Sedimentation

1 The Forward Model

We are interested in modelling sedimentation processes. In order to achieve this, the advection-diffusion equation with mean-field interaction term has to be modified to include an approximation to volume exclusion. Archer and Malijevský [1] have achieved this using the following model to describe sedimentation processes. The modelling equations are:

$$\frac{\partial \rho}{\partial t^*} = \Gamma \nabla \cdot \left(\rho \nabla \frac{\delta F[\rho]}{\delta \rho} \right),$$

where Γ is the diffusion coefficient. We can rescale this equation as done in [1] using the relationship $t = t^*/\tau_B$, where $\tau_B = \beta\sigma^2/\Gamma$ is the Brownian time scale. Applying this rescaling we get:

$$\frac{\partial \rho}{\partial t} = \beta\sigma^2 \nabla \cdot \left(\rho \nabla \frac{\delta F[\rho]}{\delta \rho} \right). \tag{1}$$

The free energy functional considered in [1] is:

$$F[\rho] = \frac{1}{\beta} \int \rho(\ln \Lambda^2 \rho - 1) + f_{HDA} dr + \frac{1}{2} \int \int \rho(r)\rho(r') V_2(|r - r'|) dr dr' + \int \rho V_{ext} dr,$$

where f_{dh} the approximate free energy density describing the volume exclusion through hard disks. The external potential is defined as:

$$V_{ext} = cy, \quad \text{for} \quad 0 < y < L,$$

where c a constant and L is the height of a rectangular domain. Outside these bounds $V_{ext} = \infty$. Furthermore, we have the pair potential:

$$V_2 = exp(-r/\sigma),$$

where σ is the particle diameter of the hard sphere particle.

1.1 The Hard Disk Approximation

The part of the free energy functional, which accounts for the hard disk approximation, is:

$$F_{HDA}[\rho] = \frac{1}{\beta} \int f_{HDA} dr = \frac{1}{\beta} \int -\rho - \rho \ln(1 - \eta) + \frac{\rho}{1 - \eta} dr,$$

where $\eta = a\rho = \frac{\pi\sigma^2}{4}\rho$. This can be thought of as the bulk fluid, one species, two dimensional approximation of Fundamental Measure Theory (FMT) [2], which is a Density Functional Theory for hard sphere mixtures. The basis of this theory is that the excess free energy functional is of the form:

$$\beta F_{ex}[\rho_i] = \int \Phi(n_\alpha(r')) d^3 r',$$

where i is the species count and Φ is a function of the weighted densities n_α. By now there are many different versions of Φ, yielding approximations of F_{ex} with different limitations, see [3]. Rosenfeld's original version is defined as:

$$\Phi = -n_0 \ln(1-n_3) + \frac{n_1 n_2 - \mathbf{n_1} \cdot \mathbf{n_2}}{1-n_3} + \frac{n_2^3 - 3n_2 \mathbf{n_2} \cdot \mathbf{n_2}}{24\pi(1-n_3)^2}.$$

The weighted densities for ν species are:

$$n_\alpha(r) = \sum_{i=1}^{\nu} \int \rho_i(r') \omega_\alpha^i(r-r'). \tag{2}$$

The weight functions chosen by Rosenfeld are:

$$\begin{aligned} \omega_3^i &= \Theta(R_i - r), \quad \omega_2^i = \delta(R_i - r), \quad \omega_{\mathbf{2}}^{\mathbf{i}} = \frac{\mathbf{r}}{r}\delta(R_i - r), \\ \omega_1^i &= \omega_2^i/(4\pi R_i), \quad \omega_0^i = \omega_2^i/(4\pi R_i^2), \quad \omega_{\mathbf{1}}^{\mathbf{i}} = \omega_{\mathbf{2}}^{\mathbf{i}}/(4\pi R_i), \end{aligned}$$

where R_i is the radius of the excluded volume, Θ is the Heaviside function and δ is the delta function. Integrating over ω_α, with $\alpha = 0, 1, 2, 3$, we get the fundamental measures of a sphere: volume, surface area, radius and the Euler characteristic [3] [2].
Based on this theory for three dimensional spheres and the fact that the theory for hard rods is known exactly [4], Rosenfeld derived a version of this approach for two dimensional hard disks [5]. However, some additional approximations have to be made when choosing the weighted densities, which is not necessary in one and three dimensions. The resulting equation is:

$$\Phi = -n_0 \ln(1-n_3) + \frac{1}{4\pi} \frac{n_2 n_2}{1-n_3} + \frac{1}{4\pi} \frac{\mathbf{n_2} \cdot \mathbf{n_2}}{1-n_3}.$$

In the uniform limit, for one particle species, we get that:

$$n_0 = \rho, \quad n_2 = 2\pi R \rho, \quad n_3 = \pi R^2 \rho,$$

by solving the integrals in (2), using spherical polar coordinates, with $\rho = \rho_{\text{bulk}}$, a constant. Substituting this in the 2D version of Φ gives:

$$\Phi = -\rho \ln(1-\pi R^2 \rho) + \frac{1}{4\pi} \frac{4\pi^2 R^2 \rho^2}{1-\pi R^2 \rho} + \frac{1}{4\pi} \frac{\mathbf{n_2} \cdot \mathbf{n_2}}{1-\pi R^2 \rho},$$

where $\mathbf{n_2} = \mathbf{0}$ in the uniform limit, since the corresponding equation in (2) is an integral over an odd function. Noting that $R = \sigma/2$ and $\eta = \pi\sigma^2\rho/4$, we get that:

$$\Phi = -\rho \ln(1-\eta) + \frac{\rho\eta}{1-\eta} = \rho\left(\ln(1-\eta) + \frac{1}{1-\eta} - 1\right). \tag{3}$$

This expression for the free energy for the bulk fluid is the same as derived by scaled particle theory (SPT) [6], [7], [8], which also coincides with the Percus-Yevic compressibility equation

[9], as detailed in [10]. While the SPT approximation (3) and its three-dimensional equivalent are used in classical DFT, see [11], [12], [13], [14], [15], [16], and other statistical mechanics approaches, see [17], [18], [19], [20], in dynamical DFT it is not commonly applied and only the work of Archer et al. [1], [21], [22], [23], is known to us in this context.

1.2 Deriving the equation of motion

Since we are interested in the equation of motion, we need to calculate $\nabla \cdot \left(\rho \nabla \frac{\delta F_{HDA}[\rho]}{\delta \rho}\right)$. We combine F_{HDA} and F_{ID} here so that we have:

$$F_N = F_{HDA} + F_{ID}.$$

Taking the functional derivative of F_N gives:

$$\begin{aligned}
\frac{\delta F_N[\rho]}{\delta \rho} &= \frac{1}{\beta}\left(1 + \ln\rho + \Lambda^2 - 2 - \ln(1-\eta) + a\frac{\rho}{1-\eta} + \frac{1}{1-\eta} + a\frac{\rho}{(1-\eta)^2}\right) \\
&= \frac{1}{\beta}\left(1 + \ln\rho + \Lambda^2 - 2 - \ln(1-\eta) + \frac{1}{(\eta-1)^2} - \frac{1}{\eta-1} - 1\right) \\
&= \frac{1}{\beta}\left(\ln\rho + \Lambda^2 - 2 - \ln(1-\eta) - \frac{\eta-2}{(\eta-1)^2}\right),
\end{aligned}$$

using partial fractions.

$$\begin{aligned}
\nabla\frac{\delta F_N[\rho]}{\delta \rho} &= \frac{1}{\beta}\left(\nabla\ln\rho + \nabla(\Lambda^2 - 2) - \nabla\ln(1-\eta) - \nabla\frac{\eta-2}{(\eta-1)^2}\right) \\
&= \frac{1}{\beta}\left(\frac{\nabla\rho}{\rho} - \frac{\nabla(1-\eta)}{1-\eta} - \nabla\frac{\eta-2}{(\eta-1)^2}\right) \\
&= \frac{1}{\beta}\left(\frac{\nabla\rho}{\rho} + \frac{\nabla\eta}{1-\eta} - \nabla\frac{\eta-2}{(\eta-1)^2}\right)
\end{aligned}$$

Then multiplying by ρ gives:

$$\begin{aligned}
\rho\nabla\frac{\delta F_N[\rho]}{\delta \rho} &= \frac{1}{\beta}\left(\nabla\rho + \frac{\rho\nabla\eta}{1-\eta} - \rho\nabla\frac{\eta-2}{(\eta-1)^2}\right) \\
&= \frac{1}{\beta}\left(\nabla\rho + \frac{\eta\nabla\rho}{1-\eta} - \rho\nabla\frac{\eta-2}{(\eta-1)^2}\right) \\
&= \frac{1}{\beta}\left(\nabla\rho + \frac{\nabla\rho}{1-\eta} - \nabla\rho - \rho\nabla\frac{\eta-2}{(\eta-1)^2}\right) \\
&= \frac{1}{\beta}\left(\frac{\nabla\rho}{1-\eta} - \rho\nabla\frac{\eta-2}{(\eta-1)^2}\right)
\end{aligned}$$

Finally we take the divergence:

$$\begin{aligned}
\nabla\cdot\left(\rho\nabla\frac{\delta F_N[\rho]}{\delta \rho}\right) &= \frac{1}{\beta}\left(\nabla\cdot\left(\frac{\nabla\rho}{1-\eta}\right) - \nabla\cdot\left(\rho\nabla\frac{\eta-2}{(\eta-1)^2}\right)\right) \\
&= \frac{1}{\beta}\left(\frac{\nabla^2\rho}{1-\eta} + \nabla\rho\cdot\nabla\frac{1}{1-\eta} - \nabla\rho\cdot\nabla\frac{\eta-2}{(\eta-1)^2} - \rho\nabla^2\frac{\eta-2}{(\eta-1)^2}\right) \\
&= \frac{1}{\beta}\left(\frac{\nabla^2\rho}{1-\eta} + \nabla\rho\cdot\nabla\frac{(3-2\eta)}{(1-\eta)^2} - \rho\nabla^2\frac{\eta-2}{(\eta-1)^2}\right)
\end{aligned}$$

2 Optimality Conditions

One optimal control problem to consider is:

$$J = \frac{1}{2}\int_0^T \int_\Omega (\rho - \widehat{\rho})^2 dr dt + \frac{\beta}{2}\int_0^T \int_\Omega \mathbf{w}(r)^2 dr$$

subject to: (4)

$$\frac{\partial \rho}{\partial t} = \beta\sigma^2 \left(\nabla \cdot (\rho \nabla V_{ext}) - \nabla(\rho \mathbf{w}) + \nabla \cdot \left(\rho \nabla \frac{\delta F_N[\rho]}{\delta \rho} \right) + \kappa \int_\Omega \rho(r)\rho(r')\mathbf{K}(r,r')dr \right),$$

where $\mathbf{K}(r,r') = \nabla V_2$. We consider the terms of the PDE and the boundary conditions separately here.

2.1 Calculating Frechét Derivatives

In order to derive the optimalty conditions for the above OCP, we need to calculate the Frechét derivatives of the following terms:

$$\nabla \cdot \left(\rho \nabla \frac{\delta F_N[\rho]}{\delta \rho} \right) = \frac{1}{\beta}\left(\frac{\nabla^2 \rho}{1-\eta} + \nabla \rho \cdot \nabla \frac{(3-2\eta)}{(1-\eta)^2} - \rho \nabla^2 \frac{\eta - 2}{(\eta-1)^2} \right),$$

where $\eta = a\rho$ and $a = \pi\sigma^2/4$. Consider:

$$F_1(\rho) = \nabla^2 \rho \frac{1}{1-a\rho},$$
$$F_2(\rho) = \nabla \rho \cdot \nabla \left(\frac{3-2a\rho}{(1-a\rho)^2} \right),$$
$$F_3(\rho) = \rho \nabla^2 \left(\frac{a\rho - 2}{(a\rho-1)^2} \right).$$

Then

$$F_1(\rho + h) - F_1(\rho) = \nabla(\rho + h)\frac{1}{1-a(\rho+h)} - \nabla \rho \frac{1}{1-a\rho}.$$

Using the expansion:

$$\frac{1}{c-x} = \frac{1}{c} + \frac{1}{c^2}x + O(x^2),$$

where $c = 1 - a\rho$, we get:

$$\begin{aligned} F_1(\rho+h) - F_1(\rho) &= \nabla^2(\rho + h)\left(\frac{1}{1-a\rho} + \frac{a}{(1-a\rho)^2}h \right) - \nabla^2 \rho \frac{1}{1-a\rho} \\ &= \nabla^2 h \left(\frac{1}{1-a\rho} \right) + \nabla^2 \rho \left(\frac{a}{(1-a\rho)^2} h \right), \end{aligned}$$

not considering higher order terms of h. For F_2 we consider the expansion:

$$\frac{1}{(c-x)^2} = \frac{1}{c^2} + \frac{2}{c^3}x + O(x^2),$$

and get:

$$
\begin{aligned}
F_2(\rho+h)-F_2(\rho) &= \nabla(\rho+h)\cdot\nabla\left(\frac{3-2a(\rho+h)}{(1-a(\rho+h))^2}\right)-\nabla\rho\cdot\nabla\left(\frac{3-2a\rho}{(1-a\rho)^2}\right)\\
&= \nabla(\rho+h)\cdot\nabla\left(\frac{3-2a(\rho+h)}{(1-a\rho)^2}+\frac{3-2a(\rho+h)}{(1-a\rho)^3}2ah\right)-\nabla\rho\cdot\nabla\left(\frac{3-2a\rho}{(1-a\rho)^2}\right)\\
&= \nabla h\cdot\nabla\left(\frac{3-2a\rho}{(1-a\rho)^2}\right)+\nabla\rho\cdot\nabla\left(h\left(\frac{-2a}{(1-a\rho)^2}+\frac{6a-4a^2\rho}{(1-a\rho)^3}\right)\right)\\
&= \nabla h\cdot\nabla\left(\frac{3-2a\rho}{(1-a\rho)^2}\right)+(\nabla h\cdot\nabla\rho)\left(\frac{-2a}{(1-a\rho)^2}+\frac{6a-4a^2\rho}{(1-a\rho)^3}\right)\\
&+ h\nabla\rho\cdot\nabla\left(\frac{-2a}{(1-a\rho)^2}+\frac{6a-4a^2\rho}{(1-a\rho)^3}\right).
\end{aligned}
$$

Finally, we have:

$$
\begin{aligned}
F_3(\rho+h)-F_3(\rho) &= (\rho+h)\nabla^2\left(\frac{a(\rho+h)-2}{(a(\rho+h)-1)^2}\right)-\rho\nabla^2\left(\frac{a\rho-2}{(a\rho-1)^2}\right)\\
&= (\rho+h)\nabla^2\left(\frac{a(\rho+h)-2}{(1-a\rho)^2}+\frac{a(\rho+h)-2}{(1-a\rho)^3}2ah\right)-\rho\nabla^2\left(\frac{a\rho-2}{(a\rho-1)^2}\right)\\
&= h\nabla^2\left(\frac{a\rho-2}{(a\rho-1)^2}\right)+\rho\nabla^2\left(h\left(\frac{a}{(1-a\rho)^2}+\frac{2a^2\rho-4a}{(1-a\rho)^3}\right)\right)\\
&= h\nabla^2\left(\frac{a\rho-2}{(a\rho-1)^2}\right)+\rho\left(\frac{a}{(1-a\rho)^2}+\frac{2a^2\rho-4a}{(1-a\rho)^3}\right)\nabla^2 h\\
&+ 2\rho\nabla\left(\frac{a}{(1-a\rho)^2}+\frac{2a^2\rho-4a}{(1-a\rho)^3}\right)\cdot\nabla h+\rho h\nabla^2\left(\frac{a}{(1-a\rho)^2}+\frac{2a^2\rho-4a}{(1-a\rho)^3}\right).
\end{aligned}
$$

2.2 Adjoint Equation

In order to derive the adjoint equation, we need to consider the Lagrangian of the above OCP and take the derivative with respect to ρ. Given that most of the analysis has been done in a different chapter, we only consider the terms derived from F_N. The Frechét derivatives of the relevant terms have been taken and are combined to give:

$$\begin{aligned}\mathcal{L}_\rho(\rho, \mathbf{w}, q)h = ... - \frac{1}{\beta}\int_0^T \int_\Omega & q\nabla^2 h\left(\frac{1}{1-a\rho}\right) + q\nabla^2\rho\left(\frac{a}{(1-a\rho)^2}h\right) \\ & + q\nabla h\cdot\nabla\left(\frac{3-2a\rho}{(1-a\rho)^2}\right) + q\left(\nabla h\cdot\nabla\rho\right)\left(\frac{-2a}{(1-a\rho)^2}+\frac{6a-4a^2\rho}{(1-a\rho)^3}\right) \\ & + qh\nabla\rho\cdot\nabla\left(\frac{-2a}{(1-a\rho)^2}+\frac{6a-4a^2\rho}{(1-a\rho)^3}\right) \\ & - qh\nabla^2\left(\frac{a\rho-2}{(a\rho-1)^2}\right) - q\rho\left(\frac{a}{(1-a\rho)^2}+\frac{2a^2\rho-4a}{(1-a\rho)^3}\right)\nabla^2 h \\ & - q\rho\nabla\left(\frac{2a}{(1-a\rho)^2}+\frac{4a^2\rho-8a}{(1-a\rho)^3}\right)\cdot\nabla h - q\rho h\nabla^2\left(\frac{a}{(1-a\rho)^2}+\frac{2a^2\rho-4a}{(1-a\rho)^3}\right).\end{aligned}$$

Rearranging gives:

$$\begin{aligned}\mathcal{L}_\rho(\rho, \mathbf{w}, q)h = ... - \frac{1}{\beta}\int_0^T \int_\Omega & h\Bigg(q\nabla^2\rho\left(\frac{a}{(1-a\rho)^2}\right) + q\nabla\rho\cdot\nabla\left(\frac{-2a}{(1-a\rho)^2}+\frac{6a-4a^2\rho}{(1-a\rho)^3}\right) - q\nabla^2\left(\frac{a\rho-2}{(a\rho-1)^2}\right) \\ & - q\rho\nabla^2\left(\frac{a}{(1-a\rho)^2}+\frac{2a^2\rho-4a}{(1-a\rho)^3}\right)\Bigg) \\ & + \nabla h\cdot\left(q\nabla\left(\frac{3-2a\rho}{(1-a\rho)^2}\right) + q\nabla\rho\left(\frac{-2a}{(1-a\rho)^2}+\frac{6a-4a^2\rho}{(1-a\rho)^3}\right) - q\rho\nabla\left(\frac{2a}{(1-a\rho)^2}+\frac{4a^2\rho-8a}{(1-a\rho)^3}\right)\right) \\ & + \nabla^2 h\Bigg(q\left(\frac{1}{1-a\rho}\right) - q\rho\left(\frac{a}{(1-a\rho)^2}+\frac{2a^2\rho-4a}{(1-a\rho)^3}\right)\Bigg).\end{aligned}$$

Integration by parts gives:

$$\begin{aligned}\mathcal{L}_\rho(\rho, \mathbf{w}, q)h = ... - \frac{1}{\beta}\int_0^T \int_\Omega & h\Bigg(q\nabla^2\rho\left(\frac{a}{(1-a\rho)^2}\right) + q\nabla\rho\cdot\nabla\left(\frac{-2a}{(1-a\rho)^2}+\frac{6a-4a^2\rho}{(1-a\rho)^3}\right) - q\nabla^2\left(\frac{a\rho-2}{(a\rho-1)^2}\right) \\ & - q\rho\nabla^2\left(\frac{a}{(1-a\rho)^2}+\frac{2a^2\rho-4a}{(1-a\rho)^3}\right)\Bigg) \\ & - h\nabla\Bigg(q\nabla\left(\frac{3-2a\rho}{(1-a\rho)^2}\right) + q\nabla\rho\left(\frac{-2a}{(1-a\rho)^2}+\frac{6a-4a^2\rho}{(1-a\rho)^3}\right) - q\rho\nabla\left(\frac{2a}{(1-a\rho)^2}+\frac{4a^2\rho-8a}{(1-a\rho)^3}\right)\Bigg) \\ & + h\nabla^2\Bigg(q\left(\frac{1}{1-a\rho}\right) - q\rho\left(\frac{a}{(1-a\rho)^2}+\frac{2a^2\rho-4a}{(1-a\rho)^3}\right)\Bigg).\end{aligned}$$

So we have:

$$\mathcal{L}_\rho(\rho,\mathbf{w},q)h = ... - \frac{1}{\beta}\int_0^T\int_\Omega h\Bigg[q\nabla^2\rho\left(\frac{a}{(1-a\rho)^2}\right) + q\nabla\rho\cdot\nabla\left(\frac{-2a}{(1-a\rho)^2}+\frac{6a-4a^2\rho}{(1-a\rho)^3}\right) - q\nabla^2\left(\frac{a\rho-2}{(a\rho-1)^2}\right)$$

$$- q\rho\nabla^2\left(\frac{a}{(1-a\rho)^2}\right) - q\rho\nabla^2\left(\frac{2a^2\rho-4a}{(1-a\rho)^3}\right)$$

$$- \nabla\cdot\left(q\nabla\left(\frac{3-2a\rho}{(1-a\rho)^2}\right)\right) - \nabla\cdot\left(q\nabla\rho\left(\frac{-2a}{(1-a\rho)^2}\right)\right) - \nabla\cdot\left(q\nabla\rho\left(\frac{6a-4a^2\rho}{(1-a\rho)^3}\right)\right)$$

$$+ \nabla\cdot\left(q\rho\nabla\left(\frac{2a}{(1-a\rho)^2}\right)\right) + \nabla\cdot\left(q\rho\nabla\left(\frac{4a^2\rho-8a}{(1-a\rho)^3}\right)\right)$$

$$+ \nabla^2\left(q\left(\frac{1}{1-a\rho}\right)\right) - \nabla^2\left(q\rho\left(\frac{a}{(1-a\rho)^2}\right)\right) - \nabla^2\left(q\rho\left(\frac{2a^2\rho-4a}{(1-a\rho)^3}\right)\right)\Bigg]drdt.$$

Combining fractions gives:

$$\mathcal{L}_\rho(\rho,\mathbf{w},q)h = ... - \frac{1}{\beta}\int_0^T\int_\Omega h\Bigg[q\nabla^2\rho\left(\frac{a}{(1-a\rho)^2}\right) + q\nabla\rho\cdot\nabla\left(\frac{2a(a\rho-2)}{(1-a\rho)^3}\right) - q\nabla^2\left(\frac{a\rho-2}{(a\rho-1)^2}\right)$$

$$- q\rho\nabla^2\left(\frac{a(3-a\rho)}{(1-a\rho)^3}\right) - \nabla\cdot\left(q\nabla\left(\frac{3-2a\rho}{(1-a\rho)^2}\right)\right) - \nabla\cdot\left(q\nabla\rho\left(\frac{2a(a\rho-2)}{(1-a\rho)^3}\right)\right)$$

$$+ \nabla\cdot\left(q\rho\nabla\left(\frac{-2a(a\rho-3)}{(1-a\rho)^3}\right)\right) + \nabla^2\left(q\left(\frac{1}{1-a\rho}\right)\right) - \nabla^2\left(q\rho\left(\frac{-a(a\rho-3)}{(1-a\rho)^3}\right)\right)\Bigg]drdt.$$

According to Mathematica this is:

$$\mathcal{L}_\rho(\rho,\mathbf{w},q)h = ... - \frac{1}{\beta}\int_0^T\int_\Omega h\left[\frac{1}{(a\rho-1)^3}\Big(4a\nabla\rho\cdot\nabla q + 2a(-1+a\rho)q\nabla^2\rho + (-1+5a\rho-2a^2\rho^2)\nabla^2 q\Big)\right]drdt.$$

And rewriting this is:

$$\mathcal{L}_\rho(\rho,\mathbf{w},q)h = ... - \frac{1}{\beta}\int_0^T\int_\Omega h\left[\frac{4a\nabla\rho\cdot\nabla q}{(a\rho-1)^3} + \frac{2aq\nabla^2\rho}{(a\rho-1)^2} + \frac{(-1+5a\rho-2a^2\rho^2)\nabla^2 q}{(a\rho-1)^3}\right]drdt.$$

Adding the other terms of the adjoint found in previous analysis, the adjoint equation is:

$$\begin{aligned}\frac{\partial q}{\partial t} =& \frac{1}{\beta}\frac{(-1+5a\rho-2a^2\rho^2)}{(a\rho-1)^3}\nabla^2 q + \frac{1}{\beta}\frac{4a\nabla\rho}{(a\rho-1)^3}\cdot\nabla q + \frac{1}{\beta}\frac{2a\nabla^2\rho}{(a\rho-1)^2}q \\ &- \mathbf{w}\cdot\nabla q + \nabla V_{ext}\cdot\nabla q - \rho + \widehat{\rho} + \int\left(\nabla_r q(r) - \nabla_{r'}q(r')\right)\rho(r').\mathbf{K}(r,r')dr'\end{aligned}$$

2.3 Frechét Derivatives for Boundary Terms

When considering no-flux boundary conditions, we have the equation:

$$-\mathbf{j}\cdot\mathbf{n} = ... - \rho\nabla\frac{\delta F_N[\rho]}{\delta\rho}\cdot\mathbf{n} = ... - \frac{1}{\beta}\left(\frac{\nabla\rho}{1-\eta} - \rho\nabla\frac{\eta-2}{(\eta-1)^2}\right)\cdot\mathbf{n},$$

omitting the other terms, as done in the previous section. The Frechét derivatives of the following terms have to be taken, similarly to the section above:

$$\begin{aligned}
F_4(\rho) &= \frac{\nabla\rho}{1-a\rho}, \\
F_5(\rho) &= \rho\nabla\frac{a\rho-2}{(a\rho-1)^2}.
\end{aligned}$$

Then for F_4 we have:

$$\begin{aligned}
F_4(\rho+h) - F_4(\rho) &= \nabla(\rho+h)\frac{1}{1-a(\rho+h)} - \nabla\rho\frac{1}{1-a\rho} \\
&= \nabla(\rho+h)\left(\frac{1}{1-a\rho} + \frac{a}{(1-a\rho)^2}h\right) \\
&= \nabla h\left(\frac{1}{1-a\rho}\right) + \nabla\rho\left(\frac{a}{(1-a\rho)^2}h\right).
\end{aligned}$$

For F_5 we get:

$$\begin{aligned}
F_5(\rho+h) - F_5(\rho) &= (\rho+h)\nabla\frac{a(\rho+h)-2}{(a(\rho+h)-1)^2} - \rho\nabla\frac{a\rho-2}{(a\rho-1)^2} \\
&= (\rho+h)\nabla\left(\frac{a(\rho+h)-2}{(1-a\rho)^2} + \frac{a(\rho+h)-2}{(1-a\rho)^3}2ah\right) - \rho\nabla\frac{a\rho-2}{(a\rho-1)^2} \\
&= h\nabla\left(\frac{a\rho-2}{(1-a\rho)^2}\right) + \rho\nabla\left(h\left(\frac{a}{(1-a\rho)^2} + \frac{2a^2\rho-4a}{(1-a\rho)^3}\right)\right) \\
&= h\nabla\left(\frac{a\rho-2}{(1-a\rho)^2}\right) + h\rho\nabla\left(\frac{a}{(1-a\rho)^2} + \frac{2a^2\rho-4a}{(1-a\rho)^3}\right) + \nabla h\left(\rho\frac{a}{(1-a\rho)^2} + \rho\frac{2a^2\rho-4a}{(1-a\rho)^3}\right).
\end{aligned}$$

2.4 Boundary Terms

Given the Frechét derivatives, the relevant boundary terms for the Lagrangian are:

$$\begin{aligned}
\mathcal{L}_{\rho,1}(\rho,\mathbf{w},q)h = ..-\frac{1}{\beta}\int_0^T\int_{\partial\Omega}\Bigg(&-q_{\partial\Omega}\nabla h\left(\frac{1}{1-a\rho}\right) - q_{\partial\Omega}\nabla\rho\left(\frac{a}{(1-a\rho)^2}h\right) + q_{\partial\Omega}h\nabla\left(\frac{a\rho-2}{(1-a\rho)^2}\right) \\
&+ hq_{\partial\Omega}\rho\nabla\left(\frac{a}{(1-a\rho)^2} + \frac{2a^2\rho-4a}{(1-a\rho)^3}\right) + q_{\partial\Omega}\nabla h\left(\rho\frac{a}{(1-a\rho)^2} + \rho\frac{2a^2\rho-4a}{(1-a\rho)^3}\right)\Bigg)\cdot\mathbf{n}dr.dt
\end{aligned}$$

From the integration by parts of the terms within the domain (in the previous section) we get:

$$\begin{aligned}\mathcal{L}_{\rho,2}(\rho,\mathbf{w},q)h = ... - \frac{1}{\beta}\int_0^T\int_{\partial\Omega}\Bigg(h\Bigg(q\nabla\left(\frac{3-2a\rho}{(1-a\rho)^2}\right) + q\nabla\rho\left(\frac{-2a}{(1-a\rho)^2}+\frac{6a-4a^2\rho}{(1-a\rho)^3}\right)\\ - q\rho\nabla\left(\frac{2a}{(1-a\rho)^2}+\frac{4a^2\rho-8a}{(1-a\rho)^3}\right)\Bigg)\\ + \nabla h\Bigg(q\left(\frac{1}{1-a\rho}\right) - q\rho\left(\frac{a}{(1-a\rho)^2}+\frac{2a^2\rho-4a}{(1-a\rho)^3}\right)\Bigg)\\ - h\nabla\Bigg(q\left(\frac{1}{1-a\rho}\right) - q\rho\left(\frac{a}{(1-a\rho)^2}+\frac{2a^2\rho-4a}{(1-a\rho)^3}\right)\Bigg)\Bigg)\cdot\mathbf{n}drdt.\end{aligned}$$

Combining all of these give all boundary terms for the Lagrangian:

$$\begin{aligned}\mathcal{L}_{\rho}(\rho,\mathbf{w},q)h = ... - \frac{1}{\beta}\int_0^T\int_{\partial\Omega}\Bigg(h\Bigg(-q_{\partial\Omega}\nabla\rho\left(\frac{a}{(1-a\rho)^2}\right) + q_{\partial\Omega}\nabla\left(\frac{a\rho-2}{(1-a\rho)^2}\right)\\ + q_{\partial\Omega}\rho\nabla\left(\frac{a}{(1-a\rho)^2}+\frac{2a^2\rho-4a}{(1-a\rho)^3}\right) + \left(q\nabla\left(\frac{3-2a\rho}{(1-a\rho)^2}\right) + q\nabla\rho\left(\frac{-2a}{(1-a\rho)^2}+\frac{6a-4a^2\rho}{(1-a\rho)^3}\right)\right.\\ \left.- q\rho\nabla\left(\frac{2a}{(1-a\rho)^2}+\frac{4a^2\rho-8a}{(1-a\rho)^3}\right)\right) - \nabla\Bigg(q\left(\frac{1}{1-a\rho}\right) - q\rho\left(\frac{a}{(1-a\rho)^2}+\frac{2a^2\rho-4a}{(1-a\rho)^3}\right)\Bigg)\Bigg)\\ + \nabla h\Bigg(-q_{\partial\Omega}\left(\frac{1}{1-a\rho}\right) + q_{\partial\Omega}\left(\rho\frac{a}{(1-a\rho)^2}+\rho\frac{2a^2\rho-4a}{(1-a\rho)^3}\right) + q\left(\frac{1}{1-a\rho}\right)\\ - q\rho\left(\frac{a}{(1-a\rho)^2}+\frac{2a^2\rho-4a}{(1-a\rho)^3}\right)\Bigg)\Bigg)\cdot\mathbf{n}drdt.\end{aligned}$$

Comparing terms in ∇h:

$$\begin{aligned}\Bigg[-q_{\partial\Omega}\left(\frac{1}{1-a\rho}\right) + q_{\partial\Omega}\left(\rho\frac{a}{(1-a\rho)^2}+\rho\frac{2a^2\rho-4a}{(1-a\rho)^3}\right)\\ + q\left(\frac{1}{1-a\rho}\right) - q\rho\left(\frac{a}{(1-a\rho)^2}+\frac{2a^2\rho-4a}{(1-a\rho)^3}\right)\Bigg]\cdot\mathbf{n} = 0.\end{aligned}$$

This holds when $q_{\partial\Omega} = q$. Then for $h \neq 0$ we get:

$$\begin{aligned}&\Bigg[-q\nabla\rho\left(\frac{a}{(1-a\rho)^2}\right) + q\nabla\left(\frac{a\rho-2}{(1-a\rho)^2}\right)\\ &+ q\rho\nabla\left(\frac{a}{(1-a\rho)^2}+\frac{2a^2\rho-4a}{(1-a\rho)^3}\right) + q\nabla\left(\frac{3-2a\rho}{(1-a\rho)^2}\right) + q\nabla\rho\left(\frac{-2a}{(1-a\rho)^2}+\frac{6a-4a^2\rho}{(1-a\rho)^3}\right)\\ &- q\rho\nabla\left(\frac{2a}{(1-a\rho)^2}+\frac{4a^2\rho-8a}{(1-a\rho)^3}\right) - \nabla\Bigg(q\left(\frac{1}{1-a\rho}\right) - q\rho\left(\frac{a}{(1-a\rho)^2}+\frac{2a^2\rho-4a}{(1-a\rho)^3}\right)\Bigg)\Bigg]\cdot\mathbf{n} = 0\end{aligned}$$

According to Mathematica this reduces to:

$$\frac{(1+a\rho)\nabla q}{(a\rho-1)^3}\cdot\mathbf{n} = 0$$

Since $a\rho > 0$ by definition, this is:

$$\frac{\partial q}{\partial n} = 0.$$

Note that the other terms of the PDE are not entering this expression, as they cancel out during the derivation. This has been shown in the derivation of a simpler set of equations and since this derivation is additive, the result remains unchanged.
Furthermore, the gradient equation remains unchanged by this equation, since F_N does not contain terms involving $\mathbf{w}$, compare to (5), and is:

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

2.5 Time-Independent Control

While the gradient equation is unchanged by the sedimentation equation, as compared to an advection diffusion equation, it is changed when we consider a time independent control. We choose the problem:

$$J = \frac{1}{2}\int_0^T \int_\Omega (\rho - \widehat{\rho})^2 dr dt + \frac{\beta}{2}\int_\Omega \mathbf{w}(r)^2 dr$$

subject to:

$$\frac{\partial \rho}{\partial t} = \beta\sigma^2\left(\nabla\cdot(\rho\nabla V_{ext}) - \nabla(\rho\mathbf{w}) + \nabla\cdot\left(\rho\nabla\frac{\delta F_N[\rho]}{\delta\rho}\right) + \kappa\int_\Omega \rho(r)\rho(r')\mathbf{K}(r,r')dr\right),$$

where $\mathbf{K}(r,r') = \nabla V_2$. Taking derivatives of the Lagrangian with respect to $\mathbf{w}$ gives:

$$\mathcal{L}_{\mathbf{w}}(\rho,\mathbf{w},q)h = \int_\Omega \beta\mathbf{w}(r)\cdot\mathbf{h}(r)dt + \int_0^T\int_\Omega \rho\mathbf{h}(r)\cdot\nabla q dr dt. \tag{5}$$

Since $\mathbf{w}$ does not depend on t, neither does $\mathbf{h}$ and so this can be taken out of the time integral:

$$\mathcal{L}_{\mathbf{w}}(\rho,\mathbf{w},q)h = \int_\Omega\left(\beta\mathbf{w}(r)\cdot\mathbf{h}(r) + \mathbf{h}(r)\cdot\int_0^T \rho\nabla q dt\right)dr.$$

Then we get:

$$\beta\mathbf{w}(r) + \int_0^T \rho\nabla q dt = 0,$$

and finally:

$$\mathbf{w}(r) = -\frac{1}{\beta}\int_0^T \rho\nabla q dt.$$

2.6 Periodic Boundary Conditions

+++ Add here when done +++

3 Numerical Results

In this section, the results in [1] are replicated. Then optimal control problems of the form (4) are solved.

3.1 Replicating examples from the paper in a periodic box

The domain in [1] is a box with lengths $L_y = 43.5\sigma$, and $L_x = 60\sigma$. The strength of the external potential is given by $\beta c = 0.1$ and the strength of the interaction term κ is given by $\beta\kappa = -3.5$, where $\beta = \frac{1}{k_B T}$. Furthermore, we have the average density of the system $\bar{\rho}\sigma^2$, calculated using $(1/L_y)\int_0^L \rho\sigma^2 dy$. The initial condition for ρ is found by considering $\bar{\rho}$ and adding a uniform random number to each location in the range $\pm\bar{\rho}/20$. The cases $\sigma\bar{\rho} = 0.072$ and $\sigma\bar{\rho} = 0.2$ are considered in [1].

Since the original simulations are done in a periodic box, we implement the problem in the periodic box as well. We expect near identical results to the paper, given that the setup is identical. We choose a periodic box that has no flux boundary conditions on the top and bottom of the box, while being periodic on the sides. We scale time as done in Equation (1), so that the time scales are comparable. In order to get qualitatively good results, we choose $n = 100$ and $N = 100$. This takes approximately five hours to solve. In Figure 1 the results for the configurations corresponding to Figure 8 in Archer's paper can be seen ($\bar{\rho} = 0.072$, choosing $\sigma = 1$, and running up to $T = 300$). In Figures 2 we see the results that correspond to the configurations in Figure 10 in Archer's paper ($\bar{\rho} = 0.2$, choosing $\sigma = 1$, running time up to $T = 300$). While the results for Archer's first result look very close to the original, the second set of results is a little different. This may have to do with slightly different initial conditions or numerical solutions.

3.2 Replicating examples from the paper in a box with noflux BCs

As above, we choose $N = n = 100$, which takes over 24 hours to run. We run up to time $T = 300$, set $\sigma = 1$ and consider the case $\bar{\rho} = 0.072$ and $\bar{\rho} = 0.2$. Note: the dimensions are switched around, which needs to be fixed with the next rerun. We can see the results for both choices of $\bar{\rho}$ in Figures 3 and 4.

3.3 Optimization Problems

3.3.1 Optimization in a Box

We have $N = 40$ and $n = 30$. We choose the ODE tolerance to be 10^{-7} and the optimization tolerance is 10^{-3}. We choose $\bar{\rho} = 0.036$. We set up a test problem which sets $\widehat{\rho}$ to be the forward

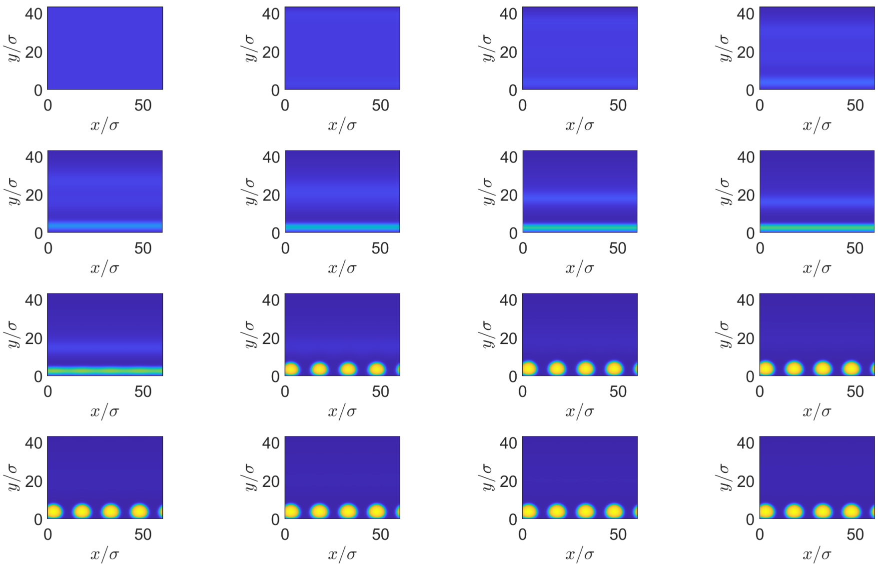

Figure 1: Figure 8 in paper, periodic domain

solution for the problem with $V_{ext} = cy$, where $c = 0.1$, as in Archer's paper. The optimization forward problem is such that $c = 0.01$ and $\mathbf{w} = \mathbf{0}$. We expect the control to act downward, since the strength of gravity c is decreased. We also expect that the cost $\mathcal{J}$ is decreasing from the baseline J_{FW} when optimizing. For $\beta = 10^{-3}$ and $\beta = 10^{-1}$ this works well. When $\beta = 10^{-3}$ we get $J_{FW} = 0.4955$ and $J_{Opt} = 0.0556$. The results can be seen in Figures 5, 6 and 7.

3.3.2 Optimization in a Box - Time-Independent Control

We consider the identical problem but now require the control to be time independent. This affects the gradient equation as discussed in Section 2.5. Therefore, we expect a $\mathbf{w}$ which is averaged over the time horizon and therefore time independent. The result is $J_{FW} = 0.4855$ and $J_{Opt} = 0.0733$ and can be seen in Figures 8, 9 and 10. We observe that, as expected, J_{opt} is larger than for the previous example where $\mathbf{w}$ was allowed to vary over time.

We wanted to see whether the time independent flow control is similar to the ∇V_{ext} of the target. The target state was influenced by $V_{ext} = 0.1y_2$. The forward state for the OCP was influenced by $V_{ext} = 0.01y_2$. Figure 11 shows the control and ∇V_{ext} of the target. We can see that one of these is positive, while the other one is negative. This is due to the opposite signs of $\mathbf{w}$ and ∇V_{ext} in the PDE.

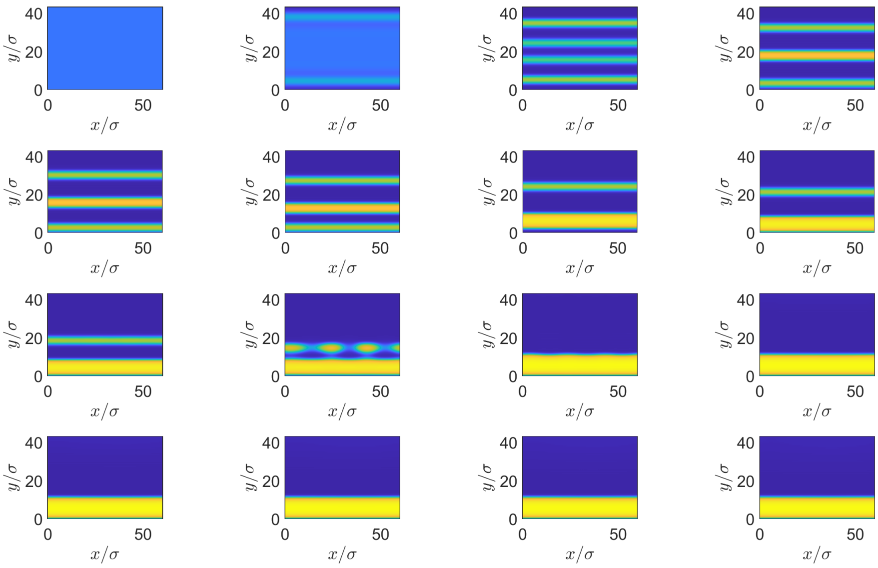

Figure 2: Figure 10 in paper, periodic domain

3.3.3 Optimization in a Periodic Box

3.3.4 Optimization in a Periodic Box - Time-Independent Control

3.3.5 Optimization in a Multishape

The first example is a simple mulitshape with two quadrilaterals. We choose $n = 30$ and $N = 20$ and run up to time $T = 30$, the parameter choices are as in the section on optimization in a box. We choose $\lambda = 0.01$ as usual. We get $J_{FW} = 0.0713$ and $J_{Opt} = 0.0059$. The results are displayed in Figures 12 and 13.

The second example is an optimization problem in a larger multishape. The setup remains the same as before, but now computed on a multishape which is comprised of four shapes, out of which three are quadrilaterals and one is a wedge. We get $J_{FW} = 0.0766$ and $J_{Opt} = 0.0116$. The results can be seen in Figures 14 and 15.

For a third example, we choose a multishape with an imposed background flow and gravity as a target, see Figure 16. The optimal control problem has the same strength of gravity $c = 0.1$ imposed, but no flow. We expect the control to act similar to the flow profile imposed to produce $\widehat{\rho}$. We choose $T = 10$ this time. We get $J_{FW} = 0.0484$ and $J_{Opt} = 0.0258$ and the results are displayed in Figures 17 and 18. Furthermore, we compare the strength of $\mathbf{w}$ of the target and the optimal control. The absolute $L_2/\ L_\infty$ norms are compared, and we get

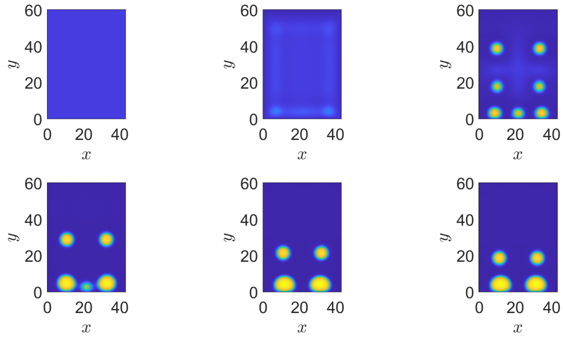

Figure 3: Figure 8 in paper, no flux BCs, ++ fix wrong dimensions ++

$||\mathbf{w}_{\widehat{\rho}}|| = 68$ and $||\mathbf{w}_{Opt}|| = 50.8965$.

3.3.6 Optimization in a Multishape - Time-Independent Control

We use the first multishape example from the previous section with two quadrilaterals with the same setup and parameter choice. Here, since this is a more difficult problem, we choose $\lambda = 0.001$, which takes considerably more iterations than problems with larger λ. We get $J_{FW} = 0.0713$ and $J_{Opt} = 0.0081$ and the result can be seen in Figures 19 and 20. If we compare with the time dependent case, as expected for the time independent control, the optimal cost is higher.

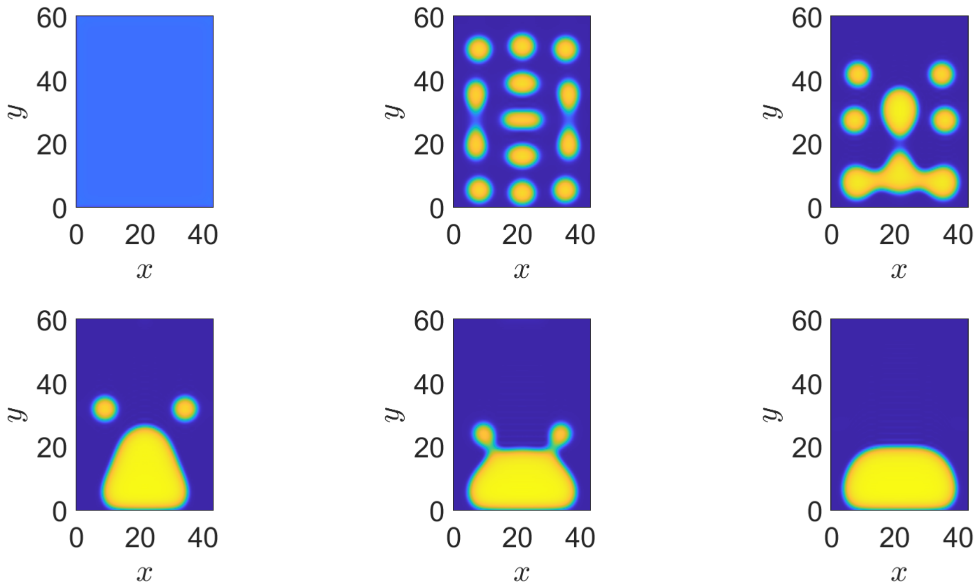

Figure 4: Figure 10 in paper, no flux BCs, ++ fix wrong dimensions ++

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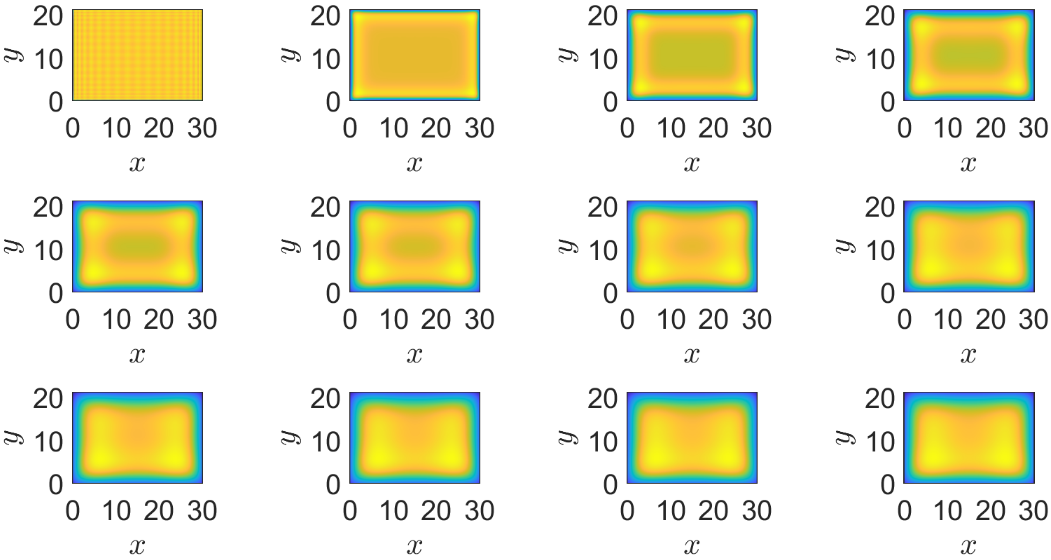

Figure 5: Forward ρ for $c = 0.01$

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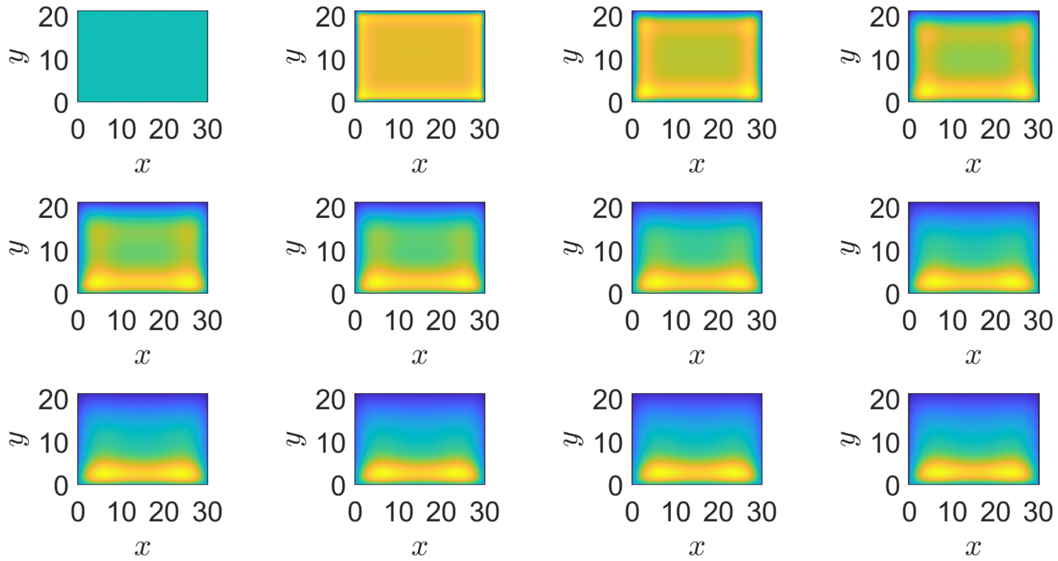

Figure 6: Optimal ρ for $c = 0.01$

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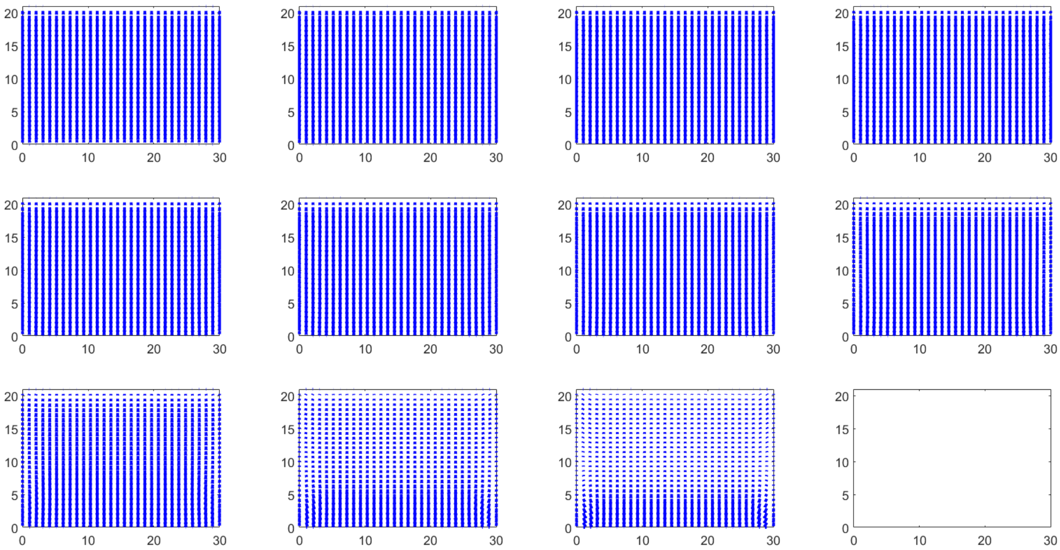

Figure 7: Optimal Control for $c = 0.01$

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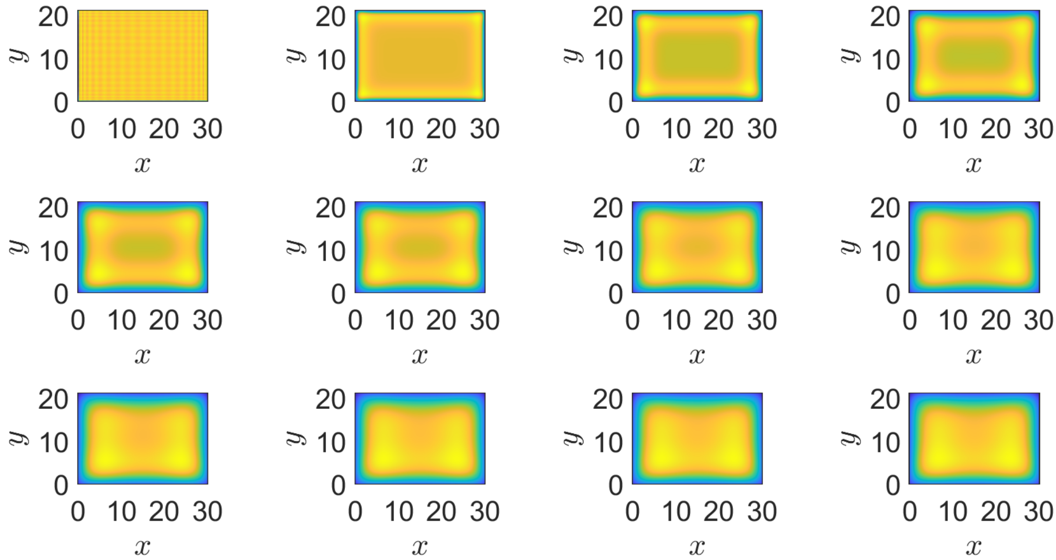

Figure 8: Time-independent; Forward ρ for $a = 0.01$

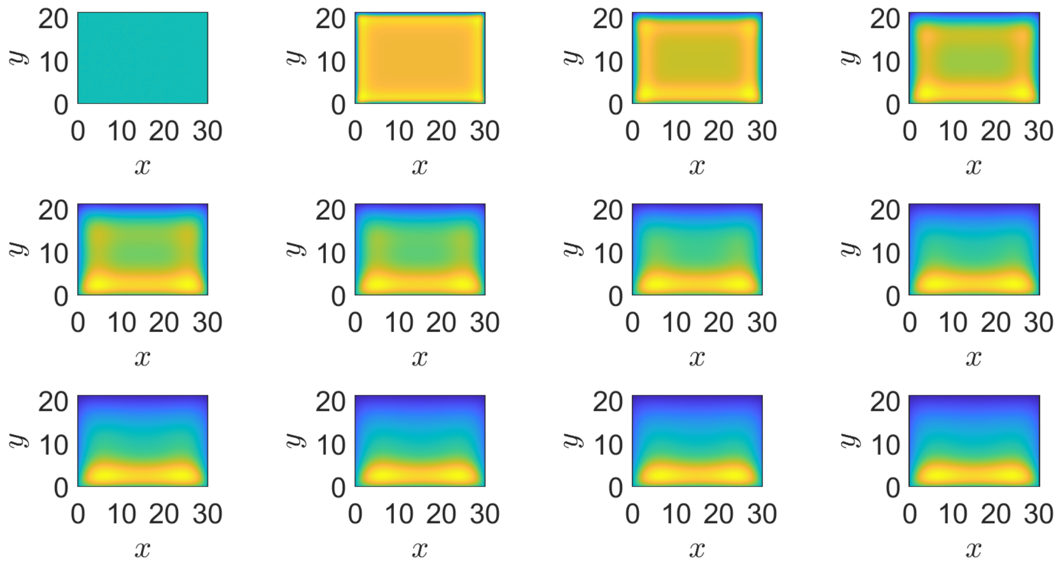

Figure 9: Time-independent; Optimal ρ for $a = 0.01$

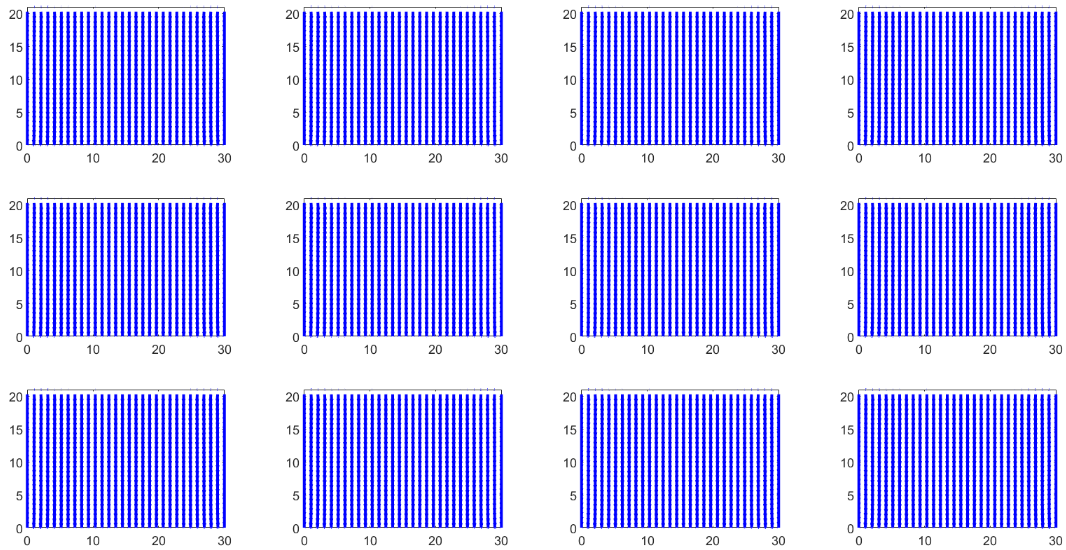

Figure 10: Time-independent; Optimal Control for $a = 0.01$

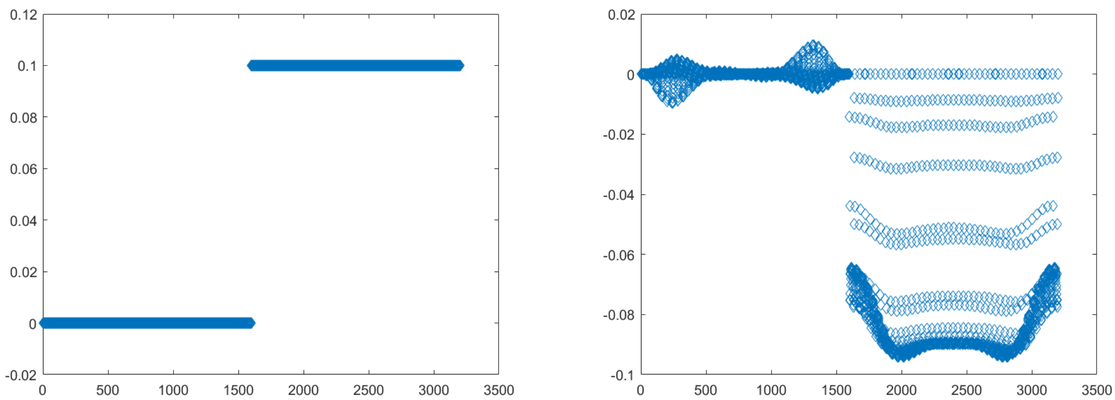

Figure 11: ∇V_{ext} of target and optimal control $\mathbf{w}$.

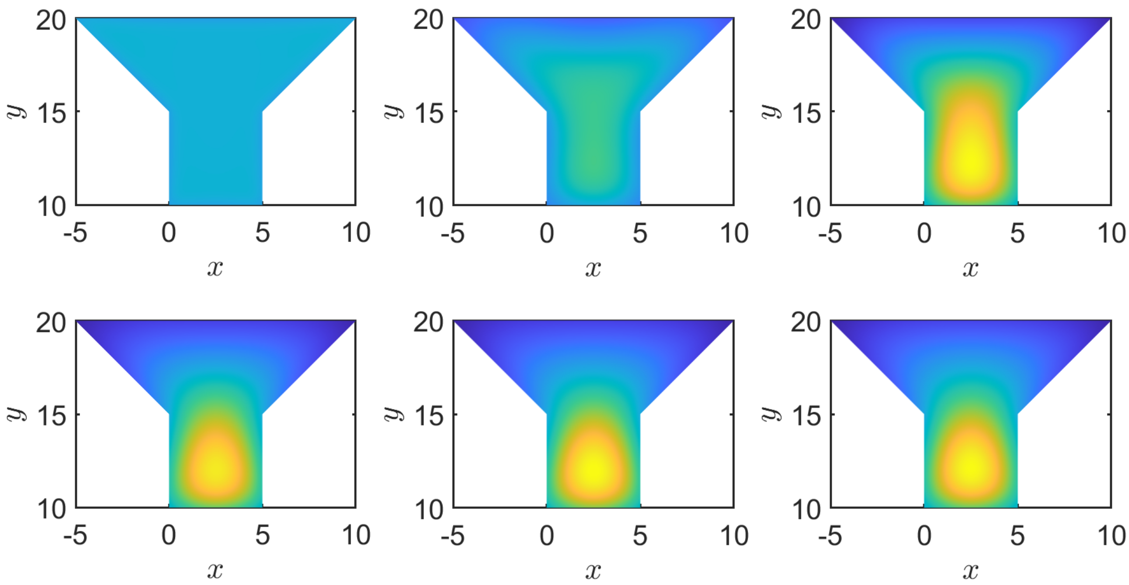

Figure 12: Multishape Example 1: Optimal ρ

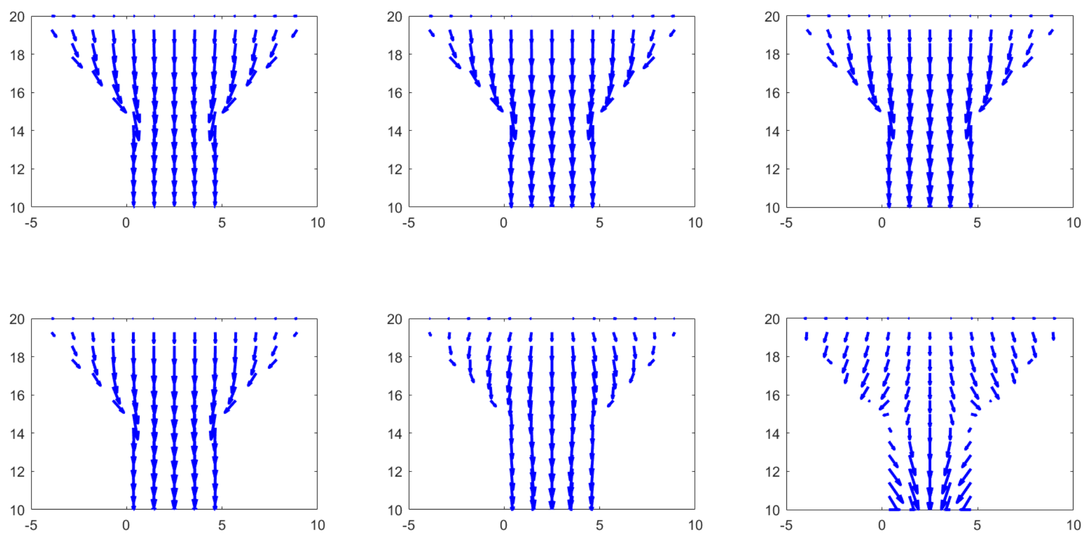

Figure 13: Multishape Example 1: Optimal control

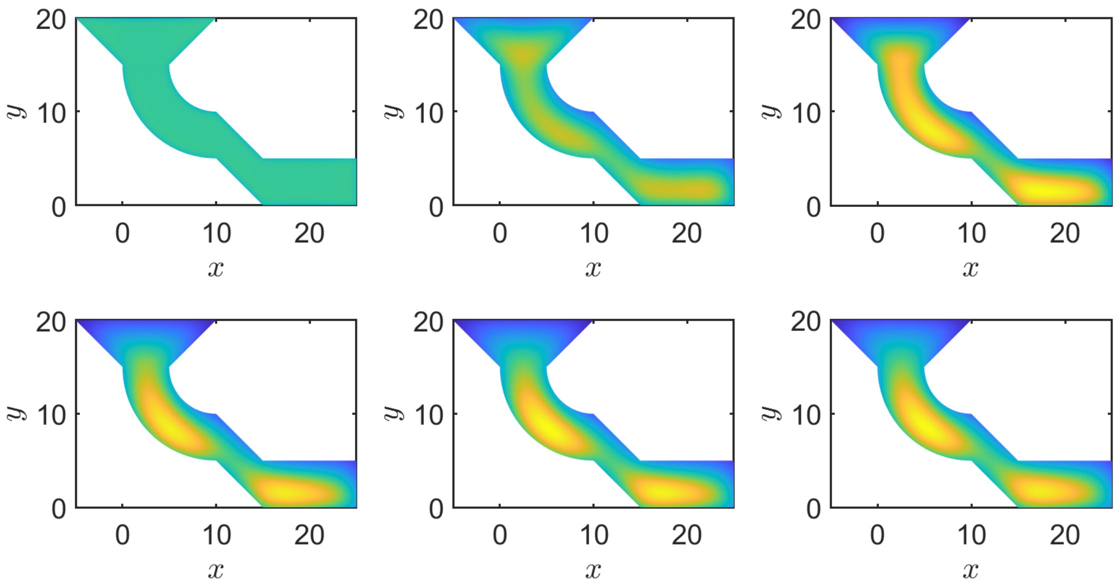

Figure 14: Multishape Example 2: Optimal ρ

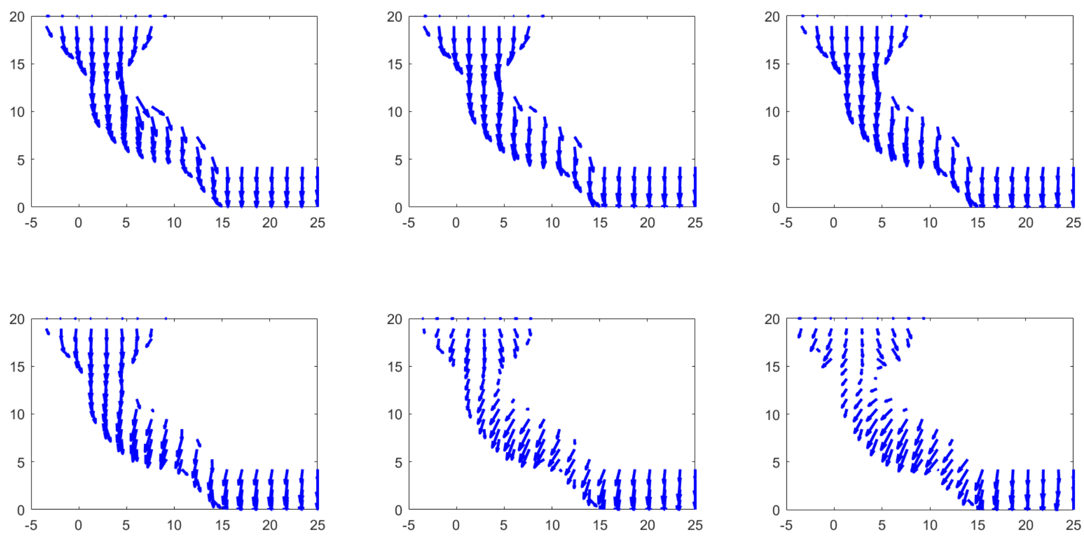

Figure 15: Multishape Example 2: Optimal control

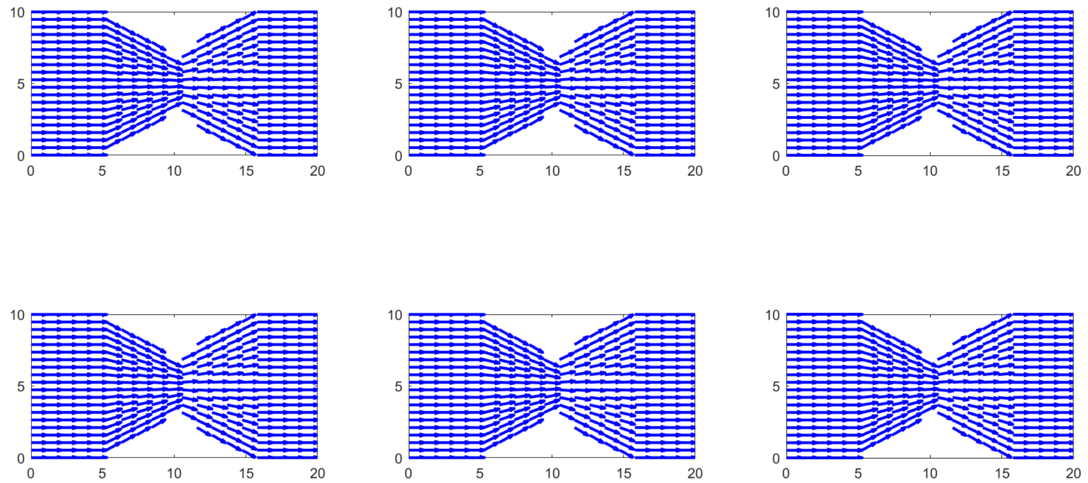

Figure 16: Multishape Example 3:Flow profile determining $\widehat{\rho}$

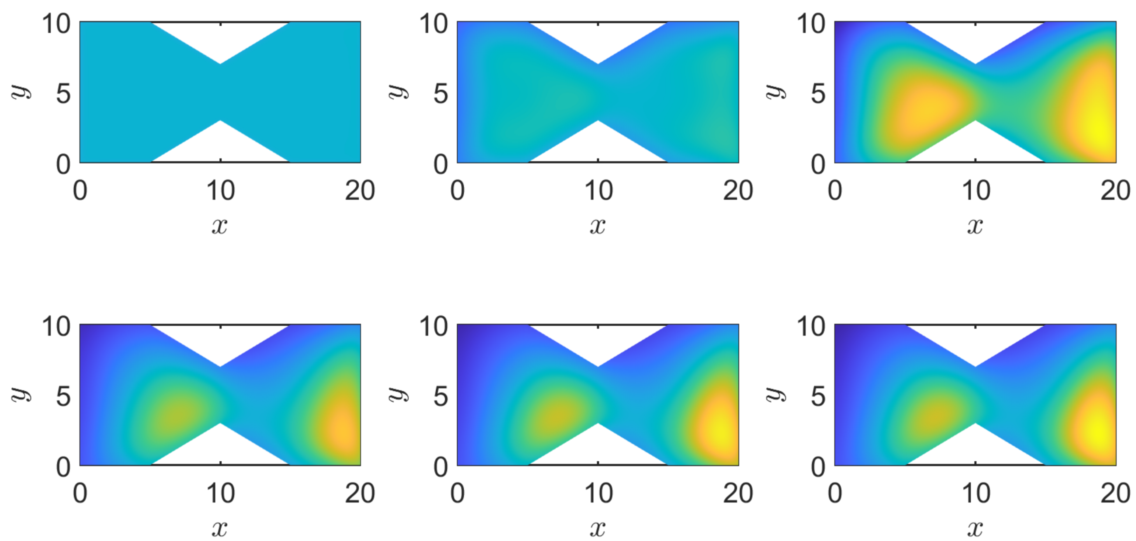

Figure 17: Multishape Example 3: Optimal ρ

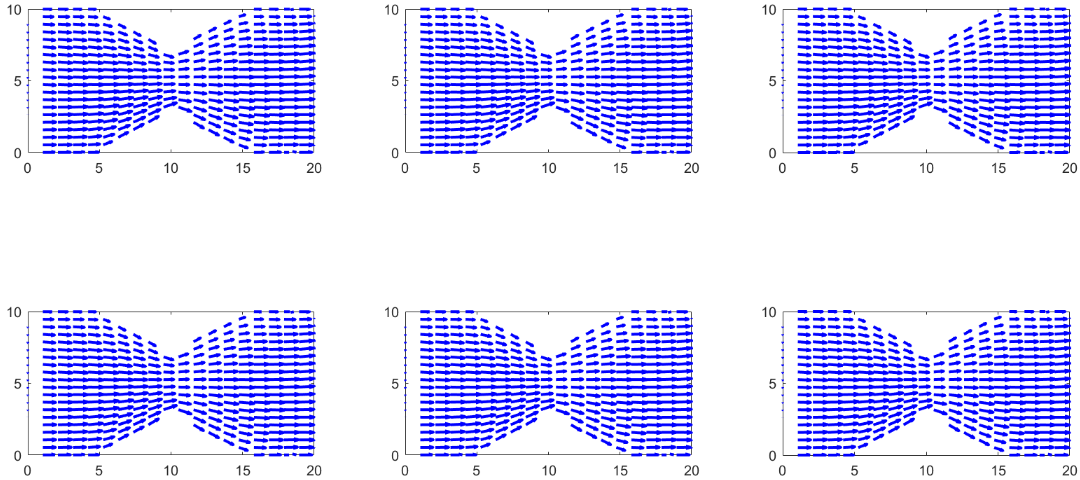

Figure 18: Multishape Example 3: Optimal control

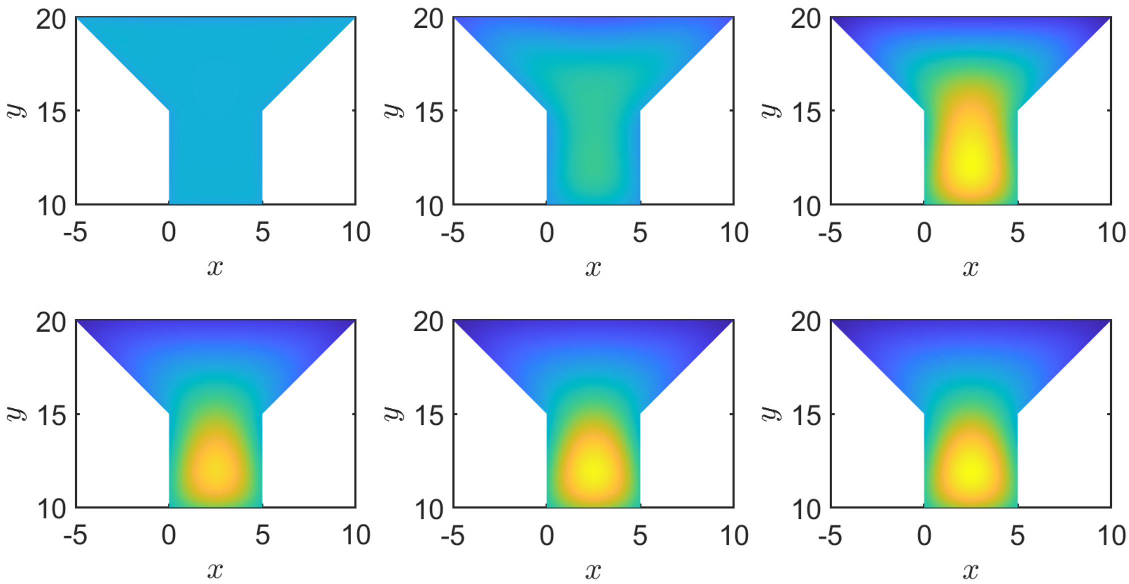

Figure 19: Multishape Example 1 (time independent control): Optimal ρ

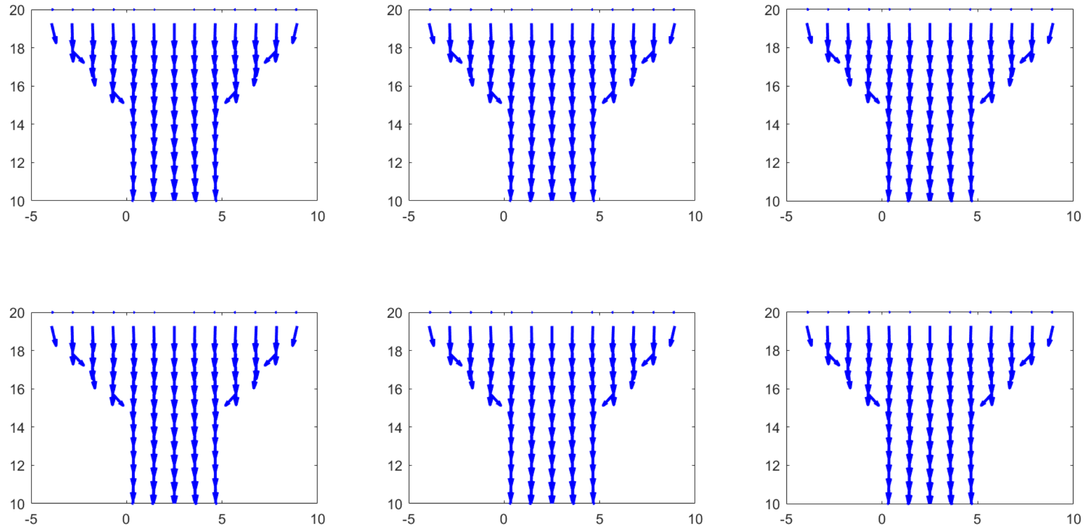

Figure 20: Multishape Example 1 (time independent control): Optimal control