1 Optimality conditions for the sedimentation equations

We consider the terms of the PDE and the boundary conditions separately here.

1.1 Terms that go into the PDE

The relevant part of the PDE is:

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

where $\eta = a\rho$ and $a = \pi\sigma^2/4$. Consider:

$$F_1(\rho) = \nabla^2 \rho \frac{1}{1 - a\rho}$$

$$F_2(\rho) = \nabla \rho \cdot \nabla \left(\frac{3 - 2a\rho}{(1 - a\rho)^2} \right)$$

$$F_3(\rho) = \rho \nabla^2 \left(\frac{a\rho - 2}{(a\rho - 1)^2} \right)$$

Then

$$F_1(\rho + h) - F_1(\rho) = \nabla(\rho + h) \frac{1}{1 - a(\rho + h)} - \nabla\rho \frac{1}{1 - a\rho}$$

Using the expansion:

$$\frac{1}{c-x} = \frac{1}{c} + \frac{1}{c^2}x + O(x^2),$$

where $c = 1 - a\rho$, we get:

$$F_1(\rho+h) - F_1(\rho) = \nabla^2(\rho+h) \left(\frac{1}{1-a\rho} + \frac{a}{(1-a\rho)^2} h \right) - \nabla^2 \rho \frac{1}{1-a\rho}$$
$$= \nabla^2 h \left(\frac{1}{1-a\rho} \right) + \nabla^2 \rho \left(\frac{a}{(1-a\rho)^2} h \right)$$

For F_2 we consider the expansion:

$$\frac{1}{(c-x)^2} = \frac{1}{c^2} + \frac{2}{c^3}x + O(x^2),$$

and get:

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

Finally, we have:

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

Combining these in the Lagrangian gives:

$$\begin{split} \mathcal{L}_{\rho}(\rho,\mathbf{w},q)h &= -\frac{1}{\beta} \int_{0}^{T} \int_{\Omega} q \nabla^{2} h \left(\frac{1}{1-a\rho} \right) + q \nabla^{2} \rho \left(\frac{a}{(1-a\rho)^{2}} h \right) \\ &+ q \nabla h \cdot \nabla \left(\frac{3-2a\rho}{(1-a\rho)^{2}} \right) + q \left(\nabla h \cdot \nabla \rho \right) \left(\frac{-2a}{(1-a\rho)^{2}} + \frac{6a-4a^{2}\rho}{(1-a\rho)^{3}} \right) \\ &+ q h \nabla \rho \cdot \nabla \left(\frac{-2a}{(1-a\rho)^{2}} + \frac{6a-4a^{2}\rho}{(1-a\rho)^{3}} \right) \\ &- q h \nabla^{2} \left(\frac{a\rho-2}{(a\rho-1)^{2}} \right) - q \rho \left(\frac{a}{(1-a\rho)^{2}} + \frac{2a^{2}\rho-4a}{(1-a\rho)^{3}} \right) \nabla^{2} h \\ &- q \rho \nabla \left(\frac{2a}{(1-a\rho)^{2}} + \frac{4a^{2}\rho-8a}{(1-a\rho)^{3}} \right) \cdot \nabla h - q \rho h \nabla^{2} \left(\frac{a}{(1-a\rho)^{2}} + \frac{2a^{2}\rho-4a}{(1-a\rho)^{3}} \right). \end{split}$$

Rearranging gives:

$$\mathcal{L}_{\rho}(\rho, \mathbf{w}, q)h = -\frac{1}{\beta} \int_{0}^{T} \int_{\Omega} h \left(q \nabla^{2} \rho \left(\frac{a}{(1 - a\rho)^{2}} \right) + q \nabla \rho \cdot \nabla \left(\frac{-2a}{(1 - a\rho)^{2}} + \frac{6a - 4a^{2}\rho}{(1 - a\rho)^{3}} \right) - q \nabla^{2} \left(\frac{a\rho - 2}{(a\rho - 1)^{2}} \right) - q\rho \nabla^{2} \left(\frac{a}{(1 - a\rho)^{2}} + \frac{2a^{2}\rho - 4a}{(1 - a\rho)^{3}} \right) \right) + \nabla h \cdot \left(q \nabla \left(\frac{3 - 2a\rho}{(1 - a\rho)^{2}} \right) + q \nabla \rho \left(\frac{-2a}{(1 - a\rho)^{2}} + \frac{6a - 4a^{2}\rho}{(1 - a\rho)^{3}} \right) - q\rho \nabla \left(\frac{2a}{(1 - a\rho)^{2}} + \frac{4a^{2}\rho - 8a}{(1 - a\rho)^{3}} \right) \right) + \nabla^{2} h \left(q \left(\frac{1}{1 - a\rho} \right) - q\rho \left(\frac{a}{(1 - a\rho)^{2}} + \frac{2a^{2}\rho - 4a}{(1 - a\rho)^{3}} \right) \right)$$

Integration by parts gives:

$$\mathcal{L}_{\rho}(\rho, \mathbf{w}, q)h = -\frac{1}{\beta} \int_{0}^{T} \int_{\Omega} h \left(q \nabla^{2} \rho \left(\frac{a}{(1 - a\rho)^{2}} \right) + q \nabla \rho \cdot \nabla \left(\frac{-2a}{(1 - a\rho)^{2}} + \frac{6a - 4a^{2}\rho}{(1 - a\rho)^{3}} \right) - q \nabla^{2} \left(\frac{a\rho - 2}{(a\rho - 1)^{2}} \right) - q\rho \nabla^{2} \left(\frac{a}{(1 - a\rho)^{2}} + \frac{2a^{2}\rho - 4a}{(1 - a\rho)^{3}} \right) \right) - h\nabla \left(q \nabla \left(\frac{3 - 2a\rho}{(1 - a\rho)^{2}} \right) + q \nabla \rho \left(\frac{-2a}{(1 - a\rho)^{2}} + \frac{6a - 4a^{2}\rho}{(1 - a\rho)^{3}} \right) - q\rho \nabla \left(\frac{2a}{(1 - a\rho)^{2}} + \frac{4a^{2}\rho - 8a}{(1 - a\rho)^{3}} \right) \right) + h\nabla^{2} \left(q \left(\frac{1}{1 - a\rho} \right) - q\rho \left(\frac{a}{(1 - a\rho)^{2}} + \frac{2a^{2}\rho - 4a}{(1 - a\rho)^{3}} \right) \right)$$

So we have:

$$\begin{split} \mathcal{L}_{\rho}(\rho,\mathbf{w},q)h &= -\frac{1}{\beta} \int_{0}^{T} \int_{\Omega} h \left[q \nabla^{2} \rho \left(\frac{a}{(1-a\rho)^{2}} \right) + q \nabla \rho \cdot \nabla \left(\frac{-2a}{(1-a\rho)^{2}} + \frac{6a-4a^{2}\rho}{(1-a\rho)^{3}} \right) - q \nabla^{2} \left(\frac{a\rho-2}{(a\rho-1)^{2}} \right) \right. \\ &\quad - q \rho \nabla^{2} \left(\frac{a}{(1-a\rho)^{2}} \right) - q \rho \nabla^{2} \left(\frac{2a^{2}\rho - 4a}{(1-a\rho)^{3}} \right) \\ &\quad - \nabla \cdot \left(q \nabla \left(\frac{3-2a\rho}{(1-a\rho)^{2}} \right) \right) - \nabla \cdot \left(q \nabla \rho \left(\frac{-2a}{(1-a\rho)^{2}} \right) \right) - \nabla \cdot \left(q \nabla \rho \left(\frac{6a-4a^{2}\rho}{(1-a\rho)^{3}} \right) \right) \\ &\quad + \nabla \cdot \left(q \rho \nabla \left(\frac{2a}{(1-a\rho)^{2}} \right) \right) + \nabla \cdot \left(q \rho \nabla \left(\frac{4a^{2}\rho - 8a}{(1-a\rho)^{3}} \right) \right) \\ &\quad + \nabla^{2} \left(q \left(\frac{1}{1-a\rho} \right) \right) - \nabla^{2} \left(q \rho \left(\frac{a}{(1-a\rho)^{2}} \right) \right) - \nabla^{2} \left(q \rho \left(\frac{2a^{2}\rho - 4a}{(1-a\rho)^{3}} \right) \right) \right] dr dt \end{split}$$

And combining fractions gives:

$$\mathcal{L}_{\rho}(\rho, \mathbf{w}, q)h = -\frac{1}{\beta} \int_{0}^{T} \int_{\Omega} h \left[q \nabla^{2} \rho \left(\frac{a}{(1 - a\rho)^{2}} \right) + q \nabla \rho \cdot \nabla \left(\frac{2a(a\rho - 2)}{(1 - a\rho)^{3}} \right) - q \nabla^{2} \left(\frac{a\rho - 2}{(a\rho - 1)^{2}} \right) \right.$$

$$\left. - q\rho \nabla^{2} \left(\frac{a(3 - a\rho)}{(1 - a\rho)^{3}} \right) - \nabla \cdot \left(q \nabla \left(\frac{3 - 2a\rho}{(1 - a\rho)^{2}} \right) \right) - \nabla \cdot \left(q \nabla \rho \left(\frac{2a(a\rho - 2)}{(1 - a\rho)^{3}} \right) \right) \right.$$

$$\left. + \nabla \cdot \left(q\rho \nabla \left(\frac{-2a(a\rho - 3)}{(1 - a\rho)^{3}} \right) \right) + \nabla^{2} \left(q \left(\frac{1}{1 - a\rho} \right) \right) - \nabla^{2} \left(q\rho \left(\frac{-a(a\rho - 3)}{(1 - a\rho)^{3}} \right) \right) \right] dr dt$$

According to Mathematica this is:

$$\mathcal{L}_{\rho}(\rho, \mathbf{w}, q) h = -\frac{1}{\beta} \int_{0}^{T} \int_{\Omega} h \left[\frac{1}{(a\rho - 1)^{3}} \left(4a\nabla\rho \cdot \nabla q + 2a(-1 + a\rho)q\nabla^{2}\rho + (-1 + 5a\rho - 2a^{2}\rho^{2})\nabla^{2}q \right) \right] dr dt$$

And rewriting this is:

$$\mathcal{L}_{\rho}(\rho, \mathbf{w}, q)h = -\frac{1}{\beta} \int_{0}^{T} \int_{\Omega} h \left[\frac{4a\nabla\rho \cdot \nabla q}{(a\rho - 1)^{3}} + \frac{2aq\nabla^{2}\rho}{(a\rho - 1)^{2}} + \frac{(-1 + 5a\rho - 2a^{2}\rho^{2})\nabla^{2}q}{(a\rho - 1)^{3}} \right] dr dt$$

1.2 Boundary Terms

We have the equation:

$$-\mathbf{j} \cdot \mathbf{n} = -\rho \nabla \frac{\delta F[\rho]}{\delta \rho} \cdot \mathbf{n} = -\frac{1}{\beta} \left(\frac{\nabla \rho}{1-\eta} - \rho \nabla \frac{\eta - 2}{(\eta - 1)^2} \right) \cdot \mathbf{n}$$

Then:

$$F_4(\rho) = \frac{\nabla \rho}{1 - a\rho}$$
$$F_5(\rho) = \rho \nabla \frac{a\rho - 2}{(a\rho - 1)^2}$$

Then for F_4 we have:

$$F_4(\rho + h) - F_4(\rho) = \nabla(\rho + h) \frac{1}{1 - a(\rho + h)} - \nabla\rho \frac{1}{1 - a\rho}$$
$$= \nabla(\rho + h) \left(\frac{1}{1 - a\rho} + \frac{a}{(1 - a\rho)^2}h\right)$$
$$= \nabla h \left(\frac{1}{1 - a\rho}\right) + \nabla\rho \left(\frac{a}{(1 - a\rho)^2}h\right)$$

For F_5 we get:

$$\begin{split} F_5(\rho+h) - F_5(\rho) &= (\rho+h) \nabla \frac{a(\rho+h) - 2}{(a(\rho+h) - 1)^2} - \rho \nabla \frac{a\rho - 2}{(a\rho - 1)^2} \\ &= (\rho+h) \nabla \left(\frac{a(\rho+h) - 2}{(1-a\rho)^2} + \frac{a(\rho+h) - 2}{(1-a\rho)^3} 2ah \right) - \rho \nabla \frac{a\rho - 2}{(a\rho - 1)^2} \\ &= h \nabla \left(\frac{a\rho - 2}{(1-a\rho)^2} \right) + \rho \nabla \left(h \left(\frac{a}{(1-a\rho)^2} + \frac{2a^2\rho - 4a}{(1-a\rho)^3} \right) \right) \\ &= h \nabla \left(\frac{a\rho - 2}{(1-a\rho)^2} \right) + h\rho \nabla \left(\frac{a}{(1-a\rho)^2} + \frac{2a^2\rho - 4a}{(1-a\rho)^3} \right) + \nabla h \left(\rho \frac{a}{(1-a\rho)^2} + \rho \frac{2a^2\rho - 4a}{(1-a\rho)^3} \right) \end{split}$$

Then the boundary terms for the Lagrangian are:

$$\mathcal{L}_{\rho,1}(\rho,\mathbf{w},q)h = -\frac{1}{\beta} \int_0^T \int_{\partial\Omega} \left(-q_{\partial\Omega} \nabla h \left(\frac{1}{1-a\rho} \right) - q_{\partial\Omega} \nabla \rho \left(\frac{a}{(1-a\rho)^2} h \right) + q_{\partial\Omega} h \nabla \left(\frac{a\rho - 2}{(1-a\rho)^2} \right) + h q_{\partial\Omega} \rho \nabla \left(\frac{a}{(1-a\rho)^2} + \frac{2a^2\rho - 4a}{(1-a\rho)^3} \right) + q_{\partial\Omega} \nabla h \left(\rho \frac{a}{(1-a\rho)^2} + \rho \frac{2a^2\rho - 4a}{(1-a\rho)^3} \right) \right) \cdot \mathbf{n} dr dt$$

From the integration by parts of the terms within the domain (in the previous section) we get:

$$\mathcal{L}_{\rho,2}(\rho, \mathbf{w}, q)h = -\frac{1}{\beta} \int_0^T \int_{\partial\Omega} \left(h \left(q \nabla \left(\frac{3 - 2a\rho}{(1 - a\rho)^2} \right) + q \nabla \rho \left(\frac{-2a}{(1 - a\rho)^2} + \frac{6a - 4a^2\rho}{(1 - a\rho)^3} \right) \right)$$

$$- q\rho \nabla \left(\frac{2a}{(1 - a\rho)^2} + \frac{4a^2\rho - 8a}{(1 - a\rho)^3} \right) \right)$$

$$+ \nabla h \left(q \left(\frac{1}{1 - a\rho} \right) - q\rho \left(\frac{a}{(1 - a\rho)^2} + \frac{2a^2\rho - 4a}{(1 - a\rho)^3} \right) \right)$$

$$- h\nabla \left(q \left(\frac{1}{1 - a\rho} \right) - q\rho \left(\frac{a}{(1 - a\rho)^2} + \frac{2a^2\rho - 4a}{(1 - a\rho)^3} \right) \right) \cdot \mathbf{n} dr dt$$

Combining all of these give all boundary terms for the Lagrangian:

$$\mathcal{L}_{\rho}(\rho, \mathbf{w}, q)h = -\frac{1}{\beta} \int_{0}^{T} \int_{\partial\Omega} \left(h \left(-q_{\partial\Omega} \nabla \rho \left(\frac{a}{(1 - a\rho)^{2}} \right) + q_{\partial\Omega} \nabla \left(\frac{a\rho - 2}{(1 - a\rho)^{2}} \right) \right) \right.$$

$$\left. + q_{\partial\Omega} \rho \nabla \left(\frac{a}{(1 - a\rho)^{2}} + \frac{2a^{2}\rho - 4a}{(1 - a\rho)^{3}} \right) + \left(q \nabla \left(\frac{3 - 2a\rho}{(1 - a\rho)^{2}} \right) + q \nabla \rho \left(\frac{-2a}{(1 - a\rho)^{2}} + \frac{6a - 4a^{2}\rho}{(1 - a\rho)^{3}} \right) \right.$$

$$\left. - q\rho \nabla \left(\frac{2a}{(1 - a\rho)^{2}} + \frac{4a^{2}\rho - 8a}{(1 - a\rho)^{3}} \right) \right) - \nabla \left(q \left(\frac{1}{1 - a\rho} \right) - q\rho \left(\frac{a}{(1 - a\rho)^{2}} + \frac{2a^{2}\rho - 4a}{(1 - a\rho)^{3}} \right) \right) \right)$$

$$+ \nabla h \left(- q_{\partial\Omega} \left(\frac{1}{1 - a\rho} \right) + q_{\partial\Omega} \left(\rho \frac{a}{(1 - a\rho)^{2}} + \rho \frac{2a^{2}\rho - 4a}{(1 - a\rho)^{3}} \right) + q \left(\frac{1}{1 - a\rho} \right) \right.$$

$$\left. - q\rho \left(\frac{a}{(1 - a\rho)^{2}} + \frac{2a^{2}\rho - 4a}{(1 - a\rho)^{3}} \right) \right) \cdot \mathbf{n} dr dt$$

Comparing terms in ∇h :

$$\left[-q_{\partial\Omega} \left(\frac{1}{1 - a\rho} \right) + q_{\partial\Omega} \left(\rho \frac{a}{(1 - a\rho)^2} + \rho \frac{2a^2\rho - 4a}{(1 - a\rho)^3} \right) + q \left(\frac{1}{1 - a\rho} \right) - q\rho \left(\frac{a}{(1 - a\rho)^2} + \frac{2a^2\rho - 4a}{(1 - a\rho)^3} \right) \right] \cdot \mathbf{n} = 0.$$

This holds when $q_{\partial\Omega}=q$. Then for $h\neq 0$ we get:

$$\begin{split} & \left[-q\nabla\rho\left(\frac{a}{(1-a\rho)^2}\right) + q\nabla\left(\frac{a\rho - 2}{(1-a\rho)^2}\right) \right. \\ & + q\rho\nabla\left(\frac{a}{(1-a\rho)^2} + \frac{2a^2\rho - 4a}{(1-a\rho)^3}\right) + q\nabla\left(\frac{3-2a\rho}{(1-a\rho)^2}\right) + q\nabla\rho\left(\frac{-2a}{(1-a\rho)^2} + \frac{6a - 4a^2\rho}{(1-a\rho)^3}\right) \\ & - q\rho\nabla\left(\frac{2a}{(1-a\rho)^2} + \frac{4a^2\rho - 8a}{(1-a\rho)^3}\right) - \nabla\left(q\left(\frac{1}{1-a\rho}\right) - q\rho\left(\frac{a}{(1-a\rho)^2} + \frac{2a^2\rho - 4a}{(1-a\rho)^3}\right)\right)\right] \cdot \mathbf{n} = 0 \end{split}$$

According to Mathematica this is:

$$\frac{(1+a\rho)\nabla q}{(a\rho-1)^3} \cdot \mathbf{n} = 0$$

Since $a\rho > 0$ by definition, this is:

$$\frac{\partial q}{\partial n} = 0.$$