(\pi x_1\right)\sin\left(\frac{\pi x_2}{2} - \frac{\pi}{2}\right) + \frac{1}{4}\right)
\end{aligned}$$

so that the problem has Dirichlet boundary conditions at 0.25 ($\rho = 0.25$ on $\partial\Omega$). We choose the domain $[-1,1]^2$ with a time horizon $(0,1)$ and $N = 20$, $n = 11$. For $\beta = 10^{-3}$, for $\kappa = -1$

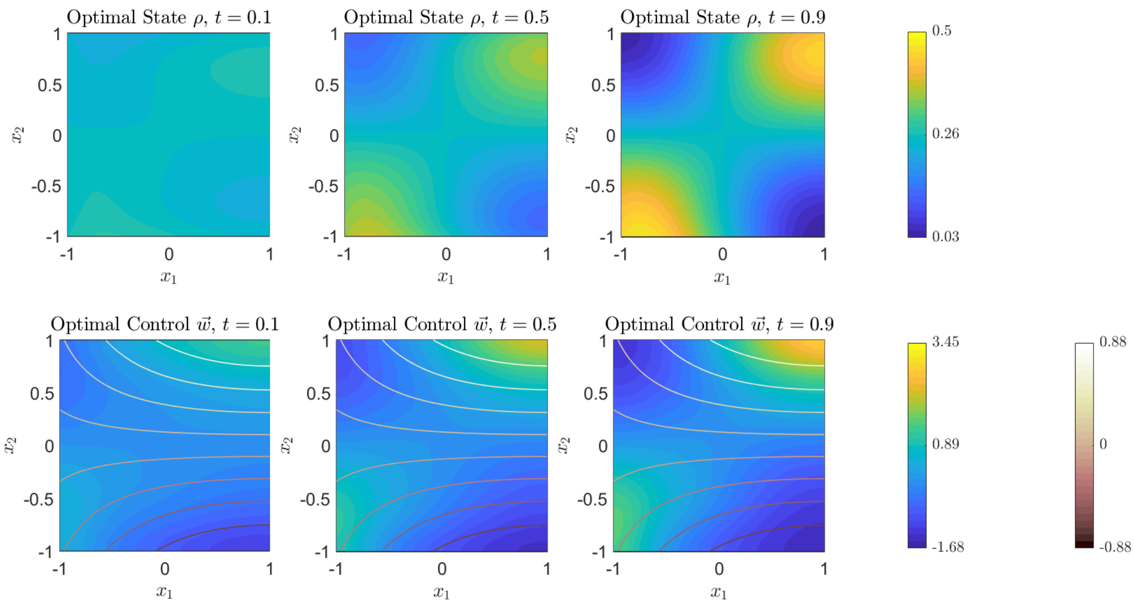

Figure 1: Neumann Source Control: Optimal ρ and optimal control for $\kappa = 0$ and $\beta = 10^{-3}$.

we have $\mathcal{J}_c = 0.0036$, for $\kappa = 0$ (compared to $\mathcal{J}_{uc} = 0.0219$ from $\beta = 10^3$), $\mathcal{J}_c = 0.0038$ and for $\kappa = 1$, $\mathcal{J}_c = 0.0043$. Each of these computations takes around 70 seconds for 10 outer iterations. The results can be seen in Figures 4, 5 and 6.

3 Neumann Flow Control

We choose

$$\begin{aligned}
\rho_0 &= \frac{1}{4} \\
V_{ext} &= \left((x_1+0.3)^2-1\right)\left((x_1-0.4)^2-0.5\right)\left((x_2+0.3)^2-1\right)\left((x_2-0.4)^2-0.5\right) \\
\widehat{\rho} &= \frac{1}{4}(1-t) + t\frac{1}{1.3791}\exp\left(-2\left((x_1+0.2)^2+(x_2+0.2)^2\right)\right)
\end{aligned}$$

We choose the domain $[-1,1]^2$ with a time horizon $(0,1)$. We have $N = 20$, $n = 11$. For $\beta = 10^{-3}$, $\kappa = 1$ we get $\mathcal{J}_c = 0.0059$ (compare to $\beta = 10^3$ with $\mathcal{J}_{uc} = 0.0336$), for $\kappa = 0$, $\mathcal{J}_c = 0.0043$, and for $\kappa = -1$ we get $\mathcal{J}_c = 0.0030$, (compare to $\beta = 10^3$ with $\mathcal{J}_{uc} = 0.0214$). Each of the problems takes around 180 seconds to solve. The results can be seen in Figures 7, 8 and 9. Note that mass is conserved.

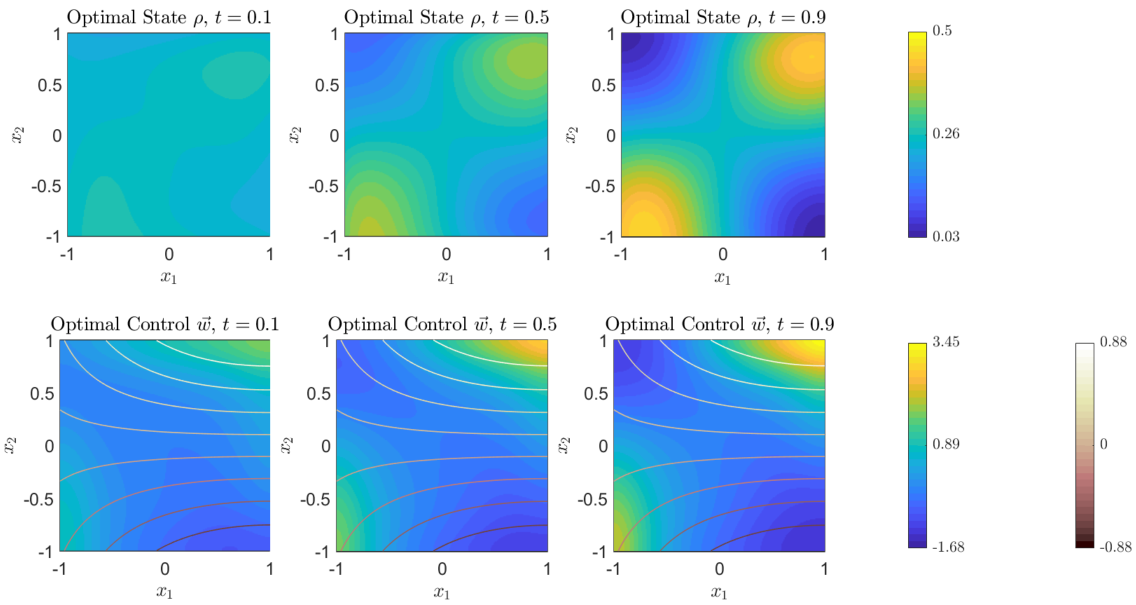

Figure 2: Neumann Source Control: Optimal ρ and optimal control for $\kappa = -1$ and $\beta = 10^{-3}$.

3.1 Dirichlet Flow Control

We add the following external potential to the above problem, see Figure **??**

$$V_{ext} = 10 \sin\left(\frac{\pi x_1}{2}\right) \sin\left(\frac{\pi x_2}{3} - \frac{\pi}{2}\right)$$

For $\beta = 10^{-3}$, $\kappa = 1$ we get $\mathcal{J}_c = 0.0130$, for $\kappa = 0$, $\mathcal{J}_c = 0.0106$, and for $\kappa = -1$ we get $\mathcal{J}_c = 0.0113$. (Compare these to $\beta = 10^3$ with $\mathcal{J}_{uc} = 0.0898$) Each of the problems takes around 50 seconds to solve. The results can be seen in Figures 10, 11 and 12.

Paper Example 3D

We choose

$$\begin{aligned}
\rho_0 &= 0.125 \\
V_{ext} &= ((x_1 + 0.3)^2 - 1)((x_1 - 0.4)^2 - 0.5) \\
&\quad ((x_2 + 0.3)^2 - 1)((x_2 - 0.4)^2 - 0.5)((x_3 + 0.3)^2 - 1)((x_3 - 0.4)^2 - 0.5) \\
\widehat{\rho} &= 0.125(1 - t) + t \left(\frac{\pi}{4}\right)^3 \cos\left(\frac{\pi x_1}{2}\right) \cos\left(\frac{\pi x_2}{2}\right) \cos\left(\frac{\pi x_3}{2}\right)
\end{aligned}$$

The external potential is shown in Figure **??**.

For $N = 20$ and $n = 11$, with $\beta = 10^{-3}$ we get for $\kappa = 0$, $\mathcal{J}_c = 0.0078$, with $\mathcal{J}_1 = 0.0071$ and $\mathcal{J}_2 = 8.5034$. This can be compared to $\mathcal{J}_{uc} = 0.0195$ from the computed forward problem with

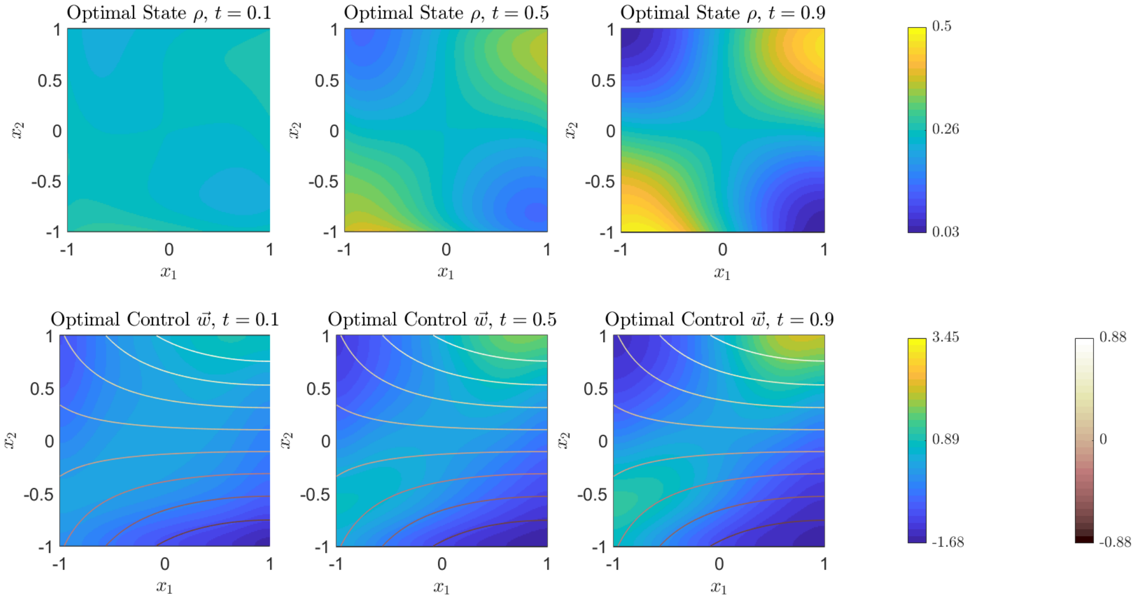

Figure 3: Optimal ρ and optimal control for $\kappa = 1$ and $\beta = 10^{-3}$.

$\mathbf{w} = \vec{0}$.
For $\kappa = 1$, we get that $\mathcal{J}_c = 0.0102$, with $\mathcal{J}_1 = 0.0097$, $\mathcal{J}_2 = 10.7306$. Compare to $\mathcal{J}_{uc} = 0.0232$. For $\kappa = -1$ we have $\mathcal{J}_c = 0.0059$, $\mathcal{J}_1 = 0.0054$, $\mathcal{J}_2 = 6.4039$. Compare to $\mathcal{J}_{uc} = 0.0477$. While the forward problem takes around 12 minutes to solve, the optimal control problem with Newton-Krylov takes about 35 hours for 10 outer iterations, which is enough for convergence. Mass is conserved to 10^{-4}. The results can be seen in Figures 13, 14 and 15.

The controls are plotted in Figures 16, 17 and 18. They are all normalized to the maximum over all three controls and scaled by a factor of 2 for visibility. The figures are still not good though. I am not sure how the scaling works – $\kappa = 0$ should have way smaller arrows by that logic.

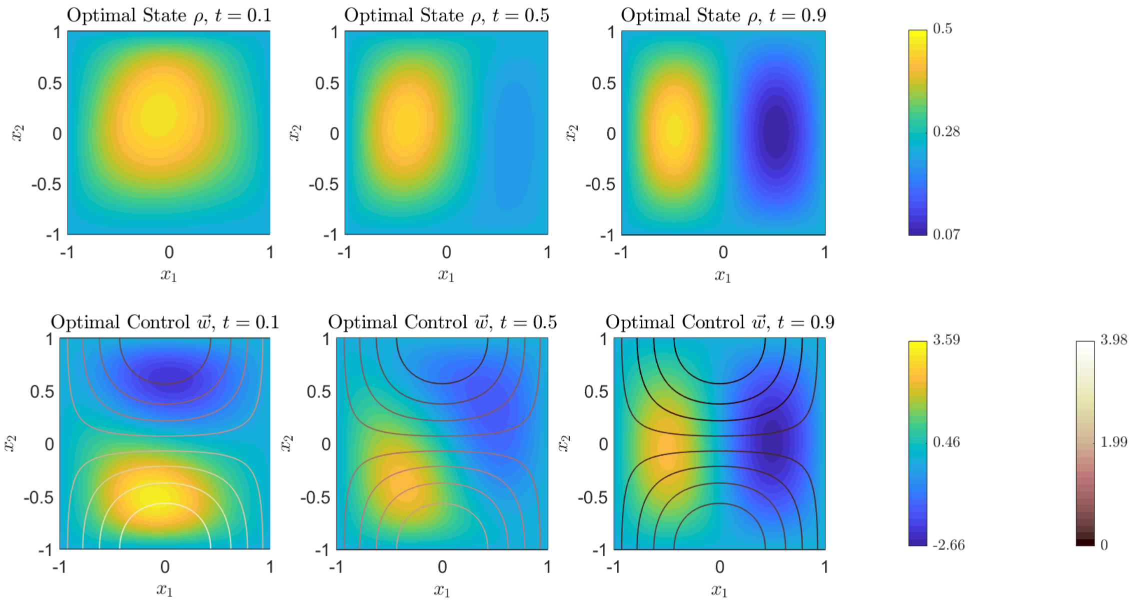

Figure 4: Dirichlet Source Control: Optimal ρ and optimal control for $\kappa = 0$ and $\beta = 10^{-3}$.

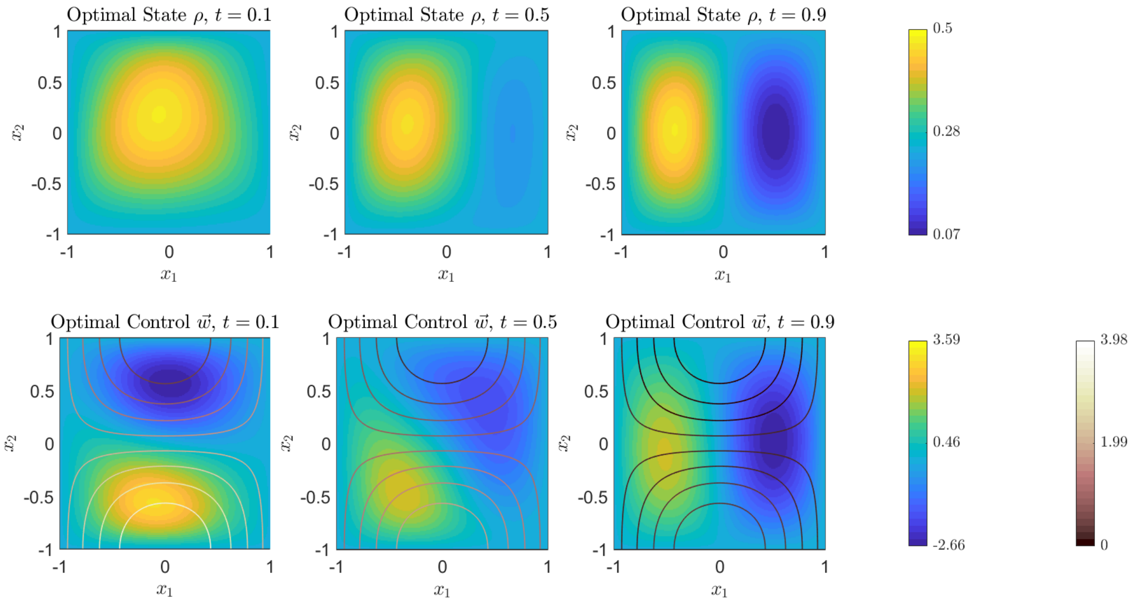

Figure 5: Dirichlet Source Control: Optimal ρ and optimal control for $\kappa = -1$ and $\beta = 10^{-3}$.

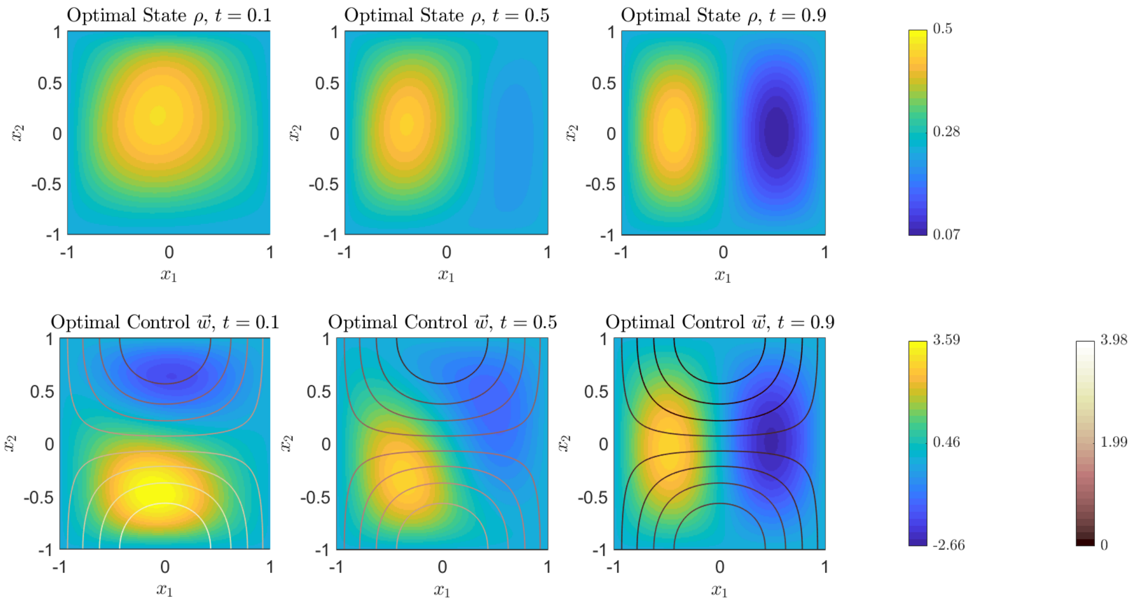

Figure 6: Dirichlet Source Control: Optimal ρ and optimal control for $\kappa = 1$ and $\beta = 10^{-3}$.

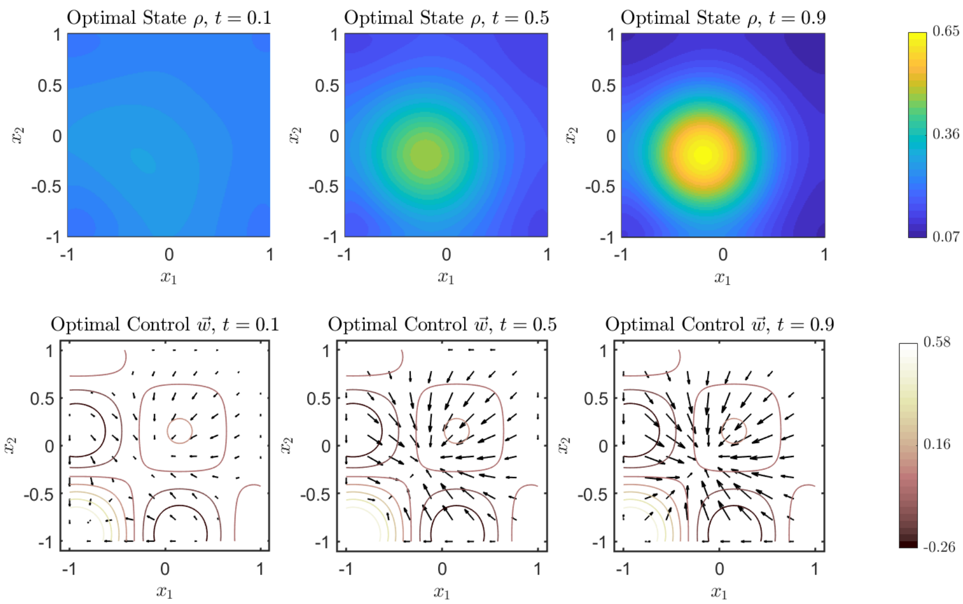

Figure 7: Neumann Flow Control: Optimal ρ and optimal control for $\kappa = 0$ and $\beta = 10^{-3}$.

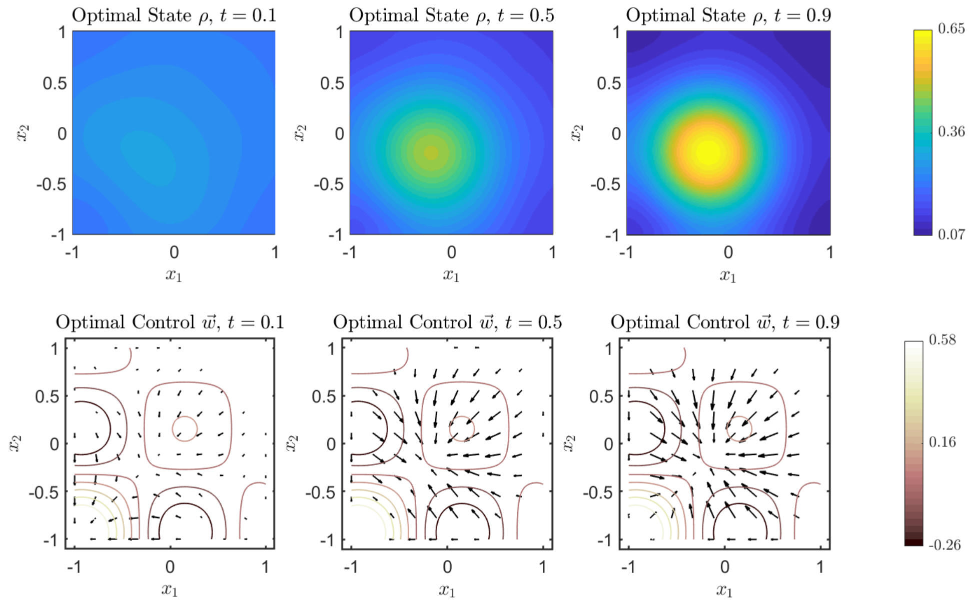

Figure 8: Neumann Flow Control: Optimal ρ and optimal control for $\kappa = -1$ and $\beta = 10^{-3}$.

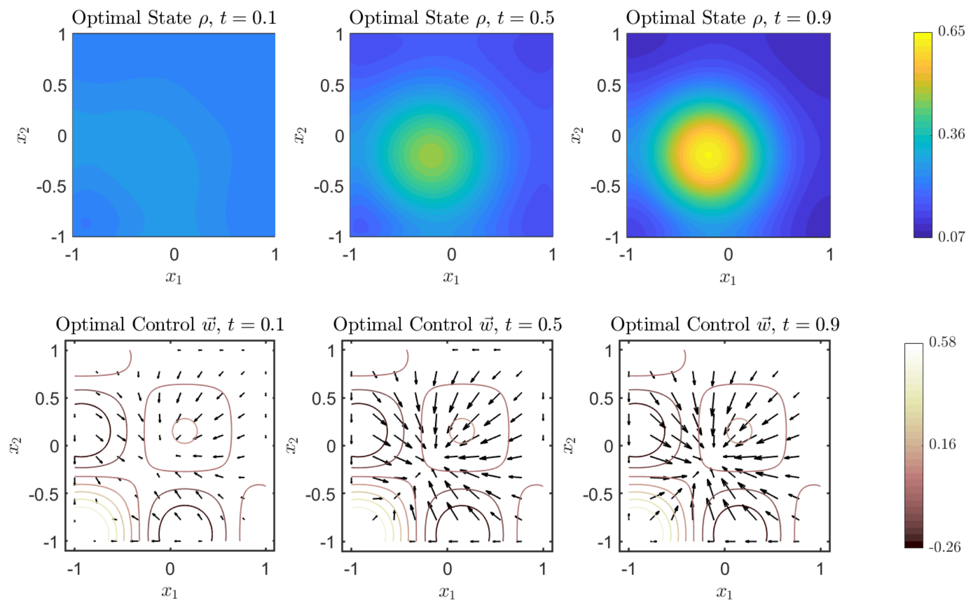

Figure 9: Neumann Flow Control: Optimal ρ and optimal control for $\kappa = 1$ and $\beta = 10^{-3}$.

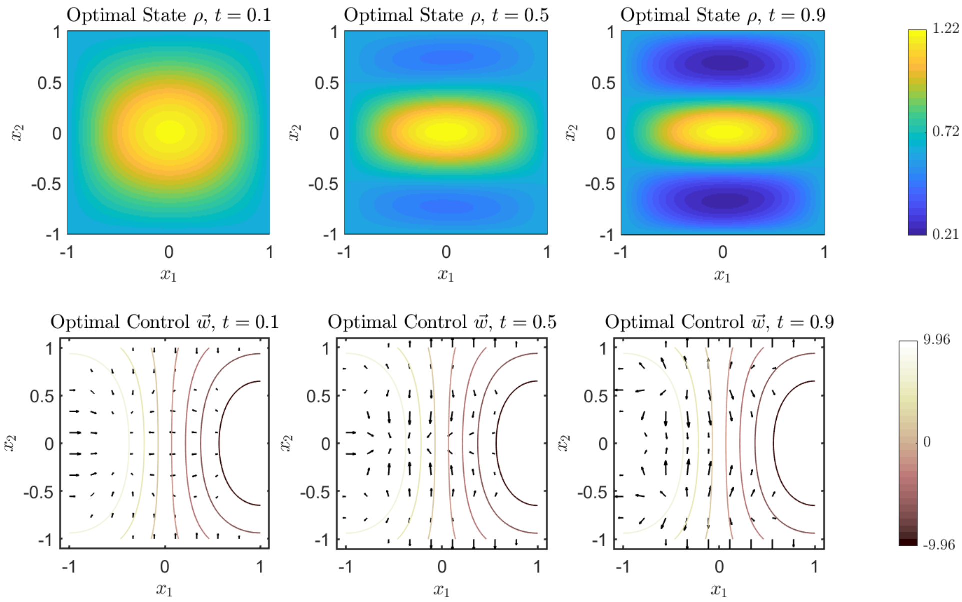

Figure 10: Dirichlet Flow Control 2: Optimal ρ and optimal control for $\kappa = 0$ and $\beta = 10^{-3}$.

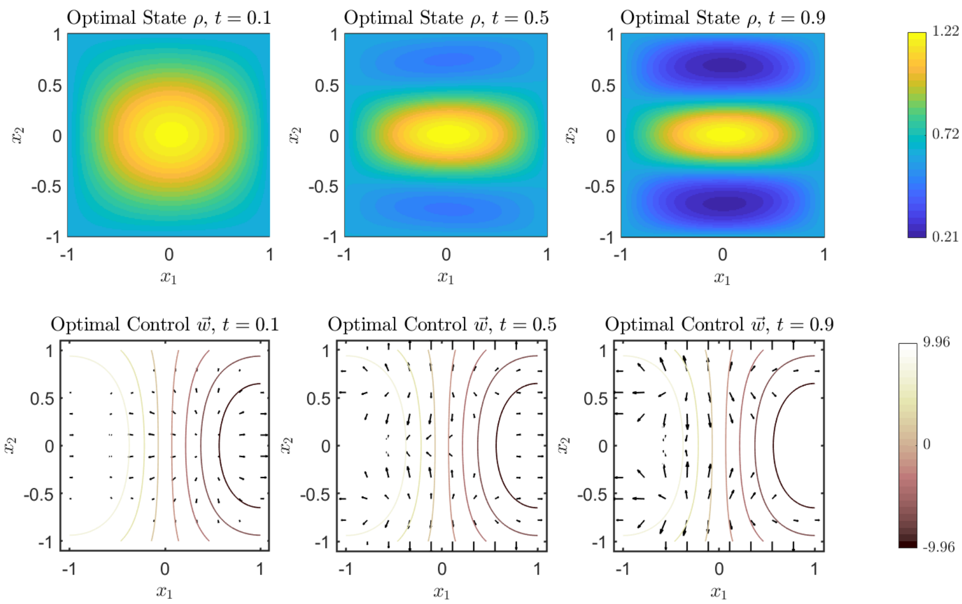

Figure 11: Dirichlet Flow Control 2: Optimal ρ and optimal control for $\kappa = -1$ and $\beta = 10^{-3}$.

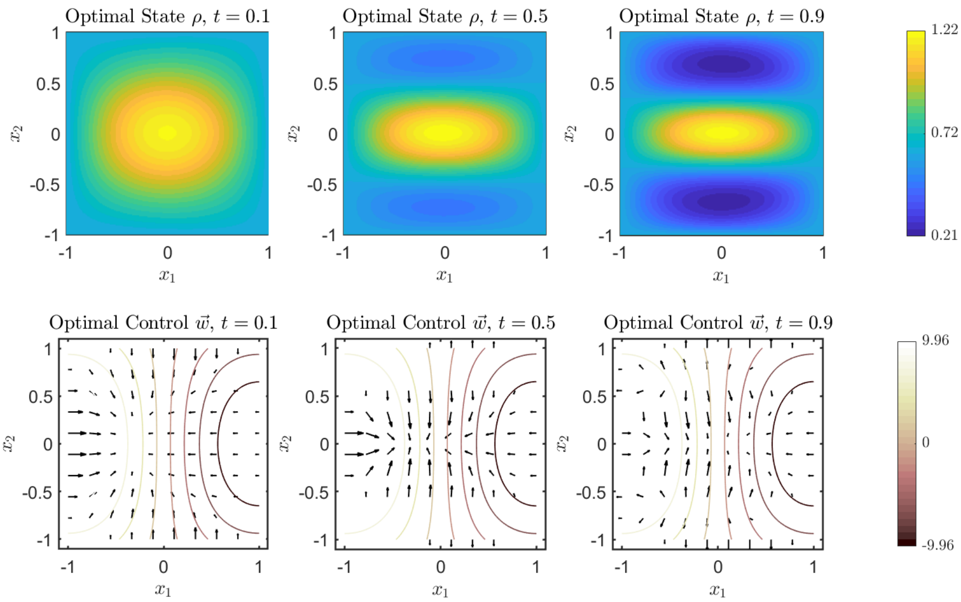

Figure 12: Dirichlet Flow Control 2: Optimal ρ and optimal control for $\kappa = 1$ and $\beta = 10^{-3}$.

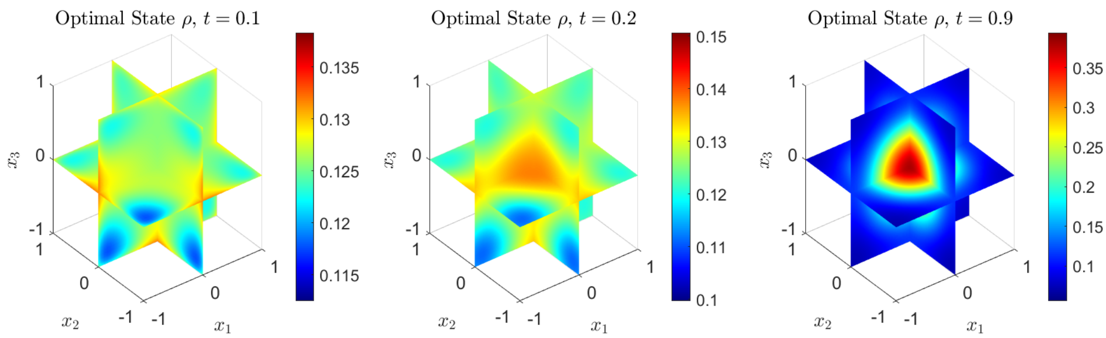

Figure 13: Optimal state ρ for $\kappa = 1$.

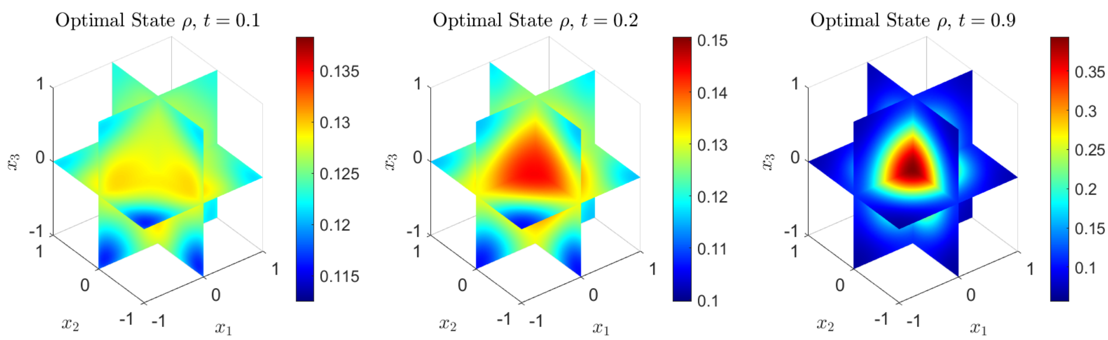

Figure 14: Optimal state ρ for $\kappa = 0$.

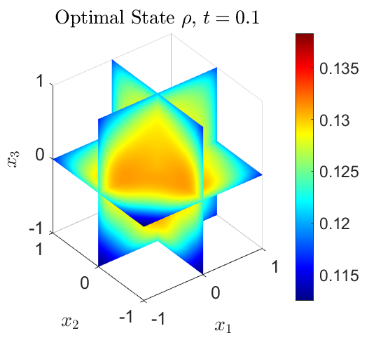

Figure 15: Optimal state ρ for $\kappa = -1$.

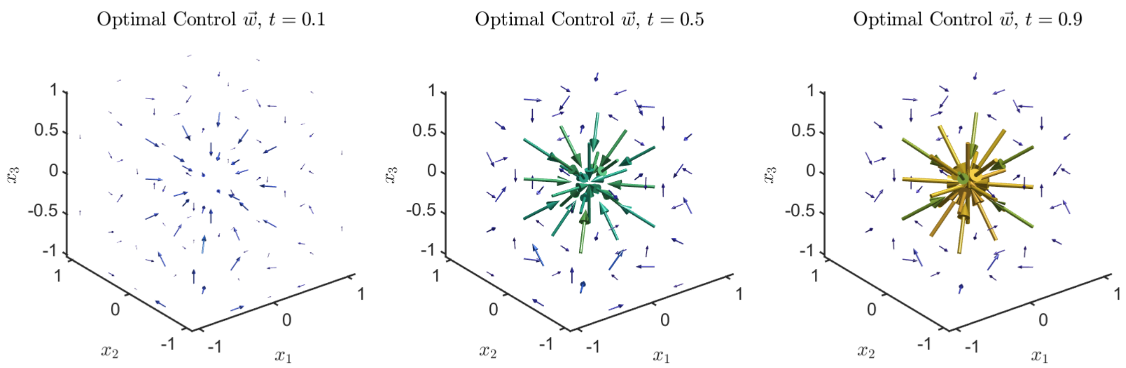

Figure 16: Optimal control $\mathbf{w}$ for $\kappa = 1$.

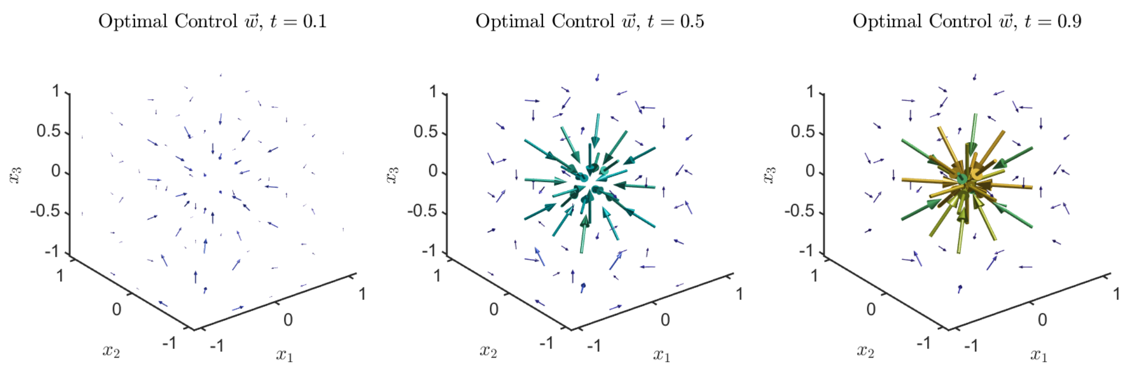

Figure 17: Optimal control $\mathbf{w}$ for $\kappa = 0$.

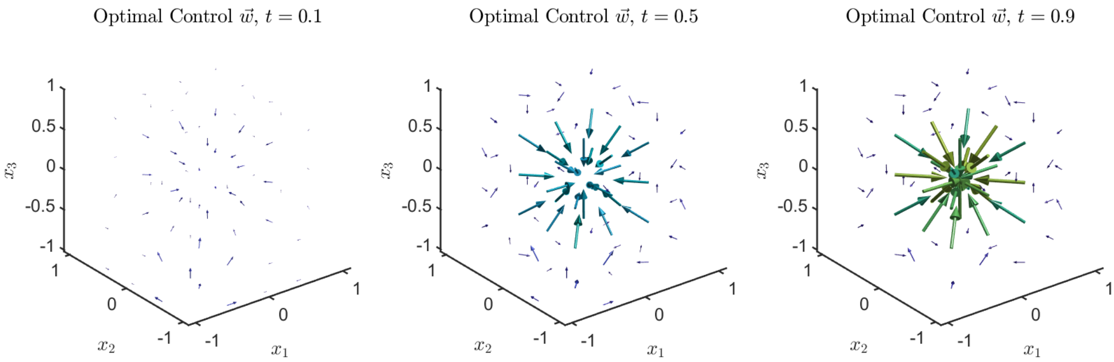

Figure 18: Optimal control $\mathbf{w}$ for $\kappa = -1$.