Step-By-Step Derivation of the Energy Balance in Equation (52)

Identities

In this derivation we make use of the following identities. For any vectors $\mathbf{x}$ and $\mathbf{y}$ we have

$$\mathbf{x}^\mathsf{T}\mathbf{y} = \mathbf{y}^\mathsf{T}\mathbf{x}. \tag{B.1}$$

For any symmetric matrix $\mathbf{D}$

$$\begin{aligned}(\mu\mathbf{x}^{n+\frac{1}{2}})^\mathsf{T}\mathbf{D}\delta\mathbf{x}^{n+\frac{1}{2}} &= (\mathbf{x}^{n+1}+\mathbf{x}^{n})^\mathsf{T}\mathbf{D}(\mathbf{x}^{n+1}-\mathbf{x}^{n})\\ &= (\mathbf{x}^{n+1})^\mathsf{T}\mathbf{D}\mathbf{x}^{n+1} - (\mathbf{x}^{n})^\mathsf{T}\mathbf{D}\mathbf{x}^{n}\\ &= \delta\left((\mathbf{x}^{n+\frac{1}{2}})^\mathsf{T}\mathbf{D}\mathbf{x}^{n+\frac{1}{2}}\right).\end{aligned} \tag{B.2}$$

In scalar form, and denoting $g^n = (x^n)^2$, the same identity reduces to

$$\begin{aligned}\mu x^{n+\frac{1}{2}}\delta x^{n+\frac{1}{2}} &= \left(x^{n+1}+x^{n}\right)\left(x^{n+1}-x^{n}\right)\\ &= (x^{n+1})^2-(x^n)^2\\ &= \delta g^{n+\frac{1}{2}}.\end{aligned} \tag{B.3}$$

Furthermore, for $z = \mathrm{b}, \mathrm{c}$ we have

$$y_z^n = \mathbf{g}_z^\mathsf{T}\bar{\mathbf{y}}^n. \tag{B.4}$$

Energy Balance

The starting point is equation (41) of the paper:

$$\delta\bar{\mathbf{q}}^{n+\frac{1}{2}} = -\mathbf{A}\mu\bar{\mathbf{y}}^{n+\frac{1}{2}} - \mathbf{B}\delta\bar{\mathbf{y}}^{n+\frac{1}{2}} + \xi\sum_{z=\mathrm{c,b,e}}\mathbf{g}_z F_z^{n+\frac{1}{2}}. \tag{B.5}$$

Multiplying the left-hand side of (B.5) with $(\mu\bar{\mathbf{q}}^{n+\frac{1}{2}})^\mathsf{T}$ and the right-hand side with $(\delta\bar{\mathbf{y}}^{n+\frac{1}{2}})^\mathsf{T}$ (these terms are equal per equation (40) of the paper) yields

$$\begin{aligned}(\mu\bar{\mathbf{q}}^{n+\frac{1}{2}})\delta\bar{\mathbf{q}}^{n+\frac{1}{2}} &= -(\delta\bar{\mathbf{y}}^{n+\frac{1}{2}})^\mathsf{T}\mathbf{A}\mu\bar{\mathbf{y}}^{n+\frac{1}{2}} - (\delta\bar{\mathbf{y}}^{n+\frac{1}{2}})^\mathsf{T}\mathbf{B}\delta\bar{\mathbf{y}}^{n+\frac{1}{2}}\\ &\quad + \xi(\delta y^{n+\frac{1}{2}})^\mathsf{T}\mathbf{g}_\mathrm{c}F_\mathrm{c}^{n+\frac{1}{2}} + \xi(\delta y^{n+\frac{1}{2}})^\mathsf{T}\mathbf{g}_\mathrm{b}F_\mathrm{b}^{n+\frac{1}{2}} + \tfrac{1}{2}\xi(\delta y^{n+\frac{1}{2}})^\mathsf{T}\mathbf{g}_\mathrm{e}\mu F_\mathrm{e}^{n+\frac{1}{2}}.\end{aligned} \tag{B.6}$$

Using (B.1),(B.2), and (B.4), and noting that the diagonal matrices $\mathbf{A}$ and $\mathbf{B}$ are per definition symmetrical, we can write this as

$$\frac{\delta(\bar{\mathbf{q}}^\mathsf{T}\bar{\mathbf{q}}+\bar{\mathbf{y}}\mathbf{A}\bar{\mathbf{y}})^{n+\frac{1}{2}}}{\xi} = -\frac{(\delta\bar{\mathbf{y}}^{n+\frac{1}{2}})^\mathsf{T}\mathbf{B}\delta\bar{\mathbf{y}}^{n+\frac{1}{2}}}{\xi} + \underbrace{\delta y_\mathrm{c}^{n+\frac{1}{2}}F_\mathrm{c}^{n+\frac{1}{2}}}_{G_\mathrm{c}} + \underbrace{\delta y_\mathrm{b}^{n+\frac{1}{2}}F_\mathrm{b}^{n+\frac{1}{2}}}_{G_\mathrm{b}} + \tfrac{1}{2}\mathbf{g}_\mathrm{e}^\mathsf{T}\delta y^{n+\frac{1}{2}}\mu F_\mathrm{e}^{n+\frac{1}{2}}. \tag{B.7}$$

Using (B.3) and equation (29) of the paper, the term G_{c} is

$$
\begin{aligned}
G_{\mathrm{c}} &= \delta y_{\mathrm{c}}^{n+\frac{1}{2}} k_{\mathrm{c}} \left(h_{\mathrm{c}} - \tfrac{1}{2}\mu y_{\mathrm{c}}^{n+\frac{1}{2}} \right) - \frac{r_{\mathrm{c}}}{\Delta t} \left(\delta y_{\mathrm{c}}^{n+\frac{1}{2}} \right)^2 \\
&= -\tfrac{1}{2} k_{\mathrm{c}} \delta \left(h_{\mathrm{c}} - y_{\mathrm{c}} \right)^{n+\frac{1}{2}} \mu (h_{\mathrm{c}} - y_{\mathrm{c}})^{n+\frac{1}{2}} - \frac{r_{\mathrm{c}}}{\Delta t} \left(\delta y_{\mathrm{c}}^{n+\frac{1}{2}} \right)^2 \\
&= -\delta \left(\tfrac{1}{2} k_{\mathrm{c}} [h_{\mathrm{c}} - y_{\mathrm{c}}]^2 \right)^{n+\frac{1}{2}} - \frac{r_{\mathrm{c}}}{\Delta t} \left(\delta y_{\mathrm{c}}^{n+\frac{1}{2}} \right)^2, \\
&= -\delta V_{\mathrm{c}}^{n+\frac{1}{2}} - \frac{r_{\mathrm{c}}}{\Delta t} \left(\delta y_{\mathrm{c}}^{n+\frac{1}{2}} \right)^2
\end{aligned}
\tag{B.8}
$$

and using equation (30) of the paper, the term G_{b} can be written

$$
G_{\mathrm{b}} = -\delta y_{\mathrm{b}} \frac{\delta V_{\mathrm{b}}^{n+\frac{1}{2}}}{\delta y_{\mathrm{b}}} = -\delta V_{\mathrm{b}}^{n+\frac{1}{2}}. \tag{B.9}
$$

Substituting back into (B.7) yields

$$
\delta \left(\xi^{-1} \left[\bar{\mathbf{q}}^{\mathsf{T}} \bar{\mathbf{q}} + \bar{\mathbf{y}} \mathbf{A} \bar{\mathbf{y}} \right] + V_{\mathrm{c}} + V_{\mathrm{b}} \right)^{n+\frac{1}{2}} = \tfrac{1}{2} \mathbf{g}_{\mathrm{e}}^{\mathsf{T}} \delta y^{n+\frac{1}{2}} \mu F_{\mathrm{e}}^{n+\frac{1}{2}} - \left[\frac{(\delta \bar{\mathbf{y}}^{n+\frac{1}{2}})^{\mathsf{T}} \mathbf{B} \delta \bar{\mathbf{y}}^{n+\frac{1}{2}}}{\xi} + \frac{r_{\mathrm{c}}}{\Delta t} \left(\delta y_{\mathrm{c}}^{n+\frac{1}{2}} \right)^2 \right]. \tag{B.10}
$$

Dividing by Δt and using equation (50) from the paper, this can be written as

$$
\frac{\delta H^{n+\frac{1}{2}}}{\Delta t} = \underbrace{\frac{\mathbf{g}_{\mathrm{e}}^{\mathsf{T}} \delta y^{n+\frac{1}{2}} \mu F_{\mathrm{e}}^{n+\frac{1}{2}}}{2\Delta t}}_{P^{n+\frac{1}{2}}} - \underbrace{\left[\frac{(\delta \bar{\mathbf{y}}^{n+\frac{1}{2}})^{\mathsf{T}} \mathbf{B} \delta \bar{\mathbf{y}}^{n+\frac{1}{2}}}{\xi \Delta t} + \frac{r_{\mathrm{c}}}{\Delta t^2} \left(\delta y_{\mathrm{c}}^{n+\frac{1}{2}} \right)^2 \right]}_{Q^{n+\frac{1}{2}}}, \tag{B.11}
$$

which matches equation (52) in the paper.