Continuum Equations

Use the basic conservation law for a conserved quantity to derive the Navier-Stokes & Energy Eqs of fluid mech, but with micro expressions for stress & heat flux.

($\mu(\partial_i u_j + \partial_j u_i)$ & $-k_T \nabla T$ are phenomenological.)

R = fixed region in 3d

$\rho(\underline{r},t)$ = density of some conserved "stuff" (mass, momentum, energy, charge ...)

Amount of stuff inside R is $M_R(t) = \int_R d^3r \, \rho(\underline{r},t)$

$$\frac{dM_R}{dt} = \int_R d^3r \, \frac{\partial \rho(\underline{r},t)}{\partial t} = - \int_{\partial R} d\underline{S} \cdot \underline{F}$$

bdry of R — "flux of stuff"

"flux" = amt. passing through ∂R per area per time

Use divergence thm: $\int_R d^3r \left(\frac{\partial \rho}{\partial t} + \nabla \cdot \underline{F} \right) = 0$

true for any R so $\frac{\partial \rho}{\partial t} + \nabla \cdot \underline{F} = 0$

w/o conservation law, rhs $\to S(\underline{r},t)$ = amt of stuff supplied or lost / vol / time

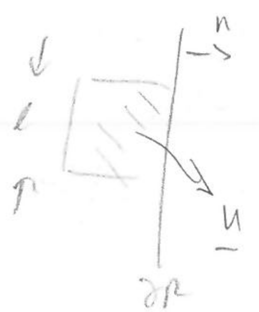
Apply to mass:

micro: $\rho(\underline{r},t) = \sum_{i=1}^{N} m_i \, \delta(\underline{r}-\underline{r}_i(t))$ N particles of mass m_i

$$\frac{\partial \rho}{\partial t} = -\sum_i m_i \dot{\underline{r}}_i \cdot \frac{\partial}{\partial \underline{r}} \delta(\underline{r}-\underline{r}_i(t))$$

$$= -\frac{\partial}{\partial \underline{r}} \cdot \underbrace{\sum_i m_i \dot{\underline{r}}_i \, \delta(\underline{r}-\underline{r}_i(t))}_{\underline{P}(\underline{r},t) \,=\, \text{momentum density} \,=\, \text{mass flux}}$$

continuum: $\underline{P} = \rho \underline{u}$



mass ρl^3 inside cube

c-s area $= l^2$

time to cross $\partial R = \dfrac{l}{\underline{u}\cdot\hat{n}}$

flux in direction $\hat{n} = \dfrac{\rho l^3}{l^2 \cdot l / \underline{u}\cdot\hat{n}} = \rho \underline{u}\cdot\hat{n}$

Micro expression for $\rho \underline{u}$:

define velocity $\underline{u} = \langle \underline{P} \rangle / \langle \rho \rangle$

$\xrightarrow{\text{MD sim}} \left(\sum_{i \in B(\underline{r})} m_i \dot{\underline{r}}_i \right) \Big/ \left(\sum_{i \in B(\underline{r})} m_i \right)$

$\langle \cdot \rangle$ = ensemble or time avg.

$B(\underline{r})$ = "sampling bin" = micro region around $\underline{r}$

Momentum   Irving + Kirkwood, J. Chem. Phys. 18, 817 (1950)

$$\frac{d}{dt}\int_R d^3r\, \underline{P}(\underline{r},t) = -\int_{\partial R} d\underline{S}\cdot\underline{\underline{\tau}}(\underline{r},t) + \int_R d^3r\, \underline{f}^{ext}(\underline{r},t)$$

ext force density

e.g. $\sum m_i \underline{g}\, \delta(\underline{r}-\underline{r}_i)$

$\underline{\underline{\tau}}$ = momentum flux

due to advection and interactions

= "pressure tensor"

also $= -\underline{\underline{\sigma}}(\underline{r},t)$, $\underline{\underline{\sigma}}$ = force/area exerted on material inside by exterior

local form: $\frac{\partial \underline{P}}{\partial t} = -\nabla\cdot\underline{\underline{\tau}} + \underline{f}^{ext} = +\nabla\cdot\underline{\underline{\sigma}} + \underline{f}^{ext}$

→ will use this eq to find $\underline{\underline{\sigma}}$.

Energy:

$\frac{d}{dt}$(energy in R) = −(energy advected through ∂R)

− (heat flux through ∂R)

+ (work done by exterior)

or $\frac{d}{dt}\mathcal{E}(\underline{r},t) = \int_{\partial R} d\underline{S}\cdot\left(-\underline{u}\mathcal{E} - \underline{J}_Q + \underline{\underline{\sigma}}\cdot\underline{u}\right)$

energy density

will find this

"force × velocity

$$\frac{\partial \underline{p}}{\partial t} = \sum_i m_i \dot{\underline{r}}_i \left(-\dot{\underline{r}}_i \cdot \frac{\partial}{\partial \underline{r}} \delta(\underline{r} - \underline{r}_i(t)) \right) + \sum_i m_i \ddot{\underline{r}}_i \, \delta(\underline{r} - \underline{r}_i(t))$$

(1) (2)

$$(1) = -\frac{\partial}{\partial \underline{r}} \sum_i m_i \dot{\underline{r}}_i \dot{\underline{r}}_i \, \delta(\underline{r} - \underline{r}_i(t))$$ momentum $m\dot{\underline{r}}$ advected by $\dot{\underline{r}}$

use later

$$= -\frac{\partial}{\partial \underline{r}} \Big[\sum_i m_i (\dot{\underline{r}}_i - \underline{u})(\dot{\underline{r}}_i - \underline{u}) \, \delta(\underline{r} - \underline{r}_i(t))$$

$$+ \Big(\sum m_i \dot{\underline{r}}_i \, \delta(\;'' \;)\Big) \cdot \underline{u} + \underline{u} \cdot \underbrace{\Big(\sum m_i \dot{\underline{r}}_i \, \delta(\cdots)\Big)}_{\rho \underline{u}}$$

$$- \underline{u}\,\underline{u} \sum_i m_i \, \delta(\;'' \;)$$

$$= -\frac{\partial}{\partial \underline{r}} \cdot \Big[\sum_i m_i (\dot{\underline{r}}_i - \underline{u})(\dot{\underline{r}}_i - \underline{u}) \, \delta(\underline{r} - \underline{r}_i(t)) + \rho \underline{u}\,\underline{u} \Big]$$

peculiar velocity

$$(2) = \sum_i \left(\underline{F}_i^{int} + \underline{F}_i^{ext} \right) \delta(\;\;)$$

$$= \sum_i \sum_{j \neq i} \underline{F}_{ij} \, \delta(\underline{r} - \underline{r}_i(t)) + \underline{f}^{ext}(\underline{r}, t)$$ interchange $i \leftrightarrow j$

$$= \frac{1}{2} \sum_{i \neq j} \Big[\underline{F}_{ij} \, \delta(\underline{r} - \underline{r}_i(t)) + \underbrace{\underline{F}_{ji}}_{= -\underline{F}_{ij}} \, \delta(\underline{r} - \underline{r}_j(t)) \Big] + \underline{f}^{ext}$$

from Newton 3rd law

$$= \frac{1}{2} \sum_{i \neq j} \underline{F}_{ij} \Big[\delta(\underline{r} - \underline{r}_i(t)) - \delta(\underline{r} - \underline{r}_j(t)) \Big] + \underline{f}^{ext}$$

Approximate $\delta(\underline{r} - \underline{r}_j) = \delta(\underline{r} - \underline{r}_i + \underline{r}_{ij}) \simeq \delta(\underline{r} - \underline{r}_i) + \underline{r}_{ij} \cdot \frac{\partial}{\partial \underline{r}} \delta(\underline{r} - \underline{r}_i)$

(improvement later) $\quad \underline{r}_{ij} = \underline{r}_i - \underline{r}_j$

so (2) $\to -\frac{1}{2}\sum_{i\neq j} \underline{F}_{ij}\underline{r}_{ij}\cdot\frac{\partial}{\partial \underline{r}}\delta(\underline{r}-\underline{r}_i) + \underline{f}^{\,ext}$

or $$\frac{\partial \underline{P}}{\partial t} + \frac{\partial}{\partial \underline{r}}\cdot\Big(\underbrace{\Big[\sum_i m_i \dot{\underline{r}}_i \dot{\underline{r}}_i + \frac{1}{2}\sum_{i\neq j}\underline{F}_{ij}\underline{r}_{ij}\Big]\delta(\underline{r}-\underline{r}_i(t))}_{=\underline{\underline{\tau}}(\underline{r},t)\ \text{momentum flux tensor}}\Big) = 0$$

Thermostat forces?

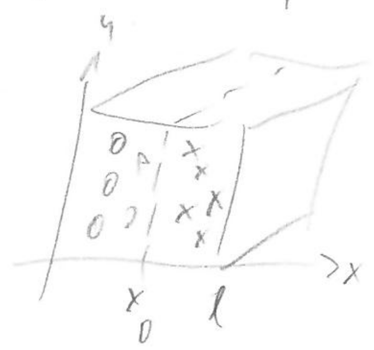
$$F_i^{\,therm} = \begin{cases} -\gamma \underline{p}_i + \underline{\eta}_i & \text{Langevin} \\ -\zeta \underline{p}_i & \text{Nosé Hoover} \end{cases}$$

this form is for equilibrium; when fluid moves need the peculiar velocity $-\gamma m_i(\dot{\underline{r}}_i - \underline{u})$ $\underline{u}$ = local avg. vel. which adds to 0 over a sampling region about $\underline{r}$

$m_i \dot{\underline{r}}_i \dot{\underline{r}}_i$ is the advected momentum

$\underline{r}_{ij}\cdot\underline{F}_{ij}$ is the "advected interaction force" - why stress?

look at a micro-box of side l^3;



+ the xx term

plane at x_0, normal $\hat{n} = \hat{x}$

find the force/area exerted on the atoms left of x_0 by those right of x_0: $\sigma_{xx}(x_0)$

$$\sigma_{xx}(x_0) = \frac{1}{l^2} \sum_{x_i < x_0} \sum_{x_j > x_0} F_{ij,x} \; ;$$

does not depend on x_0

$$\sigma_{xx} = \text{avg over the cube} = \frac{1}{l} \int_0^l dx_0 \, \sigma_{xx}(x_0)$$

$$= \frac{1}{l^3} \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} F_{ij,x} \int_{x_i}^{x_j} dx_0$$

because each term contributes only when $x_i < x_0 < x_j$

$$= -\frac{1}{V} \sum_{i<j} F_{ij,x} (x_i - x_j) = -\Pi_{xx}$$

— x —

NB: $\frac{1}{V} \leftrightarrow \delta(\underline{r} - \underline{r}_i(t))$ in averaging

What about periodicity?

suppose (ij) subject to minimum-image convention

$\underline{F}_{ij}\,\delta(\underline{r} - \underline{r}_i) \to \underline{F}_{ij'}\,\delta(\underline{r} - \underline{r}_i)$ in the original form

$\underline{F}_{ji}\,\delta(\underline{r} - \underline{r}_j) \to \underline{F}_{j'i}\,\delta(\underline{r} - \underline{r}_{j'})$ when $i \leftrightarrow j$

$$\to \frac{1}{2} \underline{F}_{ij'} \left[\delta(\underline{r} - \underline{r}_i) - \delta(\underline{r} - \underline{r}_{j'}) \right] = -\frac{1}{2} \underline{F}_{ij'}\, \underline{r}_{ij'} \, \delta(\underline{r} - \underline{r}_i)$$

$$- \underline{r}_{ij'} \cdot \frac{\partial}{\partial \underline{r}} \delta(\underline{r} - \underline{r}_i)$$

use MI calc.

— x —

Combine ① + ② + rearrange:

$$\frac{\partial}{\partial t}(\rho \underline{u}) = -\frac{\partial}{\partial \underline{r}} \cdot \Big[\sum_i m_i (\dot{\underline{r}}_i - \underline{u})(\dot{\underline{r}}_i - \underline{u})\, \delta(\underline{r} - \underline{r}_i(t)) + \rho\, \underline{u}\,\underline{u} - \quad ①$$

$$- \frac{1}{2} \sum_{i \neq j} \underline{r}_{ij} \underline{f}_{ij}\, \delta(\underline{r} - \underline{r}_i(t)) \Big] + \underline{f}^{ext} \quad ②$$

use
$$\left\{ \begin{aligned} \frac{\partial}{\partial \underline{r}} \cdot (\rho \underline{u}\,\underline{u}) \Big|_i &= \frac{\partial}{\partial r_j}(\rho u_j u_i) = \frac{\partial}{\partial r_j}(\rho u_j) \cdot u_i + \rho u_j \frac{\partial}{\partial r_j} u_i \\ &= \frac{\partial}{\partial \underline{r}} \cdot (\rho \underline{u})\, \underline{u} + \left(\rho\, \underline{u} \cdot \frac{\partial}{\partial \underline{r}}\right) \underline{u} \Big|_i \\ \frac{\partial}{\partial t}(\rho \underline{u}) &= \frac{\partial \rho}{\partial t} \underline{u} + \rho \frac{\partial \underline{u}}{\partial t} \end{aligned} \right.$$

so
$$\frac{\partial}{\partial t}(\rho \underline{u}) + \frac{\partial}{\partial \underline{r}} \cdot (\rho \underline{u}\,\underline{u}) = \rho \underbrace{\left(\frac{\partial}{\partial t} + \underline{u} \cdot \frac{\partial}{\partial \underline{r}} \right)}_{\frac{D\underline{u}}{Dt}} \underline{u} + \underbrace{\left(\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial \underline{r}} \cdot (\rho \underline{u}) \right)}_{=0} \underline{u}$$

$$\rho \frac{D\underline{u}}{Dt} = \nabla \cdot \Big[- \sum_i m_i (\dot{\underline{r}}_i - \underline{u})(\dot{\underline{r}}_i - \underline{u}) - \frac{1}{2} \sum_{i \neq j} \underline{r}_{ij} \underline{f}_{ij}\, \delta(\underline{r} - \underline{r}_i) \Big]$$
$$+ \underline{f}^{ext}$$

so $[\;] =$ + stress tensor $\underline{\underline{\sigma}} = -$ pressure tensor $\underline{\underline{\pi}}$

$$\leftrightarrow -p \underline{\underline{1}} + \mu \left(\frac{\partial}{\partial \underline{r}} \underline{u} + \underline{u} \overleftarrow{\frac{\partial}{\partial \underline{r}}} \right) \quad ??$$

Check: if $\underline{u} = \underline{F} = 0$, $\langle \sum m_i \dot{\underline{r}}_i \dot{\underline{r}}_i\, \delta(\,) \rangle$

$$\rightarrow N \cdot m \cdot \frac{1}{3} \underline{v}^2 \cdot \frac{1}{V} = \rho k_B T \quad \text{ideal gas}$$

Why? $\delta(\underline{r}-\underline{r}_i) \to \frac{1}{V}$ uniform in space

$\langle v_\alpha v_\beta \rangle = \lambda \delta_{\alpha\beta}$ isotropy $-$ $\delta_{\alpha\beta}$ is the only 2nd rank tensor

$\to \langle \underline{v}^2 \rangle = 3\lambda$

$\langle \underline{v}^2 \rangle = 3k_B T/m$ equipartition

$\sim \lambda \sim$

What about the approx for the $\underline{r}_{ij}\underline{F}_{ij}$ term?

$$\delta(\underline{r}-\underline{r}_j) = \delta(\underline{r}-\underline{r}_i+\underline{r}_{ij}) = \sum_{n=0}^{\infty} \frac{1}{n!}\left(\underline{r}_{ij}\cdot\frac{\partial}{\partial \underline{r}}\right)^n \delta(\underline{r}-\underline{r}_i)$$

exactly

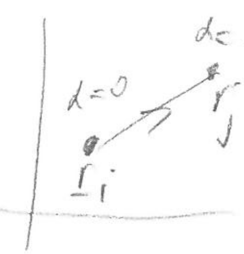
$$\text{\& use } \frac{1}{n!} = \frac{1}{(n-1)!}\int_0^1 d\alpha\, \alpha^{n-1}$$

$$\underline{F}_{ij}\left[\delta(\underline{r}-\underline{r}_i) - \delta(\underline{r}-\underline{r}_j)\right] =$$

$$\equiv - \underline{F}_{ij}\underline{r}_{ij}\cdot\frac{\partial}{\partial \underline{r}}\int_0^1 d\alpha \sum_{n=1}^{\infty}\frac{1}{(n-1)!}\left(\alpha \underline{r}_{ij}\cdot\frac{\partial}{\partial \underline{r}}\right)^{n-1}\delta(\underline{r}-\underline{r}_i)$$

$$\text{let } k=n-1,\ k: 0 \to \infty;\ \sum_{k=0}^{\infty}\frac{1}{k!}\left(\alpha\frac{\partial}{\partial x}\right)^k f(x) = f(x+\alpha)$$

$$= - \underline{F}_{ij}\underline{r}_{ij}\cdot\frac{\partial}{\partial \underline{r}}\int_0^1 d\alpha\, \delta(\underline{r}-\underline{r}_i+\alpha\underline{r}_{ij})$$



$\to$ stress is uniformly distributed along the line $\underline{r}_i \to \underline{r}_j$

Alternate form: let $\underline{r}' = \underline{r}_i - \alpha \underline{r}_{ij}$

$$= + \underline{F}_{ij}\frac{\partial}{\partial \underline{r}}\cdot\int_{\underline{r}_i}^{\underline{r}_j} d\underline{r}'\, \delta(\underline{r}-\underline{r}')$$

Energy Eq:

$$\mathcal{E}(\underline{r},t) = \sum_i \frac{1}{2} m_i \dot{\underline{r}}_i^2 \,\delta(\underline{r}-\underline{r}_i)$$

even split btw i & j

$$+ \frac{1}{2} \sum_{i\neq j} U(r_{ij}) \left[\frac{1}{2}\delta(\underline{r}-\underline{r}_i) + \frac{1}{2}\delta(\underline{r}-\underline{r}_j)\right]$$

sum over pairs

switch $i \leftrightarrow j$

$$= \sum_i \left(\frac{1}{2} m_i \dot{\underline{r}}_i^2 + \frac{1}{2} \sum_{i\neq j} U(r_{ij}) \right) \delta(\underline{r}-\underline{r}_i)$$

$$\frac{\partial \mathcal{E}}{\partial t} = -\frac{\partial}{\partial \underline{r}} \cdot \sum_i \dot{\underline{r}}_i \left(\frac{1}{2} m \dot{\underline{r}}_i^2 + \frac{1}{2} \sum_{i\neq j} U(r_{ij}) \right) \delta(\underline{r}-\underline{r}_i) + \quad (1)$$

$$+ \sum_i \left(\dot{\underline{r}}_i \cdot \underline{F}_i + \frac{1}{2} \sum_{i\neq j} \dot{r}_{ij} U'(r_{ij}) \right) \delta(\underline{r}-\underline{r}_i) \quad (2)$$

$$r_{ij} = \sqrt{(\underline{r}_i - \underline{r}_j)^2} \quad \text{so} \quad \dot{r}_{ij} = \frac{1}{r_{ij}} \underline{r}_{ij} \cdot \dot{\underline{r}}_{ij}$$

$$\dot{r}_{ij} U'(r_{ij}) = -\dot{\underline{r}}_{ij} \cdot \left[-\frac{1}{r_{ij}} \underline{r}_{ij} U'(r_{ij}) \right]$$

$\hookrightarrow -\frac{\partial}{\partial \underline{r}_i} U(r_{ij})$

$$= -\dot{\underline{v}}_{ij} \cdot \underline{F}_{ij}$$

$$(2) \rightarrow \sum_i \left[\dot{\underline{r}}_i \cdot \left(\sum_{j\neq i} \underline{F}_{ij} \right) - \frac{1}{2} \sum_{i\neq j} \dot{\underline{r}}_{ij} \cdot \underline{F}_{ij} \right] \delta(\underline{r}-\underline{r}_i)$$

$$= \sum_{i\neq j} \frac{1}{2} \left[\dot{\underline{r}}_i \cdot \underline{F}_{ij} + \dot{\underline{r}}_j \cdot \underline{F}_{ij} \right] \delta(r - r_i)$$

switch $i \leftrightarrow j$; use $\underline{F}_{ji} = -\underline{F}_{ij}$; use approx for $\delta - \delta$

$$\frac{\partial \mathcal{E}}{\partial t} = -\frac{\partial}{\partial \underline{r}} \cdot \sum_i \delta(\underline{r}-\underline{r}_i) \Big[\Big(\tfrac{1}{2} m_i \dot{\underline{r}}_i^2 + \tfrac{1}{2} \sum_{i \neq j} U(r_{ij}) \Big) \dot{\underline{r}}_i + \tfrac{1}{2} \sum_{i \neq j} \underline{r}_{ij} \left(\dot{\underline{r}}_i \cdot \underline{F}_{ij} \right) \Big]$$

1st term: energy of i advected by $\dot{\underline{r}}_i$

2nd term: work done by intermolecular forces

looks asymmetric due to $\dot{\underline{r}}_i$, but if the "correct" expression for $\delta-\delta$ is used it can be replaced by $\frac{1}{2}(\dot{\underline{r}}_i + \dot{\underline{r}}_j)$

Compare to the continuum eq:

$$\frac{\partial \mathcal{E}}{\partial t} = -\frac{\partial}{\partial \underline{r}} \cdot \left(\underline{u}\, \mathcal{E} + \underline{J}_Q - \underline{\underline{\sigma}} \cdot \underline{u} \right)$$

similar to 1st + 2nd terms above with $\underline{u} \to \dot{\underline{r}}_i$

$$\underline{J}_Q = \text{difference}$$

$$= \sum_i \delta(\underline{r}-\underline{r}_i) \Big[\Big(\tfrac{1}{2} m_i \dot{\underline{r}}_i^2 + \tfrac{1}{2} \sum_{j \neq i} U(r_{ij}) \Big) (\dot{\underline{r}}_i - \underline{u}) - m_i (\dot{\underline{r}}_i - \underline{u}) (\dot{\underline{r}}_i - \underline{u}) \cdot \underline{u} + \tfrac{1}{2} \sum_{j \neq i} \underline{r}_{ij}\, \underline{F}_{ij} (\dot{\underline{r}}_i - \underline{u}) \Big]$$

Note $\frac{1}{2} \dot{\underline{r}}^2 (\dot{\underline{r}} - \underline{u}) - (\dot{\underline{r}} - \underline{u})(\dot{\underline{r}} - \underline{u}) \cdot \underline{u}$

$$= \tfrac{1}{2} \left((\dot{\underline{r}} - \underline{u})^2 + \cancel{\underline{u}^2} \right) (\dot{\underline{r}} - \underline{u})$$

sums to zero

so $$\underline{J}_Q = \sum_i \delta(\underline{r}-\underline{r}_i)\left[e_i(\dot{\underline{r}}_i - \underline{u}) + \frac{1}{2}\sum_{j\neq i} \underline{r}_{ij}\underline{F}_{ij}\cdot(\dot{\underline{r}}_i - \underline{u})\right]$$

$$e_i \downarrow \quad \frac{1}{2}m_i(\dot{\underline{r}}_i - \underline{u})^2 + \frac{1}{2}\sum_{j\neq i} u(r_{ij})$$

= "peculiar energy of i"

— x —

NB - Usual form of energy eq:

Here $\mathcal{E}$ = energy/vol $= \rho\cdot\hat{\mathcal{E}}$, $\hat{\mathcal{E}}$ = energy/mass

$= \rho\left(\frac{1}{2}\underline{v}^2 + \mathcal{U}\right)$, $\mathcal{U}$ = internal energy/mass

Note $$\rho\frac{Df(\underline{r},t)}{Dt} = \rho\frac{\partial f}{\partial t} + \rho\,\underline{u}\cdot\frac{\partial}{\partial \underline{r}}f$$

$$\rho\frac{\partial f}{\partial t} \to \frac{\partial}{\partial t}(\rho f) - f\frac{\partial \rho}{\partial t}, \qquad -f\frac{\partial \rho}{\partial t} \to f\,\underline{u}\cdot\frac{\partial}{\partial \underline{r}}(\rho\underline{u})$$

$$= \frac{\partial}{\partial t}(\rho f) + \frac{\partial}{\partial \underline{r}}\cdot(\rho\underline{u}f)$$

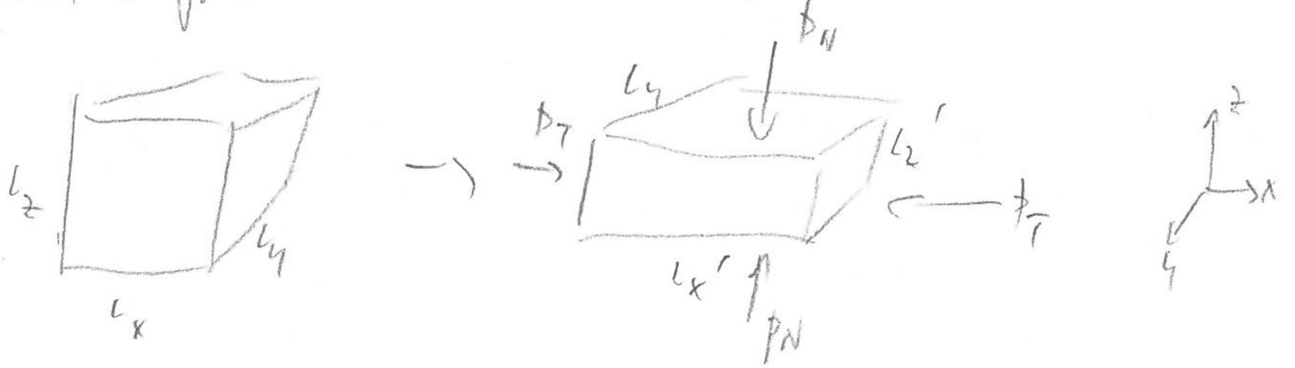
so $$\rho\frac{D\hat{\mathcal{E}}}{Dt} = \frac{\partial}{\partial t}(\rho\hat{\mathcal{E}}) + \frac{\partial}{\partial \underline{r}}\cdot(\underline{u}\rho\hat{\mathcal{E}}) = -\frac{\partial}{\partial \underline{r}}\cdot(\underline{J}_Q - \underline{\underline{\sigma}}\cdot\underline{u})$$

$$\to \cancel{\rho\,\underline{u}\cdot\frac{D\underline{u}}{Dt}} + \rho\frac{D\mathcal{U}}{Dt} = -\frac{\partial}{\partial \underline{r}}\cdot\underline{J}_Q + \cancel{\left(\frac{\partial}{\partial \underline{r}}\cdot\underline{\underline{\sigma}}\right)\cdot\underline{u}} + \underline{\underline{\sigma}}:\left(\frac{\partial \underline{u}}{\partial \underline{r}}\right)$$

+ if $\mathcal{U} = C_V T$ + constant + $\underline{J}_Q = -k_T\frac{\partial T}{\partial \underline{r}}$

$$\rho C_V\frac{\partial T}{\partial t} = k_T\nabla^2 T + \underline{\underline{\sigma}}:\frac{\partial \underline{u}}{\partial \underline{r}}$$

Revisit surface tension calculation:



$$dF = \gamma\, dA = đW = -p_N A_N\, dz - p_T A_T\, dx$$

or $$\gamma L_y\, dx = -\sigma_{zz} L_x L_y\, dz - \sigma_{xx} L_y L_z\, dx$$

$$\rightarrow \quad \gamma = -\sigma_{zz} L_x \frac{dz}{dx} - \sigma_{xx} L_z$$

Volume conservation $\rightarrow$

$$L_x' L_y L_z' = (L_x + dx) L_y (L_z + dz) = L_x L_y L_z + L_y(\underbrace{L_z\, dx + L_x\, dz}_{=0}) + \dots$$
$$= L_x L_y L_z$$

$$\rightarrow \quad \gamma = (\sigma_{zz} - \sigma_{xx}) L_z$$

This applies to a particular slab, but should be used for a sequence of narrow slabs, because σ_{ij} varies across the interface. So

$$\gamma = \int_{-\infty}^{\infty} dz\, \left(\sigma_{zz}(z) - \sigma_{xx}(z)\right)$$

only the interface contributes, so limits $\rightarrow \infty$

Substitute for σ_{ij} + this reduces to the previous formula