Following the meeting on 09/07/2020

1 Question 1 (John):

Considering the OCP discussed yesterday, where we add a term into the cost functional (where $\mathbf{f}$ is an imposed, fixed flow, $\mathbf{w}$ is the control flow):

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

subject to:

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

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

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

Considering the relevant part of the Lagrangian:

$$\mathcal{L}(\rho,\mathbf{v},q,\mathbf{p}_\Sigma,\mathbf{w}) = ... + \frac{\eta}{2}\int_0^T\int_\Omega\Big(\nabla\mathbf{v}\Big)^2 drdt + ...$$

In 1D this is:

$$\mathcal{L}(\rho,v,q,p,w) = ... + \frac{\eta}{2}\int_0^T\int_\Omega\Big(\frac{\partial v}{\partial x}\Big)^2 dxdt + ... = ... + \int_0^T\int_\Omega\Big(\frac{\partial v}{\partial x}\Big)\Big(\frac{\partial v}{\partial x}\Big)dxdt + ...$$

Then, taking the derivative and using the product rule:

$$\mathcal{L}_v(\rho,v,q,p,w)h = ... + \frac{\eta}{2}\int_0^T\int_\Omega\Big(\frac{\partial h}{\partial x}\Big)\Big(\frac{\partial v}{\partial x}\Big) + \Big(\frac{\partial v}{\partial x}\Big)\Big(\frac{\partial h}{\partial x}\Big)dxdt + ...$$

Integrating by parts gives:

$$\begin{aligned}\mathcal{L}_v(\rho,v,q,p,w)h &= ... + \frac{\eta}{2}\Big[\int_0^T\int_{\partial\Omega}h\Big(\frac{\partial v}{\partial n}\Big) + \Big(\frac{\partial v}{\partial n}\Big)hdxdt - \int_0^T\int_\Omega h\Big(\frac{\partial^2 v}{\partial x^2}\Big) + \Big(\frac{\partial^2 v}{\partial x^2}\Big)hdxdt\Big] + ... \\ &= ... + \eta\Big[\int_0^T\int_{\partial\Omega}\Big(\frac{\partial v}{\partial n}\Big)hdxdt - \int_0^T\int_\Omega\Big(\frac{\partial^2 v}{\partial x^2}\Big)hdxdt\Big] + ...\end{aligned}$$

So going through the derivation, we would get a boundary term $\frac{\partial v}{\partial x}$ and a term $\frac{\partial^2 v}{\partial x^2}$ in the second adjoint equation. In particular, from the boundary terms we get that the relationship between the adjoints p, $p_{\partial\Sigma}$ and q is:

$$mvp + p_{\partial\Sigma} + q + \eta\frac{\partial v}{\partial n} = 0$$

And from the interior terms we get that the second adjoint equation is:

$$\begin{aligned} m\rho\frac{\partial p}{\partial t} &= -\eta\frac{\partial^2 v}{\partial x^2} - m\frac{\partial \rho}{\partial t}p - \rho\nabla q + m\rho\frac{\partial v}{\partial x}p + m\gamma\rho p \\ &- m\rho\left(v\frac{\partial}{\partial x}\right)p - m\rho\frac{\partial v}{\partial x}p - m(v\frac{\partial \rho}{\partial x})p \qquad \text{in} \quad \Sigma \\ p(T) &= 0. \end{aligned} \tag{2}$$

So we get the negative Laplacian for v. But in the meeting we said it will be $\mathbf{v} - \nabla\mathbf{v}$, i.e. $v - \frac{\partial^2 v}{\partial x^2}$. I do not get an additional term for v, so I either misunderstood something in the meeting or something in my derivation is wrong. (side note: the other equations are not listed because they're not affected by this change of the cost functional. They can be seen in the document I sent two weeks ago 'ThesisEndOfYear1', under Archer Optimality Conditions.)

2 Question 2 (Ben):

Considering this version of the problem instead (where $\mathbf{f}$ is an imposed flow, $\mathbf{w}$ is the control flow and there is the smoothing term $\eta\nabla^2\mathbf{v}$ for $\mathbf{v}$ in the PDE):

$$\begin{aligned} &\min_{\rho,\mathbf{v},\mathbf{w}} \quad \frac{1}{2}||\rho - \hat{\rho}||^2_{L_2(\Sigma)} + \frac{\beta}{2}||\mathbf{w}||^2_{L_2(\Sigma)} \\ &\text{subject to:} \\ &m\rho\frac{\partial \mathbf{v}}{\partial t} = \Big(- m\rho(\mathbf{v}\cdot\nabla)\mathbf{v} - \rho\nabla V^{ext} - \rho\mathbf{f} - \rho\mathbf{w} - \nabla\rho - m\gamma\rho\mathbf{v} + \eta\nabla^2\mathbf{v}\Big) \qquad \text{in} \quad \Sigma \\ &\frac{\partial \rho}{\partial t} = -\nabla\cdot(\rho\mathbf{v}) \\ &\rho\mathbf{v}\cdot\mathbf{n} = 0 \qquad \text{on } \partial\Omega \end{aligned} \tag{3}$$

We discussed yesterday that we can rewrite the PDE system in terms of $\rho = e^s$. However, in this case we get:

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

So then we have e^{-s} in the problem and that's not really the point of the transformation, right? Equation (39) in the Archer paper doesn't multiply $\eta\nabla^2\mathbf{v}$ by ρ so I think doing that would change the meaning of the term?

The same question actually applies to the adjoint equation for the setup in question 1 (see Equation 2). In Setup 1 (Equation 1), the adjoint equation becomes a problem because of the extra Laplacian term from the cost functional. Since this term in Equation 2 doesn't have a ρ term, we can't readily make the transformation there.
In Setup 2 (Equation 3) the adjoint equation isn't a problem for rewriting $\rho = e^s$, but the forward equation is. Long story short: Does it make sense in either Setup (Equation 1 or Equation 3), to apply this transformation and keep the negative exponential e^{-s} in the equation, or is it better to just leave the variable as ρ?

3 Question 2.5

I think I forgot to double check this yesterday (or I forgot that I did...): In the adjoint equations (e.g. Equation 2 above) I have $\frac{\partial\rho}{\partial t}$ terms. Is it correct to take the first differentiation matrix from the 'time line' TDC? I have implemented it this way:

```
Difft = this.TDC.ComputeDifferentiationMatrix();
Dt = Difft.Dy;
Dtrho = Dt*rho;
```

and then interpolate as normal onto the correct time in the ODE solver.