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 $\kappa = -1$

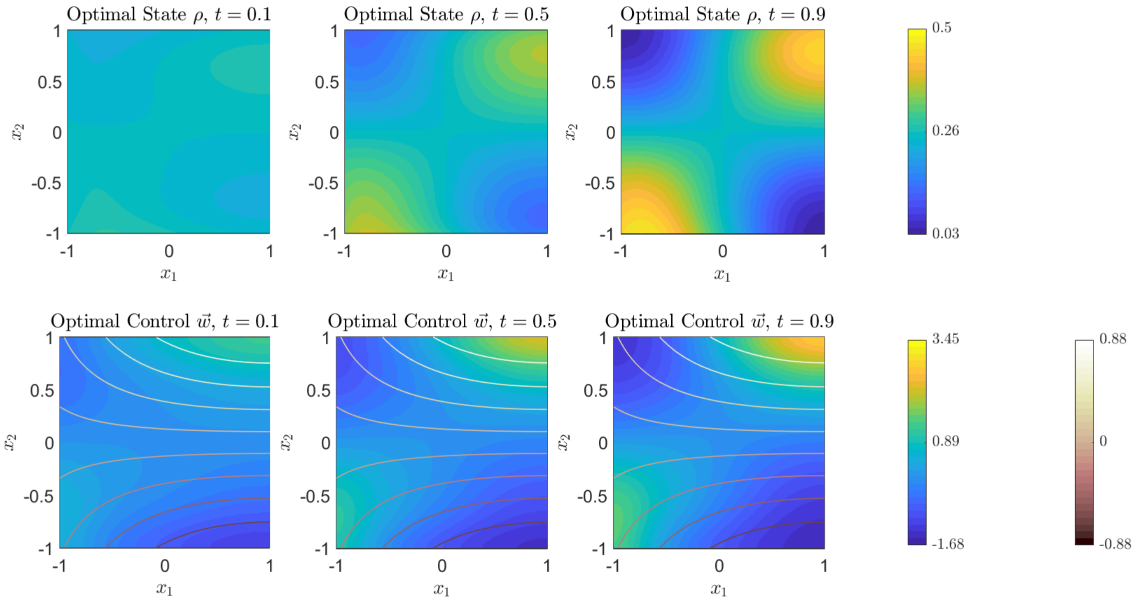

Figure 1: Neumann Source Control: Optimal ρ and optimal control for $\kappa = 0$ and $\beta = 10^{-3}$.

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.

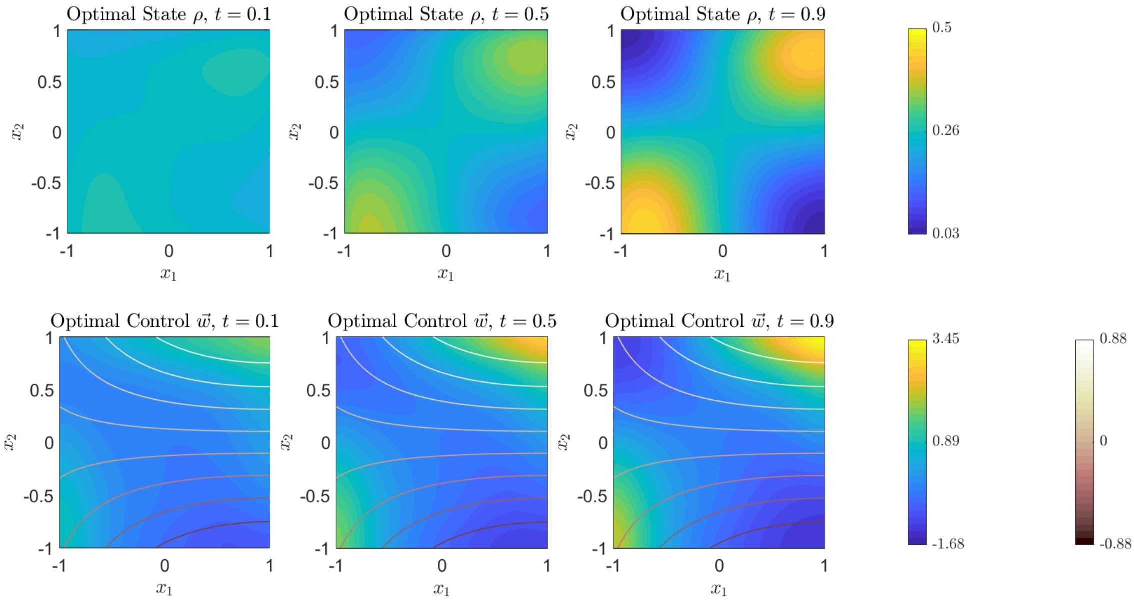

Figure 2: Neumann Source Control: Optimal ρ and optimal control for $\kappa = -1$ and $\beta = 10^{-3}$.

3.1 Dirichlet Flow Control

We choose

$$\rho_0 = \left(\frac{\pi}{4}\right)^2 \cos\left(\frac{\pi x_1}{2}\right) \cos\left(\frac{\pi x_2}{2}\right) + \left(\frac{\pi}{4}\right)^2$$

$$\widehat{\rho} = (1-t)\left(\left(\frac{\pi}{4}\right)^2 \cos\left(\frac{\pi x_1}{2}\right) \cos\left(\frac{\pi x_2}{2}\right) + \left(\frac{\pi}{4}\right)^2\right) + t\left(\left(\frac{\pi}{4}\right)^2 \cos\left(\frac{\pi x_1}{2}\right) \cos\left(\frac{3\pi x_2}{2}\right) + \left(\frac{\pi}{4}\right)^2\right)$$

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

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.

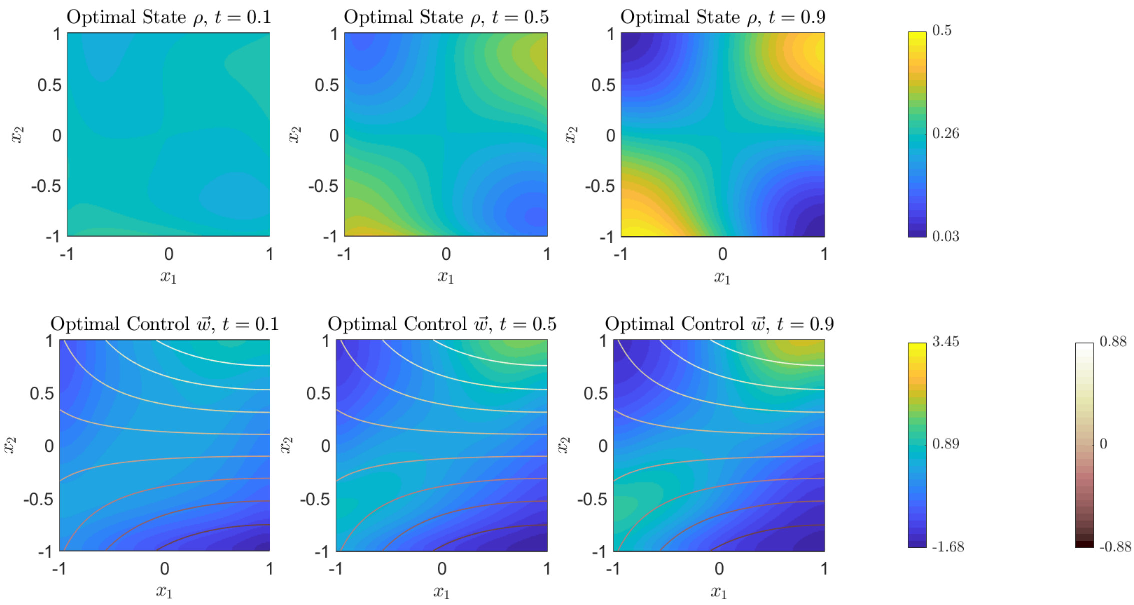

Figure 3: Optimal ρ and optimal control for $\kappa = 1$ and $\beta = 10^{-3}$.

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 13.
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 $\mathbf{w} = \vec{0}$.
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 14, 15 and 16.

The controls are plotted in Figures 17, 18 and 19. They are all normalized to the maximum

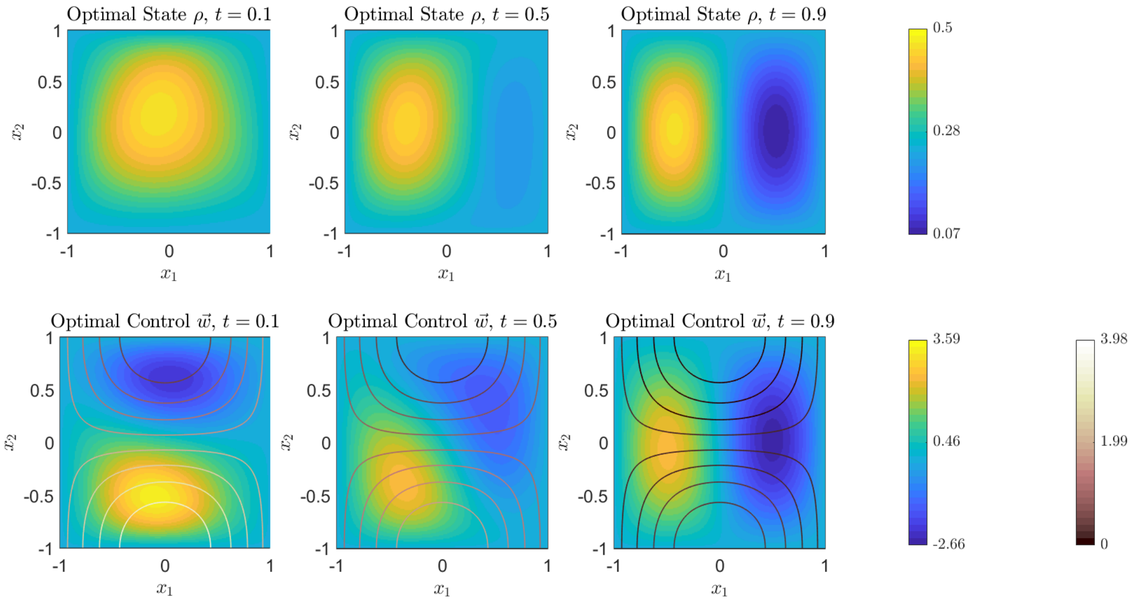

Figure 4: Dirichlet Source Control: Optimal ρ and optimal control for $\kappa = 0$ and $\beta = 10^{-3}$.

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.

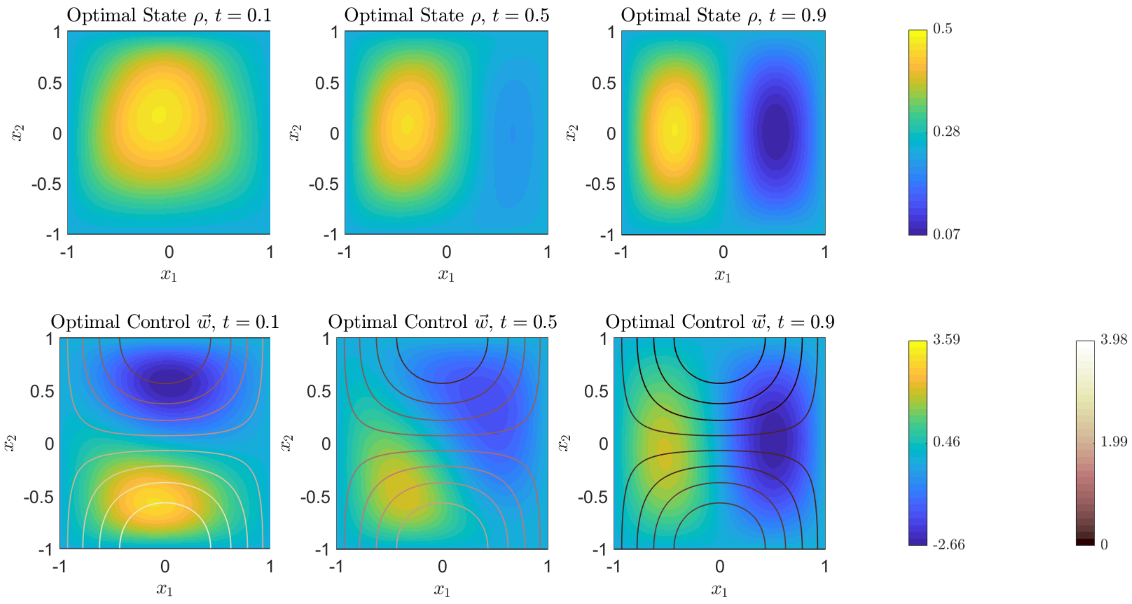

Figure 5: Dirichlet Source Control: Optimal ρ and optimal control for $\kappa = -1$ and $\beta = 10^{-3}$.

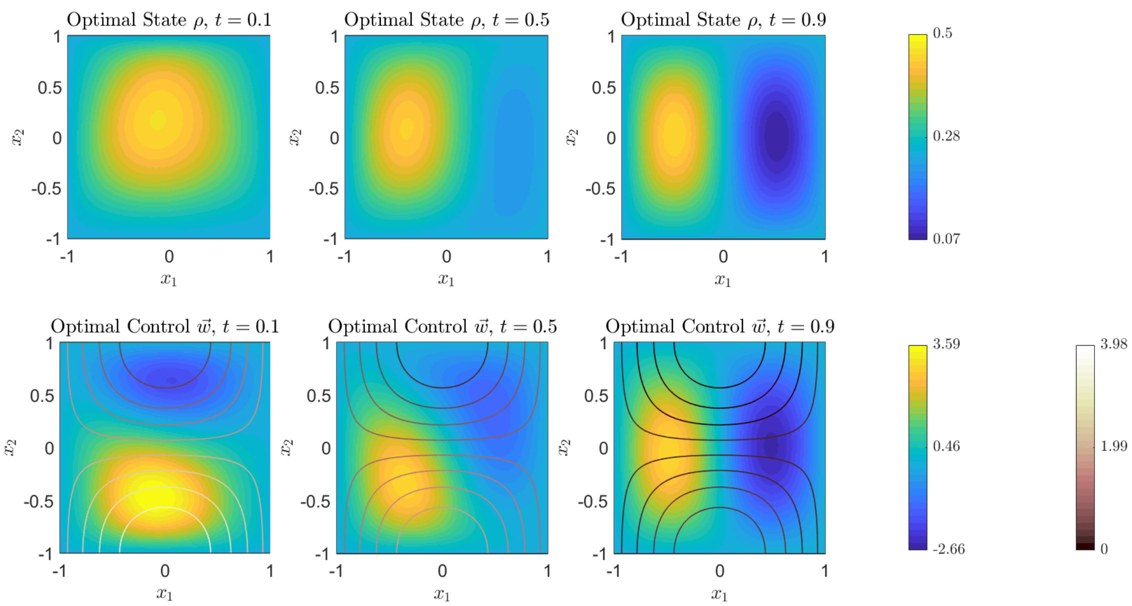

Figure 6: Dirichlet Source Control: Optimal ρ and optimal control for $\kappa = 1$ and $\beta = 10^{-3}$.

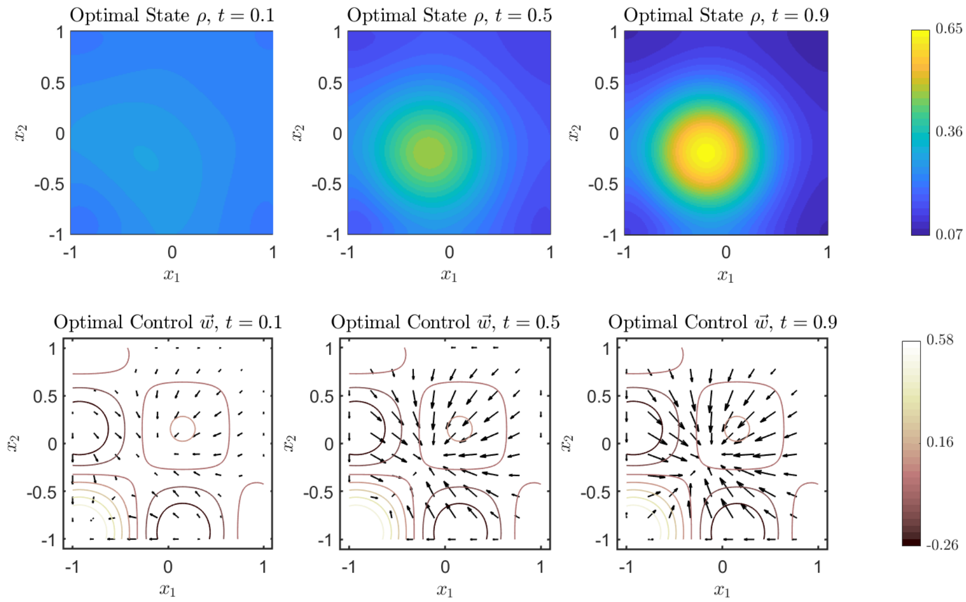

Figure 7: Neumann Flow Control: Optimal ρ and optimal control for $\kappa = 0$ and $\beta = 10^{-3}$.

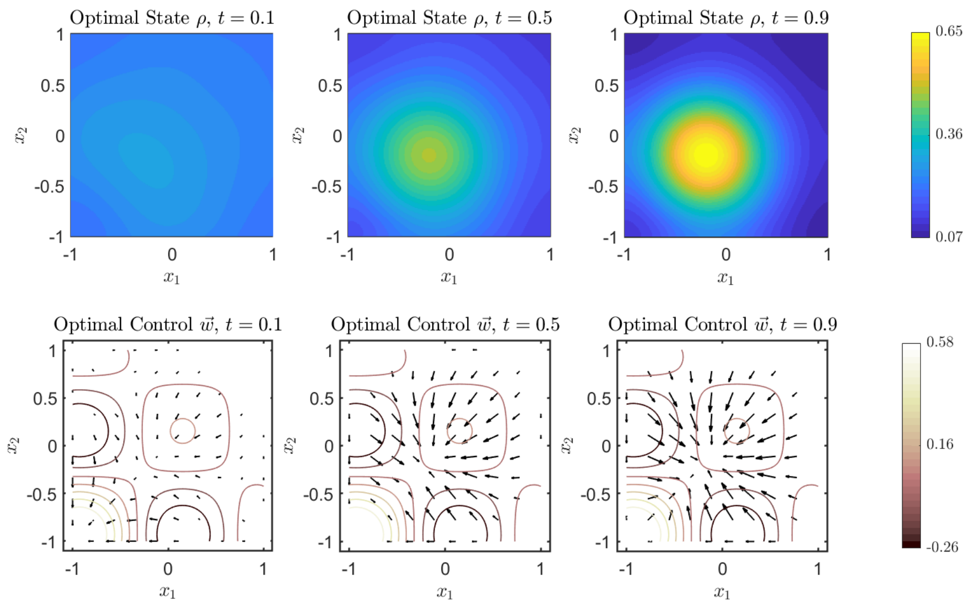

Figure 8: Neumann Flow Control: Optimal ρ and optimal control for $\kappa = -1$ and $\beta = 10^{-3}$.

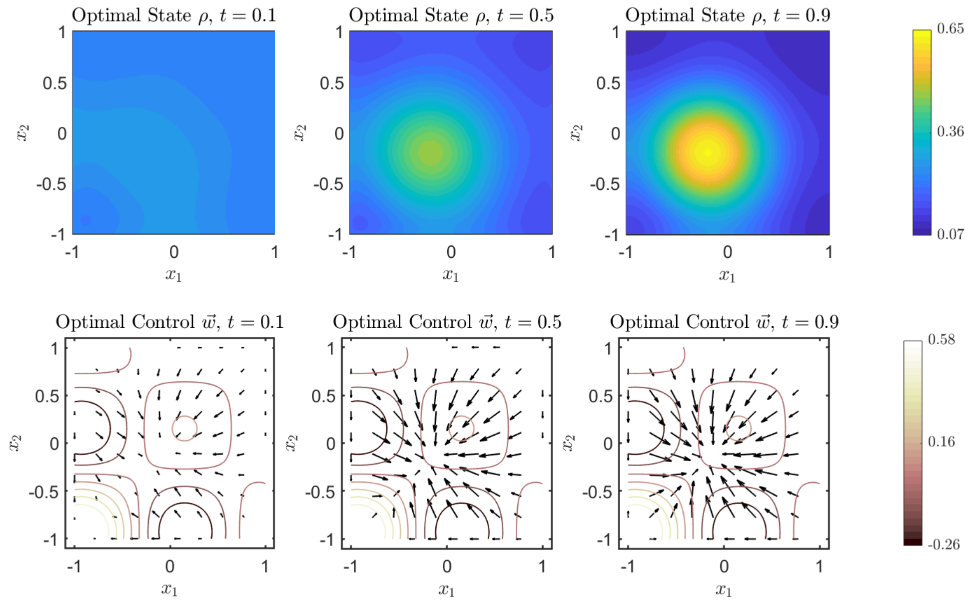

Figure 9: Neumann Flow Control: Optimal ρ and optimal control for $\kappa = 1$ and $\beta = 10^{-3}$.

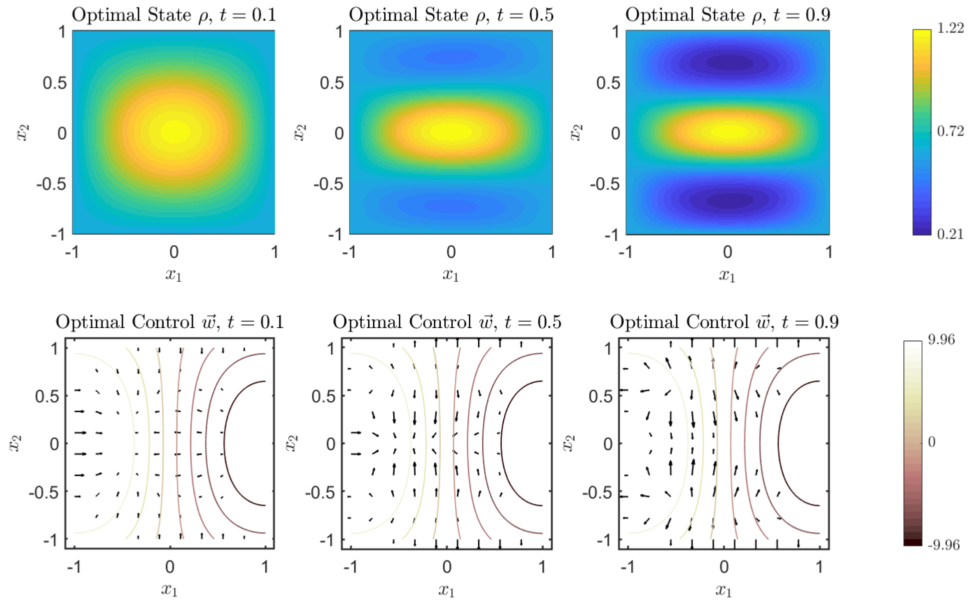

Figure 10: Dirichlet Flow Control 2: Optimal ρ and optimal control for $\kappa = 0$ and $\beta = 10^{-3}$.

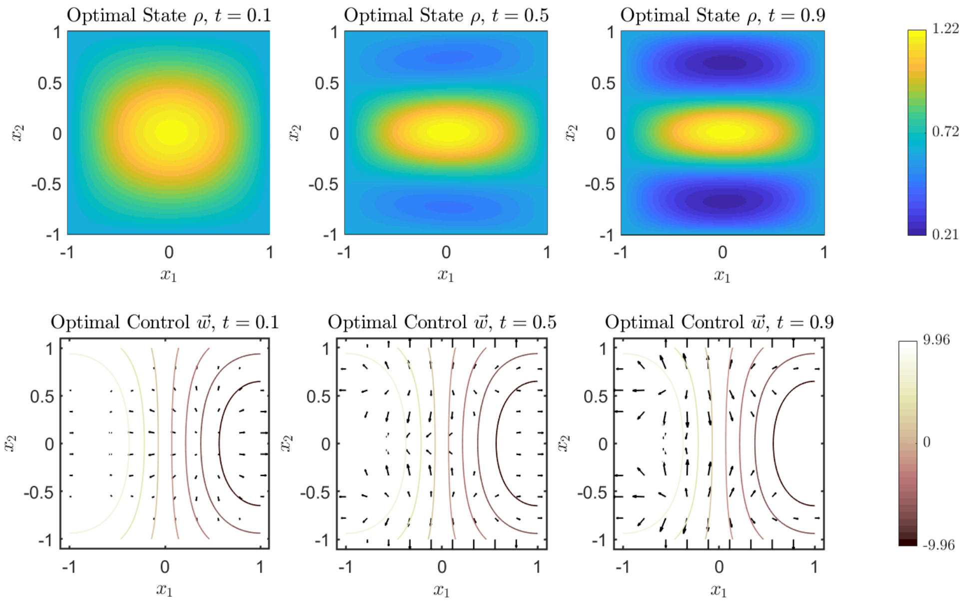

Figure 11: Dirichlet Flow Control 2: Optimal ρ and optimal control for $\kappa = -1$ and $\beta = 10^{-3}$.

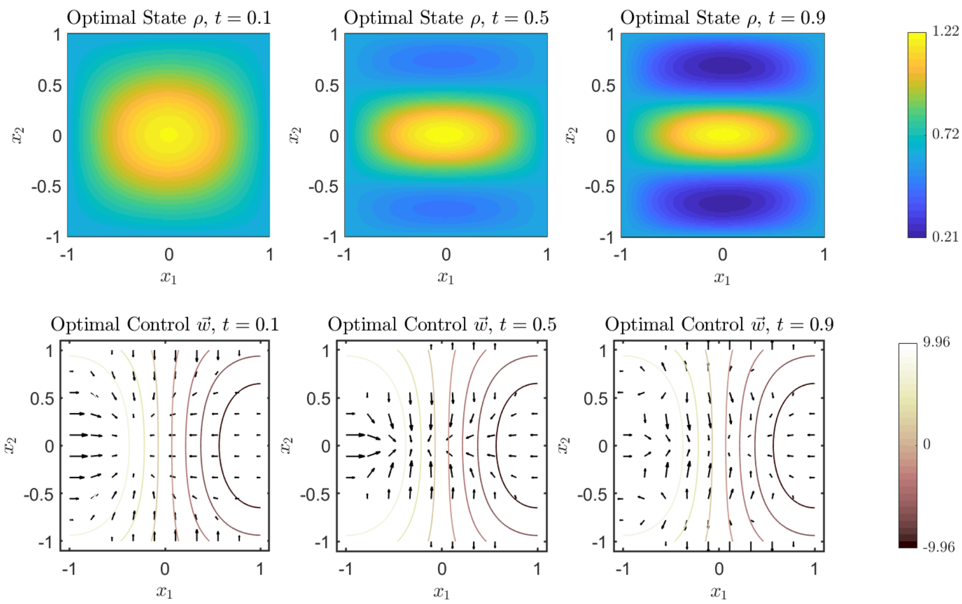

Figure 12: Dirichlet Flow Control 2: Optimal ρ and optimal control for $\kappa = 1$ and $\beta = 10^{-3}$.

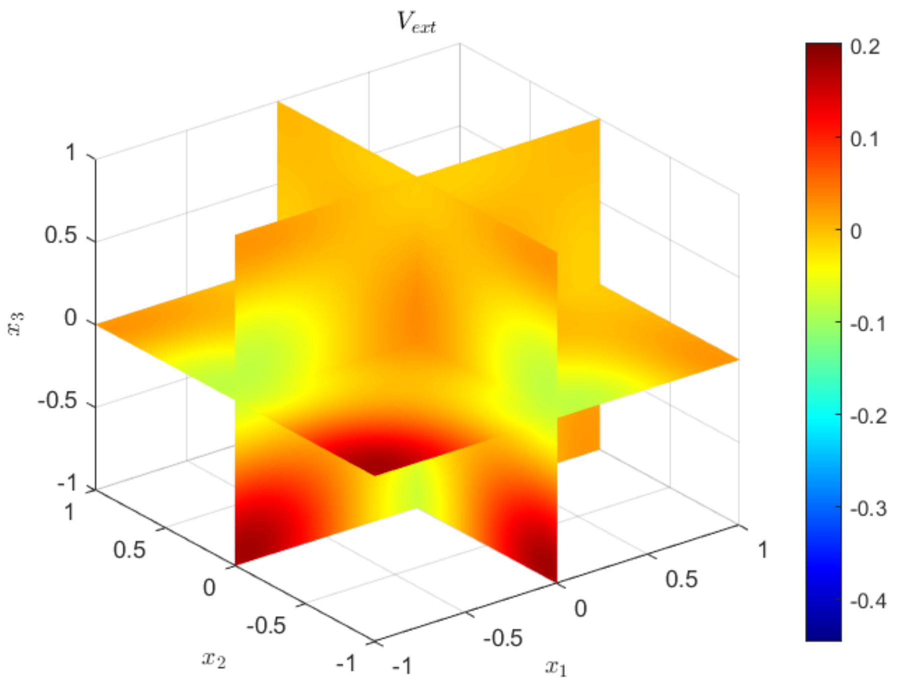

Figure 13: External Potential V_{ext}

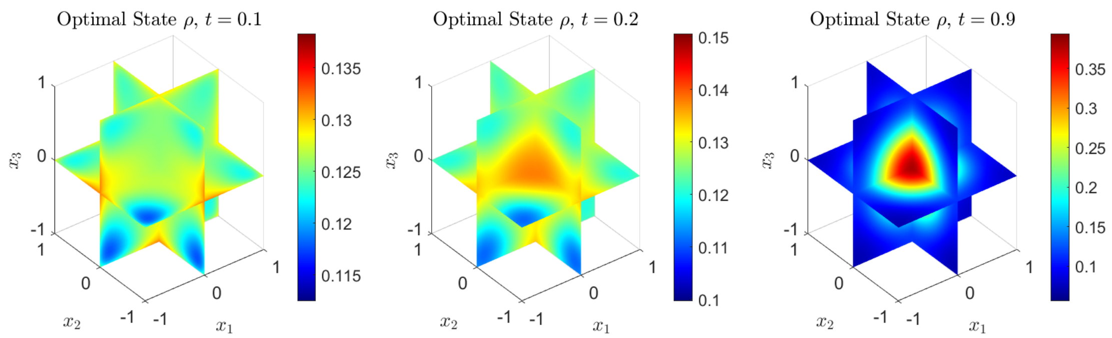

Figure 14: Optimal state ρ for $\kappa = 1$.

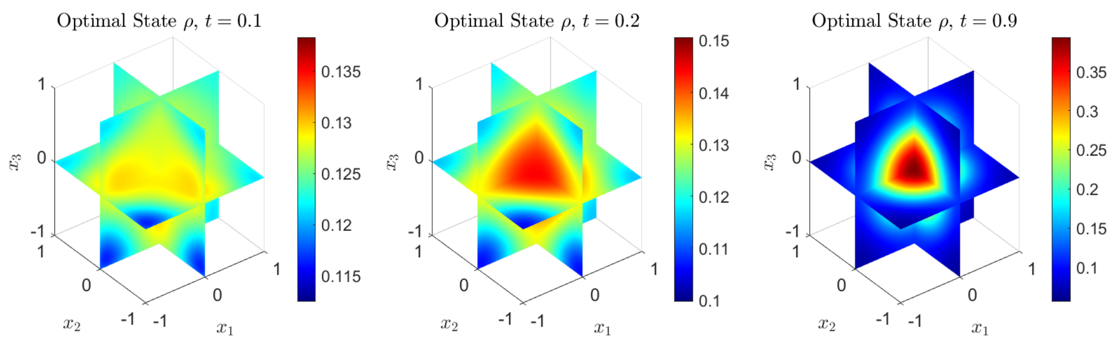

Figure 15: Optimal state ρ for $\kappa = 0$.

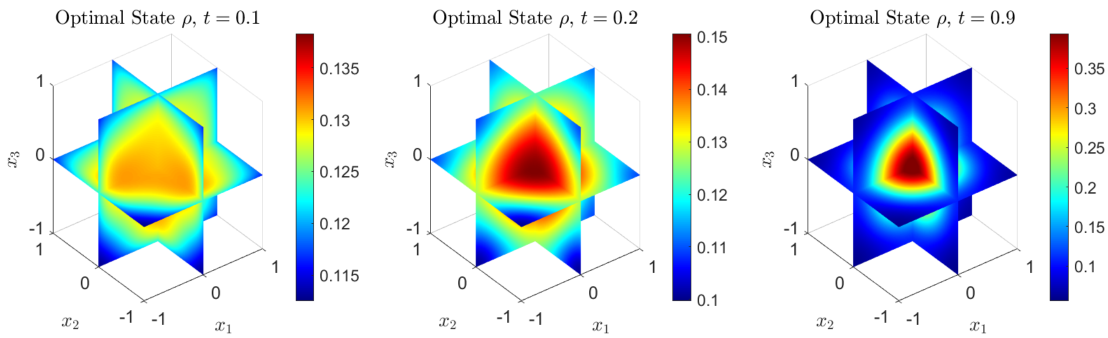

Figure 16: Optimal state ρ for $\kappa = -1$.

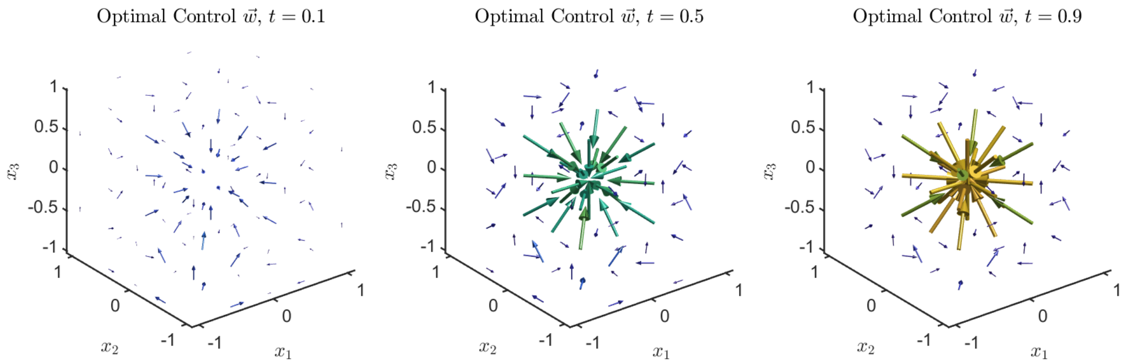

Figure 17: Optimal control $\mathbf{w}$ for $\kappa = 1$.

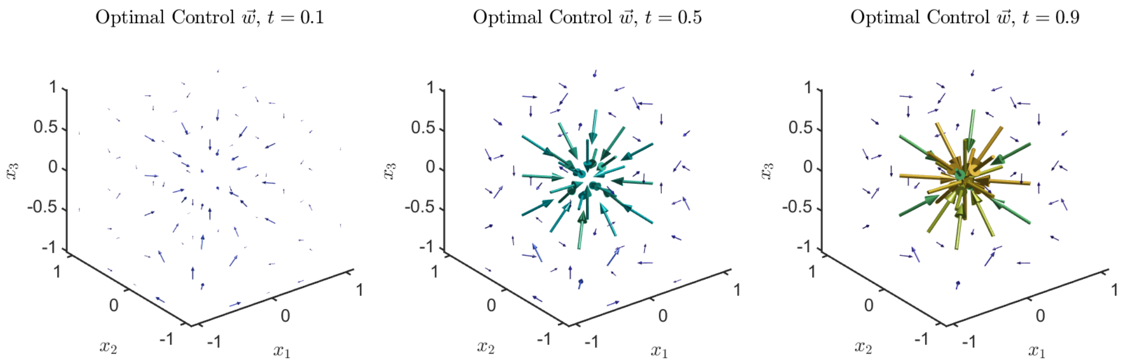

Figure 18: Optimal control $\mathbf{w}$ for $\kappa = 0$.

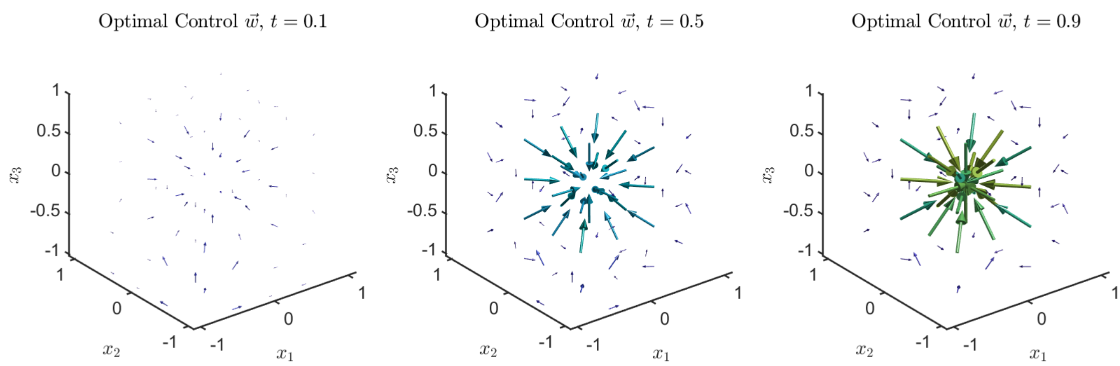

Figure 19: Optimal control $\mathbf{w}$ for $\kappa = -1$.