Annual Review (in particular structure) and Extension Request.
Paper: added required terms, code snippet. Too long?

1 Newton-Krylov Investigation

1.1 'Final time independent' solutions

We investigate whether the time scaling has an effect on the odd behaviour of the Neumann exact solution. We choose the following inputs

$$\rho = 0.25\beta^{1/2}\exp(t/T)(\cos(\pi x)+1),$$
$$q = 0.25\beta^{1/2}(\exp(T/T) - \exp(t/T))\cos(\pi x)$$

For $n = 10$, $N = 30$, we have for $T = 1$, the exact error for ρ and q is of order 10^{-15} and 10^{-14}, for $T = 5$, we get an error of 10^{-14} and 10^{-13} respectively. For $T = 0.1$ we get errors of order 10^{-15}. For $n = 20$, $N = 30$, for $T = 1$ we have errors of order 10^{-15}, for $T = 5$, the error is 10^{-14} and 10^{-13} and for $T = 0.1$ we only get 10^{-6}.
For $n = 25$, $N = 30$, for $T = 1$ we only get 10^{-7}/ 10^{-6} accuracy, while for $T = 5$, we get 10^{-14} (ans for $T = 0.1$ we only get $10^{-3}/10^{-4}$). This is not changed by increasing N to 40. For $n = 30$, $N = 40$, $T = 5$ is also not that accurate anymore, and only $T = 20$ results in $10^{-11}/10^{-9}$. For $N = 35$ it improves to 10^{-13}.

1.2 Perturbation in Time

We take the perturbation from the second year review. We consider multiplying the exact solution by $1 + \epsilon p(t)$, where $p(t)$ is the perturbation at time t. For $\epsilon = 0$, the algorithm converges immediately. For $n = 30$, $N = 35$, for $\epsilon = 0.0001$ we get an error of 10^{-7} and the algorithm reaches 100 inner iterations each time. For $\epsilon = 0.01$ we get errors of 10^{-5}. For $n = 20$ and $N = 30$, we get 10^{-15}, even for $\epsilon = 0.1$. So this suggests that the time scaling thing from the previous section is more of a problem.

1.3 Increasing number of iterations

However, if we instead increase the maximum number of iterations, this also improves convergence. For $n = 30$, $N = 35$, we get for $\epsilon = 0.01$, instead of an error of 10^{-5}, with max 200 iterations we get an error of 10^{-14}. The same result holds for $\epsilon = 0.1$.

We investigate the same relationship between maximum iterations and time scaling. Giving again the initial conditions as initial guess, we get for $n = 30$ and $N = 35$, for $T = 1$ with 20 iterations we get an error of 10^{-14} instead of 10^{-3}. The inner iteration still reaches this maximum sometimes, but not each time as is the case for 100 maximum iterations. For $T = 0.1$ we improve to 10^{-8}, but reach the maximum iterations often. For maximum of 300 iterations, we get down to 10^{-15}.

So overall I would conclude that some things are harder and therefore need more inner iterations.

The issue with $T = 0.1$ and $n = 30/\ N = 35$ can be observed for the Dirichlet problem, too. However, the solution is still 10^{-8} accurate (as opposed to 10^{-3} for Neumann). Increasing the number of iterations to 200, we get 10^{-15} accuracy. For $T = 1$, we don't have a problem for Dirichlet.
For the perturbation with $n = 30$ and $N = 35$ we don't have a problem, even for large ϵ, which makes sense because this is computed at $T = 1$, which didn't cause problems for the initial condition as initial guess (which is further from the exact solution than the perturbed problem).

Increasing the number of iterations does not improve the difference in the paper example (between Newton-Krylov and Fixed Point Algorithms). The error between the two approaches furthermore is consistent for different values of β.

2 Comparing Fixed Point with Newton-Krylov (from last week - for reference)

2.1 1D Problems

I apply this observation to one of the paper examples (Example 2), with $\kappa = 1$. When I run the problem with $N = 50$ and $n = 10$, and then with the old code with $n = 30$ and interpolate to $n = 10$ in time, We get an error of 0.0362. If I run both versions with $n = 30$ we get an error of 3.8640×10^{-4}, which seems to contradict the above observation.
For $n = 30$, we get for $\kappa = -1$ and error of 0.0013 and for $\kappa = 0$ and error of 1.2519×10^{-8}. These problems take 56 seconds to solve.

For the paper example 1, we again choose $N = 50$ and $n = 30$. We get for $\kappa = 0$ an error of 1.5563×10^{-13}, for $\kappa = -1$ we have the error 0.0174 and for $\kappa = 1$, the error is 0.0037. The same error results from comparing NK to fsolve for this problem set up with $n = 20$, $N = 30$. The error between fixed point and fsolve is of order 10^{-7}.

For the third example, we have Dirichlet BCs and again choose $N = 50$ and $n = 30$. We

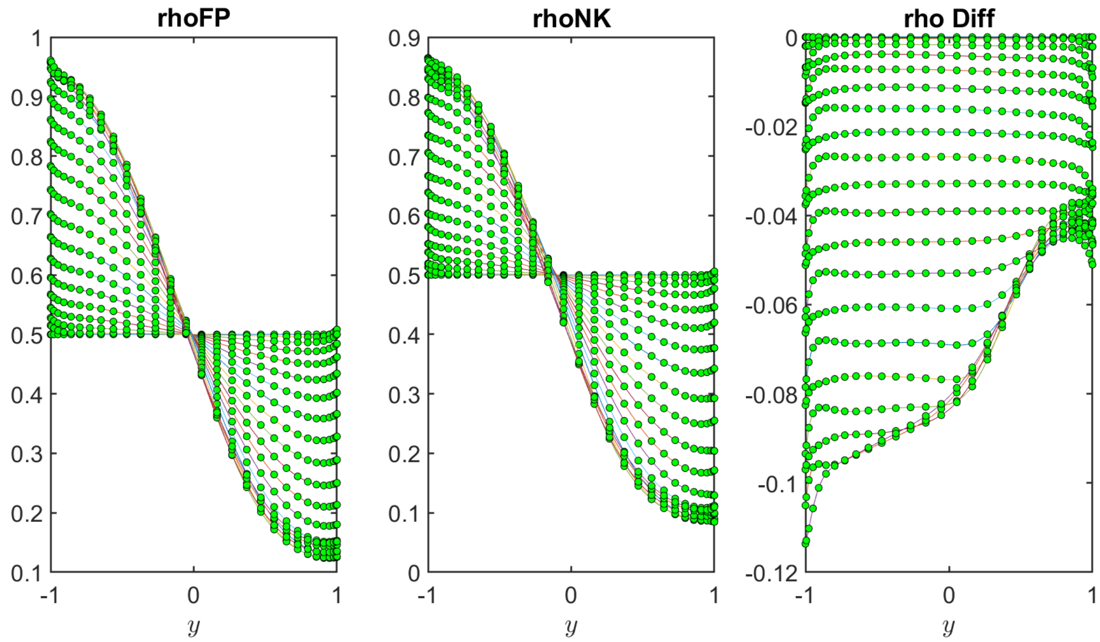

Figure 1: Paper Example 1 with $\kappa = 1$, $n = 20$, $N = 30$, Comparison between fix point and Newton Krylov

get for $\kappa = 0$ the eroor is 1.8015×10^{-7}, for $\kappa = -1$ the error is 1.6645×10^{-7} and for $\kappa = 1$ the error is 1.9485×10^{-7}.

2.2 2D Problems

The exact 2D Dirichlet problem (with and without external potential), for $N = 20$ and $n = 10$, has an error of 10^{-15} for both u and v and is solved in 40 and 60 seconds respectively. The exact Neumann problem reduces the error in u to 10^{-8} and in v to 10^{-7}. The inner iterations reach 100 and it takes 170 seconds. For the first paper problem, we have the following results. For $\kappa = -1$ the error is 0.0032, for $\kappa = 0$, the error is 3.6813×10^{-9} and for $\kappa = 1$ the error is 0.0014. For the second paper problem, we have the following results. For $\kappa = -1$ the error is 0.0062, for $\kappa = 0$, the error is 3.1640×10^{-4} and for $\kappa = 1$ the error is 0.0017. All of these problems take 300 to 500 seconds.

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

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

More importantly, we know that

$$\nabla \times \mathbf{w} = \nabla \cdot \mathbf{w}_\perp, \tag{1}$$

where $\mathbf{w}_\perp = (w_2, -w_1)$, the result of a rotation of $\mathbf{w}$ by $\pi/2$. Then the Lagrangian is

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

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

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

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

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

Then we integrate by parts (or divergence theorem) to get

$$\mathcal{L}_\mathbf{w}(\rho, \mathbf{w}, q)h = \int_0^T \int_\Omega \beta \mathbf{w} \cdot \mathbf{h} + \rho \nabla q \cdot \mathbf{h} - \eta \nabla \left(\nabla \cdot \mathbf{w}_\perp \right) \cdot \mathbf{h}_\perp d\mathbf{x}dt + \int_0^T \int_{\partial\Omega} \eta \left(\nabla \cdot \mathbf{w}_\perp \right) \mathbf{h}_\perp \cdot \mathbf{n} d\mathbf{x}dt.$$

Finally we need to rewrite the equations in terms of $\mathbf{h}$. We note that

$$\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \mathbf{h} = \mathbf{h}_{\perp}.$$

Furthermore,

$$\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \mathbf{n} \cdot \mathbf{h} = \mathbf{h}_{\perp} \cdot \mathbf{n}.$$

Replacing these in the Lagrangian gives

$$\begin{aligned} \mathcal{L}_{\mathbf{w}}(\rho, \mathbf{w}, q)h = & \int_0^T \int_\Omega \beta \mathbf{w} \cdot \mathbf{h} + \rho \nabla q \cdot \mathbf{h} - \eta \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \nabla \left(\nabla \cdot \mathbf{w}_{\perp} \right) \cdot \mathbf{h} d\mathbf{x} dt \\ & + \int_0^T \int_{\partial\Omega} \eta \left(\nabla \cdot \mathbf{w}_{\perp} \right) \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \mathbf{n} \cdot \mathbf{h} d\mathbf{x} dt. \end{aligned}$$

Finally, using (1) we get

$$\begin{aligned} \mathcal{L}_{\mathbf{w}}(\rho, \mathbf{w}, q)h = & \int_0^T \int_\Omega \beta \mathbf{w} \cdot \mathbf{h} + \rho \nabla q \cdot \mathbf{h} - \eta \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \nabla \left(\nabla \times \mathbf{w} \right) \cdot \mathbf{h} d\mathbf{x} dt \\ & + \int_0^T \int_{\partial\Omega} \eta \left(\nabla \times \mathbf{w} \right) \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \mathbf{n} \cdot \mathbf{h} d\mathbf{x} dt. \end{aligned}$$

Since this holds for all admissible $\mathbf{h}$ we get the gradient equation

$$\begin{aligned} \beta \mathbf{w} + \rho \nabla q - \eta \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \nabla \left(\nabla \times \mathbf{w} \right) &= 0 \quad \text{in} \quad \Omega \\ \eta \left(\nabla \times \mathbf{w} \right) \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \mathbf{n} &= 0 \quad \text{on} \quad \partial\Omega. \end{aligned}$$

In component form this is

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

and

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