

## Paper Examples

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  $\kappa$  are visible in the initial times, while also scaling the colormap for the overall maximum of  $\rho$  over all times and  $\kappa$ . The controls are also scaled for all times and  $\kappa$  (for flow control we use the largest value over all times and  $\kappa$  as the scaling for the arrow).

### 1 Neumann Source Control

We choose

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

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 2, 3 and 4 and the external potential acting on  $\rho$  is displayed in Figure 1.

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. The results are displayed in Figures 5, 6 and 7. The controls are larger, but the difference in dynamics is smaller for different interactions.

### 2 Dirichlet Source Control

We choose

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

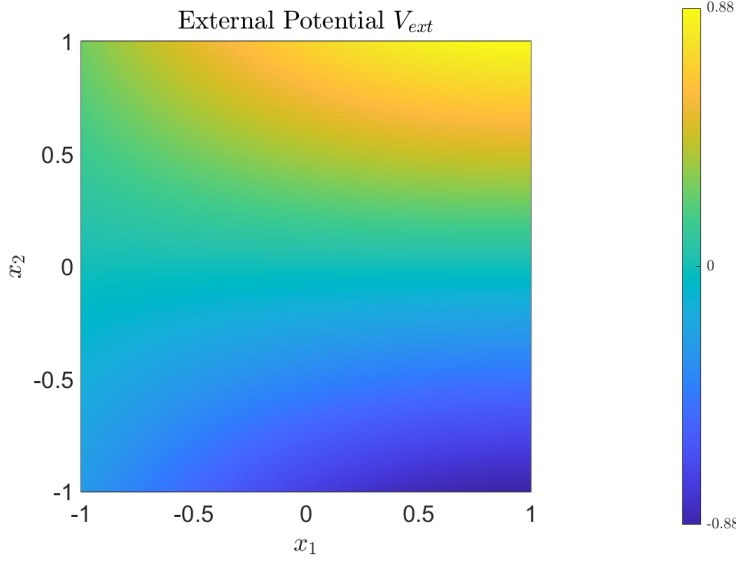


Figure 1: Neumann Source Control: External Potential  $V_{ext}$  acting on  $\rho$ .

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  $\kappa = -1$  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 9, 10 and 11 and the external potential acting on  $\rho$  is displayed in Figure 8.

### 3 Neumann Flow Control

We choose

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

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 13,

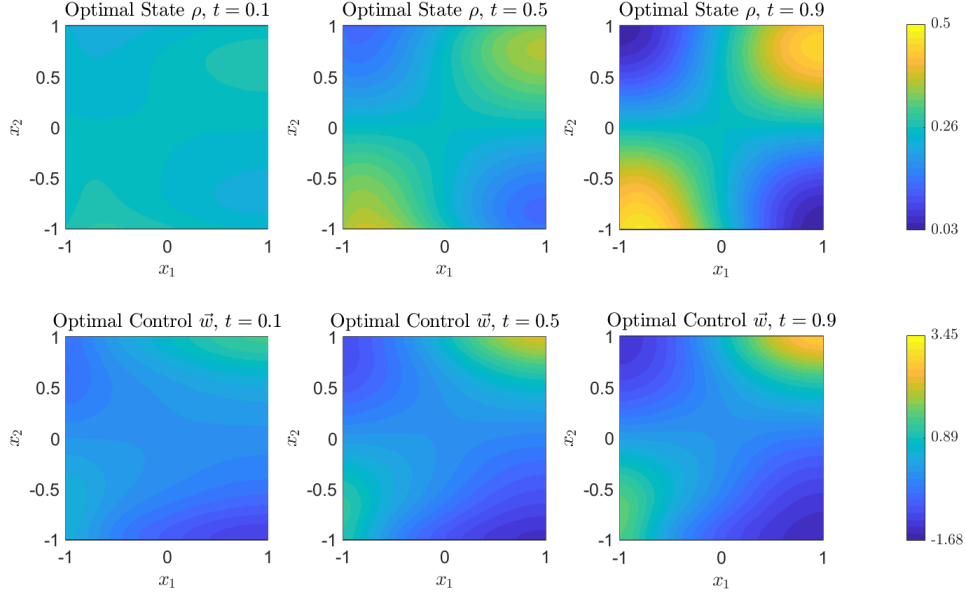


Figure 2: Neumann Source Control: Optimal  $\rho$  and optimal control for  $\kappa = 0$  and  $\beta = 10^{-3}$ .

14 and 15 and the external potential associated with it is shown in Figure 12. Note that mass is conserved.

## 4 Dirichlet Flow Control

I computed the Dirichlet example once with and once without  $V_{ext}$ . I think we can just use the one that has  $V_{ext}$  included.

### 4.1 Dirichlet Flow Control without $V_{ext}$

We choose

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

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

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  $\mathcal{J}_c = 0.0121$ , for  $\kappa = 0$ ,  $\mathcal{J}_c = 0.0095$ , and for  $\kappa = -1$  we get  $\mathcal{J}_c = 0.0104$ , (compare to  $\beta = 10^3$  with  $\mathcal{J}_{uc} = 0.5272$ ). Each of the problems takes around 50 seconds to solve. The results can be seen in Figures 16, 17 and 18.

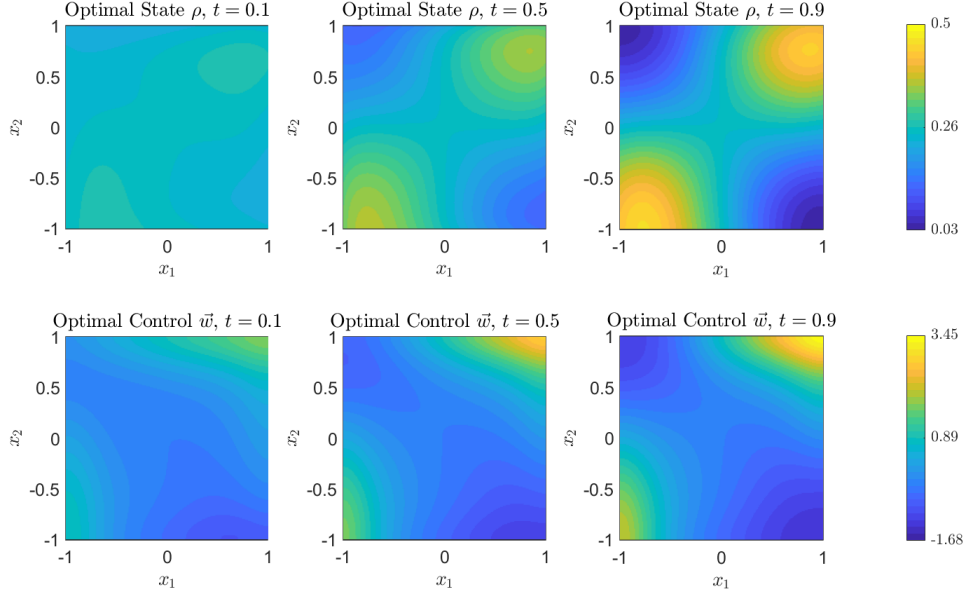


Figure 3: Neumann Source Control: Optimal  $\rho$  and optimal control for  $\kappa = -1$  and  $\beta = 10^{-3}$ .

#### 4.2 Dirichlet Flow Control with $V_{ext}$

We add the following external potential to the above problem, see Figure 19

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

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 20, 21 and 22.

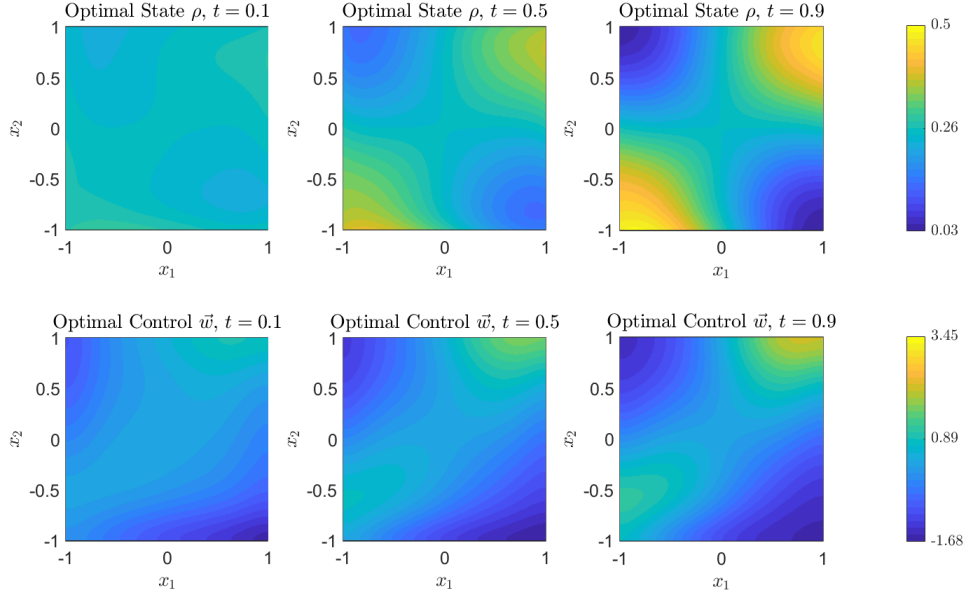


Figure 4: Optimal  $\rho$  and optimal control for  $\kappa = 1$  and  $\beta = 10^{-3}$ .

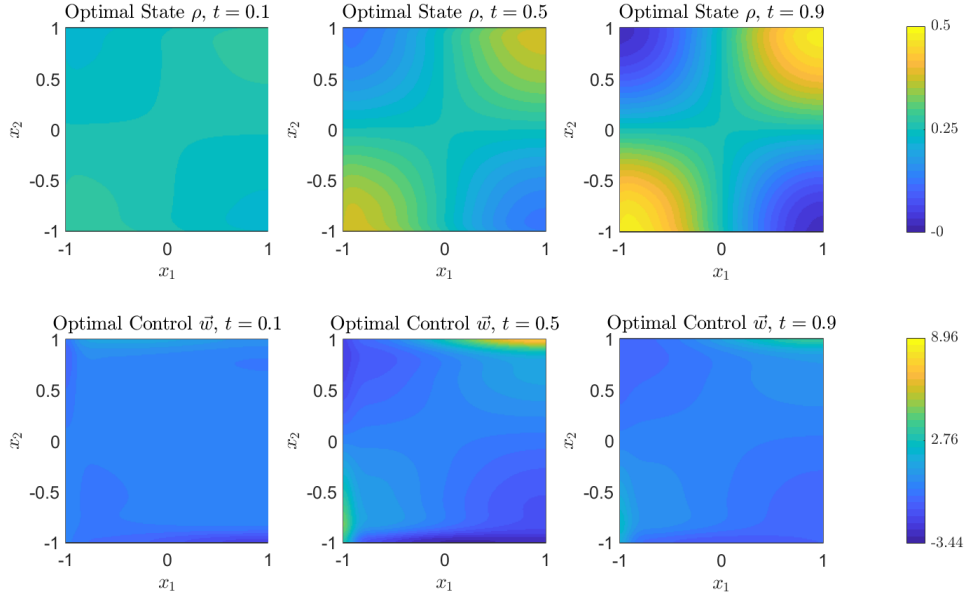


Figure 5: Neumann Source Control: Optimal  $\rho$  and optimal control for  $\kappa = 0$  and  $\beta = 10^{-5}$ .

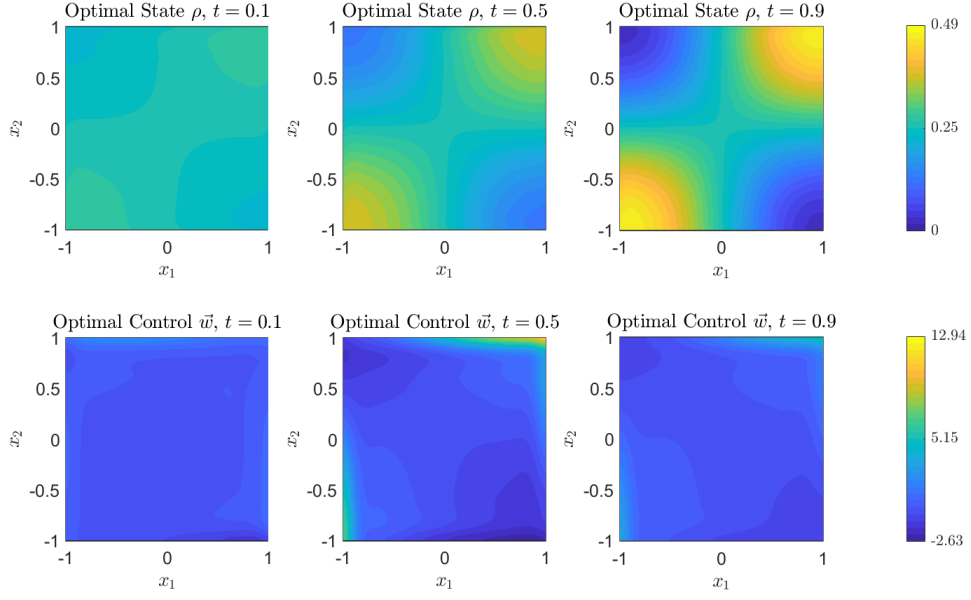


Figure 6: Neumann Source Control: Optimal  $\rho$  and optimal control for  $\kappa = -1$  and  $\beta = 10^{-5}$ .

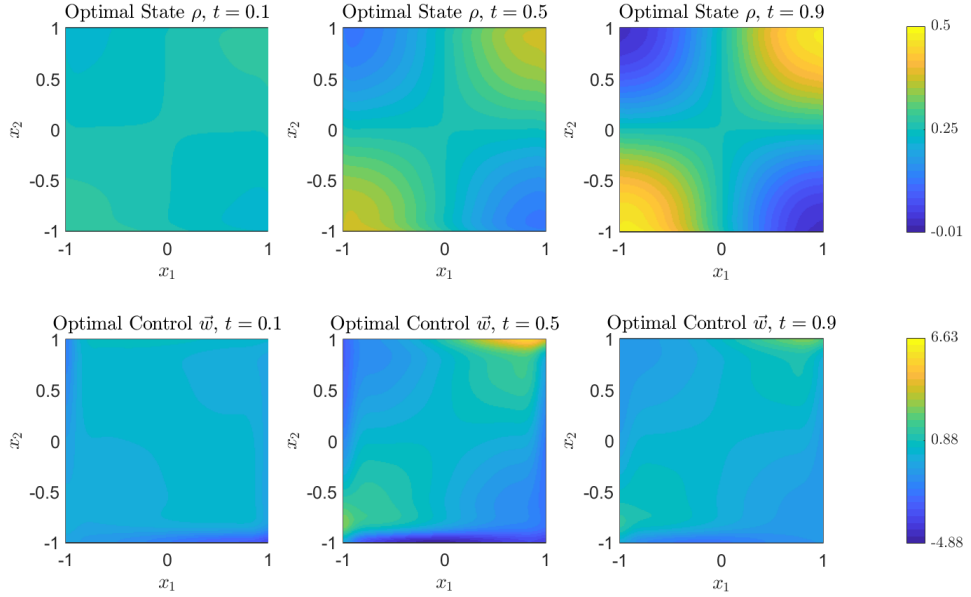


Figure 7: Neumann Source Control: Optimal  $\rho$  and optimal control for  $\kappa = 1$  and  $\beta = 10^{-5}$ .

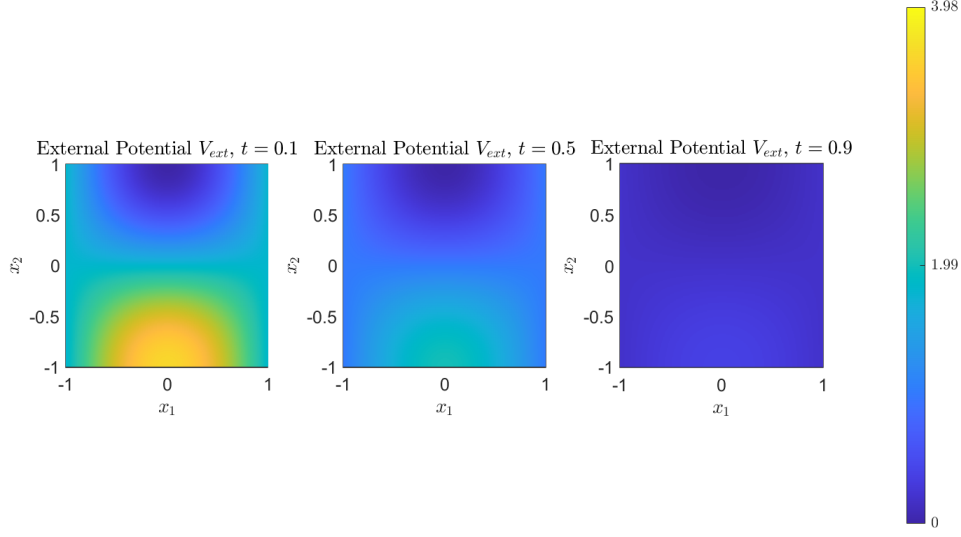


Figure 8: Dirichlet Source Control: External Potential  $V_{ext}$  acting on  $\rho$ .

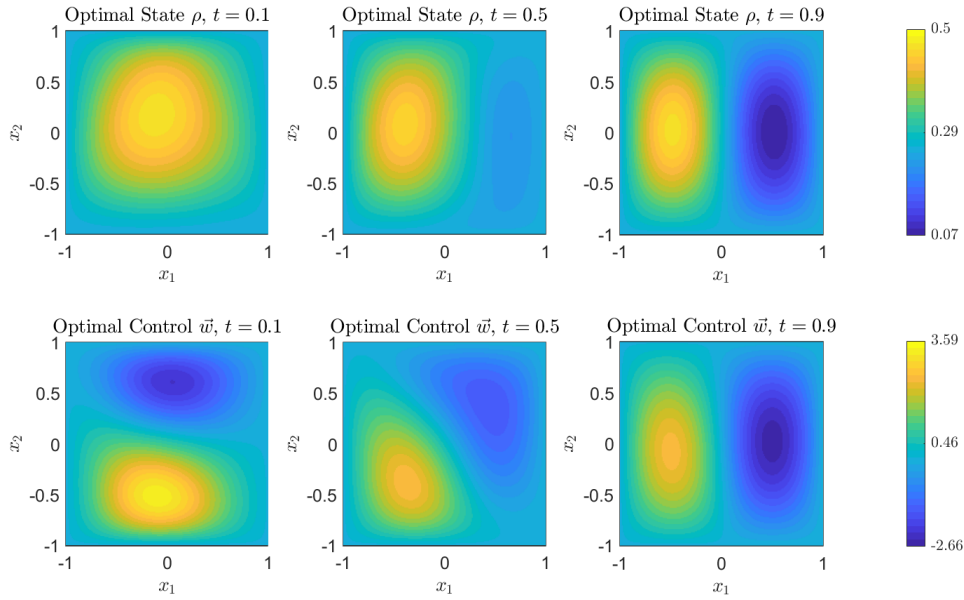


Figure 9: Dirichlet Source Control: Optimal  $\rho$  and optimal control for  $\kappa = 0$  and  $\beta = 10^{-3}$ .

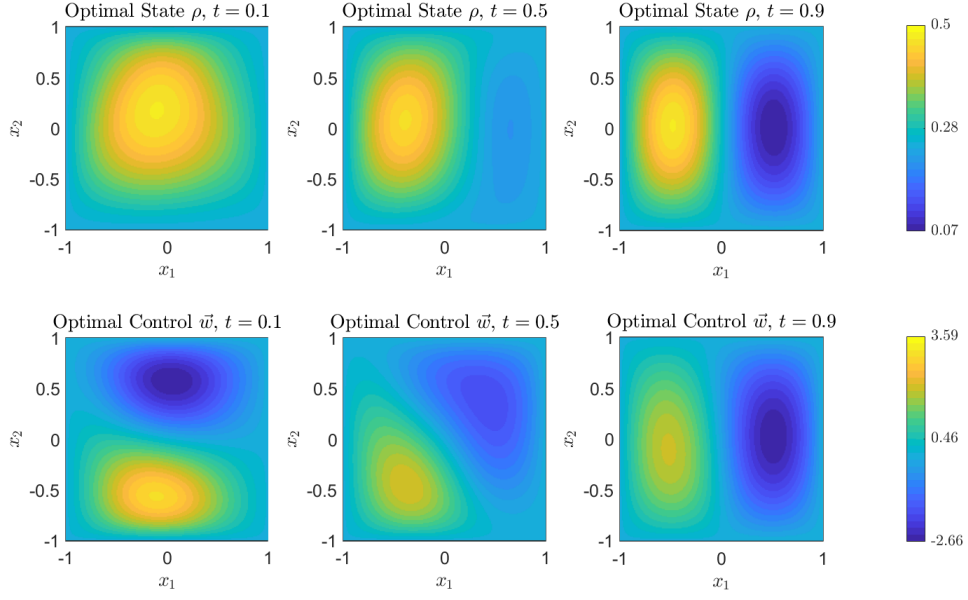


Figure 10: Dirichlet Source Control: Optimal  $\rho$  and optimal control for  $\kappa = -1$  and  $\beta = 10^{-3}$ .

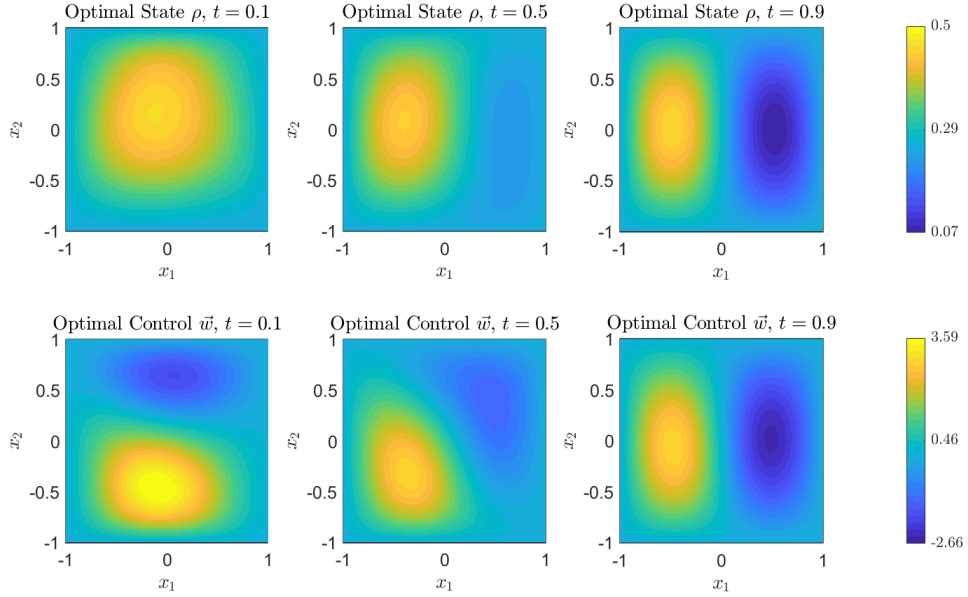


Figure 11: Dirichlet Source Control: Optimal  $\rho$  and optimal control for  $\kappa = 1$  and  $\beta = 10^{-3}$ .



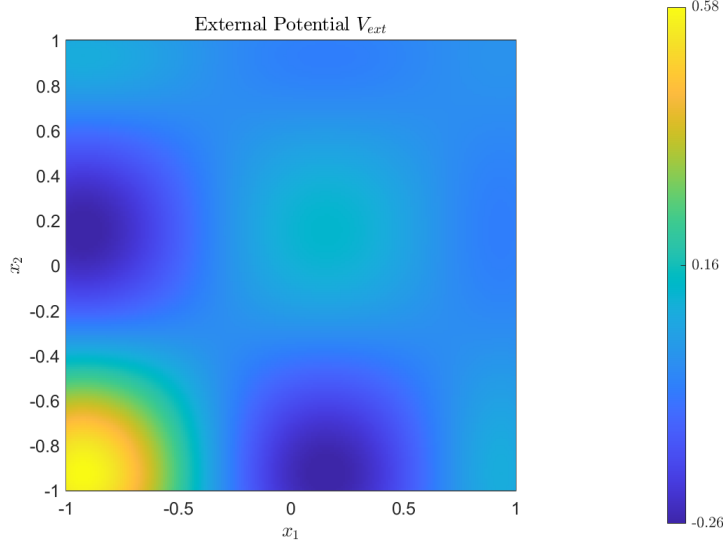


Figure 12: Neumann Flow Control: External Potential  $V_{ext}$  acting on  $\rho$ .

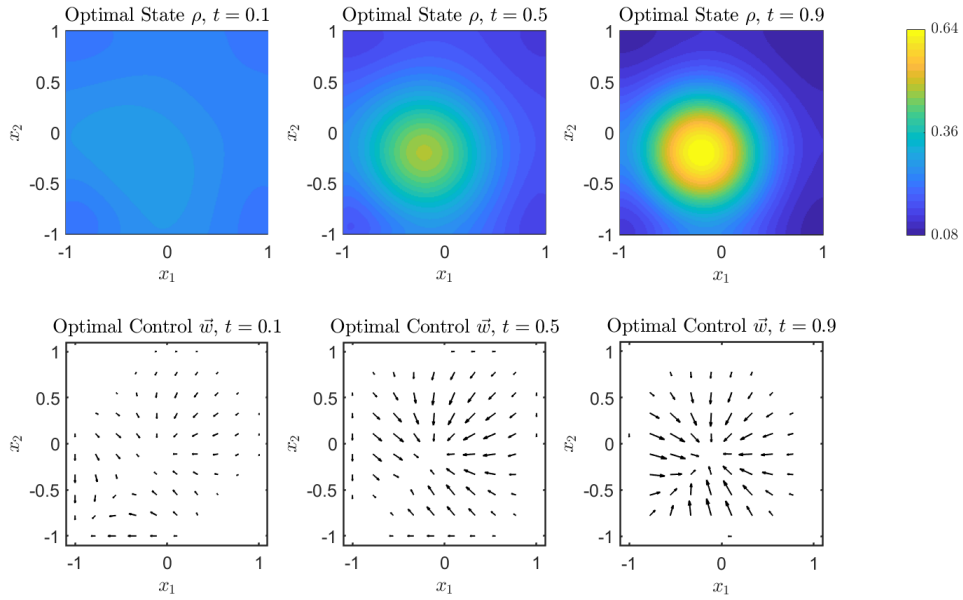


Figure 13: Neumann Flow Control: Optimal  $\rho$  and optimal control for  $\kappa = 0$  and  $\beta = 10^{-3}$ .

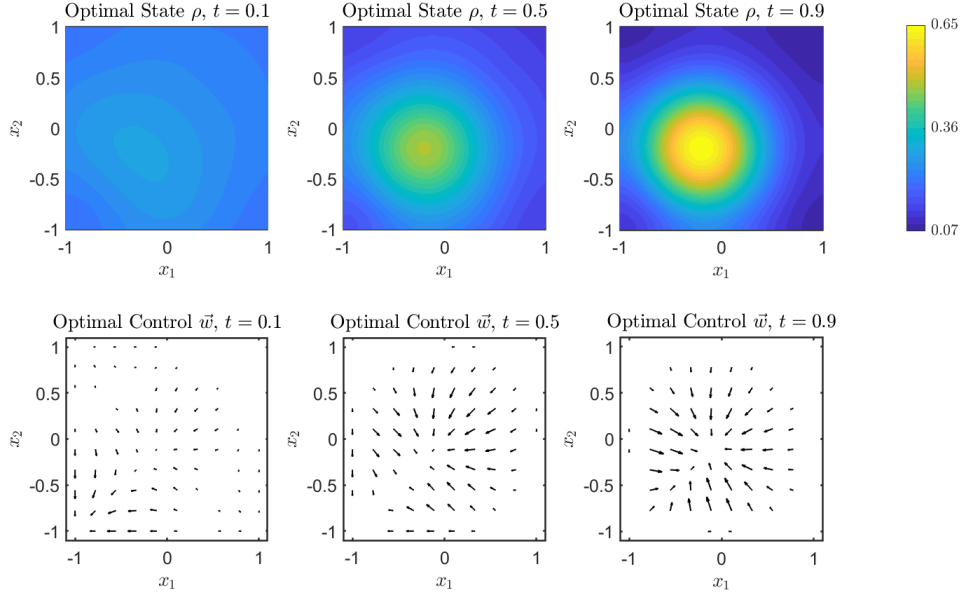


Figure 14: Neumann Flow Control: Optimal  $\rho$  and optimal control for  $\kappa = -1$  and  $\beta = 10^{-3}$ .

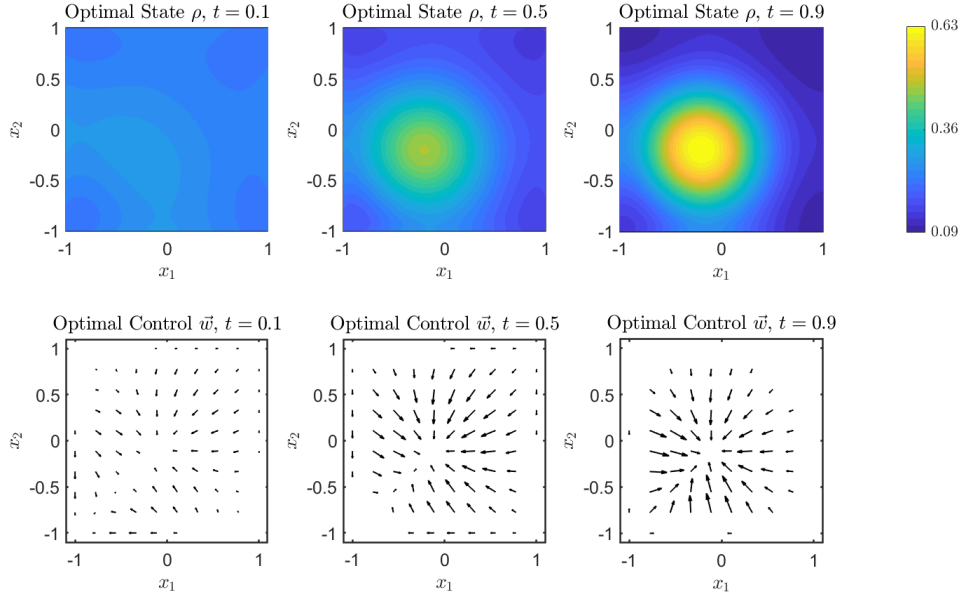


Figure 15: Neumann Flow Control: Optimal  $\rho$  and optimal control for  $\kappa = 1$  and  $\beta = 10^{-3}$ .

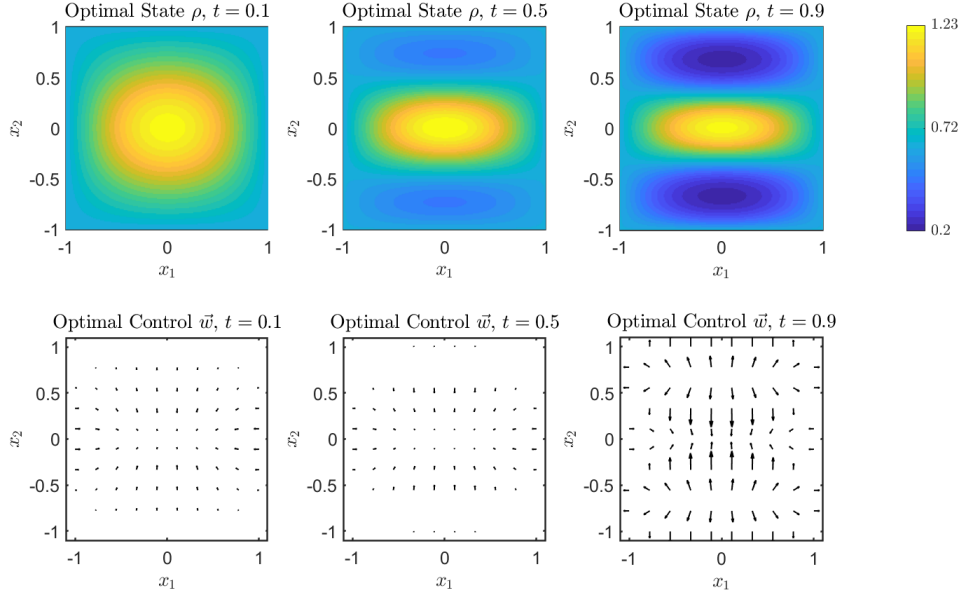


Figure 16: Dirichlet Flow Control: Optimal  $\rho$  and optimal control for  $\kappa = 0$  and  $\beta = 10^{-3}$ .

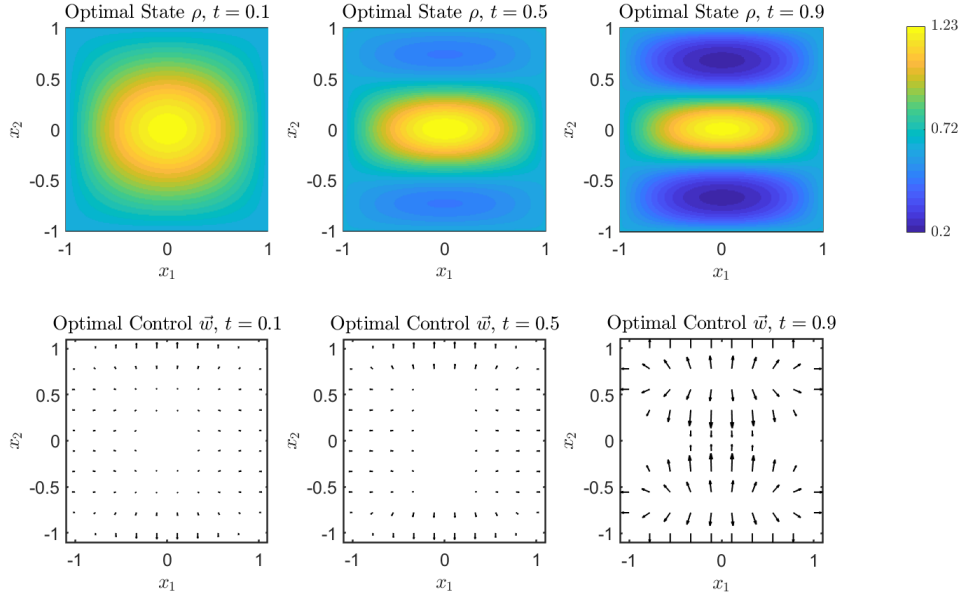


Figure 17: Dirichlet Flow Control: Optimal  $\rho$  and optimal control for  $\kappa = -1$  and  $\beta = 10^{-3}$ .

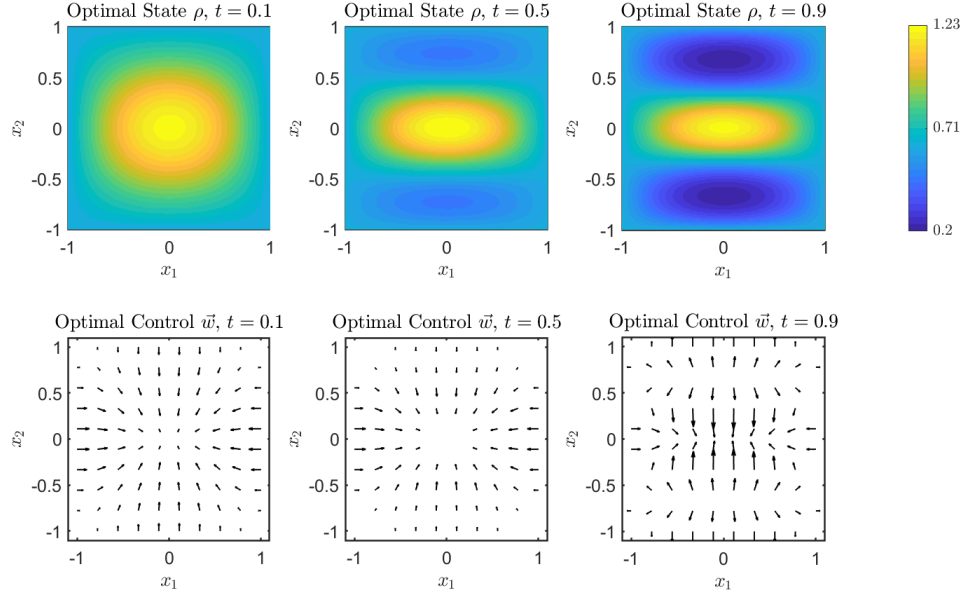


Figure 18: Dirichlet Flow Control: Optimal  $\rho$  and optimal control for  $\kappa = 1$  and  $\beta = 10^{-3}$ .

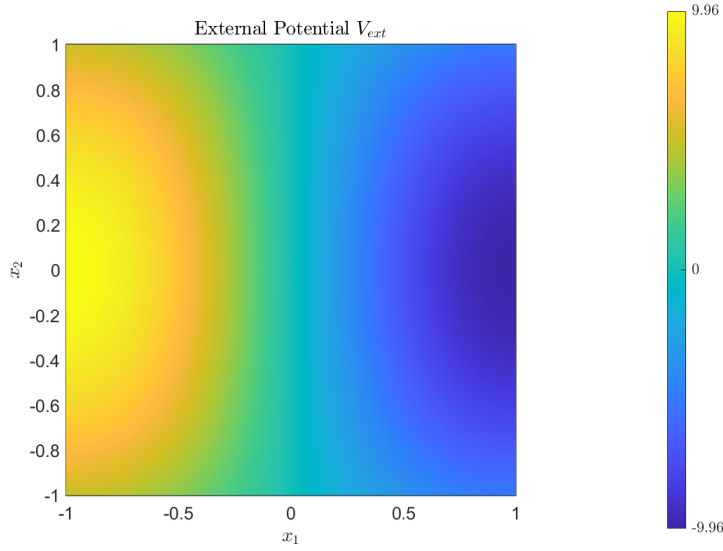


Figure 19: Dirichlet Flow Control 2: External Potential  $V_{ext}$  acting on  $\rho$ .

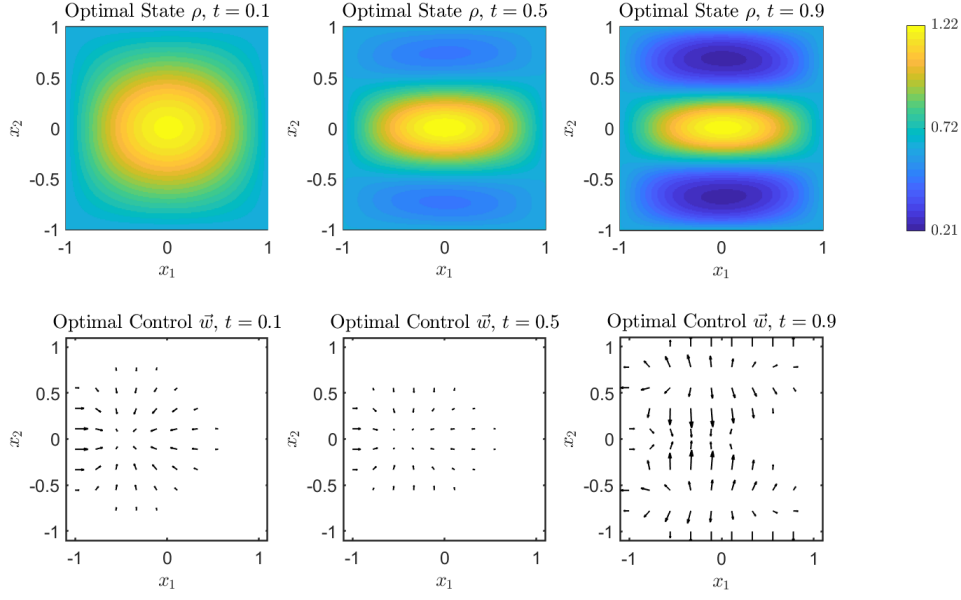


Figure 20: Dirichlet Flow Control 2: Optimal  $\rho$  and optimal control for  $\kappa = 0$  and  $\beta = 10^{-3}$ .

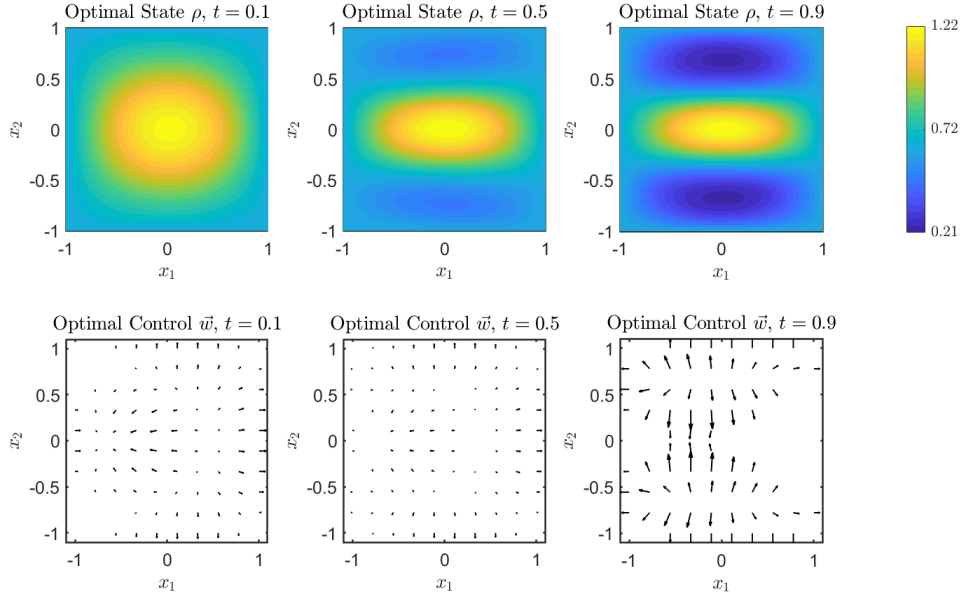


Figure 21: Dirichlet Flow Control 2: Optimal  $\rho$  and optimal control for  $\kappa = -1$  and  $\beta = 10^{-3}$ .

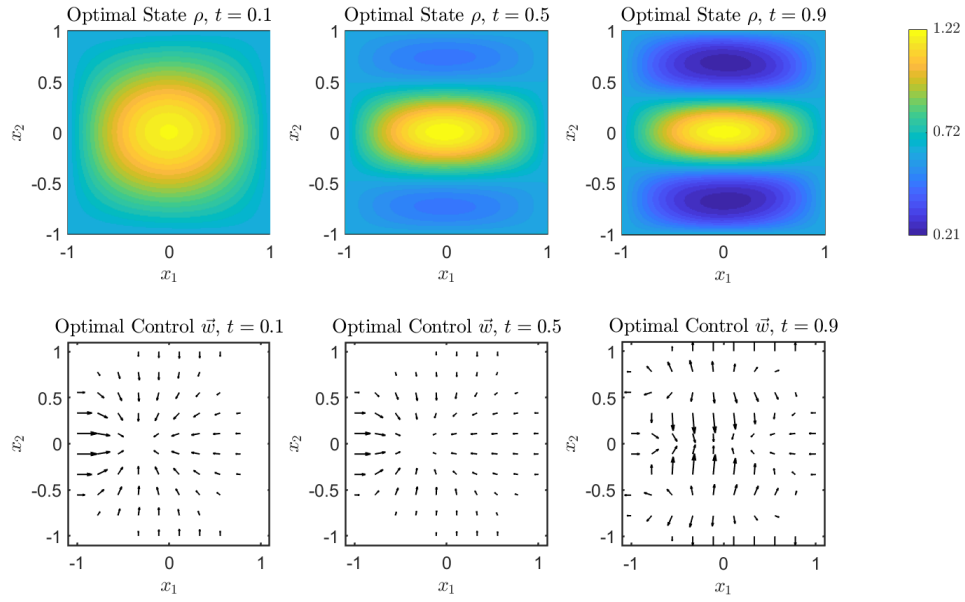


Figure 22: Dirichlet Flow Control 2: Optimal  $\rho$  and optimal control for  $\kappa = 1$  and  $\beta = 10^{-3}$ .