1 Optimality conditions for the sedimentation equations

The relevant part of the equation is:

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

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:

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

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:

$$F_{2}(\rho+h) - F_{2}(\rho) = \nabla(\rho+h) \cdot \nabla\left(\frac{3-2a(\rho+h)}{(1-a(\rho+h))^{2}}\right) - \nabla\rho \cdot \nabla\left(\frac{3-2a\rho}{(1-a\rho)^{2}}\right)$$

$$= \nabla(\rho+h) \cdot \nabla\left(\frac{3-2a(\rho+h)}{(1-a\rho)^{2}} + \frac{3-2a(\rho+h)}{(1-a\rho)^{3}}2ah\right) - \nabla\rho \cdot \nabla\left(\frac{3-2a\rho}{(1-a\rho)^{2}}\right)$$

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

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

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

Finally, we have:

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

Combining these in the Lagrangian gives:

$$\begin{split} \mathcal{L}_{\rho}(\rho,\mathbf{w},q)h &= -\frac{1}{\beta} \int_{0}^{T} \int_{\Omega} q \nabla^{2} h \left(\frac{1}{1-a\rho} \right) + q \nabla^{2} \rho \left(\frac{a}{(1-a\rho)^{2}} h \right) \\ &+ q \nabla h \cdot \nabla \left(\frac{3-2a\rho}{(1-a\rho)^{2}} \right) + q \left(\nabla h \cdot \nabla \rho \right) \left(\frac{-2a}{(1-a\rho)^{2}} + \frac{6a-4a^{2}\rho}{(1-a\rho)^{3}} \right) \\ &+ q h \nabla \rho \cdot \nabla \left(\frac{-2a}{(1-a\rho)^{2}} + \frac{6a-4a^{2}\rho}{(1-a\rho)^{3}} \right) \\ &- q h \nabla^{2} \left(\frac{a\rho-2}{(a\rho-1)^{2}} \right) - q \rho \left(\frac{a}{(1-a\rho)^{2}} + \frac{2a^{2}\rho-4a}{(1-a\rho)^{3}} \right) \nabla^{2} h \\ &- q \rho \nabla \left(\frac{2a}{(1-a\rho)^{2}} + \frac{4a^{2}\rho-8a}{(1-a\rho)^{3}} \right) \cdot \nabla h - q \rho h \nabla^{2} \left(\frac{a}{(1-a\rho)^{2}} + \frac{2a^{2}\rho-4a}{(1-a\rho)^{3}} \right). \end{split}$$

Rearranging gives:

$$\begin{split} \mathcal{L}_{\rho}(\rho,\mathbf{w},q)h &= -\frac{1}{\beta} \int_{0}^{T} \int_{\Omega} h\bigg(q\nabla^{2}\rho\left(\frac{a}{(1-a\rho)^{2}}\right) + q\nabla\rho\cdot\nabla\left(\frac{-2a}{(1-a\rho)^{2}} + \frac{6a-4a^{2}\rho}{(1-a\rho)^{3}}\right) - q\nabla^{2}\left(\frac{a\rho-2}{(a\rho-1)^{2}}\right) \\ &- q\rho\nabla^{2}\left(\frac{a}{(1-a\rho)^{2}} + \frac{2a^{2}\rho-4a}{(1-a\rho)^{3}}\right) \bigg) \\ &+ \nabla h\cdot\left(q\nabla\left(\frac{3-2a\rho}{(1-a\rho)^{2}}\right) + q\nabla\rho\left(\frac{-2a}{(1-a\rho)^{2}} + \frac{6a-4a^{2}\rho}{(1-a\rho)^{3}}\right) - q\rho\nabla\left(\frac{2a}{(1-a\rho)^{2}} + \frac{4a^{2}\rho-8a}{(1-a\rho)^{3}}\right) \right) \\ &+ \nabla^{2}h\bigg(q\left(\frac{1}{1-a\rho}\right) - q\rho\left(\frac{a}{(1-a\rho)^{2}} + \frac{2a^{2}\rho-4a}{(1-a\rho)^{3}}\right) \bigg) \end{split}$$

Integration by parts gives:

$$\mathcal{L}_{\rho}(\rho, \mathbf{w}, q)h = -\frac{1}{\beta} \int_{0}^{T} \int_{\Omega} h \left(q \nabla^{2} \rho \left(\frac{a}{(1 - a\rho)^{2}} \right) + q \nabla \rho \cdot \nabla \left(\frac{-2a}{(1 - a\rho)^{2}} + \frac{6a - 4a^{2}\rho}{(1 - a\rho)^{3}} \right) - q \nabla^{2} \left(\frac{a\rho - 2}{(a\rho - 1)^{2}} \right) - q\rho \nabla^{2} \left(\frac{a}{(1 - a\rho)^{2}} + \frac{2a^{2}\rho - 4a}{(1 - a\rho)^{3}} \right) \right) - h\nabla \left(q \nabla \left(\frac{3 - 2a\rho}{(1 - a\rho)^{2}} \right) + q \nabla \rho \left(\frac{-2a}{(1 - a\rho)^{2}} + \frac{6a - 4a^{2}\rho}{(1 - a\rho)^{3}} \right) - q\rho \nabla \left(\frac{2a}{(1 - a\rho)^{2}} + \frac{4a^{2}\rho - 8a}{(1 - a\rho)^{3}} \right) \right) + h\nabla^{2} \left(q \left(\frac{1}{1 - a\rho} \right) - q\rho \left(\frac{a}{(1 - a\rho)^{2}} + \frac{2a^{2}\rho - 4a}{(1 - a\rho)^{3}} \right) \right)$$

So we have:

$$\begin{split} \mathcal{L}_{\rho}(\rho,\mathbf{w},q)h &= -\frac{1}{\beta} \int_{0}^{T} \int_{\Omega} h \bigg[q \nabla^{2} \rho \left(\frac{a}{(1-a\rho)^{2}} \right) + q \nabla \rho \cdot \nabla \left(\frac{-2a}{(1-a\rho)^{2}} + \frac{6a-4a^{2}\rho}{(1-a\rho)^{3}} \right) - q \nabla^{2} \left(\frac{a\rho-2}{(a\rho-1)^{2}} \right) \\ &- q \rho \nabla^{2} \left(\frac{a}{(1-a\rho)^{2}} \right) - q \rho \nabla^{2} \left(\frac{2a^{2}\rho-4a}{(1-a\rho)^{3}} \right) \\ &- \nabla \cdot \left(q \nabla \left(\frac{3-2a\rho}{(1-a\rho)^{2}} \right) \right) - \nabla \cdot \left(q \nabla \rho \left(\frac{-2a}{(1-a\rho)^{2}} \right) \right) - \nabla \cdot \left(q \nabla \rho \left(\frac{6a-4a^{2}\rho}{(1-a\rho)^{3}} \right) \right) \\ &+ \nabla \cdot \left(q \rho \nabla \left(\frac{2a}{(1-a\rho)^{2}} \right) \right) + \nabla \cdot \left(q \rho \nabla \left(\frac{4a^{2}\rho-8a}{(1-a\rho)^{3}} \right) \right) \\ &+ \nabla^{2} \left(q \left(\frac{1}{1-a\rho} \right) \right) - \nabla^{2} \left(q \rho \left(\frac{a}{(1-a\rho)^{2}} \right) \right) - \nabla^{2} \left(q \rho \left(\frac{2a^{2}\rho-4a}{(1-a\rho)^{3}} \right) \right) \bigg] dr dt \end{split}$$

And combining fractions gives:

$$\mathcal{L}_{\rho}(\rho, \mathbf{w}, q)h = -\frac{1}{\beta} \int_{0}^{T} \int_{\Omega} h \left[q \nabla^{2} \rho \left(\frac{a}{(1 - a\rho)^{2}} \right) + q \nabla \rho \cdot \nabla \left(\frac{2a(a\rho - 2)}{(1 - a\rho)^{3}} \right) - q \nabla^{2} \left(\frac{a\rho - 2}{(a\rho - 1)^{2}} \right) \right.$$

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

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

According to Mathematica this is:

$$\mathcal{L}_{\rho}(\rho,\mathbf{w},q)h = -\frac{1}{\beta} \int_{0}^{T} \int_{\Omega} h \left[\frac{1}{(a\rho-1)^{3}} \left(4a\nabla\rho \cdot \nabla q + 2a(-1+a\rho)q\nabla^{2}\rho + (-1+5a\rho-2a^{2}\rho^{2})\nabla^{2}q \right) \right] dr dt$$

And rewriting this is:

$$\mathcal{L}_{\rho}(\rho, \mathbf{w}, q)h = -\frac{1}{\beta} \int_{0}^{T} \int_{\Omega} h \left[\frac{4a\nabla\rho \cdot \nabla q}{(a\rho - 1)^{3}} + \frac{2aq\nabla^{2}\rho}{(a\rho - 1)^{2}} + \frac{(-1 + 5a\rho - 2a^{2}\rho^{2})\nabla^{2}q}{(a\rho - 1)^{3}} \right] dr dt$$

1.1 Boundary Terms

We have the equation:

$$\rho \nabla \frac{\delta F[\rho]}{\delta \rho} = \frac{1}{\beta} \left(\frac{\nabla \rho}{1 - \eta} - \rho \nabla \frac{\eta - 2}{(\eta - 1)^2} \right)$$

Then:

$$F_4(\rho) = \frac{\nabla \rho}{1 - a\rho}$$
$$F_5(\rho) = \rho \nabla \frac{a\rho - 2}{(a\rho - 1)^2}$$

Then for F_4 we have:

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

For F_5 we get:

$$F_{5}(\rho + h) - F_{5}(\rho) = (\rho + h)\nabla\frac{a(\rho + h) - 2}{(a(\rho + h) - 1)^{2}} - \rho\nabla\frac{a\rho - 2}{(a\rho - 1)^{2}}$$

$$= (\rho + h)\nabla\left(\frac{a(\rho + h) - 2}{(1 - a\rho)^{2}} + \frac{a(\rho + h) - 2}{(1 - a\rho)^{3}}2ah\right) - \rho\nabla\frac{a\rho - 2}{(a\rho - 1)^{2}}$$

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

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

Then the boundary terms for the Lagrangian are:

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

From the integration by parts of the terms within the domain we get:

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

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

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

$$- h\nabla \left(q \left(\frac{1}{1 - a\rho} \right) - q\rho \left(\frac{a}{(1 - a\rho)^2} + \frac{2a^2\rho - 4a}{(1 - a\rho)^3} \right) \right) \cdot \mathbf{n} dr dt$$

Combining all of these give all boundary terms for the Lagrangian

$$\mathcal{L}_{\rho}(\rho, \mathbf{w}, q)h = -\frac{1}{\beta} \int_{0}^{T} \int_{\partial\Omega} \left(h \left(q_{\partial\Omega} \nabla \rho \left(\frac{1}{(1 - a\rho)^{2}} \right) - q_{\partial\Omega} \nabla \left(\frac{a\rho - 2}{(1 - a\rho)^{2}} \right) \right) \right.$$

$$\left. - q_{\partial\Omega} \rho \nabla \left(\frac{a}{(1 - a\rho)^{2}} + \frac{2a^{2}\rho - 4a}{(1 - a\rho)^{3}} \right) + \left(q \nabla \left(\frac{3 - 2a\rho}{(1 - a\rho)^{2}} \right) + q \nabla \rho \left(\frac{-2a}{(1 - a\rho)^{2}} + \frac{6a - 4a^{2}\rho}{(1 - a\rho)^{3}} \right) \right.$$

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

$$+ \nabla h \left(q_{\partial\Omega} \left(\frac{1}{1 - a\rho} \right) - q_{\partial\Omega} \left(\rho \frac{a}{(1 - a\rho)^{2}} + \rho \frac{2a^{2}\rho - 4a}{(1 - a\rho)^{3}} \right) + q \left(\frac{1}{1 - a\rho} \right) \right.$$

$$\left. - q\rho \left(\frac{a}{(1 - a\rho)^{2}} + \frac{2a^{2}\rho - 4a}{(1 - a\rho)^{3}} \right) \right) \right) \cdot \mathbf{n} dr dt$$

Comparing terms in ∇h (there should be $\cdot \mathbf{n}$ everywhere in the below):

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

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

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

According to Mathematica this is:

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

Rearranging in terms of q gives:

$$\left[q\frac{(a-1)\nabla\rho}{(a\rho-1)^2} + \nabla q\frac{(1+a\rho)}{(a\rho-1)^3}\right] \cdot \mathbf{n} = 0$$

2 Constriction Flow

2.1 Equilibrium

We choose N = 50, n = 30 and a box from -3 to 3 in both directions. We choose the strength of V_{ext} to be 10 instead of 1000 as in the paper. We vary constriction width b and interaction strength κ in equilibrium.

For b = 0.6 and varying interaction strengths, the results are shown in Figures 1, 2 and 3.

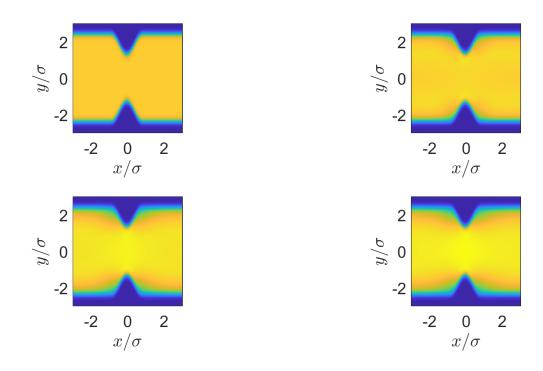


Figure 1: b = 0.6, $\kappa = -0.2$

In Figure 4 we see how the dynamics changes for a wider constriction (compare to Figure 2).

2.2 Non-Equilibrium

We impose a flow of size 1 on the equilibrium setup.

For b = 0.6 the results are displayed in Figures 5, 6, 7 and 8.

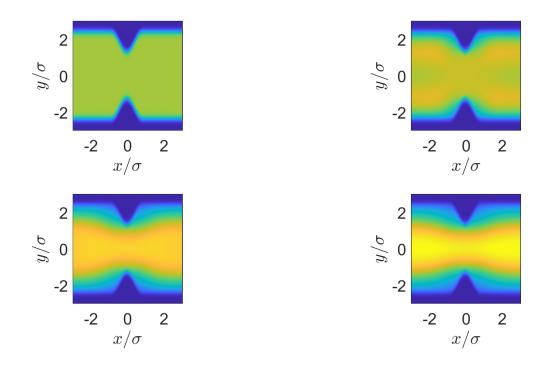


Figure 2: $b = 0.6, \, \kappa = -0.5$

3 Sedimentation

The result for the configurations as in Figure 8 in Archer's paper can be seen in Figure 9 (needs more points).

The result for the configurations as in Figure 10 in Archer's paper can be seen in Figures 10 and 11 (needs more points).

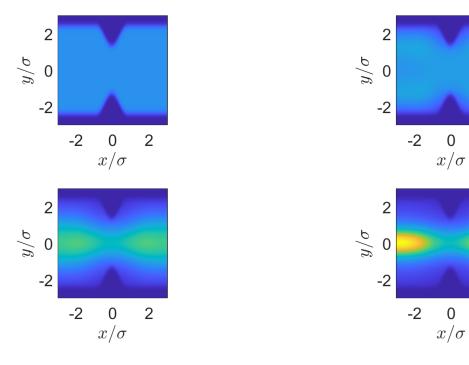


Figure 3: $b = 0.6, \kappa = -0.8$

2

2

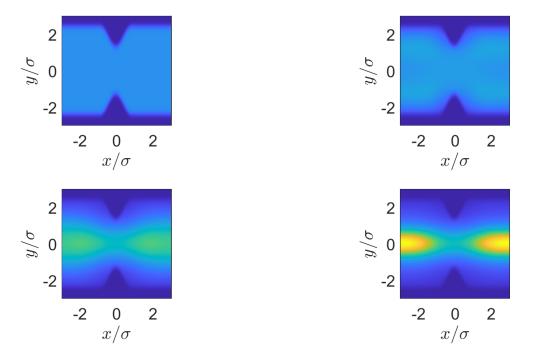


Figure 4: $b = 0.8, \, \kappa = -0.5$

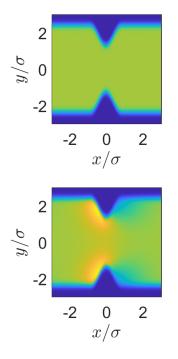


Figure 5: $b = 0.6, \kappa = 0$

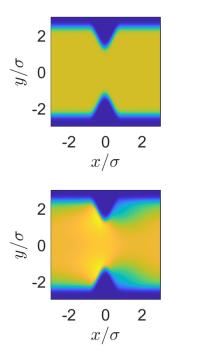
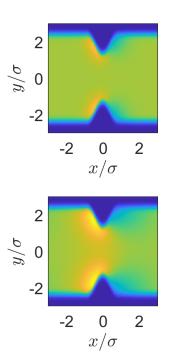
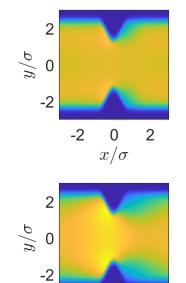


Figure 6: $b = 0.6, \, \kappa = -0.2$





 $0 \ x/\sigma$

2

-2

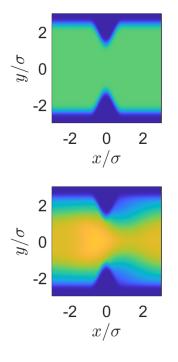


Figure 7: $b = 0.6, \, \kappa = -0.5$

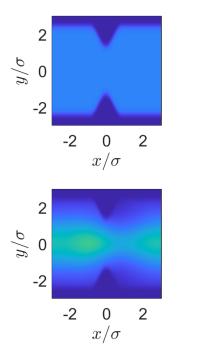
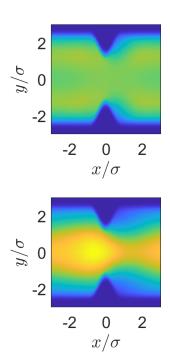
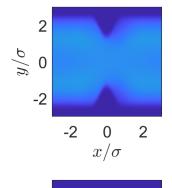
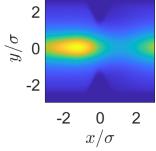


Figure 8: $b = 0.6, \, \kappa = -0.8$







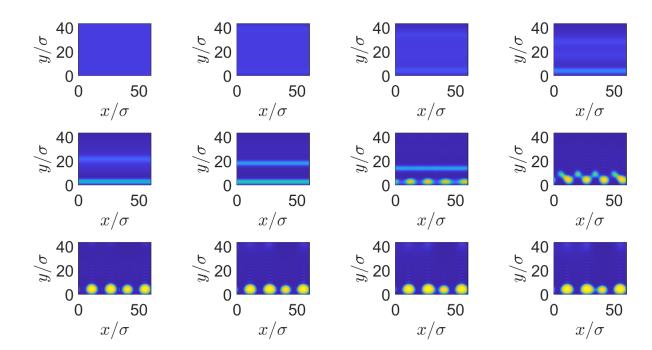


Figure 9: Result corresponding to Figure 8 in Archer's paper

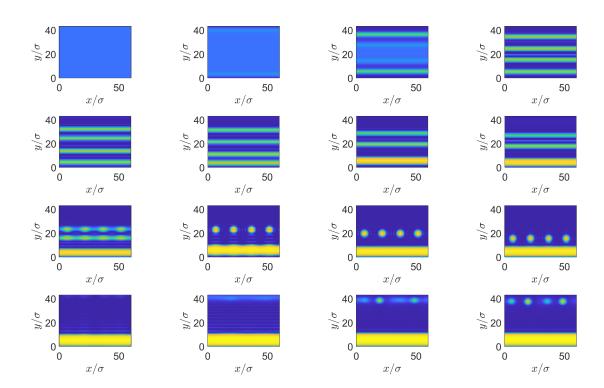


Figure 10: Result corresponding to Figure 10 in Archer's paper, at equispaced times

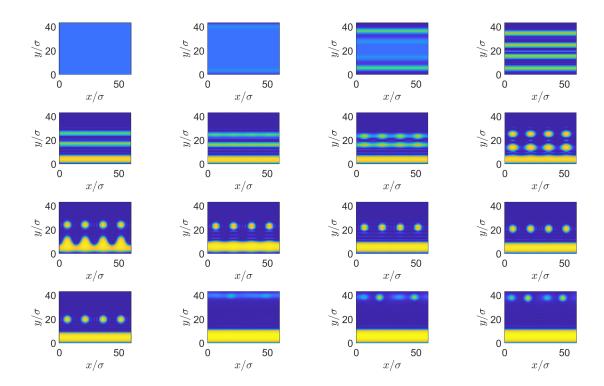


Figure 11: Result corresponding to Figure 10 in Archer's paper, at times 1,3,6,9,22,23,24,25,26,27,28,29,30, 43,46,49