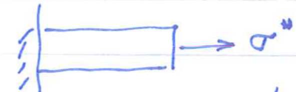
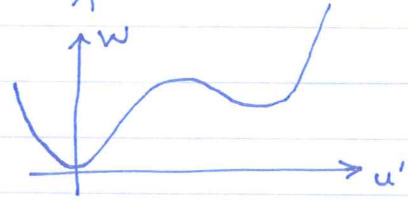
5/8/14 Kinetics and evolution (Quasistatics)

Return to Ericksen's bar



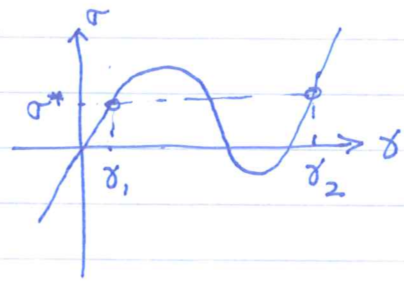
Many equilibria!

The correct on depends on history!

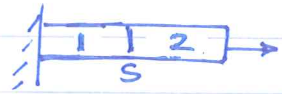


Need to prescribe evolution or kinetic laws!

Many (essentially identical) approaches



1/ "<u>Gradient flow</u>" (Cahn, ...)



$$\mathcal{E}(u,s) = \int_0^L W(u')\,dx - \sigma^* u(L)$$ Let (u,s) be eq.

Perturb the system $u_\varepsilon \mapsto u+\varepsilon v$, $s_\varepsilon \mapsto s+\varepsilon r$

$$0 = \frac{d\,\mathcal{E}(u+\varepsilon v, s+\varepsilon r)}{d\varepsilon}\Bigg|_{\varepsilon=0} = \frac{d}{d\varepsilon}\left(\int_0^{s+\varepsilon r} W(u'+\varepsilon v')\,dx + \int_{s+\varepsilon r}^{L} W(u'+\varepsilon v')\,dx - \sigma^*(u(L)+\varepsilon v(L))\right)\Bigg|_{\varepsilon=0}$$

$$= \underbrace{\int_0^s \overbrace{\frac{dW}{d\gamma}}^{\sigma}\cdot v'\,dx}_{\underbrace{\int_0^s \frac{d}{dx}(\sigma v)\,dx}_{\sigma v\big|_0^{s^-}} - \int_0^s \frac{d\sigma}{dx}\cdot v\,dx} + W(\gamma|_{s^-})\,r + \int_s^L \frac{dW}{d\gamma}\cdot v'\,dx - W(\gamma|_{s^+})\,r - \sigma^* v(L)$$

$$\boxed{[\![q]\!]_s = q^+ - q^-}$$

$$= \int_0^L \frac{d\sigma}{dx} v\,dx - [\![W]\!]_s\, r - [\![\sigma v]\!]_s - \sigma(0)\cancelto{0}{v(0)}$$
$$+ \left(\sigma(L) - \sigma^*\right) v(L)$$

Since v is arbitrary, $$\boxed{\begin{aligned}\frac{d\sigma}{dx} &= 0 \\ \sigma(L) &= \sigma^*\end{aligned}}$$

Further, we want u_ε to be continuous!

$$\therefore \quad u_\varepsilon(s_\varepsilon^-, \varepsilon) = u_\varepsilon(s_\varepsilon^+, \varepsilon)$$

differentiate w.r.t. ε and evaluate at $\varepsilon = 0$

$$\left.\frac{du_\varepsilon}{d\varepsilon}\right|_{s^-,0} + \left.\frac{du}{dx}\right|_{s^-,0} \left.\frac{ds_\varepsilon}{d\varepsilon}\right|_{\varepsilon=0} = \left.\frac{du_\varepsilon}{d\varepsilon}\right|_{s^+,0} + \left.\frac{du}{dx}\right|_{s^+,0} \left.\frac{ds_\varepsilon}{d\varepsilon}\right|_{\varepsilon=0}$$

or $[\![v]\!] + r[\![\gamma]\!] = 0$

Also $[\![ab]\!] = [\![a]\!]\langle b\rangle + \langle a\rangle[\![b]\!]$

$$\therefore \; 0 = -[\![W]\!]_s r - [\![\sigma]\!]_s \langle v\rangle - [\![v]\!]\langle\sigma\rangle$$

Again v arbitrary $\Rightarrow \boxed{[\![\sigma]\!] = 0}$

$$\therefore \; 0 = -\underbrace{\left([\![W_s]\!] - [\![\sigma\gamma]\!]\right)}_{-\delta_s E \;\ldots\; \text{"thermodynamic driving force"} \; d} r$$

Postulate: $\boxed{\frac{ds}{dt} = f(d)}$

2/ <u>Dissipation inequality</u> (Knowles ...)

Consider an evolution $u(x,t)$, $s(t)$

Rate of dissipation = Rate of working − Rate of change of stored energy

$$= \sigma^* \dot{u}(L) - \frac{d}{dt}\int_0^L W(\gamma)\,dx$$

$$= \sigma(L)\,\dot{u}(L) - \sigma(0)\,\dot{u}(0) - \frac{d}{dt}\left(\int_0^{s(t)} W(\gamma)\,dx + \int_{s(t)}^L W(\gamma)\,dx\right)$$

$$- \sigma(s^-)\,\dot{u}(s^-) + \sigma(s^+)\,\dot{u}(s^+)$$

$$+ \sigma(s^-)\,\dot{u}(s^-) - \sigma(s^+)\,\dot{u}(s^+)$$

$$= \int_0^L \underbrace{\frac{d}{dx}(\sigma \dot{u})}_{\frac{d\sigma}{dx}\dot{u} + \sigma\dot{\gamma}} dx - \int_0^L \frac{\partial W}{\partial \gamma}\dot{\gamma}\, dx + \underbrace{[\![\sigma \dot{u}]\!]}_{\langle\sigma\rangle \underbrace{[\![\dot{u}]\!]}_{-[\![\gamma]\!]\dot{s}} + [\![\sigma]\!]\langle \dot{u}\rangle} + [\![W]\!]\dot{s}$$

$\frac{d\sigma}{dx} \to 0$ by equilibrium

$[\![\sigma]\!] \to 0$ by equilibrium

$$= \int_0^L \left(\sigma - \frac{\partial W}{\partial \gamma}\right)\dot{\gamma}\, dx + \left([\![W]\!] - [\![\sigma\gamma]\!]\right)\dot{s}$$

≥ 0 for all equilibrium processes.

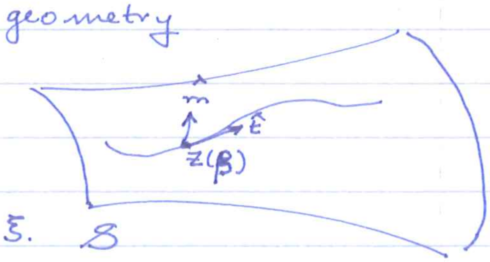
$\Rightarrow \sigma = \frac{\partial W}{\partial \gamma}$ (Coleman-Noll), $\underbrace{\left([\![W]\!] - [\![\sigma\gamma]\!]\right)}_{\text{Force conjugate to } \dot{s}, \ \ldots \text{"driving force" } d}\dot{s} \geq 0$

Postulate $\boxed{\dot{s} = f(d)}$.

Higher dimensions (Include chemical composition and surface effects.)

Brief introduction to surface geometry

- Consider a smooth surface $\mathcal{S} \subset \mathbb{R}^3$ and some curve $\underset{\sim}{z}(\xi)$ on the surface parametrized by an arc length parameter ξ.



Let $\psi : \mathcal{S} \to \mathbb{R}$ and $\underset{\sim}{g} : \mathcal{S} \to \mathbb{R}^3$ be smooth scalar and vector fields defined on $\mathcal{S}$. Then, the surface gradients are defined through the chain rule:

$$\frac{\partial \psi}{\partial \xi} = \nabla_s \psi \cdot \frac{\partial \underset{\sim}{z}}{\partial \xi}, \qquad \frac{\partial \underset{\sim}{g}}{\partial \xi} = \left(\nabla_s \underset{\sim}{g}\right)\frac{\partial \underset{\sim}{z}}{\partial \xi}$$

$$\underset{\sim}{\nabla_s}\psi \cdot \hat{m} = 0 \qquad \left(\nabla_s \underset{\sim}{g}\right)\hat{m} = 0$$

for any smooth curve $\underset{\sim}{z}(\xi)$ on $\mathcal{S}$ parametrized by an arc-length parameter and $\hat{m}$ normal to $\mathcal{S}$.

Note $\underset{\sim}{\nabla_s}\psi$ is a vector in the tangent plane and $\nabla_s \underset{\sim}{g}$ a tensor that acts on vectors in the tangent plane.

The <u>surface divergence</u> of a vector field $\underset{\sim}{g}$ is $\nabla_S \cdot \underset{\sim}{g} = \mathrm{tr}(\nabla_S \underset{\sim}{g})$
and that of a tensor field $\underset{\sim}{S}$ is defined through

$$\underset{\sim}{a} \cdot (\nabla_S \cdot \underset{\sim}{S}) = \nabla_S \cdot (\underset{\sim}{S}^T \underset{\sim}{a}) \quad \forall \; a \in \mathbb{R}^3.$$

<u>Curvature tensor</u> $\underset{\sim}{L} = -\nabla_S \hat{m}$, total curvature $\kappa = \mathrm{tr}\, L = -\nabla_S \cdot \hat{m}$

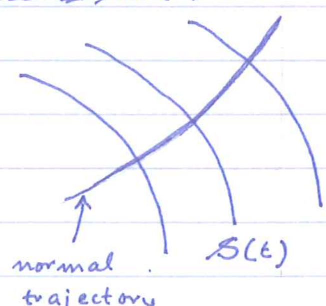
Projection operator $\underset{\sim}{P} = \underset{\sim}{I} - \hat{m} \otimes \hat{m}$.

- Consider a <u>smooth evolving surface</u> $S(t) \subset \mathbb{R}^3$

  Let $\underset{\sim}{z}(t)$ define a normal trajectory: $\dot{\underset{\sim}{z}} = v_m \hat{m}$

  v_m ↑ normal velocity.

  i.e. the trajectory is normal to the surface at each time.

  <u>Normal time derivative</u> $\underset{\sim}{g}^{\circ}$ of a superficial field g is the time derivative of g following a normal trajectory.

  For any spatial field $\underset{\sim}{g}: \Omega \to \mathbb{R}^3$, $\underset{\sim}{g}^{\circ} = \dot{\underset{\sim}{g}} + v_m (\nabla \underset{\sim}{g}) \hat{m}$.

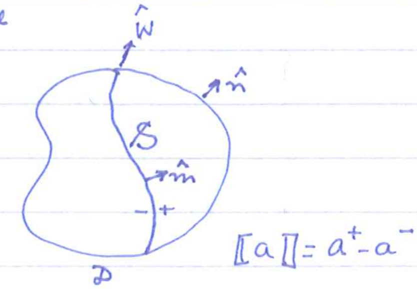
- Consider a <u>smooth curve</u> $\mathcal{C}$ parametrized by the arc length parameter ξ: $\mathcal{C} = \{ \underset{\sim}{x}(\xi) \}$. We have

  $$\underset{\sim}{x}_{\xi} = \hat{t}, \quad \hat{t}_{\xi} = \kappa \hat{n}, \quad \hat{n}_{\xi} = \tau \hat{b} - \kappa \hat{t} \quad \hat{b}_{\xi} = -\tau \hat{n} \quad \text{(Frenét-Servet formula)}$$

  $\hat{t}$: tangent; κ: curvature; $\hat{n}$: normal; τ: torsion; $\hat{b}$: binormal

- Divergence theorem

  $$\int_{\mathcal{D}} \nabla \cdot \underset{\sim}{a} \, dV = \int_{\partial \mathcal{D}} \underset{\sim}{a} \cdot \hat{n} \, dA - \int_{S} [\![\underset{\sim}{a}]\!] \cdot \hat{m} \, dA$$

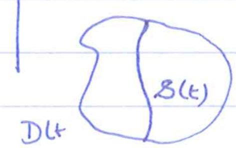
  $$\int_S \nabla_S \cdot \underset{\sim}{a} \, dA = \int_{\partial S} \underset{\sim}{a} \cdot \hat{w} \, dl$$

  $\hat{w}$: normal to ∂S

• Transport theorem. Consider a moving control volume $D(t)$ with a moving surface $S(t)$

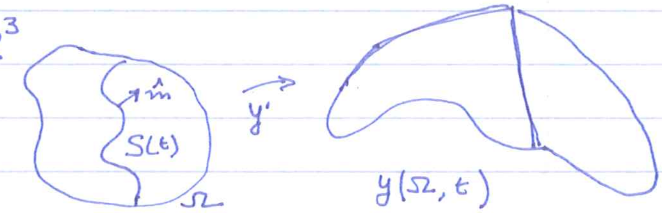
$$\frac{d}{dt}\int_{D(t)} \varphi\, dV = \int_{D(t)} \dot{\varphi}\, dV + \int_{\partial D} \varphi\, v_n\, dA - \int_{S(t)} [\![\varphi]\!]\, v_m\, dA$$

$$\frac{d}{dt}\int_{S(t)} \psi\, dA = \int_{S(t)} (\psi^{\circ} - \psi\, v_m K)\, dA + \int_{\partial S(t)} \psi\, \underset{\sim}{v}\cdot\hat{w}\, d\ell$$



• Deformation $\underset{\sim}{y} : \Omega \times [0, \bar{T}] \to \mathbb{R}^3$

$\underset{\sim}{y}$ continuous across evolving interface $S(t)$



a/ Fix $t = t_0$. Let $\underset{\sim}{x}(\xi)$ be a curve on $S(t_0)$.

Continuity $\Rightarrow$ $y(x^+(\xi), t_0) = y(x^-(\xi), t_0)$

Differentiate w.r.t. ξ : $\nabla y\big|_{x^+, t_0} \hat{t} = \nabla y\big|_{x^-, t_0} \hat{t}$ $\qquad \hat{t} = \underset{\sim}{x}_{\xi}$

This holds for all smooth curves $\Rightarrow [\![\underset{\sim}{F}]\!]\hat{t} = 0 \quad \forall\ \hat{t}\cdot\hat{m} = 0$ $\qquad \underset{\sim}{F} = \nabla \underset{\sim}{y}$

$\Rightarrow [\![\underset{\sim}{F}]\!] = \underset{\sim}{a} \otimes \hat{m}$

b/ Now consider a (smooth) trajectory $\underset{\sim}{x}(t) \in S(t)$.

Continuity $\Rightarrow$ $y(x^+(t), t) = y(x^-(t), t) \quad \forall\ t$

Diff. w.r.t. $\underset{\sim}{F}^+ \dot{x} + \dot{y}^+ = F^- \dot{x} + \dot{y}^-$

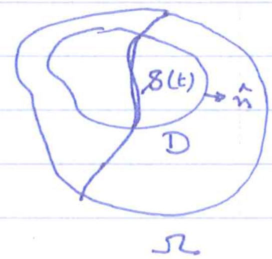
$\Rightarrow [\![\dot{y}]\!] + v_m [\![F]\!]\hat{m} = 0$

c/ Define <u>superficial deformation gradient</u> $\nabla_s \underset{\sim}{y} = \underset{\sim}{\bar{F}}$

Can show $\underset{\sim}{\bar{F}} = \langle \underset{\sim}{F} \rangle \underset{\sim}{P}$

or $\underset{\sim}{\bar{F}}\hat{t} = \underset{\sim}{F}^+\hat{t} = \underset{\sim}{F}^-\hat{t} = \langle \underset{\sim}{F} \rangle \hat{t}$

- Balance of mass/species. Consider a solid made of N species. Let ρ^i denote ~~the~~ the reference density of species i, and let $\underset{\sim}{j}^i$ be it's flux. Consider a region D with a moving interface $\mathcal{S}(t)$.



Balance of species i (assuming no reactions/sources)

$$0 = \frac{d}{dt}\int_D \rho^i dV - \int_{\partial D} \underset{\sim}{j}^i \cdot \hat{n}\, dA$$

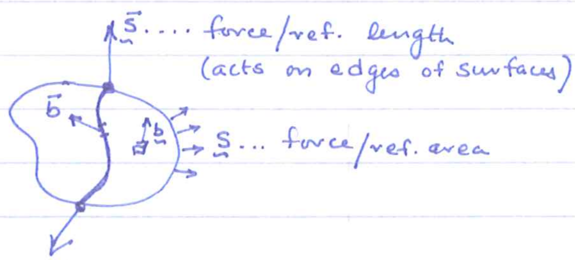
$$= \int_D \dot{\rho}^i\, dV - \int_{D\cap\mathcal{S}(t)} [\![\rho]\!]\, v_m\, dA \qquad \text{(transport thm)}$$

$$- \int_D \nabla\cdot \underset{\sim}{j}^i\, dV + \int_{D\cap\mathcal{S}(t)} [\![\underset{\sim}{j}^i]\!]\, \hat{m}\, dA$$

This holds for all D $\Rightarrow$

$$\boxed{\begin{array}{ll} \dot{\rho}^i = \nabla\cdot \underset{\sim}{j}^i & \text{in } \Omega \\ [\![\rho^i]\!]\, v_m = [\![\underset{\sim}{j}^i]\!]\cdot \hat{m} & \text{on } S(t) \end{array}}$$

- Balance of linear momentum (ignoring inertia)



$$\int_{\partial D} \underset{\sim}{s}\, dA + \int_D \underset{\sim}{b}\, dV + \int_{\partial(D\cap\mathcal{S})} \bar{\underset{\sim}{s}}\, dl + \int_{\mathcal{S}} \bar{b}\, dA = 0$$

Using the usual tetrahedron/triangle argument, $\exists$

$\exists$ $\underset{\approx}{S}$ ... Piola-Kirchhoff stress tensor ... s.t. $\boxed{\underset{\sim}{s} = \underset{\approx}{S}\hat{n}}$

$\bar{\underset{\approx}{S}}$ ... superficial SK " " s.t. $\boxed{\bar{\underset{\sim}{s}} = \bar{\underset{\approx}{S}}\hat{w}}$

$$\therefore \underbrace{\int_{\partial D} \underset{\approx}{S}\hat{n}\, dA}_{\int_D \nabla\cdot \underset{\approx}{S}\, dV + \int_{\mathcal{S}} [\![\underset{\approx}{S}]\!]\hat{m}\, dA} + \int_D \underset{\sim}{b}\, dV + \underbrace{\int_{\partial(D\cap\mathcal{S})} \bar{\underset{\approx}{S}}\hat{w}\, dl}_{\int_{\mathcal{S}} \nabla_S\cdot \bar{\underset{\approx}{S}}\, dA} + \int_{\mathcal{S}} \bar{b}\, dA = 0 \qquad \forall\ D$$

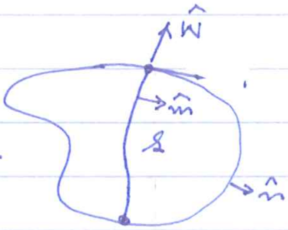
$$\Rightarrow \boxed{\begin{array}{l} \nabla\cdot \underset{\approx}{S} + \underset{\sim}{b} = 0 \\ \nabla_S\cdot \bar{\underset{\approx}{S}} + [\![\underset{\approx}{S}]\!]\hat{m} + \bar{\underset{\sim}{b}} = 0 \end{array}}$$

• Balance of angular momentum (ignoring inertia)

$$\int_{\partial D} y \times S\, dA + \int_{D} y \times b\, dV + \int_{\partial(D\cap \mathcal{S})} y \times \bar{S}\, dA + \int_{\mathcal{S}\cap D} y \times \bar{b}\, dA = 0$$

By the usual argument,
$$\boxed{\begin{aligned} F S^T &= S F^T \\ \bar{F}\bar{S}^T &= \bar{S}\bar{F}^T \end{aligned}}$$

• Rate of dissipation



$$\dot{\mathcal{D}} = \int_{\partial\Omega} S\cdot \dot{y}\, dA + \int_{\partial \mathcal{S}} \bar{S}\hat{w}\cdot\left(\langle \dot{y}\rangle + \langle \nabla y\rangle (v_m \hat{m} + v_w \hat{w})\right) d\ell$$

$$- \int_{\partial\Omega} \sum \underset{\uparrow\ \text{chemical potential}}{\mu^i} j^i\cdot \hat{n}\, dA - \frac{d}{dt}\int_{\Omega} W(s^i, F)\, dV - \frac{d}{dt}\int_{\mathcal{S}} \psi(\bar{F}, \hat{m})\, dA$$

$$= \mathrm{I} + \mathrm{II} + \mathrm{III} + \mathrm{IV} + \mathrm{V}$$

$$\mathrm{I} = \int_{\partial\Omega} S\hat{n}\cdot \dot{y}\, dA = \int_{\Omega} \nabla\cdot(S^T \dot{y})\, dV + \int_{\mathcal{S}} [\![S^T \dot{y}]\!]\cdot \hat{m}\, dA$$

$$= \int_{\Omega} \underbrace{(\nabla\cdot S)}_{0}\cdot \dot{y}\, dV + \int_{\Omega} S\cdot \dot{F}\, dV + \int_{\mathcal{S}} ([\![S]\!]\hat{m})\cdot\langle \dot{y}\rangle\, dA + \int_{\mathcal{S}} \langle S\rangle \hat{m}\cdot(-[\![F]\!]\hat{m}) v_m\, dA$$

$$\mathrm{II} = \int_{\partial\mathcal{S}} \hat{w}\cdot \bar{S}^T(\langle \dot{y}\rangle + \langle \nabla y\rangle v_m \hat{m})\, d\ell + \int_{\partial\mathcal{S}} (\bar{S}\hat{w}\cdot v_w \langle \nabla y\rangle \hat{w})\, d\ell$$

$$= \int_{\mathcal{S}} \nabla_s\cdot\left(\bar{S}^T(\langle \dot{y}\rangle + \langle \nabla y\rangle v_m \hat{m})\right) dA + \quad -\;''\;-$$

$$= \int_{\mathcal{S}} (\nabla_s\cdot \bar{S})\cdot\langle \dot{y}\rangle\, dA + \int_{\mathcal{S}} (\nabla_s\cdot \bar{S})\cdot(\langle \nabla y\rangle \hat{m})\, v_m\, dA$$

$$+ \int_{\mathcal{S}} \bar{S}\cdot \underbrace{\left(\nabla_s(\langle \dot{y}\rangle + \langle \nabla y\rangle \hat{m}\, v_m\right)}_{(\langle \mathring{F}\rangle - \langle F\rangle \hat{m}\otimes \mathring{\hat{m}} - v_m\langle F\rangle L)P} dA + \int_{\partial\mathcal{S}} (\bar{S}\hat{w}\cdot\langle \nabla y\rangle \hat{w})\, v_w\, d\ell$$

$$\underline{\text{III}} = -\int_\Omega \sum \nabla\cdot(\mu^i j^i)\, dV - \int_S \sum [\![\mu^i j^i]\!]\cdot\hat{m}\, dA$$

$$= -\int_\Omega \sum \nabla\mu^i\cdot j^i\, dV - \int_\Omega \sum \mu^i \underbrace{\nabla\cdot j^i}_{\dot{s}^i} dV - \int_S \Big(\sum \big([\![\mu^i]\!]\langle j^i\rangle\cdot\hat{m} + \langle\mu^i\rangle \underbrace{[\![j^i]\!]\cdot\hat{m}}_{[\![s^i]\!]v_m}\big)\Big) dA$$

$$\underline{\text{IV}} = -\int_\Omega \frac{\partial W}{\partial F}\cdot\dot{F}\, dV - \int_\Omega \sum \frac{\partial W}{\partial s^i}\dot{s}^i + \int_S [\![W]\!]\, v_m\, dA$$

$$\underline{\text{V}} = -\int_S \frac{\partial \psi}{\partial \bar{F}}\cdot \overset{\circ}{F}\, dA - \int_S \frac{\partial\psi}{\partial\hat{m}}\cdot\overset{\circ}{\hat{m}}\, dA + \int_S \psi\, v_m \kappa\, dA + \int_{\partial S}\psi(v\cdot\hat{w})\, dl$$

~~Putting these together~~ Finally, introduce 'surface shear' q and a constitutive relation $q = q(\hat{m})$

$$0 = \int_S \underbrace{\nabla_s\cdot(v_m q)}_{v_m\nabla_s\cdot q\, -\, q\cdot\overset{\circ}{m}} dA - \int_{\partial S}(q\cdot\hat{w})\, v_m\, dl$$

$$\overset{\circ}{m} = -\nabla_s v_m$$

Adding $\text{I} - \text{V} + 0$:

$$\dot{\mathcal{D}} = \int_\Omega \Big(\dot{F}\cdot\Big(S - \frac{\partial W}{\partial F}\Big) - \sum \dot{s}^i\Big(\mu^i + \frac{\partial W}{\partial s^i}\Big) - \nabla\mu^i\cdot j^i\Big) dV$$

$$+ \int_S v_m\Big(\hat{m}\cdot\underbrace{[\![W I - F^T S]\!]}_{-\sum\langle\mu^i\rangle s^i I}\hat{m} + (\psi P - \bar{F}^T\bar{S})\cdot L + \nabla_s\cdot q\Big) dA$$

$$+ \int_S \Big(\overset{\circ}{F}\cdot\Big(\bar{S} - \frac{\partial W}{\partial\bar{F}}\Big) - \Big(q + \frac{\partial\psi}{\partial\hat{m}} + \bar{S}^T\langle F\rangle\hat{m}\Big)\cdot\overset{\circ}{m} - \sum[\![\mu^i]\!]\langle j^i\rangle\cdot\hat{m}\Big) dA$$

$$+ \int_{\partial S}\Big\{(q\cdot\hat{w})\, v_m + \big(\psi - \bar{S}w\cdot\langle F\rangle w\big) v_w\Big\} dl$$