- Dante: where does the 1/2 come from??

- BCs?
- Dt?
-$\nabla \mathbf{v}$ transpose implementation
- division by rho?
- 'good' test problem?
- what is a small beta here?
- naming convention for things?
- I think that maybe high friction is good for the FW problem but bad for the adjoint. Not 100 percent sure but it looks a bit like this...
- Convergence fluctuates (FixPt) – never did this in the AD problems. Why?
- Fun 1 worked with friction = 5 and beta = 10 but not for lower beta
- I think solving 4 instead of 2 PDEs makes it slower with increasing number of points
- generally quite unstable at the moment but it's just the beginning :)
- Is there an exact solution? (- i.e. does it make sense at this point to look for one...)

1 Archer forward problem

$$
\begin{aligned}
m\rho \frac{\partial \mathbf{v}}{\partial t} &= -m\rho(\mathbf{v}\cdot\nabla)\mathbf{v} - \rho\nabla V_{ext} - \nabla\rho - m\gamma\rho\mathbf{v} \qquad && \text{in} \quad \Sigma \\
\frac{\partial \rho}{\partial t} &= -\nabla\cdot(\rho\mathbf{v})
\end{aligned}
$$

$$
\rho\mathbf{v}\cdot\mathbf{n} = 0 \qquad \text{on } \partial\Omega
$$

- Problem: we need to divide by ρ, which means that it can never be zero
- Problem: one boundary condition for the system.

$$
\begin{aligned}
\frac{\partial \mathbf{v}}{\partial t} &= \frac{1}{m\rho}\Big(- m\rho(\mathbf{v}\cdot\nabla)\mathbf{v} - \rho\nabla V_{ext} - \nabla\rho - m\gamma\rho\mathbf{v}\Big) \qquad && \text{in} \quad \Sigma \\
\frac{\partial \rho}{\partial t} &= -\nabla\cdot(\rho\mathbf{v})
\end{aligned}
$$

$$
\rho\mathbf{v}\cdot\mathbf{n} = 0 \qquad \text{on } \partial\Omega
$$

- Running the FW problem like this. Using initial conditions for ρ and $\mathbf{v}$:

$$\rho_0 = (1/2.2)(\sin(\pi y) + 1.1)$$
$$\mathbf{v}_0 = ((1/2)\cos(\pi y) + 1/2)$$

  The focus was that ρ_0 integrates to one and that $\mathbf{v}_0$ is zero on the boundary.

- Applying the boundary condition to the equation for ρ works, doing it for both equations or for the $\mathbf{v}$ equation does not ($DAE > 1$). Increasing points changes nothing.
- Chose $\nabla V^{ext} = 2y$.
- If γ gets too small we get the error with the integration tolerance. Can't be solved by more points. Doesn't solve the PDEs for more than a few time points (if even) then. With the choice of variables above, this cutoff is somewhere between $\gamma = 10$ and $\gamma = 1$. With increasing ∇V^{ext}, this cut-off needs to be even higher as far as I can tell.

Test to rewrite the problem using $\rho = e^q$:

$$\frac{\partial \mathbf{v}}{\partial t} = \frac{1}{m}\Big(- m(\mathbf{v}\cdot\nabla)\mathbf{v} - \nabla V_{ext} - q - m\gamma\mathbf{v}\Big) \qquad \text{in} \quad \Sigma$$
$$\frac{\partial q}{\partial t} = -\mathbf{v}\cdot\nabla q - \nabla \mathbf{v}$$

$$e^q \mathbf{v}\cdot\mathbf{n} = 0 \qquad \text{on } \partial\Omega$$

This actually doesn't change anything, at least as seen in the plots.

1.1 Forward Problem – some 'results'

Choosing

$$\rho_0 = (1/2.2)(\sin(\pi y) + 1.1)$$
$$\mathbf{v}_0 = ((1/2)\cos(\pi y) + 1/2)$$
$$\nabla V_1^{ext} = 2y$$

we get the following results (with ODE tolerance 10^{-3}, $N = 30$, $n = 20$), see Figures 1, 2 and 3 for $\gamma = 5000, 100, 10$. For $\nabla V_2^{ext} = 1$, see Figures 4,5, and 6. There is a small effect from ∇V_1^{ext} to ∇V_2^{ext} visible.

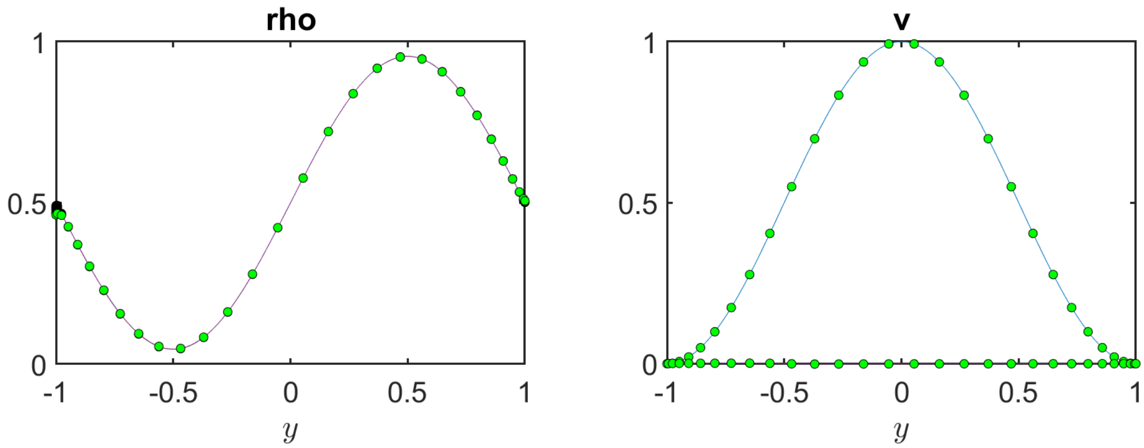

Figure 1: Result for ∇V_1^{ext} with $\gamma = 5000$

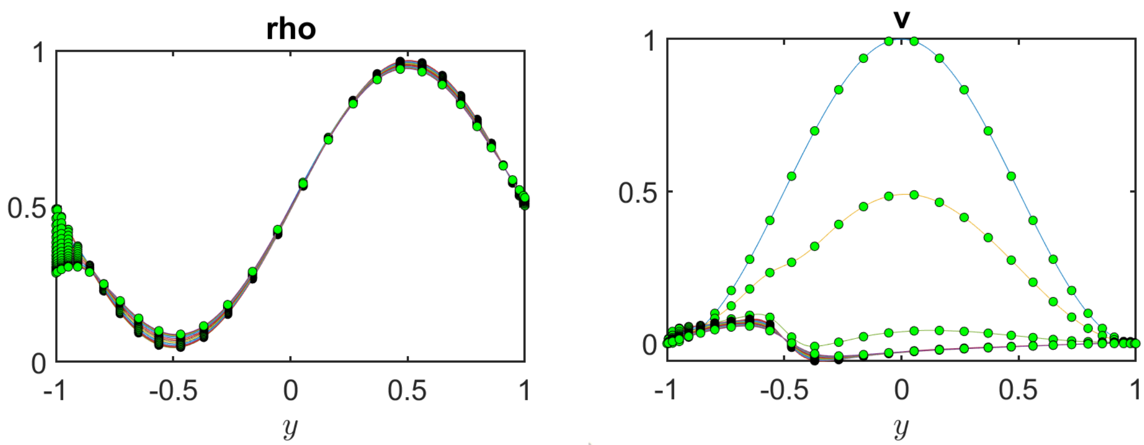

Figure 2: Result for ∇V_1^{ext} with $\gamma = 100$

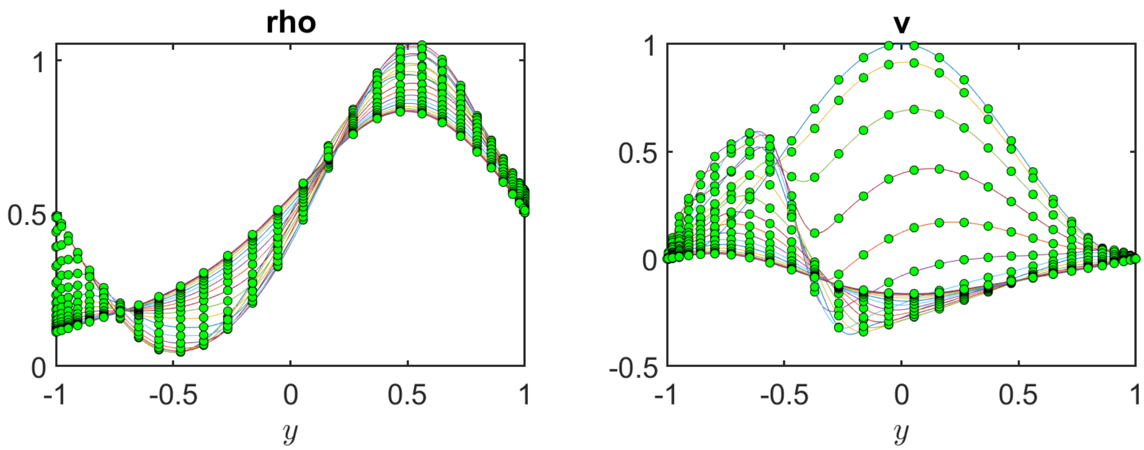

Figure 3: Result for ∇V_1^{ext} with $\gamma = 10$

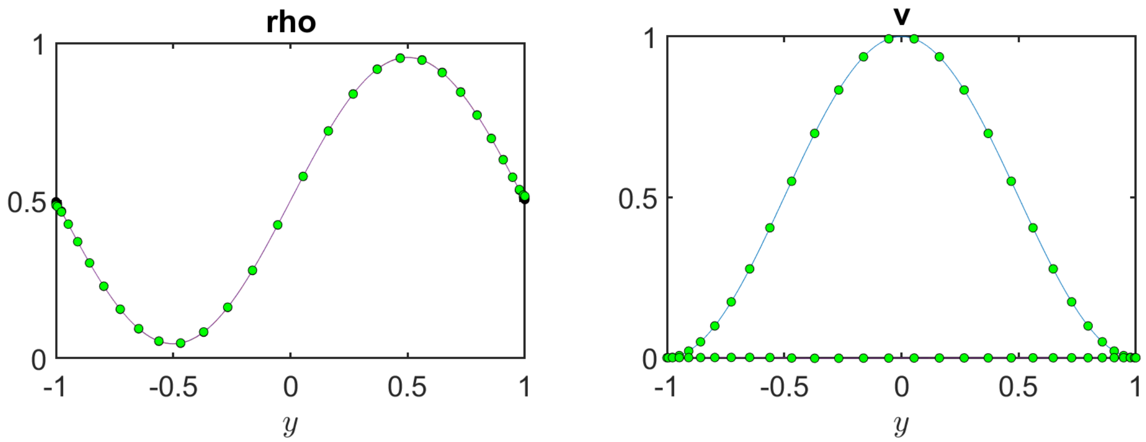

Figure 4: Result for ∇V_2^{ext} with $\gamma = 5000$

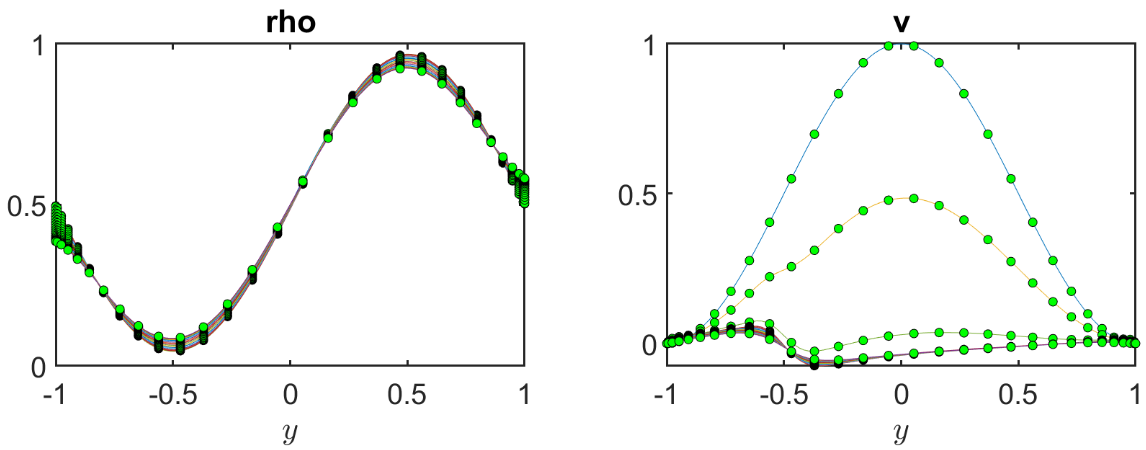

Figure 5: Result for ∇V_2^{ext} with $\gamma = 100$

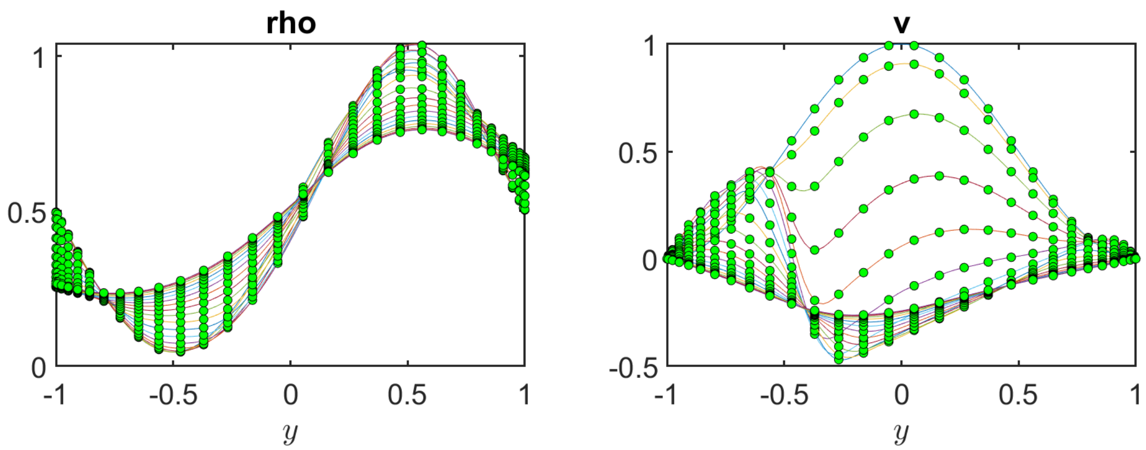

Figure 6: Result for ∇V_2^{ext} with $\gamma = 10$

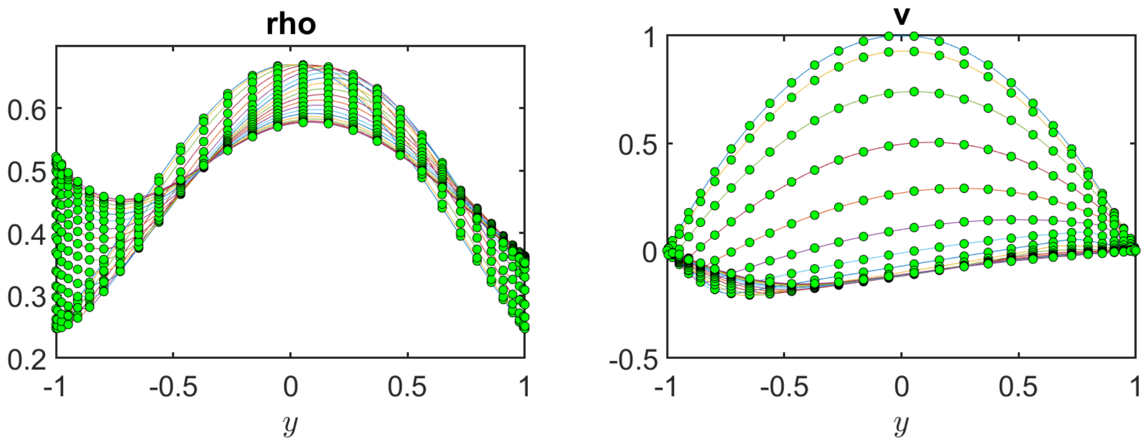

Figure 7: Result for ∇V_2^{ext} with $\gamma = 10$

Choosing instead:

$$\rho_0 = (1/1.4937)e^{-y.^2}$$
$$\mathbf{v}_0 = -y^2 + 1$$
$$\nabla V_2^{ext} = 1$$

We get the following result for $\gamma = 10$, see Figure 7.

2 Optimal Control Problem - 'Potential Control'

$$\min_{\rho,\mathbf{v},\nabla V^{ext}} \quad \frac{1}{2}||\rho - \hat{\rho}||^2_{L_2(\Sigma)} + \frac{\alpha}{2}||\mathbf{v} - \hat{\mathbf{v}}||^2_{L_2(\Sigma)} + \frac{\beta}{2}||\nabla V^{ext}||^2_{L_2(\Sigma)}$$

subject to:

$$\frac{\partial \mathbf{v}}{\partial t} = \frac{1}{m\rho}\Big(- m\rho(\mathbf{v}\cdot\nabla)\mathbf{v} - \rho\nabla V^{ext} - \nabla\rho - m\gamma\rho\mathbf{v}\Big) \qquad \text{in} \quad \Sigma$$

$$\frac{\partial \rho}{\partial t} = -\nabla\cdot(\rho\mathbf{v})$$

$$\rho\mathbf{v}\cdot\mathbf{n} = 0 \qquad \text{on } \partial\Omega$$

2.1 Optimality Conditions

Adjoint Equation 1:

$$
\begin{aligned}
&\frac{\partial q}{\partial t} = (\rho - \hat{\rho}) + m\frac{\partial \mathbf{v}}{\partial t} \cdot \mathbf{p}_\Sigma + m((\mathbf{v} \cdot \nabla)\mathbf{v}) \cdot \mathbf{p}_\Sigma + \nabla V_{ext} \cdot \mathbf{p}_\Sigma - \nabla \cdot \mathbf{p}_\Sigma - \ \nabla q \cdot \mathbf{v} \\
&+ m\gamma \mathbf{v} \cdot \mathbf{p}_\Sigma \qquad\qquad\qquad\qquad \text{in} \quad \Sigma \\
&\mathbf{p}_\Sigma \cdot \mathbf{n} = 0 \qquad \text{on} \quad \partial\Sigma \\
&q(T) = 0
\end{aligned}
$$

Adjoint Equation 2:

$$
\begin{aligned}
&\frac{\partial \mathbf{p}_\Sigma}{\partial t} = \frac{1}{m\rho}\Big(\alpha(\mathbf{v} - \hat{\mathbf{v}}) - m\frac{\partial \rho}{\partial t}\mathbf{p}_\Sigma - \rho\nabla q + m\rho(\nabla \mathbf{v})^\top \mathbf{p}_\Sigma + m\gamma\rho\mathbf{p}_\Sigma \\
&- m\rho(\mathbf{v} \cdot \nabla)\mathbf{p}_\Sigma - m\rho(\nabla \cdot \mathbf{v})\mathbf{p}_\Sigma - m(\mathbf{v} \cdot \nabla\rho)\mathbf{p}_\Sigma\Big) \qquad\qquad \text{in} \quad \Sigma \\
&\mathbf{p}_\Sigma(T) = \mathbf{0}.
\end{aligned}
$$

Gradient Equation:

$$\nabla V^{ext} = \frac{1}{\beta}\rho\mathbf{p}$$

2.2 First Results (provided correct implementation?)

Choosing (ρ mass 1, $\mathbf{v}$ BCs zero, ∇V^{ext} sort of in line with gradient eqation, i.e. something containing ρ and final time condition for $\mathbf{p}$ satisfied):

$$
\begin{aligned}
\rho_0 &= (1/2.2)(\sin(\pi y) + 1.1) \\
\mathbf{v}_0 &= -y^2 + 1 \\
\nabla V_3^{ext} &= (1/\beta)(e^T - e^t)((1/2)\cos(\pi y) + 1/2)
\end{aligned}
$$

The targets are:

$$
\begin{aligned}
rhoTarget &= (1-t)(1/2.2)(\sin(\pi y) + 1.1) + t(1/1.4937)\exp(-y^2) \\
vTarget &= (1-t)(-y^2 + 1) + t(((1/2)\cos(\pi y) + 1/2))
\end{aligned}
$$

Then choosing very easy settings: $\beta = 10$, ODE tols $= 10^{-6}$, optimality tols $= 10^{-3}$, $\gamma = 5$ and $\alpha = m = 1$, $N = 30$, $n = 20$, $\lambda = 0.01$ this converges, see Figure 8. Converges in around $700 - 800$ iterations but the results are $J_{FW} = 0.6868$, $J_{Opt} = 2.1045$. So something is wrong. (And smaller β diverge quickly.)

Next try rhoHat, vHat from forward problem. The results are $J_{FW} = 0.0466$ and $J_{Opt} = 6.5415e - 04$, so that's good. the results are in Figure 9. It converges in about 500 iterations.

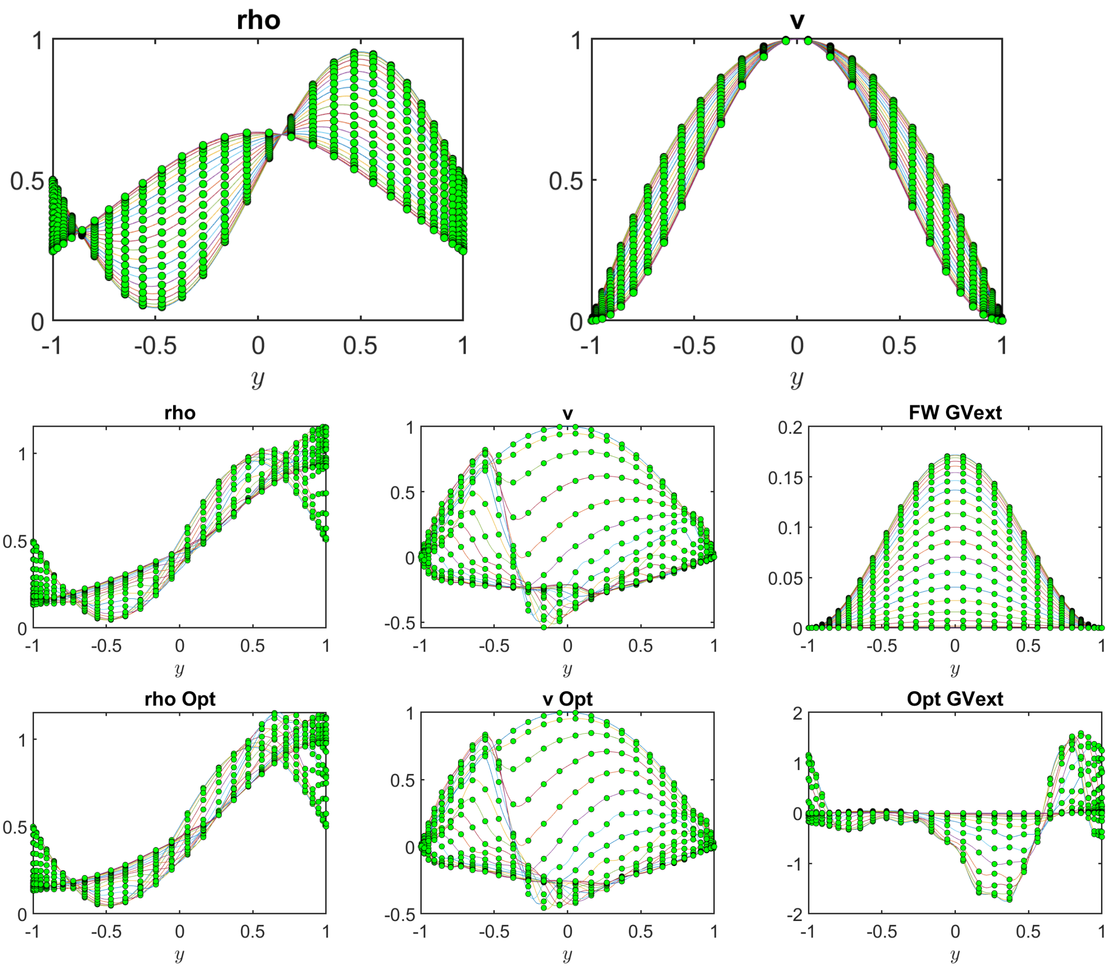

Figure 8: targets (top), FW Result OCP (middle), Opt (bottom) for ∇V_3^{ext} with $\gamma = 10$

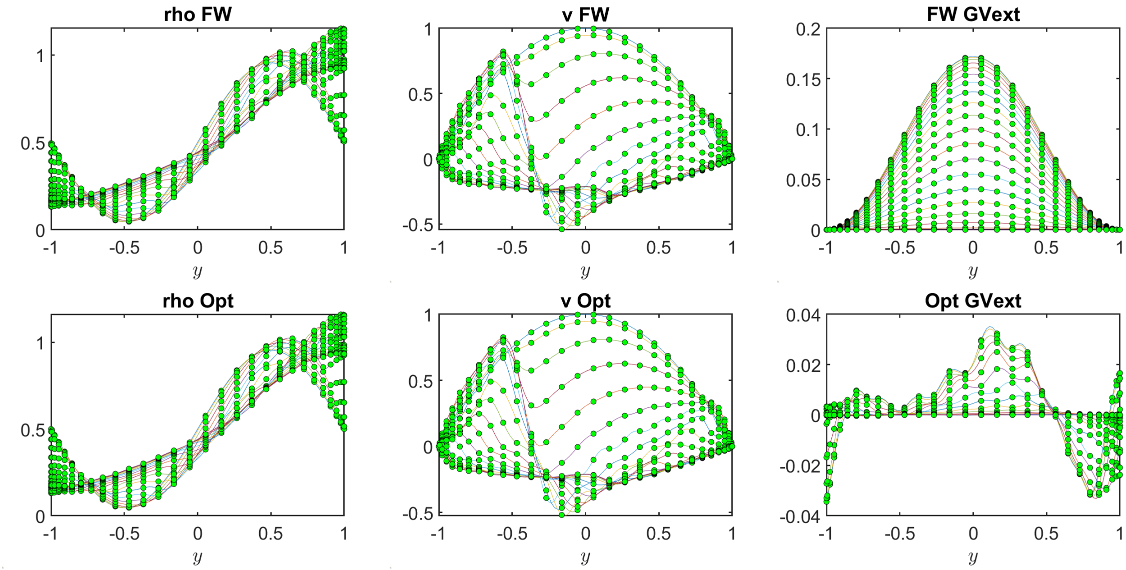

Figure 9: FW Result OCP (top), Opt (bottom) for ∇V_3^{ext} with $\beta = 10$ and FW result is target

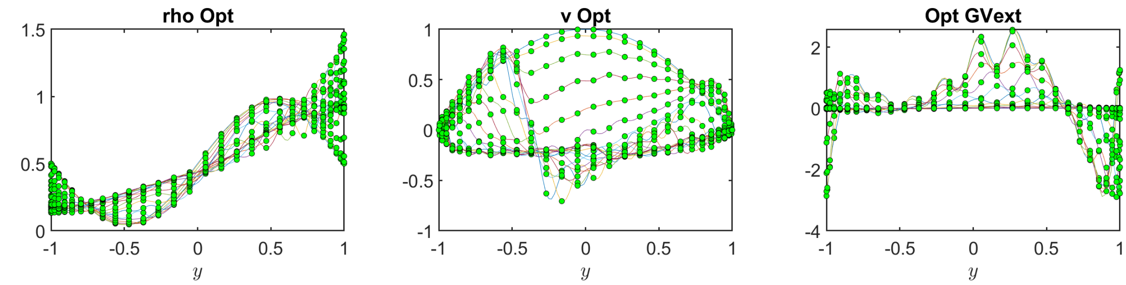

Figure 10: FW Result OCP (top), Opt (bottom) for ∇V_3^{ext} with $\beta = 1$ and FW result is target

For $\beta = 1$ this converges too, but it takes 1000 iterations and looks much more unstable, see Figure 10. With these configurations $\beta = 10^{-1}$ doesn't even work for the forward problem. It is clear that the choice of initial inputs isn't very good, some of the solutions aren't so stable. However, it doesn't help to increase the points or decrease the tolerances.

2.3 Change ∇V^{ext}

Change it to be independent of β this stabilizes the forward problem. Consequently also the OCP. Choose same as before, minus beta dependence.

$$\begin{aligned}\rho_0 &= (1/2.2)(\sin(\pi y) + 1.1)\\ \mathbf{v}_0 &= -y^2 + 1\\ \nabla V_3^{ext} &= (e^T - e^t)((1/2)\cos(\pi y) + 1/2)\end{aligned}$$

The targets come from forward problem. $\beta = 10^{-1}$ still doesn't work (diverges). Observation (again): the forward problem likes larger γ, but the OCP diverges faster if γ is larger. Still works for $\beta = 1$.

3 Optimal Control Problem - Force Control

The OCP:

$$\begin{aligned}&\min_{\rho,\mathbf{v},\mathbf{f}} \quad \frac{1}{2}||\rho - \hat{\rho}||^2_{L_2(\Sigma)} + \frac{\alpha}{2}||\mathbf{v} - \hat{\mathbf{v}}||^2_{L_2(\Sigma)} + \frac{\beta}{2}||\mathbf{f}||^2_{L_2(\Sigma)}\\ &\text{subject to:}\\ &\frac{\partial \mathbf{v}}{\partial t} = \frac{1}{m\rho}\Big(- m\rho(\mathbf{v}\cdot\nabla)\mathbf{v} - \rho\nabla V_{ext} - \nabla\rho - m\gamma\rho\mathbf{v} - \mathbf{f}\Big) \qquad \text{in} \quad \Sigma\\ &\frac{\partial \rho}{\partial t} = -\nabla\cdot(\rho\mathbf{v})\\ &\\ &\rho\mathbf{v}\cdot\mathbf{n} = 0 \qquad \text{on } \partial\Omega\end{aligned}$$

3.1 Optimality Conditions

Adjoint Equation 1:

$$\begin{aligned}&\frac{\partial q}{\partial t} = (\rho - \hat{\rho}) + m\frac{\partial \mathbf{v}}{\partial t}\cdot\mathbf{p}_\Sigma + m((\mathbf{v}\cdot\nabla)\mathbf{v})\cdot\mathbf{p}_\Sigma + \nabla V_{ext}\cdot\mathbf{p}_\Sigma - \nabla\cdot\mathbf{p}_\Sigma - \nabla q\cdot\mathbf{v}\\ &+ m\gamma\mathbf{v}\cdot\mathbf{p}_\Sigma \qquad \text{in} \quad \Sigma\\ &\mathbf{p}_\Sigma\cdot\mathbf{n} = 0 \qquad \text{on} \quad \partial\Sigma\\ &q(T) = 0\end{aligned}$$

Adjoint Equation 2:

$$\frac{\partial \mathbf{p}_\Sigma}{\partial t} = \frac{1}{m\rho}\bigg(\alpha(\mathbf{v}-\hat{\mathbf{v}}) - m\frac{\partial \rho}{\partial t}\mathbf{p}_\Sigma - \rho\nabla q + m\rho(\nabla\mathbf{v})^\top\mathbf{p}_\Sigma + m\gamma\rho\mathbf{p}_\Sigma$$
$$- m\rho(\mathbf{v}\cdot\nabla)\mathbf{p}_\Sigma - m\rho(\nabla\cdot\mathbf{v})\mathbf{p}_\Sigma - m(\mathbf{v}\cdot\nabla\rho)\mathbf{p}_\Sigma\bigg) \qquad \text{in} \quad \Sigma$$
$$\mathbf{p}_\Sigma(T) = \mathbf{0}.$$

Gradient Equation:

$$\mathbf{f} = -\frac{1}{\beta}\mathbf{p}$$

3.2 First Results (with care)

Choose:

$$\rho_0 = 5(1/2.2)(\sin(\pi y) + 1.1)$$
$$\mathbf{v}_0 = -y^2 + 1$$
$$\mathbf{f} = (T-t)y$$
$$\nabla V^{ext} = \cos(\pi y)$$

Note that the control is $\mathbf{f}$ and ∇V^{ext} is just an input now. The friction coefficient is set to 10 now because a lower value results in failing the forward problem. Higher values mess with the convergence of the optimality system. We have $\beta = 10$ and $\lambda = 0.01$. Choose again $10^{-6}/10^{-3}$ tolerances. This converges in around 800 iterations. The result is $J_{FW} = 1.1111$ and $J_{Opt} = 0.6193$. Figure 11 shows the result. The targets are the forward results. It can be seen that the optimal control is becoming 'wiggly' at times.
Redoing this exact problem with $N = 60$ and $n = 50$, it takes almost 1000 iterations to converge, but looks a little more stable, see Figure 12. The result is $J_{FW} = 1.1111$ and $J_{Opt} = 0.8655$. This is considerably different from the case with less points. So it has to be checked how many points are necessary. We can see that one of the suspected problems is that the control becomes very steep on the boundaries.

3.3 Quick sanity check

After solving the above, we get $\mathbf{f}_{Opt}$. Now, giving the code this optimal value of $\mathbf{f}$, with the same target, ICs etc, we expect so solve the problem in one iteration. This indeed happens. So at least we found something that the system considers optimal, what ever that may mean in practice.

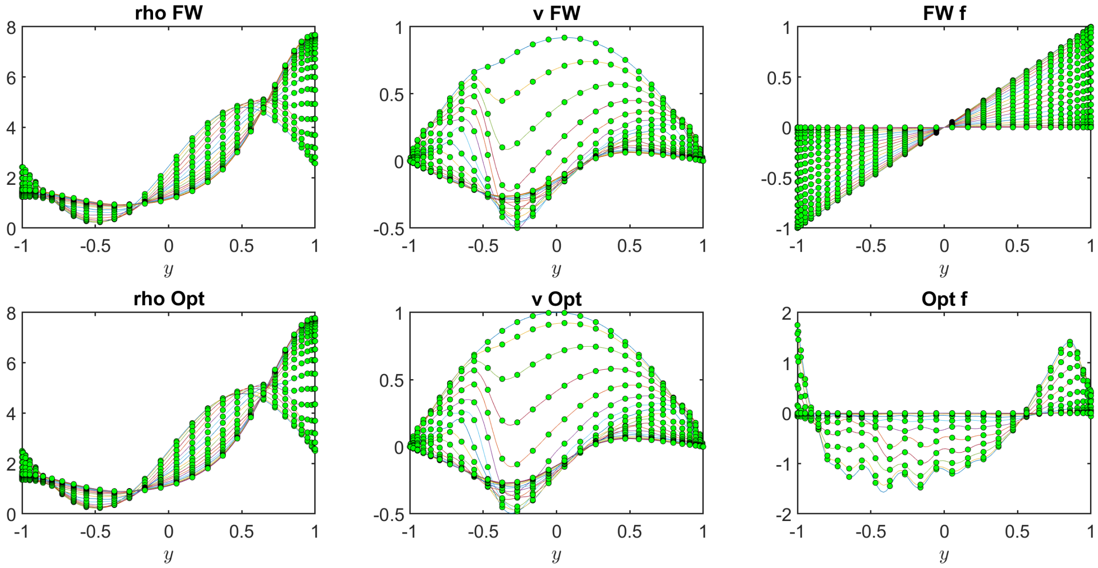

Figure 11: FW Result OCP (top), Opt (bottom) for $\mathbf{f}$, force control, with $\gamma = 10$ and FW result is target

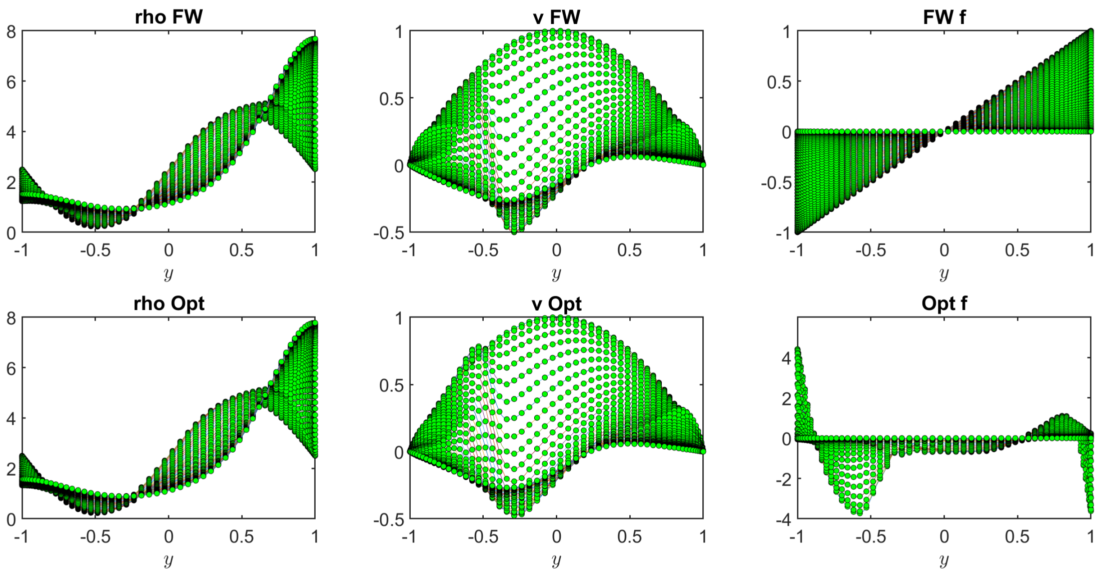

Figure 12: FW Result OCP (top), Opt (bottom) for $\mathbf{f}$, force control, with $\gamma = 10$ and FW result is target, more points