1 The Multiple Species Gradient Equation

We consider the derivative of the Lagrangian with respect to $\mathbf{w}$. However, we will need to consider the Frechét derivative of terms involving $F(\mathbf{w})$ first. If F is a function of $\mathbf{w}$ only and not of the position variable r, we can do the following. Otherwise, we will have to work with the definition of the Frechét derivative and derive the gradient equation like that. We consider the first order term of the Taylor expansion, so that we have:

$$F(\mathbf{w}+\mathbf{h}) - F(\mathbf{w}) = \left(\nabla_{\mathbf{w}} F(\mathbf{w})^T\right)\mathbf{h}$$

Then:

$$\begin{aligned}
\mathcal{L}_{\mathbf{w}}(\rho_a, \rho_b, \mathbf{w}, q_a, q_b)\mathbf{h} &= \int_0^T \int_\Omega \Big(\beta\mathbf{w}\cdot\mathbf{h} - D_a\nabla\cdot(\rho_a\left(\nabla_{\mathbf{w}} F_a(\mathbf{w})^T\right)\mathbf{h})q_a - D_b\nabla\cdot(\rho_b\left(\nabla_{\mathbf{w}} F_b(\mathbf{w})^T\right)\mathbf{h})q_b\Big) drdt \\
&+ \int_0^T \int_{\partial\Omega} \Big(D_a\rho_a\left(\nabla_{\mathbf{w}} F_a(\mathbf{w})^T\right)\mathbf{h}q_{a,\partial\Omega} + D_b\rho_b\left(\nabla_{\mathbf{w}} F_b(\mathbf{w})^T\right)\mathbf{h}q_{b,\partial\Omega}\Big)\cdot\mathbf{n}drdt \\
&= \int_0^T \int_\Omega \Big(\beta\mathbf{w}\cdot\mathbf{h} + D_a\rho_a\left(\left(\nabla_{\mathbf{w}} F_a(\mathbf{w})^T\right)\mathbf{h}\right)\cdot\nabla q_a \\
&+ D_b\rho_b\left(\left(\nabla_{\mathbf{w}} F_b(\mathbf{w})^T\right)\mathbf{h}\right)\cdot\nabla q_b\Big) drdt \\
&- \int_0^T \int_{\partial\Omega} \Big(D_a\rho_a\left(\nabla_{\mathbf{w}} F_a(\mathbf{w})^T\right)\mathbf{h}q_a + D_b\rho_b\left(\nabla_{\mathbf{w}} F_b(\mathbf{w})^T\right)\mathbf{h}q_b\Big)\cdot\mathbf{n}drdt \\
&+ \int_0^T \int_{\partial\Omega} \Big(D_a\rho_a\left(\nabla_{\mathbf{w}} F_a(\mathbf{w})^T\right)\mathbf{h}q_{a,\partial\Omega} + D_b\rho_b\left(\nabla_{\mathbf{w}} F_b(\mathbf{w})^T\right)\mathbf{h}q_{b,\partial\Omega}\Big)\cdot\mathbf{n}drdt \\
&= \int_0^T \int_\Omega \Big(\beta\mathbf{w}\cdot\mathbf{h} + D_a\rho_a\left(\left(\nabla_{\mathbf{w}} F_a(\mathbf{w})^T\right)\mathbf{h}\right)\cdot\nabla q_a \\
&+ D_b\rho_b\left(\left(\nabla_{\mathbf{w}} F_b(\mathbf{w})^T\right)\mathbf{h}\right)\cdot\nabla q_b\Big) drdt,
\end{aligned}$$

since $q_a = q_{a,\partial\Omega}$ and $q_b = q_{b,\partial\Omega}$ from the adjoint derivation.
Now we use the relation $((\nabla\mathbf{a})^T)\mathbf{b})\cdot\mathbf{c} = ((\mathbf{c}\cdot\nabla)\mathbf{a})\cdot\mathbf{b}$ (from year end review) to find that:

$$\begin{aligned}
\mathcal{L}_{\mathbf{w}}(\rho_a, \rho_b, \mathbf{w}, q_a, q_b)\mathbf{h} = \int_0^T \int_\Omega \Big(&\beta\mathbf{w}\cdot\mathbf{h} + D_a\rho_a\left(\left(\nabla_r q_a\cdot\nabla_{\mathbf{w}}\right)F_a(\mathbf{w})\right)\cdot\mathbf{h} \\
&+ D_b\rho_b\left(\left(\nabla_r q_b\cdot\nabla_{\mathbf{w}}\right)F_b(\mathbf{w})\right)\cdot\mathbf{h}\Big) drdt,
\end{aligned}$$

Setting this to zero and since this holds for all permissible $\mathbf{h}$, we get:

$$\beta\mathbf{w} + D_a\rho_a\left(\left(\nabla_r q_a\cdot\nabla_{\mathbf{w}}\right)F_a(\mathbf{w})\right) + D_b\rho_b\left(\left(\nabla_r q_b\cdot\nabla_{\mathbf{w}}\right)F_b(\mathbf{w})\right) = 0.$$

Using that $\nabla\cdot(\mathbf{b}\mathbf{a}^T) = \mathbf{a}(\nabla\cdot\mathbf{b}) + (\mathbf{b}\cdot\nabla)\mathbf{a}$, and observing that $\nabla_{\mathbf{w}}\cdot(\nabla_r q) = 0$, we get:

$$\beta\mathbf{w} + D_a\rho_a\nabla_{\mathbf{w}}\cdot\left(\nabla q_a F_a(\mathbf{w})^T\right) + D_b\rho_b\nabla_{\mathbf{w}}\cdot\left(\nabla q_b F_b(\mathbf{w})^T\right) = 0.$$

Since $\nabla_r q$ does not depend on $\mathbf{w}$ we can rearrange this to get:

$$\beta \mathbf{w} + D_a \rho_a \left(\nabla_{\mathbf{w}} F_a(\mathbf{w})\right)^T \nabla q_a + D_b \rho_b \left(\nabla_{\mathbf{w}} F_b(\mathbf{w})\right)^T \nabla q_b = 0.$$

And finally we have:

$$\mathbf{w} = -\frac{1}{\beta}\left(D_a \rho_a \left(\nabla_{\mathbf{w}} F_a(\mathbf{w})\right)^T \nabla q_a + D_b \rho_b \left(\nabla_{\mathbf{w}} F_b(\mathbf{w})\right)^T \nabla q_b\right).$$

As an example, take $F_a(\mathbf{w}) = c_a \mathbf{w}$ and $F_b(\mathbf{w}) = c_b \mathbf{w}$. We get:

$$\mathbf{w} = -\frac{1}{\beta}\Bigg(D_a \rho_a c_a \mathbf{1} \nabla q_a + D_b \rho_b c_b \mathbf{1} \nabla q_b\Bigg).$$

2 Sedimentation

2.1 Free Energy Frechét Derivative

We have the general expression:

$$\begin{aligned}
\nabla \cdot \left(\rho \nabla \frac{\delta F[\rho]}{\delta \rho}\right) &= \frac{1}{\beta}\left(\nabla \cdot \left(\frac{\nabla \rho}{1-\eta}\right) - \nabla \cdot \left(\rho \nabla \frac{\eta - 2}{(\eta-1)^2}\right)\right) \\
&= \frac{1}{\beta}\left(\frac{\nabla^2 \rho}{1-\eta} + \nabla \rho \cdot \nabla \frac{1}{1-\eta} - \nabla \rho \cdot \nabla \frac{\eta-2}{(\eta-1)^2} - \rho \nabla^2 \frac{\eta-2}{(\eta-1)^2}\right) \\
&= \frac{1}{\beta}\left(\frac{\nabla^2 \rho}{1-\eta} + \nabla \rho \cdot \nabla \frac{(3-2\eta)}{(1-\eta)^2} - \rho \nabla^2 \frac{\eta-2}{(\eta-1)^2}\right)
\end{aligned}$$

We want to take the Frechét derivative of these terms. We set:

$$\begin{aligned}
F_1 &= \frac{\nabla^2 \rho}{1-\eta} = \frac{\nabla^2 \rho}{1-a\rho} \\
F_2 &= \nabla \rho \cdot \nabla \frac{(3-2\eta)}{(1-\eta)^2} = \nabla \rho \cdot \nabla \frac{(3-2a\rho)}{(1-a\rho)^2} \\
F_3 &= \rho \nabla^2 \frac{\eta-2}{(\eta-1)^2} = \rho \nabla^2 \frac{a\rho-2}{(a\rho-1)^2}.
\end{aligned}$$

We are looking at $F(\rho+h) - F(\rho)$. We use the expansions:

$$\begin{aligned}
\frac{1}{1-x} &= 1 + x + O(x^2) \\
\frac{1}{(1-x)^2} &= 1 + 2x + O(x^2).
\end{aligned}$$

For F_1 we get:

$$\begin{aligned}
F_1(\rho+h) - F_1(\rho) &= \frac{\nabla^2(\rho+h)}{1-a(\rho+h)} - \frac{\nabla^2 \rho}{1-a\rho} \\
&= \nabla^2(\rho+h)(1+a(\rho+h)) - \nabla^2 \rho(1+a\rho) \\
&= (\nabla^2 \rho)(1+a\rho+ah-1-a\rho) + (\nabla^2 h)(1+a\rho+ah) \\
&= (\nabla^2 \rho)(ah) + (\nabla^2 h)(1+a\rho)
\end{aligned}$$

For F_2 we have:

$$
\begin{aligned}
F_2(\rho+h)-F_2(\rho) &= \nabla(\rho+h)\cdot\nabla\frac{(3-2a(\rho+h))}{(1-a(\rho+h))^2}-\nabla\rho\cdot\nabla\frac{(3-2a\rho)}{(1-a\rho)^2} \\
&= \nabla(\rho+h)\cdot\nabla\big((3-2a(\rho+h))(1+2a(\rho+h))\big)-\nabla\rho\cdot\nabla\big((3-2a\rho)(1+2a\rho)\big) \\
&= \nabla(\rho+h)\cdot\nabla\left(3+6a(\rho+h)-2a(\rho+h)-4a^2(\rho+h)^2\right) \\
&-\nabla\rho\cdot\nabla\left(3+6a\rho-2a\rho-4a^2\rho^2\right) \\
&= \nabla\rho\cdot\nabla\left(3+4a(\rho+h)-4a^2(\rho+h)^2-\left(3+4a\rho-4a^2\rho^2\right)\right) \\
&+\nabla h\cdot\nabla\left(3+6a(\rho+h)-2a(\rho+h)-4a^2(\rho+h)^2\right) \\
&= \nabla\rho\cdot\nabla\left(4ah-8a^2\rho h\right)+\nabla h\cdot\nabla\left(3+6a\rho-2a\rho-4a^2\rho^2\right) \\
&= \nabla\rho\cdot\nabla\left((4a-8a^2\rho)h\right)+\nabla h\cdot\nabla\left(4a\rho-4a^2\rho^2\right) \\
&= \nabla\rho\cdot h\nabla\left(4a-8a^2\rho\right)+\nabla\rho\cdot(4a-8a^2\rho)\nabla h+\nabla h\cdot\nabla\left(4a\rho-4a^2\rho^2\right) \\
&= -8a^2h\nabla\rho\cdot\nabla\rho+\nabla h\cdot\left(\nabla\rho(4a-8a^2\rho)+\nabla\left(4a\rho-4a^2\rho^2\right)\right) \\
&= -8a^2h\left(\nabla\rho\right)^2+\nabla h\cdot\left(8a\nabla\rho-16a^2\rho\nabla\rho\right)
\end{aligned}
$$

Finally F_3 is:

$$
\begin{aligned}
F_3(\rho+h)-F_3(\rho) &= (\rho+h)\nabla^2\left(\frac{a(\rho+h)-2}{(a(\rho+h)-1)^2}\right)-\rho\nabla^2\left(\frac{a\rho-2}{(a\rho-1)^2}\right) \\
&= (\rho+h)\nabla^2\big((a(\rho+h)-2)(1+2a(\rho+h))\big)-\rho\nabla^2\big((a\rho-2)(1+2a\rho)\big) \\
&= (\rho+h)\nabla^2\left(-2-3a(\rho+h)+2a^2(\rho+h)^2\right)-\rho\nabla^2\left(-2-3a\rho+2a^2\rho^2\right) \\
&= \rho\nabla^2\left(-3ah+4a^2\rho h\right)+h\nabla^2\left(-3a\rho+2a^2\rho^2\right) \\
&= -3a\rho\nabla^2h+4a^2\rho\nabla^2(\rho h)-3ah\nabla^2\rho+2a^2h\nabla^2\rho^2
\end{aligned}
$$

2.2 Lagrangian

We consider the part of the Lagrangian that is relevant:

$$
\mathcal{L}(\rho,\mathbf{w},q)=-\int_0^T\int_\Omega\left(\frac{1}{\beta}\left(\frac{\nabla^2\rho}{1-\eta}+\nabla\rho\cdot\nabla\frac{(3-2\eta)}{(1-\eta)^2}-\rho\nabla^2\frac{\eta-2}{(\eta-1)^2}\right)q\right)drdt
$$

Taking the derivatives with respect to ρ gives:

$$
\begin{aligned}
\mathcal{L}_\rho(\rho,\mathbf{w},q)h=-\frac{1}{\beta}\int_0^T\int_\Omega&\Big((\nabla^2\rho)(ah)+(\nabla^2h)(1+a\rho)-8a^2h\left(\nabla\rho\right)^2+\nabla h\cdot\left(8a\nabla\rho-16a^2\rho\nabla\rho\right) \\
&+a\rho\nabla^2h-2a^2\rho\nabla^2(\rho h)+ah\nabla^2\rho-a^2h\nabla^2\rho^2\Big)qdrdt
\end{aligned}
$$

Integrate by parts the term involving $\nabla^2(\rho h)$:

$$\begin{aligned}
\int_0^T \int_\Omega q\rho\nabla^2(\rho h) dr dt &= \int_0^T \int_{\partial\Omega} q\rho\nabla(\rho h)\cdot \mathbf{n} dr dt - \int_0^T \int_\Omega \nabla(q\rho)\cdot\nabla(\rho h) dr dt \\
&= \int_0^T \int_{\partial\Omega} q\rho\left(\rho\nabla h + h\nabla\rho\right)\cdot \mathbf{n} dr dt - \int_0^T \int_{\partial\Omega} \rho h\nabla(q\rho)\cdot \mathbf{n} dr dt + \int_0^T \int_\Omega \rho h\nabla^2(q\rho) dr dt \\
&= \int_0^T \int_{\partial\Omega} \Big(q\rho^2\nabla h + q\rho h\nabla\rho - \rho^2 h\nabla q - q\rho h\nabla\rho\Big)\cdot \mathbf{n} dr dt + \int_0^T \int_\Omega \rho h\nabla^2(q\rho) dr dt \\
&= \int_0^T \int_{\partial\Omega} \Big(q\rho^2\nabla h - \rho^2 h\nabla q\Big)\cdot \mathbf{n} dr dt + \int_0^T \int_\Omega \rho h\nabla^2(q\rho) dr dt
\end{aligned}$$

Then we have the terms involving $\nabla^2 h$:

$$\begin{aligned}
\int_0^T \int_\Omega (\nabla^2 h)(q + 2aq\rho) dr dt &= \int_0^T \int_{\partial\Omega} (\nabla h)(q + 2aq\rho)\cdot \mathbf{n} dr dt - \int_0^T \int_\Omega (\nabla h)\cdot\nabla(q + 2aq\rho) dr dt \\
&= \int_0^T \int_{\partial\Omega} \big((\nabla h)(q + 2aq\rho) - h\nabla q - 2ah\nabla(q\rho)\big)\cdot \mathbf{n} dr dt \\
&+ \int_0^T \int_\Omega h\nabla^2 q + 2ah\nabla^2(q\rho) dr dt \\
&= \int_0^T \int_{\partial\Omega} \big((\nabla h)(q + 2aq\rho) - h\nabla q - 2ah\nabla(q\rho)\big)\cdot \mathbf{n} dr dt \\
&+ \int_0^T \int_\Omega h\nabla^2 q + 2ahq\nabla^2\rho + 2ah\rho\nabla^2 q + 2ah\nabla\rho\cdot\nabla q dr dt
\end{aligned}$$

Finally, the terms involving ∇h:

$$\begin{aligned}
\int_0^T \int_\Omega \nabla h\cdot\Big(8aq\nabla\rho - 16a^2 q\rho\nabla\rho\Big) dr dt &= \int_0^T \int_{\partial\Omega} h\Big(8aq\nabla\rho - 16a^2 q\rho\nabla\rho\Big)\cdot \mathbf{n} dr dt \\
&- \int_0^T \int_\Omega h\nabla\cdot\Big(8aq\nabla\rho - 16a^2 q\rho\nabla\rho\Big) dr dt \\
&= \int_0^T \int_{\partial\Omega} h\Big(8aq\nabla\rho - 16a^2 q\rho\nabla\rho\Big)\cdot \mathbf{n} dr dt \\
&- \int_0^T \int_\Omega h\Big(8a\nabla\cdot(q\nabla\rho) - 16a^2\nabla\cdot(q\rho\nabla\rho)\Big) dr dt \\
&= \int_0^T \int_{\partial\Omega} h\Big(8aq\nabla\rho - 16a^2 q\rho\nabla\rho\Big)\cdot \mathbf{n} dr dt \\
&- \int_0^T \int_\Omega h\Big(8a\nabla q\cdot\nabla\rho + 8aq\nabla^2\rho \\
&- 16a^2 q(\nabla\rho)^2 - 16a^2\rho\nabla\rho\cdot\nabla q - 16a^2 q\rho\nabla^2\rho\Big) dr dt
\end{aligned}$$

Combining all of these gives:

$$\mathcal{L}_\rho(\rho, \mathbf{w}, q)h = -\frac{1}{\beta}\int_0^T \int_\Omega \Bigg((\nabla^2\rho)(aqh) + h\nabla^2 q + 2ahq\nabla^2\rho + 2ah\rho\nabla^2 q + 2ah\nabla\rho\cdot\nabla q - 8a^2hq\,(\nabla\rho)^2$$
$$- h\Bigg(8a\nabla q\cdot\nabla\rho + 8aq\nabla^2\rho - 16a^2q(\nabla\rho)^2 - 16a^2\rho\nabla\rho\cdot\nabla q - 16a^2q\rho\nabla^2\rho\Bigg)$$
$$- 2a^2\rho h\nabla^2(q\rho) + qah\nabla^2\rho - qa^2h\nabla^2\rho^2\Bigg)drdt$$

Rearranging and cancelling results in:

$$\mathcal{L}_\rho(\rho, \mathbf{w}, q)h = -\frac{1}{\beta}\int_0^T \int_\Omega q\Bigg(a\nabla^2\rho + 2a\nabla^2\rho - 8a^2\,(\nabla\rho)^2 - 8a\nabla^2\rho$$
$$+ 16a^2(\nabla\rho)^2 + 16a^2\rho\nabla^2\rho + a\nabla^2\rho - a^2\nabla^2\rho^2 - 2a^2\rho\nabla^2\rho\Bigg)$$
$$+ \nabla q\cdot\Bigg(2a\nabla\rho - 8a\nabla\rho + 16a^2\rho\nabla\rho - 4a^2\rho\nabla\rho\Bigg)$$
$$+ \nabla^2 q\Bigg(1 + 2a\rho - 2a^2\rho^2\Bigg)drdt$$

$$\mathcal{L}_\rho(\rho, \mathbf{w}, q)h = -\frac{1}{\beta}\int_0^T \int_\Omega q\Bigg(6a^2\,(\nabla\rho)^2 - 4a\nabla^2\rho + 13a^2\rho\nabla^2\rho\Bigg)$$
$$+ \nabla q\cdot\Bigg(-6a\nabla\rho + 12a^2\rho\nabla\rho\Bigg) + \nabla^2 q\Bigg(1 + 2a\rho - 2a^2\rho^2\Bigg)drdt$$