1 Newton-Krylov

One question I have is why the solver needs more than one iteration, if the given solution is exact. Check that no-flux interacting is correct.

We have the following problems, differences measured with the L_1/L_2 norm, with $N = 16$, and with optimality tolerance 10^{-4} in the old code:
Dirichlet exact, Error $= 2.1631 \times 10^{-16}$, time $= 120$ s,
Dirichlet with $\kappa = 1$, Error $= 4.8164 \times 10^{-6}$, time $= 120$ s va 480 s,
Dirichlet exact with V_{ext}, Error $= 0.0027$, time $= 130$ s.
Then for the Neumann problems we have, with $N = 20$:
Neumann exact, Error $= 2.3286 \times 10^{-15}$, time $= 1.0824 \times 10^{3}$ s,
I ran the original code for this, which gives 228 s. I think I messed with the timing of the algorithm somehow...
(++ note: we fix the slowness by choosing to eliminate the flags. We get 4.1841×10^{-9} for the interacting Neumann case)

2 Hodge Helmholtz Decomposition

We choose a basis of Lagrange polynomials (dimension $2(p-1)p$) and choose an element v from this basis. We then note that if v satisfies $\nabla \times v = 0$, we can write $Dv = 0$, where D is the discretized curl. Then we can split this into two parts, such that $Dv = D_1 v_1 + D_2 v_2 = 0$. We determine that $(p-1)^2$ is the degree of interpolation polynomial and furthermore, this implies that $(p-1)^2$ rows of D are linearly independent. Therefore, we split up D such that D_2 has $(p-1)^2$ rows and is invertible. We can then see that

$$v_2 = -D_2^{-1} D_1 u_1,$$

which provides a formula for creating a vector $\mathbf{v} = (v_1, v_2)$ satisfying that $\nabla \times v = 0$. We can then choose $p^2 - 1$ of such vectors as a basis of the curl free vector space. Any curl free vector field $\mathbf{w}$ can then be described as a linear combination of these, i.e. $\mathbf{w} = \sum_i \alpha_i v_i$.
A similar argument can be used to construct a divergence free basis. The harmonic part of the vector field is found by subtracting the curl free and divergence free parts from the original field.

3 Curl free control

We consider

$$\min_{\rho,\mathbf{w}} \frac{1}{2}\int_0^T \int_\Omega (\rho-\widehat{\rho})^2 \, d\mathbf{x}dt + \frac{\beta}{2}\int_0^T \int_\Omega \mathbf{w}^2 d\mathbf{x}dt + \frac{\eta}{2}\int_0^T \int_\Omega (\nabla\times\mathbf{w})^2 \, d\mathbf{x}dt$$

subject to:

$$\frac{\partial\rho}{\partial t} = \nabla^2\rho - \nabla\cdot(\rho\mathbf{w})$$
$$\frac{\partial\rho}{\partial n} - \rho\mathbf{w}\cdot\mathbf{n} = 0$$

We know that in two dimensions

$$\nabla\times\mathbf{w} = \frac{\partial w_2}{\partial x_1} - \frac{\partial w_1}{\partial x_2},$$

and so the Lagrangian is

$$\begin{aligned}\mathcal{L}(\rho,\mathbf{w},q_1,q_2) =& \frac{1}{2}\int_0^T \int_\Omega (\rho-\widehat{\rho})^2 \, d\mathbf{x}dt + \frac{\beta}{2}\int_0^T \int_\Omega \mathbf{w}^2 d\mathbf{x}dt + \frac{\eta}{2}\int_0^T \int_\Omega \left(\frac{\partial w_2}{\partial x_1} - \frac{\partial w_1}{\partial x_2}\right)^2 d\mathbf{x}dt \\ &- \int_0^T \int_\Omega q_1 \left(\frac{\partial\rho}{\partial t} - \nabla^2\rho + \nabla\cdot(\rho\mathbf{w})\right) d\mathbf{x}dt \\ &- \int_0^T \int_{\partial\Omega} q_2 \left(\frac{\partial\rho}{\partial n} - \rho\mathbf{w}\cdot\mathbf{n}\right) d\mathbf{x}dt.\end{aligned}$$

Then, since we know that $q_1 = q_2$, we get

$$\begin{aligned}\mathcal{L}(\rho,\mathbf{w},q) =& \frac{1}{2}\int_0^T \int_\Omega (\rho-\widehat{\rho})^2 \, d\mathbf{x}dt + \frac{\beta}{2}\int_0^T \int_\Omega \mathbf{w}^2 d\mathbf{x}dt + \frac{\eta}{2}\int_0^T \int_\Omega \left(\frac{\partial w_2}{\partial x_1} - \frac{\partial w_1}{\partial x_2}\right)^2 d\mathbf{x}dt \\ &- \int_0^T \int_\Omega -\rho\frac{\partial q}{\partial t} - \rho\nabla^2 q - \nabla q\cdot(\rho\mathbf{w}) \, d\mathbf{x}dt - \int_\Omega q(T)\rho(T) - q(0)\rho(0) d\mathbf{x} \\ &- \int_0^T \int_{\partial\Omega} -\rho\nabla q\cdot\mathbf{n} d\mathbf{x}dt.\end{aligned}$$

For the adjoint equation, we find the usual results. We take the derivative with respect to $\mathbf{w}$

$$\mathcal{L}_\mathbf{w}(\rho,\mathbf{w},q)h = \int_0^T \int_\Omega \beta\mathbf{w}\cdot\mathbf{h} + \rho\nabla q\cdot\mathbf{h} + \eta\left(\frac{\partial w_2}{\partial x_1}\frac{\partial h_2}{\partial x_1} - \frac{\partial w_2}{\partial x_1}\frac{\partial h_1}{\partial x_2} - \frac{\partial h_2}{\partial x_1}\frac{\partial w_1}{\partial x_2} + \frac{\partial w_1}{\partial x_2}\frac{\partial h_1}{\partial x_2}\right) d\mathbf{x}dt.$$

Collecting terms in h_1 and h_2 we get

$$\begin{aligned}
\mathcal{L}_{\mathbf{w}}(\rho, \mathbf{w}, q)h = &\int_0^T \int_\Omega h_1 \left(\beta w_1 + \rho \frac{\partial q}{\partial x_1}\right) + h_2 \left(\beta w_2 + \rho \frac{\partial q}{\partial x_2}\right) \\
&+ \frac{\partial h_1}{\partial x_2}\eta \left(-\frac{\partial w_2}{\partial x_1} + \frac{\partial w_1}{\partial x_2}\right) + \frac{\partial h_2}{\partial x_1}\eta \left(\frac{\partial w_2}{\partial x_1} - \frac{\partial w_1}{\partial x_2}\right) d\mathbf{x}dt \\
= &\int_0^T \int_\Omega h_1 \left(\beta w_1 + \rho \frac{\partial q}{\partial x_1}\right) + h_2 \left(\beta w_2 + \rho \frac{\partial q}{\partial x_2}\right) \\
&- h_1 \eta \left(-\frac{\partial^2 w_2}{\partial x_1 x_2} + \frac{\partial^2 w_1}{\partial x_2^2}\right) - h_2 \eta \left(\frac{\partial^2 w_2}{\partial x_1^2} - \frac{\partial^2 w_1}{\partial x_1 x_2}\right) d\mathbf{x}dt \\
&+ \int_0^T \int_{\partial\Omega} h_1 \eta \left(-\frac{\partial w_2}{\partial n_1} + \frac{\partial w_1}{\partial n_2}\right) + h_2 \eta \left(\frac{\partial w_2}{\partial n_1} - \frac{\partial w_1}{\partial n_2}\right) d\mathbf{x}dt.
\end{aligned}$$

Then

$$\begin{aligned}
\mathcal{L}_{\mathbf{w}}(\rho, \mathbf{w}, q)h = &\int_0^T \int_\Omega \mathbf{h}\left(\beta \mathbf{w} + \rho \nabla q\right) + \eta \mathbf{h} \left(\frac{\partial^2 w_2}{\partial x_1 x_2}, \frac{\partial^2 w_1}{\partial x_1 x_2}\right) - \eta \mathbf{h} \left(\frac{\partial^2 w_1}{\partial x_2^2}, \frac{\partial^2 w_2}{\partial x_1^2}\right) d\mathbf{x}dt \\
&+ \int_0^T \int_{\partial\Omega} \eta \mathbf{h} \left(-\frac{\partial w_2}{\partial n_1} + \frac{\partial w_1}{\partial n_2}, \frac{\partial w_2}{\partial n_1} - \frac{\partial w_1}{\partial n_2}\right) d\mathbf{x}dt
\end{aligned}$$

So we can extract

$$\begin{aligned}
\beta \mathbf{w} + \rho \nabla q + \eta \left(\frac{\partial^2 w_2}{\partial x_1 x_2} - \frac{\partial^2 w_1}{\partial x_2^2}, \frac{\partial^2 w_1}{\partial x_1 x_2} - \frac{\partial^2 w_2}{\partial x_1^2}\right) &= 0 \quad \text{in} \quad \Omega \\
\eta \left(-\frac{\partial w_2}{\partial n_1} + \frac{\partial w_1}{\partial n_2}, \frac{\partial w_2}{\partial n_1} - \frac{\partial w_1}{\partial n_2}\right) &= 0 \quad \text{on} \quad \partial\Omega
\end{aligned}$$

The first components give

$$\begin{aligned}
&\beta w_1 - \eta \frac{\partial^2 w_1}{\partial x_2^2} = \rho \frac{\partial q}{\partial x_1} - \eta \frac{\partial^2 w_2}{\partial x_1 x_2} \quad \text{in} \quad \Omega \\
&\eta \left(-\frac{\partial w_2}{\partial n_1} + \frac{\partial w_1}{\partial n_2}\right) = 0 \quad \text{on} \quad \partial\Omega
\end{aligned}$$

and the second are

$$\begin{aligned}
&\beta w_2 - \eta \frac{\partial^2 w_2}{\partial x_1^2} = \rho \frac{\partial q}{\partial x_2} - \eta \frac{\partial^2 w_1}{\partial x_1 x_2} \quad \text{in} \quad \Omega \\
&\eta \left(\frac{\partial w_2}{\partial n_1} - \frac{\partial w_1}{\partial n_2}\right) = 0 \quad \text{on} \quad \partial\Omega.
\end{aligned}$$