Report 03/12/2020

1 Time independent control

We have the following OCP:

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

subject to:

$$\frac{\partial \rho}{\partial t} = \nabla^2 \rho - \nabla \cdot (\rho \mathbf{w}(r))$$

Then the Lagrangian is:

$$\begin{aligned}\mathcal{L}(\rho, \mathbf{w}, q) = &\frac{1}{2}\int_0^T \int_\Omega (\rho - \widehat{\rho})^2 dr dt + \frac{\beta}{2}\int_\Omega \mathbf{w}(r)^2 dr \\ &- \int_0^T \int_\Omega q\frac{\partial \rho}{\partial t} - q\nabla^2\rho + q\nabla \cdot (\rho \mathbf{w}) dr dt.\end{aligned}$$

And after integrating by parts (neglecting the BCs because we know them already):

$$\begin{aligned}\mathcal{L}(\rho, \mathbf{w}, q) = &\frac{1}{2}\int_0^T \int_\Omega (\rho - \widehat{\rho})^2 dr dt + \frac{\beta}{2}\int_\Omega \mathbf{w}(r)^2 dr \\ &- \int_0^T \int_\Omega q\frac{\partial \rho}{\partial t} - q\nabla^2\rho - \rho \mathbf{w} \cdot \nabla q dr dt.\end{aligned}$$

Taking derivatives with respect to $\mathbf{w}$ gives:

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

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

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

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 V_{ext} control

We have the following OCP:

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

subject to:

$$\frac{\partial \rho}{\partial t} = \nabla^2 \rho + \nabla \cdot (\rho \nabla V_{ext})$$

The Lagrangian is:

$$\begin{aligned}\mathcal{L}(\rho, V_{ext}, q) = &\frac{1}{2}\int_0^T \int_\Omega (\rho - \widehat{\rho})^2 dr dt + \frac{\beta}{2}\int_0^T \int_\Omega V_{ext}^2 dr \\ &- \int_0^T \int_\Omega q\frac{\partial \rho}{\partial t} - q\nabla^2 \rho - q\nabla \cdot (\rho \nabla V_{ext}) dr dt.\end{aligned}$$

We need to integrate by parts twice to get the term in V_{ext} into the necessary form:

$$\begin{aligned}\int_0^T \int_\Omega \nabla \cdot (\rho \nabla V_{ext}) dr dt &= \int_0^T \int_{\partial\Omega} q\rho\nabla V_{ext} \cdot \mathbf{n} dr dt - \int_0^T \int_\Omega \rho \nabla V_{ext} \cdot \nabla q dr dt \\ &= \int_0^T \int_{\partial\Omega} q\rho\nabla V_{ext} \cdot \mathbf{n} - \rho V_{ext} \nabla q \cdot \mathbf{n} dr dt + \int_0^T \int_\Omega V_{ext} \nabla(\rho \nabla q) dr dt\end{aligned}$$

We will also have

$$\int_0^T \int_\Omega q\nabla^2 \rho = \int_0^T \int_{\partial\Omega} q\nabla \rho \cdot \mathbf{n} - \rho \nabla q \cdot \mathbf{n} dr dt + \int_0^T \int_\Omega \rho \nabla^2 q dr dt$$

2.1 Boundary Conditions

And the boundary conditions:

$$\int_0^T \int_{\partial\Omega} q_{\partial\Omega} \nabla \rho \cdot \mathbf{n} + q_{\partial\Omega} \rho \nabla V_{ext} \cdot \mathbf{n} dr dt$$

Combining these:

$$\int_0^T \int_{\partial\Omega} q\rho\nabla V_{ext} \cdot \mathbf{n} - \rho V_{ext} \nabla q \cdot \mathbf{n} + q\nabla \rho \cdot \mathbf{n} - \rho \nabla q \cdot \mathbf{n} + q_{\partial\Omega} \nabla \rho \cdot \mathbf{n} + q_{\partial\Omega} \rho \nabla V_{ext} \cdot \mathbf{n} dr dt$$

During the derivation of the adjoint equation we have:

$$\int_0^T \int_{\partial\Omega} \mathbf{n} \cdot h\Big(q\nabla V_{ext} - V_{ext}\nabla q - \nabla q + q_{\partial\Omega} \nabla V_{ext}\Big) + \nabla h \cdot \mathbf{n}\Big(q + q_{\partial\Omega}\Big) dr dt$$

Then from the ∇h terms we get $q_{\partial\Omega} = -q$ and so:

$$(q\nabla V_{ext} - V_{ext}\nabla q - \nabla q - q\nabla V_{ext}) \cdot \mathbf{n} = 0$$

And therefore:

$$(1 + V_{ext})\frac{\partial q}{\partial n} = 0$$

Can we divide by $1 + V_{ext}$, is $V_{ext} > 0$.

2.2 Gradient Equation

We take the derivative of the Lagrangian with respect to V_{ext}:

$$\mathcal{L}_{V_{ext}}(\rho, V_{ext}, q)h = \int_0^T \int_\Omega \beta V_{ext} h + \nabla(\rho \nabla q) h dr dt + \int_0^T \int_{\partial\Omega} (q\rho\nabla h - \rho h \nabla q - q\rho\nabla h) \cdot \mathbf{n} dr dt$$

The boundary conditions just give (as before) $\frac{\partial q}{\partial n} = 0$ since $\rho > 0$. (+++ We don't do this, do we? But it would support my hypothesis that $1 + V_{ext}) > 0$ +++) Then from the terms within the domain we have:

$$\beta V_{ext} + \nabla(\rho \nabla q) = 0$$

And finally

$$V_{ext} = -\frac{1}{\beta}\nabla(\rho\nabla q).$$

3 Target at final time

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

subject to:

$$\frac{\partial \rho}{\partial t} = \nabla^2 \rho - \nabla \cdot (\rho \mathbf{w})$$

Then the Lagrangian is:

$$\mathcal{L}(\rho, \mathbf{w}, q) = \frac{1}{2}\int_\Omega (\rho(T) - \widehat{\rho}(T))^2 dr + \frac{\beta}{2}\int_0^T \int_\Omega \mathbf{w}^2 dr - \int_0^T \int_\Omega q\frac{\partial \rho}{\partial t} - q\nabla^2 \rho + q\nabla \cdot (\rho \mathbf{w}) dr dt.$$

From integrating by parts we get:

$$\int_0^T \int_\Omega -q\frac{\partial \rho}{\partial t} dr dt = -\int_\Omega q(T)\rho(T) - q(0)\rho(0) dr + \int_0^T \int_\Omega \rho \frac{\partial q}{\partial t} dr dt$$

$$\mathcal{L}(\rho, \mathbf{w}, q) = \frac{1}{2}\int_\Omega (\rho(T) - \widehat{\rho}(T))^2 dr + \frac{\beta}{2}\int_0^T \int_\Omega \mathbf{w}^2 dr - \int_\Omega q(T)\rho(T) - q(0)\rho(0) dr + \int_0^T \int_\Omega \rho\frac{\partial q}{\partial t} + q\nabla^2 \rho - q\nabla \cdot (\rho \mathbf{w}) dr dt.$$

Taking the derivative with respect to ρ gives:

$$\mathcal{L}_\rho(\rho, \mathbf{w}, q)h = \int_\Omega (\rho(T) - \widehat{\rho}(T))h(T)dr - \int_\Omega q(T)h(T)dr + \int_0^T \int_\Omega h\frac{\partial q}{\partial t} + q\nabla^2 h - q\nabla \cdot (h\mathbf{w})drdt.$$

Considering the terms for $h(T)$ gives:

$$(\rho(T) - \widehat{\rho}(T)) - q(T) = 0,$$

and so

$$q(T) = (\rho(T) - \widehat{\rho}(T))$$

The adjoint PDE remains unchanged.

4 Sedimentation

I ran the two different configurations with N = 100. I computed the mass in both cases and plotted the outcome. We can see that mass is still not constant but it is better than with $N = 70$.

```
  1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000

Columns 9 through 16

  1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000

Columns 17 through 24

  1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000

Columns 25 through 32

  1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000

Columns 33 through 40

  1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000

Columns 41 through 48

  1.0000    1.0000    1.0000    1.0001    1.0001    1.0001    1.0001    1.0002

Columns 49 through 56

  1.0002    1.0003    1.0003    1.0004    1.0005    1.0005    1.0006    1.0006

Columns 57 through 64

  1.0006    1.0005    1.0004    1.0006    1.0005    1.0004    1.0005    1.0007

Columns 65 through 72

  1.0008    1.0006    1.0003    1.0000    0.9996    0.9993    0.9989    0.9986

Columns 73 through 80

  0.9982    0.9979    0.9976    0.9973    0.9970    0.9967    0.9964    0.9961

Columns 81 through 88

  0.9959    0.9956    0.9954    0.9952    0.9950    0.9948    0.9946    0.9945

Columns 89 through 96

  0.9943    0.9942    0.9941    0.9939    0.9938    0.9938    0.9937    0.9936

Columns 97 through 100

  0.9936    0.9936    0.9935    0.9935
```

Figure 1: Figure 8 in paper, mass for each time

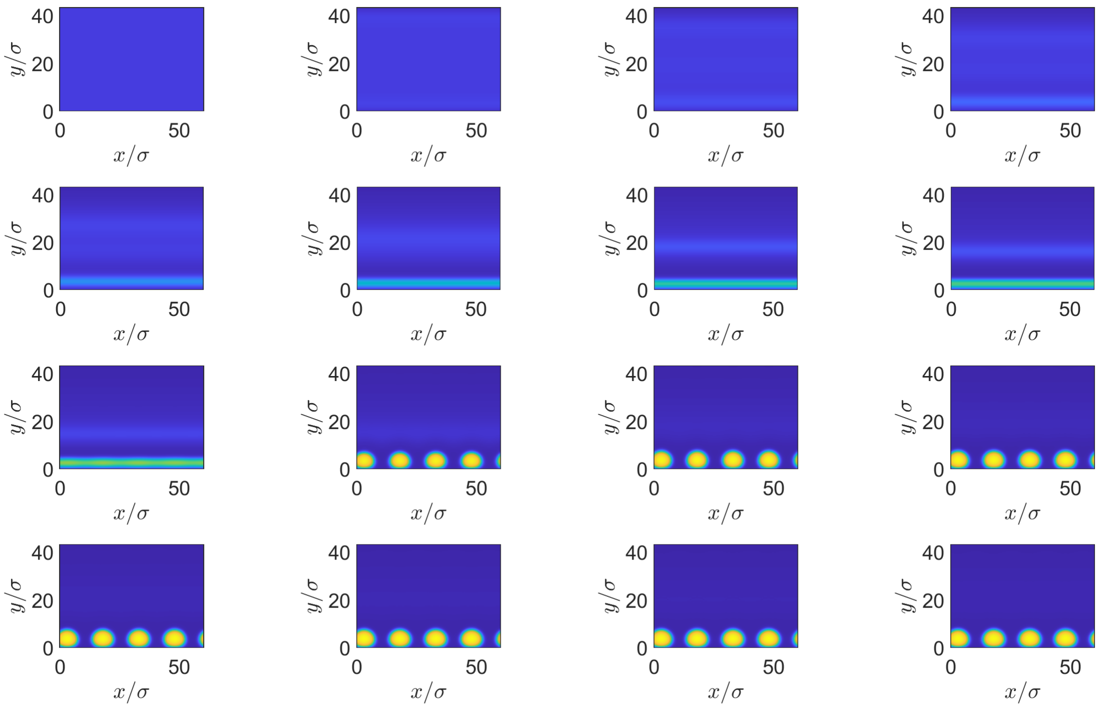

Figure 2: Figure 8 in paper, result at each time

5 MultipleSpecies forward problem

The forward problem is showing weird oscillations. Maybe I implemented this incorrectly. Figure 7 shows what happens with diffusion only. Figure 8 and 9 shows what happens with advection in opposite direction, attraction to the own species and repulsion with the other

6 Other

- sedimentation optimality conditions - next week - holiday

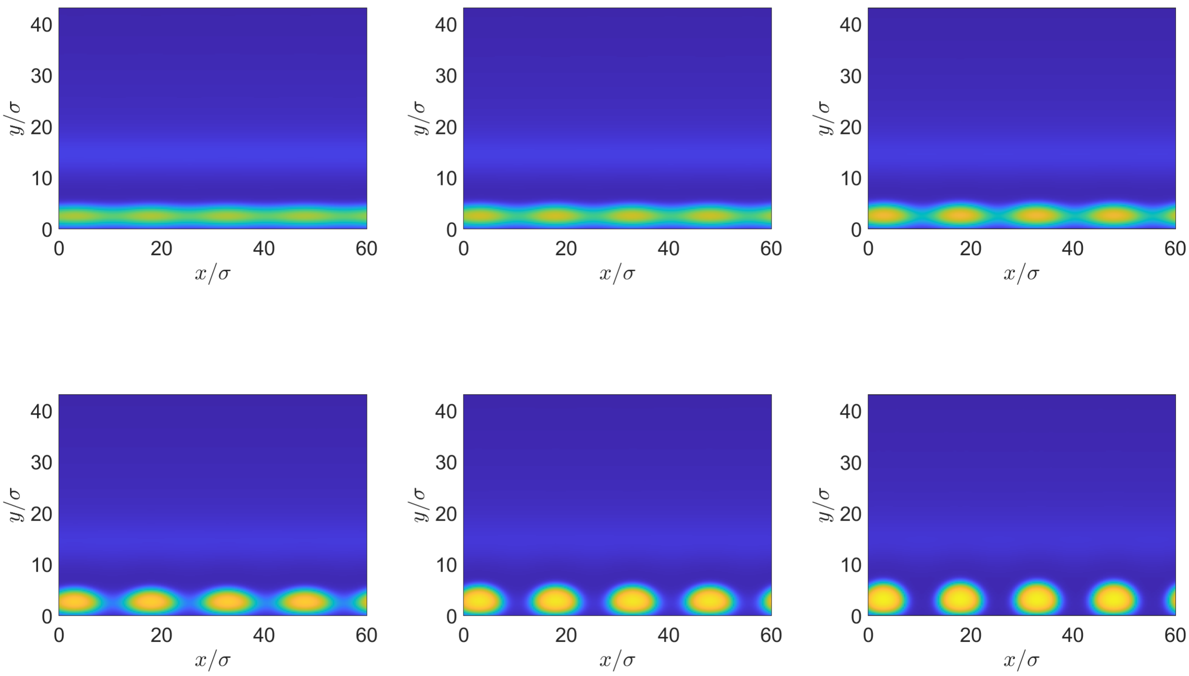

Figure 3: Figure 8 in paper, result at times 57 - 62 out of 100

```
Columns 1 through 8

  1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000

Columns 9 through 16

  1.0000    1.0000    1.0000    1.0000    0.9999    0.9999    0.9999    0.9998

Columns 17 through 24

  0.9998    0.9997    0.9997    0.9999    0.9999    0.9996    0.9999    1.0005

Columns 25 through 32

  1.0021    1.0020    1.0004    1.0005    1.0022    1.0018    1.0000    1.0009

Columns 33 through 40

  1.0020    1.0003    1.0003    1.0014    1.0005    1.0006    1.0005    1.0014

Columns 41 through 48

  0.9999    1.0017    1.0017    1.0000    1.0022    1.0008    1.0005    1.0032

Columns 49 through 56

  1.0031    1.0021    1.0024    1.0010    1.0001    1.0004    0.9988    0.9983

Columns 57 through 64

  0.9985    0.9969    0.9972    0.9972    0.9966    0.9979    0.9983    0.9986

Columns 65 through 72

  0.9986    0.9987    0.9985    0.9980    0.9986    1.0007    1.0034    1.0062

Columns 73 through 80

  1.0091    1.0118    1.0144    1.0169    1.0193    1.0215    1.0235    1.0254

Columns 81 through 88

  1.0272    1.0288    1.0303    1.0317    1.0330    1.0341    1.0351    1.0360

Columns 89 through 96

  1.0368    1.0375    1.0382    1.0387    1.0392    1.0396    1.0399    1.0402

Columns 97 through 100
```

Figure 4: Figure 10 in paper, mass for each time

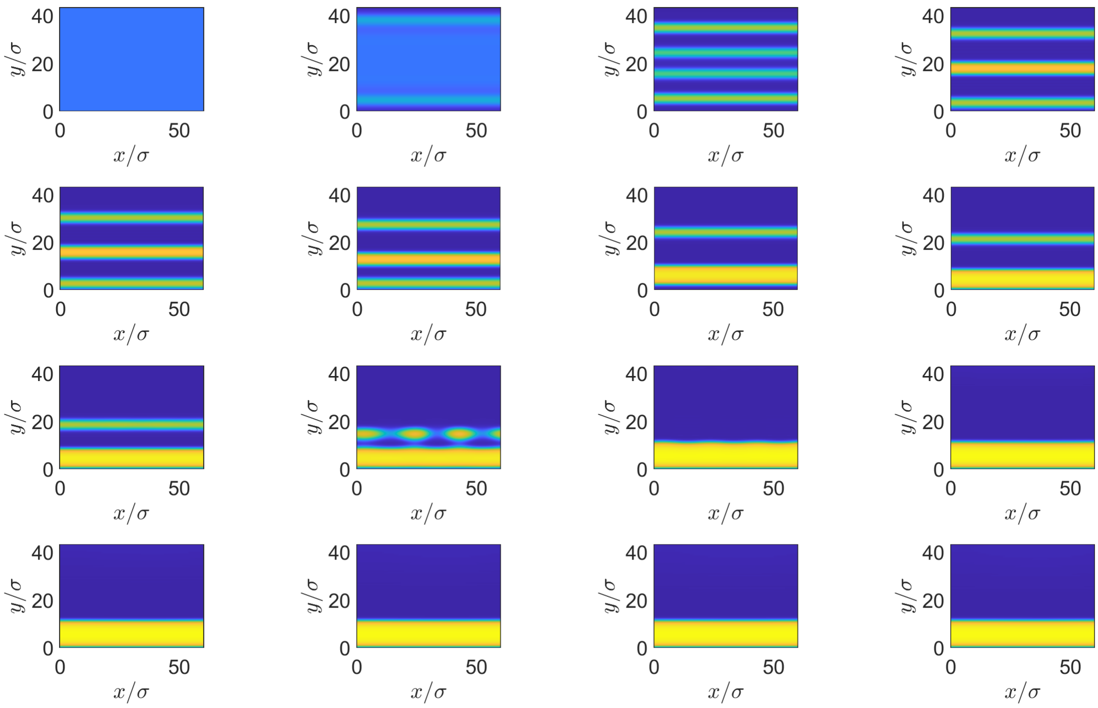

Figure 5: Figure 10 in paper, result at each time

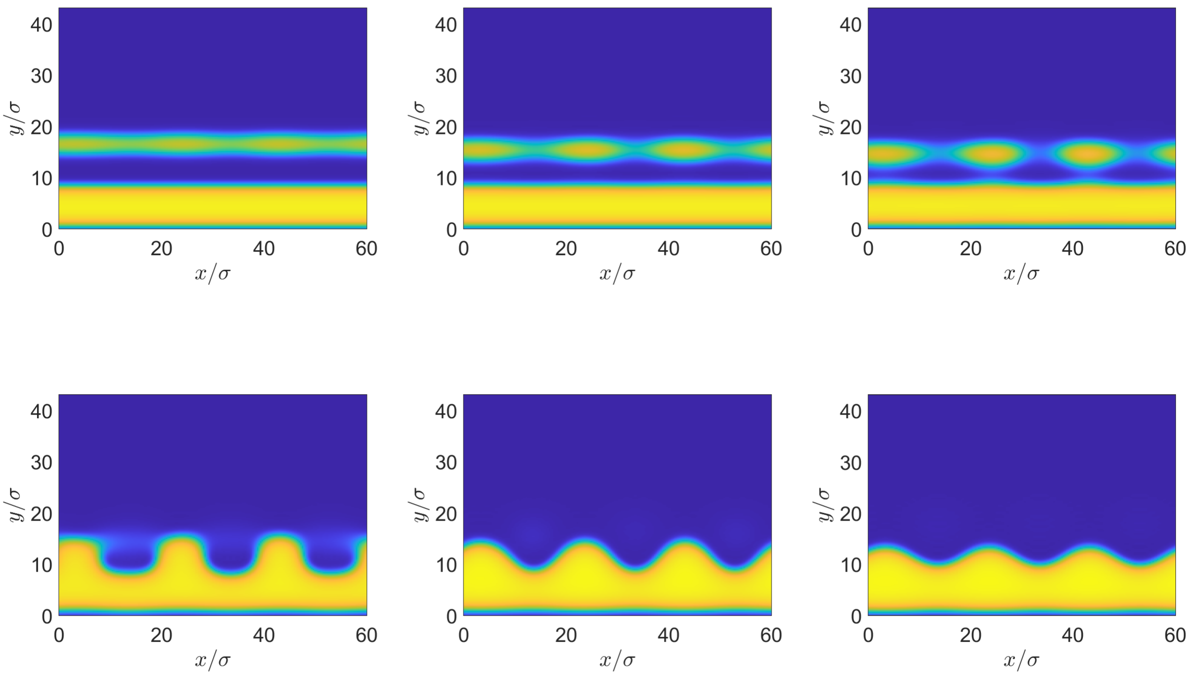

Figure 6: Figure 8 in paper, result at times 60 - 66 out of 100

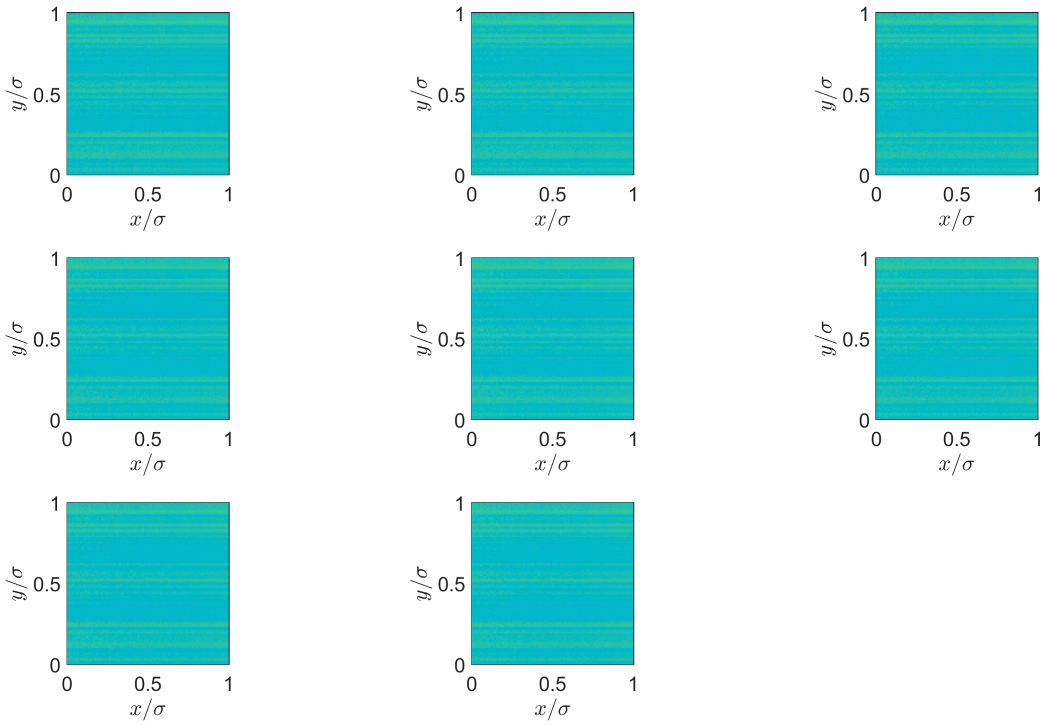

Figure 7: Weird Oscillations for diffusion only

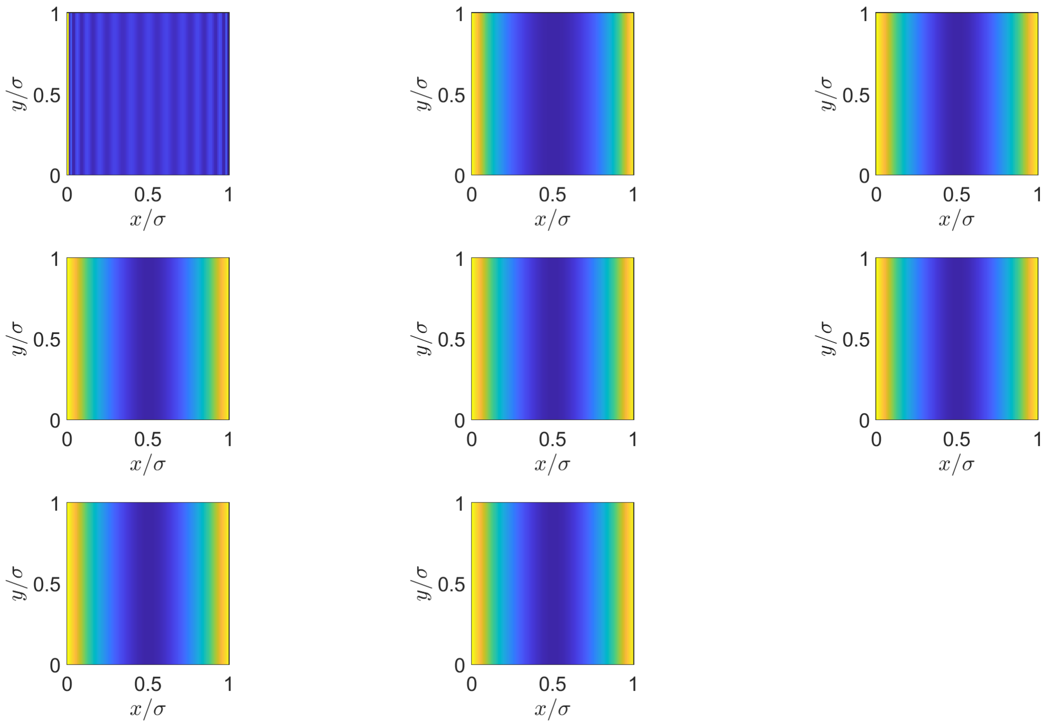

Figure 8: Maybe plausible behaviour ρ_a

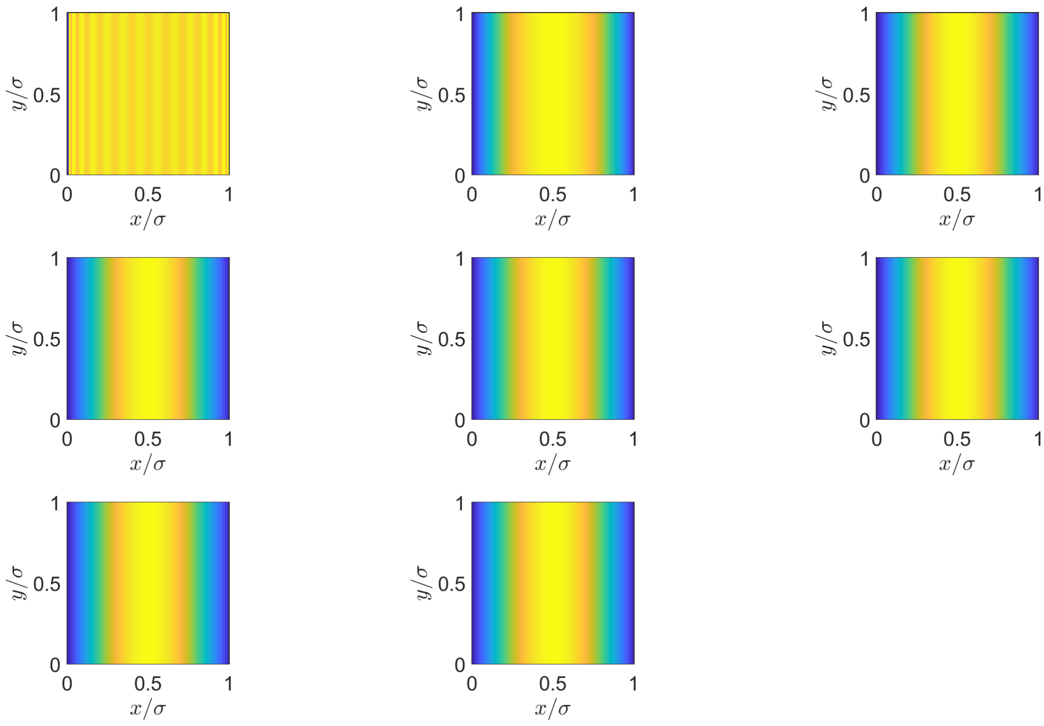

Figure 9: Maybe plausible behaviour ρ_b