We consider the following optimal control problem:

$$\mathcal{J}(\rho, \mathbf{w}) = \frac{1}{2}||\rho - \widehat{\rho}||^2_{L_2(\Sigma)} + \frac{\beta}{2}||\mathbf{w}||^2_{L_2(\Sigma)}$$

subject to:

$$\frac{\partial \rho}{\partial t} = \nabla^2 \rho - \nabla(\rho \mathbf{w}) + \kappa \nabla \int_{\Omega} \rho(r)\rho(r')\mathbf{K}(r, r')dr'.$$

1 Example 1

The initial configuration for this example is:

$$\rho_0 = exp(-2((y_1 - 0.5)^2 + (y_2 + 0.5)^2))$$
$$\mathbf{w} = \mathbf{0}.$$

The target $\widehat{\rho}$ is set by running a forward problem with the same ρ_0 but with constant velocity $\mathbf{w} = \mathbf{1}$. The domain for this example is a quadrilateral and a wedge and can be seen in Figure 1. The tolerances are $10^{-3}/10^{-7}$. Per shape

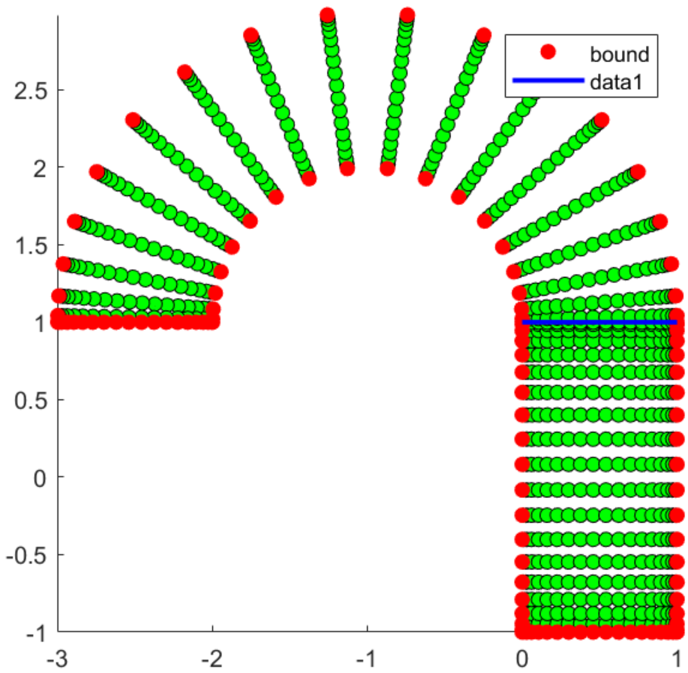


Figure 1: Domain Example 1

Choosing $\kappa = -1$, we get $J_{FW} = 0.0251$, $J_{Opt} = 0.0020$. In Figure 2 $\widehat{\rho}$ and corresponding $\mathbf{w}$ are plotted, while in Figure 3, the optimal result is displayed. Choosing $\kappa = 1$, we get

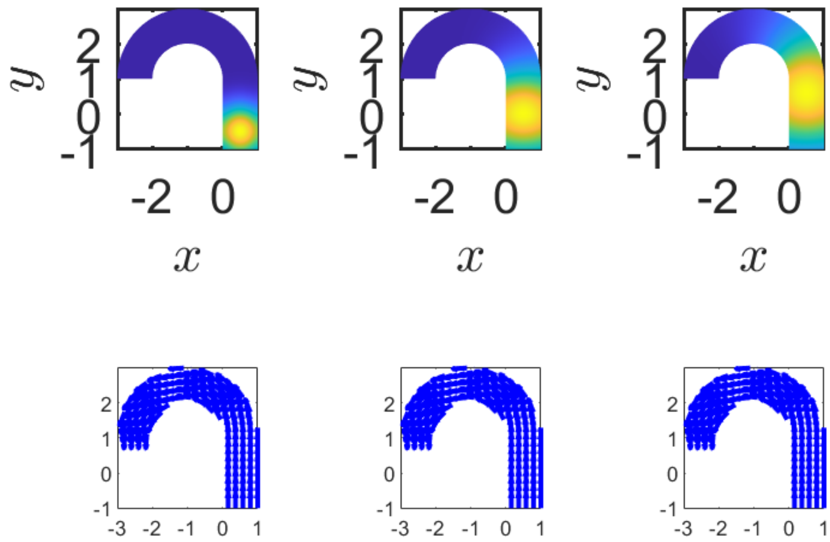


Figure 2: Example 1, $\widehat{\rho}$, $\kappa = -1$

$J_{FW} = 0.0176$, $J_{Opt} = 0.0020$. In Figure 4 $\widehat{\rho}$ and corresponding $\mathbf{w}$ are plotted, while in Figure 5, the optimal result is displayed. It can be seen that while the attractive particles clump in the middle, the repulsive particles are clustered at the boundaries. (Note to self: this corresponds to Test10/ Example5a in code.)

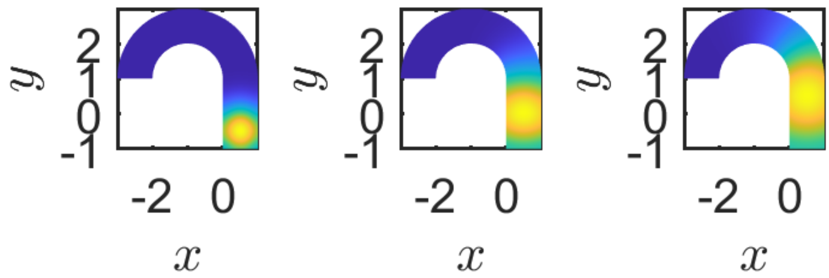
2 Example 2

As initial configuration we choose:

$$\rho_0 = exp(-2((y_1 - 0.5)^2 + (y_2 + 0.5)^2))$$
$$\mathbf{w} = \mathbf{0}.$$

The target is a forward problem run with the same ρ_0 but with a constant background flow $\mathbf{w} = \mathbf{5}$. We run the problem up to time 2, as opposed to time 1 as usual. This is more stable than increasing the strength of the background flow. The domain of the problem is a channel, see Figure 6.

Choosing $\kappa = -1$, we get $J_{FW} = 0.4111$, $J_{Opt} = 0.0807$. In Figure 7 $\widehat{\rho}$ and corresponding $\mathbf{w}$ are plotted, while in Figure 8, the optimal result is displayed. Choosing $\kappa = 1$, we get $J_{FW} = 0.3501$, $J_{Opt} = 0.0821$. In Figure 9 $\widehat{\rho}$ and corresponding $\mathbf{w}$ are plotted, while in Figure



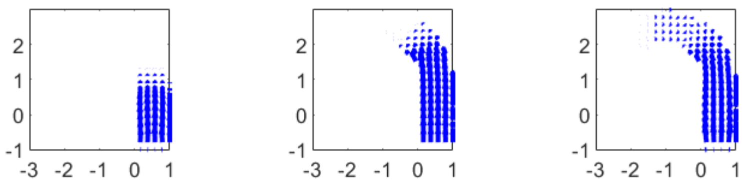


Figure 3: Example 1, optimal ρ and $\mathbf{w}$, $\kappa = -1$

10, the optimal result is displayed. Again, the difference between attractive and repulsive interaction is clearly displayed by the clustering of the particles in the channel.

3 Example 3

As initial configuration we choose:

$$\rho_0 = exp(-2((y_1 + 1)^2 + (y_2 + 0.3)^2))$$
$$\mathbf{w} = \mathbf{0}.$$

The target is a forward problem run with the same ρ_0 but with a background flow of constant one, shaped along the domain. This and the domain of the problem can be seen in Figure 11.

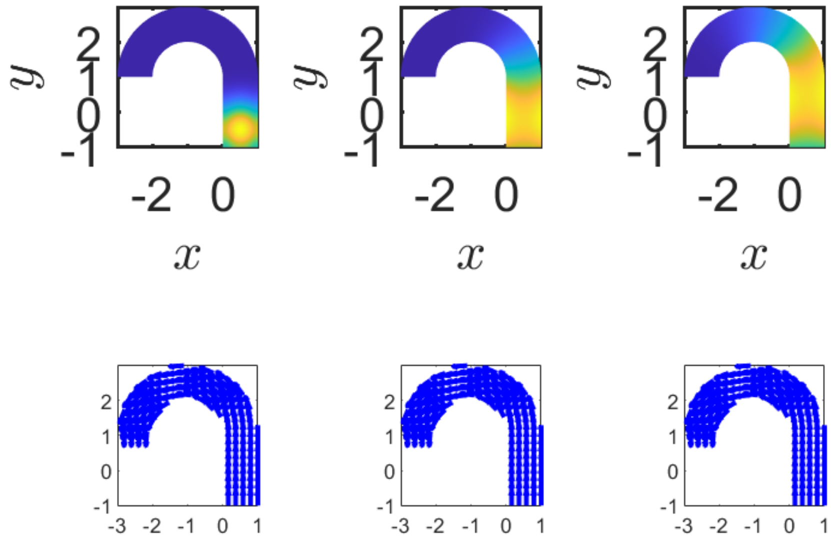


Figure 4: Example 1, $\widehat{\rho}$, $\kappa = 1$

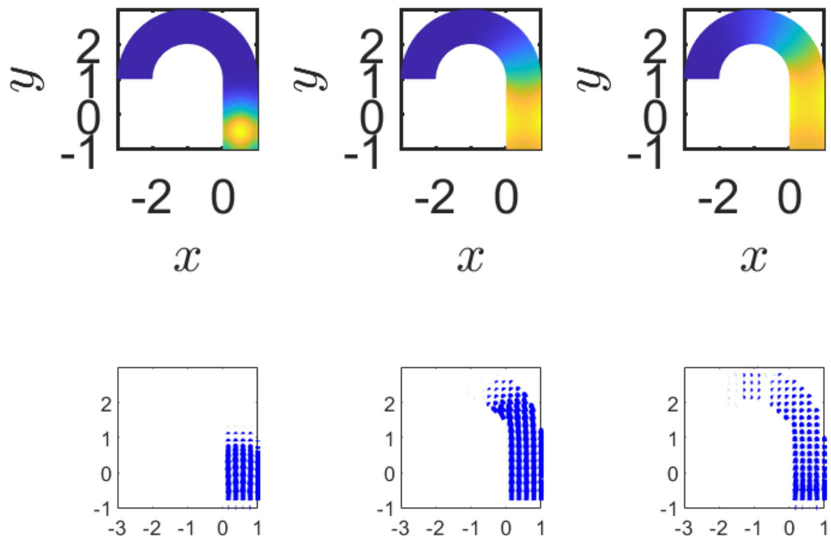


Figure 5: Example 1, optimal ρ, $\mathbf{w}$, $\kappa = 1$

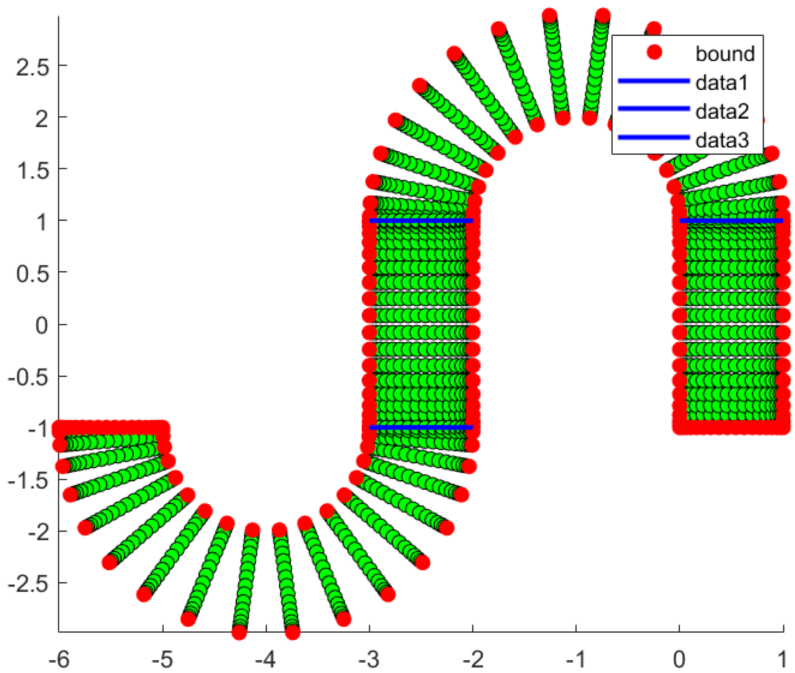


Figure 6: Domain Example 2

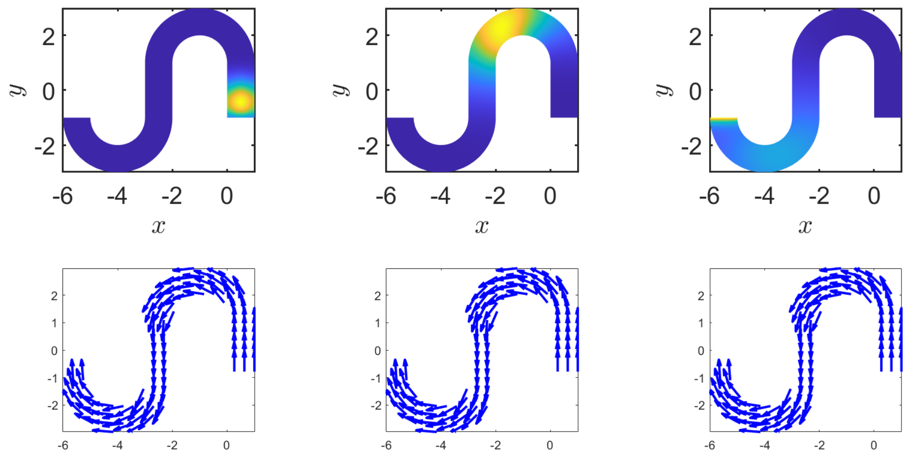


Figure 7: Example 2, $\widehat{\rho}$, $\kappa = -1$

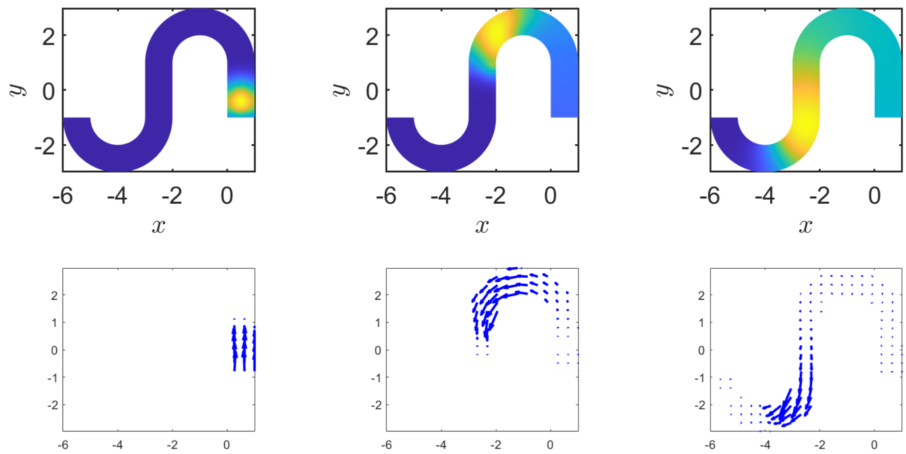


Figure 8: Example 2, optimal ρ and $\mathbf{w}$, $\kappa = -1$

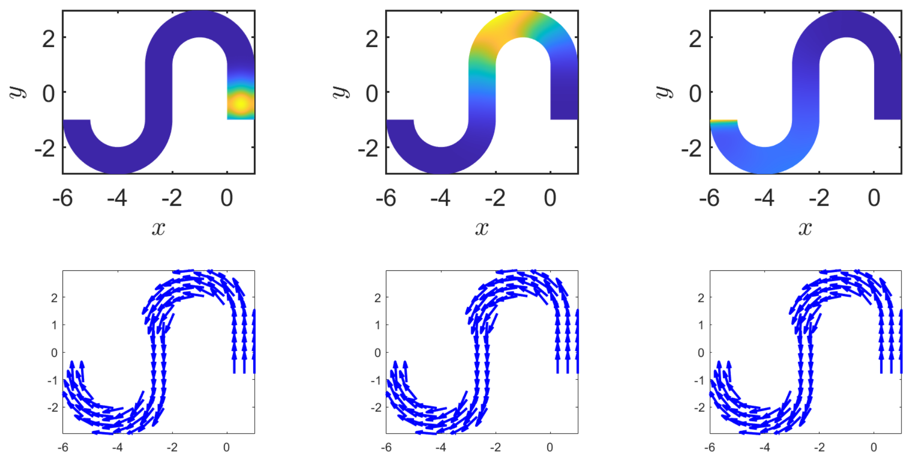


Figure 9: Example 2, $\widehat{\rho}$, $\kappa = 1$

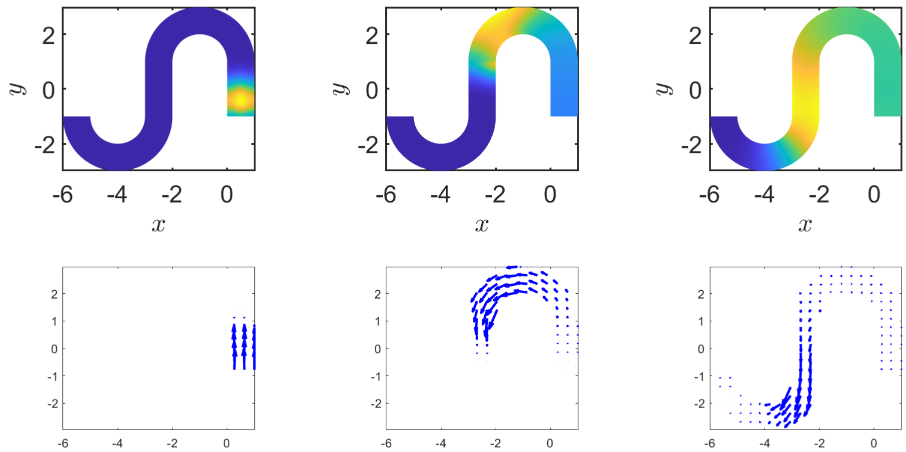


Figure 10: Example 2, optimal ρ and $\mathbf{w}$, $\kappa = 1$

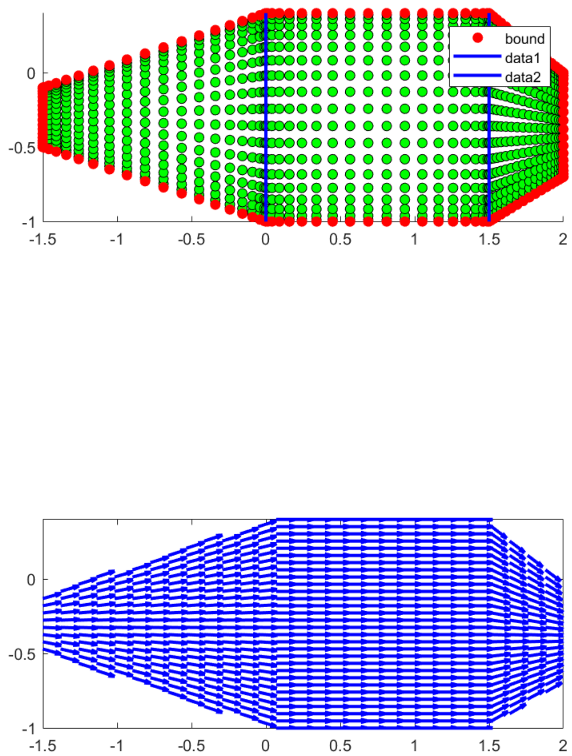


Figure 11: Domain and Flow Example 3