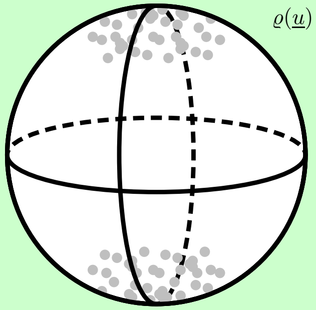
Slide 1

Balance of angular momentum in the presence of microstructure

Second rank alignment tensor

Slide 2

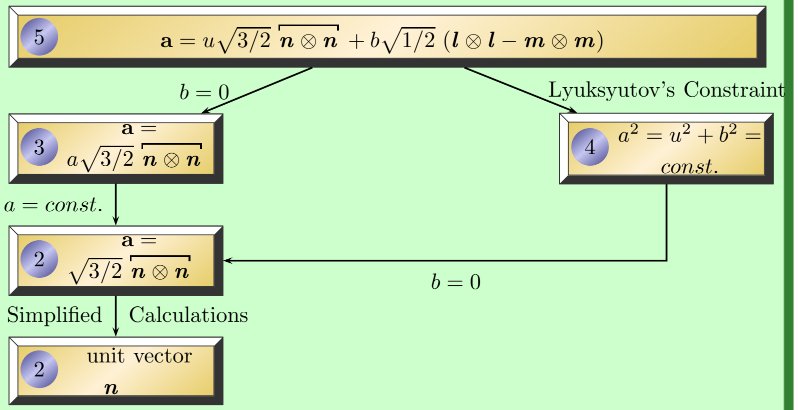
Choice of Order Parameter



- $\langle f\rangle = \oint_{S^2} f\,\varrho(\boldsymbol{u})d^2\boldsymbol{u}$
- $\varrho(\boldsymbol{u}) = \varrho(-\boldsymbol{u})$
- $\varrho(\boldsymbol{u}) \;=\; \frac{1}{4\pi}\left(1+\sum a_{\mu_1\ldots\mu_l}\phi_{\mu_1\ldots\mu_l}\right)$ with $a_{\mu_1\ldots\mu_l} = \langle\phi_{\mu_1\ldots\mu_l}\rangle \propto \langle\overline{u_{\mu_1}\cdots u_{\mu_l}}\rangle$
- $\mathbf{a} = \sqrt{\frac{15}{2}}\langle\boldsymbol{u}\otimes\boldsymbol{u} - \frac{1}{3}\delta\rangle$
- $\epsilon = \epsilon^{iso}\,\delta + \Delta\epsilon\,\mathbf{a}$

Slide 3

The Alignment Tensor and its Descendants



Slide 4

Time Derivatives

- Material time derivative $\dot{\mathbf{a}} = \frac{\partial \mathbf{a}}{\partial t} + (\nabla \mathbf{a})\boldsymbol{v}$
- …of the gradient $(\nabla \mathbf{a})^{\cdot} = \nabla \dot{\mathbf{a}} - (\nabla \mathbf{a})\nabla \boldsymbol{v}$
- Frame indifferent time derivatives:
  - Co-rotational: $\mathring{\mathbf{a}} = \dot{\mathbf{a}} - 2\,\overline{\mathbf{Wa}}$
  - Co-deformational: $\mathring{\mathbf{a}} = \dot{\mathbf{a}} - 2\,\overline{\mathbf{Wa}} - 2\sigma\,\overline{\mathbf{Da}}$

with $\mathbf{D} = \frac{1}{2}(\nabla \boldsymbol{v} + (\nabla \boldsymbol{v})^T)$ and $\mathbf{W} = \frac{1}{2}(\nabla \boldsymbol{v} - (\nabla \boldsymbol{v})^T)$

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Free Energy

$$\mathcal{F} = \int \left\{ \frac{1}{2}\rho \boldsymbol{v}^2 + \rho\kappa(\mathbf{a}, \dot{\mathbf{a}}) + \chi(\mathbf{a}) + W(\mathbf{a}, \nabla \mathbf{a}) \right\} \mathrm{d}V$$

- ρ: mass density
- κ: kinetic energy of $\dot{\mathbf{a}}$
- χ: potential energy for external actions on $\mathbf{a}$
- W: elastic free energy of the alignment
- NOT here:
  - potential energy of the compressibility ($\operatorname{div} \boldsymbol{v} = 0$)
  - body force

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Elastic Energy: Material Frame Indifference

$$\boldsymbol{x}^* = \mathbf{Q}(t)\boldsymbol{x} + \boldsymbol{b}(t)$$

$$W(a_{ij},\ a_{ij,k}) = W(Q_{ip}Q_{jq}a_{pq},\ Q_{ip}Q_{jq}Q_{kr}a_{pq,r})$$

$$\Downarrow$$

$$\epsilon_{ijk}\left(2a_{jp}\frac{\partial W}{\partial a_{pk}} + 2a_{jp,q}\frac{\partial W}{\partial a_{pk,q}} + a_{pq,j}\frac{\partial W}{\partial a_{pq,k}}\right) = 0$$

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Kinetic Energy: Inertial Frame Indifference

$$\boldsymbol{x}^* = \mathbf{Q}\boldsymbol{x} + t\boldsymbol{u}_0 + p_0$$

$$\kappa(\mathbf{a}, \dot{\mathbf{a}}) = \kappa(\mathbf{Q}\mathbf{a}\mathbf{Q}^T, \mathbf{Q}\dot{\mathbf{a}}\mathbf{Q}^T)$$

$$\Downarrow$$

$$\epsilon_{ijk}\left(a_{jp}\frac{\partial \kappa}{\partial a_{pk}} + \dot{a}_{jp}\frac{\partial \kappa}{\partial \dot{a}_{pk}}\right) = 0$$

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How to ... (Ericksen, 1961)

$$\mathbf{b} := (\mathbf{I}+\varepsilon\boldsymbol{\Omega})\,\mathbf{a}\,(\mathbf{I}+\varepsilon\boldsymbol{\Omega})^T = \mathbf{a}+\varepsilon(\boldsymbol{\Omega}\mathbf{a}-\mathbf{a}\boldsymbol{\Omega})+\mathcal{O}(\varepsilon^2), \qquad \boldsymbol{\Omega}^T = -\boldsymbol{\Omega}$$

$$\dot{\mathbf{b}} = \dot{\mathbf{a}}+\varepsilon(\boldsymbol{\Omega}\dot{\mathbf{a}}-\dot{\mathbf{a}}\boldsymbol{\Omega})+\mathcal{O}(\varepsilon^2)$$

$$\chi(\mathbf{b},\dot{\mathbf{b}})-\chi(\mathbf{a},\dot{\mathbf{a}}) = \frac{\partial\chi}{\partial\mathbf{a}}\cdot(\mathbf{b}-\mathbf{a})+\frac{\partial\chi}{\partial\dot{\mathbf{a}}}\cdot(\dot{\mathbf{b}}-\dot{\mathbf{a}})+\mathcal{O}(\varepsilon^2)$$

$$\lim_{\varepsilon\to 0}\left[\frac{\partial\chi}{\partial\mathbf{a}}\cdot(\boldsymbol{\Omega}\mathbf{a}-\mathbf{a}\boldsymbol{\Omega})+\frac{\partial\chi}{\partial\dot{\mathbf{a}}}\cdot(\boldsymbol{\Omega}\dot{\mathbf{a}}-\dot{\mathbf{a}}\boldsymbol{\Omega})+\mathcal{O}(\varepsilon)\right]=0$$

$$0 = 2\,\boldsymbol{\Omega}^T\cdot\left(\mathbf{a}\frac{\partial\chi}{\partial\mathbf{a}}+\dot{\mathbf{a}}\frac{\partial\chi}{\partial\dot{\mathbf{a}}}\right)$$

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15 Invariants Bilinear in $\mathring{a}$ and D

$\mathring{a}^2$	$\mathbf{D}\cdot\mathring{\mathbf{a}}$	D^2
$\mathring{\mathbf{a}}\cdot(\mathring{\mathbf{a}}\,\mathbf{a})$	$\mathring{\mathbf{a}}\cdot(\mathbf{D}\mathbf{a})$	$\mathbf{D}\cdot(\mathbf{D}\mathbf{a})$
$(\mathring{\mathbf{a}}\cdot\mathbf{a})^2$	$(\mathbf{D}\cdot\mathbf{a})(\mathring{\mathbf{a}}\cdot\mathbf{a})$	$(\mathbf{D}\cdot\mathbf{a})^2$
$(\mathring{\mathbf{a}}\,\mathbf{a})\cdot(\mathring{\mathbf{a}}\,\mathbf{a})$	$(\mathbf{D}\mathbf{a})\cdot(\mathring{\mathbf{a}}\,\mathbf{a})$	$(\mathbf{D}\mathbf{a})\cdot(\mathbf{D}\mathbf{a})$
$a^2\,\mathring{a}^2$	$a^2\,\mathbf{D}\cdot\mathring{\mathbf{a}}$	$a^2 D^2$

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Balance of Forces

Total mechanical power $\mathcal{W} = \dot{\mathcal{F}} = X\cdot\dot{q}$

$\downarrow$

Balance of forces $X+Y=0$

Constitutive Assumption: $\downarrow$ $Y = \dfrac{\partial R}{\partial\dot{q}}$

Equations of motion $X+\dfrac{\partial R}{\partial\dot{q}}=0$

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Power Input

$$\begin{aligned}\dot{\mathcal{F}} &= \int\left\{\rho\dot{\boldsymbol{v}}\cdot\boldsymbol{v}+\left(\rho\frac{\partial\kappa}{\partial\mathbf{a}}+\frac{\partial\chi}{\partial\mathbf{a}}+\frac{\partial W}{\partial\mathbf{a}}\right)\cdot\dot{\mathbf{a}}+\rho\frac{\partial\kappa}{\partial\dot{\mathbf{a}}}\cdot\ddot{\mathbf{a}}+\frac{\partial W}{\partial\nabla\mathbf{a}}\cdot(\nabla\mathbf{a})^{\cdot}\right\}\mathrm{d}V\\ &= \int\left\{\left[\rho\dot{\boldsymbol{v}}+\operatorname{div}\left(p\mathbf{I}+\nabla\mathbf{a}\odot\frac{\partial W}{\partial\nabla\mathbf{a}}\right)\right]\cdot\boldsymbol{v}\right.\\ &\quad+\left.\left[\rho\mathbf{M}+\frac{\partial\chi}{\partial\mathbf{a}}+\frac{\partial W}{\partial\mathbf{a}}-\operatorname{div}\frac{\partial W}{\partial\nabla\mathbf{a}}\right]\cdot\dot{\mathbf{a}}\right\}\mathrm{d}V+\text{s.t.}\end{aligned}$$

☞ $\left(\nabla\mathbf{a}\odot\dfrac{\partial W}{\partial\nabla\mathbf{a}}\right)_{ij} := a_{kl,i}\dfrac{\partial W}{\partial a_{kl,j}}$

☞ $\mathbf{M} := \left(\dfrac{\partial\kappa}{\partial\dot{\mathbf{a}}}\right)^{\cdot}-\dfrac{\partial\kappa}{\partial\mathbf{a}}$

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Fluxes and Forces

$\dot{q}$	X
$\boldsymbol{v}$	$\rho\dot{\boldsymbol{v}} + \operatorname{div}\left(p\,\mathbf{I} + \nabla\mathbf{a}\odot\dfrac{\partial W}{\partial\nabla\mathbf{a}}\right)$
$\dot{\mathbf{a}}$	$\rho\mathbf{M} + \dfrac{\partial\chi}{\partial\mathbf{a}} + \dfrac{\partial W}{\partial\mathbf{a}} - \operatorname{div}\dfrac{\partial W}{\partial\nabla\mathbf{a}}$

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Dissipation

$$\mathcal{R} = \int R(\mathbf{a}, \mathring{\mathbf{a}}, \mathbf{D})\mathrm{d}V$$

$$\Big\downarrow\ \delta(\nabla\boldsymbol{v}) = \nabla(\delta\boldsymbol{v})$$

$$\delta\mathcal{R} = \int\left\{\frac{\partial R}{\partial\dot{\mathbf{a}}}\cdot\delta\dot{\mathbf{a}} + \frac{\partial R}{\partial\nabla\boldsymbol{v}}\cdot\nabla(\delta\boldsymbol{v})\right\}\mathrm{d}V$$

$$\Big\downarrow\ \text{integration by parts}$$

$$\delta\mathcal{R} = \int\left\{\frac{\partial R}{\partial\dot{\mathbf{a}}}\cdot\delta\dot{\mathbf{a}} - \operatorname{div}\left(\frac{\partial R}{\partial\nabla\boldsymbol{v}}\right)\cdot\delta\boldsymbol{v}\right\}\mathrm{d}V + \text{s.t.}$$

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Chain Rule

$$\frac{\partial R}{\partial\nabla\boldsymbol{v}} = \frac{\partial R}{\partial\mathbf{D}} + \mathbf{a}\,\frac{\partial R}{\partial\,\mathring{\mathbf{a}}} - \frac{\partial R}{\partial\,\mathring{\mathbf{a}}}\,\mathbf{a}$$

$$\frac{\partial R}{\partial\dot{\mathbf{a}}} = \frac{\partial R}{\partial\,\mathring{\mathbf{a}}}$$

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Equations of Motion

$$\rho\dot{\boldsymbol{v}} = \operatorname{div}\mathbf{T}$$

$$\rho\mathbf{M} + \frac{\partial\chi}{\partial\mathbf{a}} + \frac{\partial W}{\partial\mathbf{a}} - \operatorname{div}\frac{\partial W}{\partial\nabla\mathbf{a}} + \frac{\partial R}{\partial\,\mathring{\mathbf{a}}} = \mathbf{0}$$

$$\mathbf{T} = -p\,\mathbf{I} - \nabla\mathbf{a}\odot\frac{\partial W}{\partial\nabla\mathbf{a}} + \frac{\partial R}{\partial\mathbf{D}} + \mathbf{a}\,\frac{\partial R}{\partial\,\mathring{\mathbf{a}}} - \frac{\partial R}{\partial\,\mathring{\mathbf{a}}}\,\mathbf{a}$$

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Angular Momentum Balance

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\mathcal{C}} \rho \boldsymbol{v}\,\mathrm{d}V = \int_{\mathcal{C}} \rho \boldsymbol{f}\,\mathrm{d}V + \int_{\partial\mathcal{C}} \boldsymbol{t}\,\mathrm{d}A$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\mathcal{C}} \rho(\boldsymbol{m} + \boldsymbol{x}\times\boldsymbol{v})\mathrm{d}V = \int_{\mathcal{C}} \rho(\boldsymbol{x}\times\boldsymbol{f} + \boldsymbol{k})\mathrm{d}V + \int_{\partial\mathcal{C}} (\boldsymbol{x}\times\boldsymbol{t} + \boldsymbol{l})\mathrm{d}A$$

$$\boldsymbol{t} = \mathbf{T}\boldsymbol{\nu}, \qquad \boldsymbol{l} = \mathbf{L}\boldsymbol{\nu}$$

$$\rho\dot{\boldsymbol{m}} = \rho\boldsymbol{k} - \boldsymbol{\tau} + \operatorname{div}\mathbf{L}$$

$$\tau_i = \epsilon_{ijk}T_{jk}$$

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Skew part of the stress

$$\begin{aligned}
\tau_i &= \epsilon_{ijk}\left(2a_{jl}\frac{\partial R}{\partial\,\mathring{a}_{lk}} - a_{lm,j}\frac{\partial W}{\partial a_{lm,k}}\right)\\
&= 2\,\epsilon_{ijk}\left(a_{jl}\frac{\partial R}{\partial\,\mathring{a}_{lk}} + a_{jl}\frac{\partial W}{\partial a_{lk}} + a_{jl,m}\frac{\partial W}{\partial a_{lk,m}}\right)
\end{aligned}$$

inserting the alignment tensor balance:

$$\begin{aligned}
\tau_i &= 2\epsilon_{ijk}\left\{-\rho a_{jl}M_{lk} - a_{jl}\frac{\partial\chi}{\partial a_{lk}} + a_{jl}\left(\frac{\partial W}{\partial a_{lk,m}}\right)_{,m} + a_{jl,m}\frac{\partial W}{\partial a_{lk,m}}\right\}\\
&= 2\epsilon_{ijk}\left\{\left(a_{jl}\frac{\partial W}{\partial a_{lk,m}}\right)_{,m} - \rho a_{jl}M_{lk} - a_{jl}\frac{\partial\chi}{\partial a_{lk}}\right\}
\end{aligned}$$

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Identifying the Parts

$$L_{ij} = 2\epsilon_{ikl}a_{km}\frac{\partial W}{\partial a_{ml,j}}$$

$$\dot{m}_i = 2\epsilon_{ijk}a_{jl}M_{lk}$$

$$\rho k_i = -2\epsilon_{ijk}a_{jl}\frac{\partial\chi}{\partial a_{lk}}$$

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Intrinsic Angular Momentum

$$m_i := 2\,\epsilon_{ijk}a_{jl}\frac{\partial\kappa}{\partial\dot{a}_{lk}}$$

$$\begin{aligned}
\dot{m}_i &= 2\,\epsilon_{ijk}\left[\dot{a}_{jl}\frac{\partial\kappa}{\partial\dot{a}_{lk}} + a_{jl}\left(\frac{\partial\kappa}{\partial a_{lk}}\right)^{\cdot}\right]\\
&= 2\,\epsilon_{ijk}\left[-a_{jl}\frac{\partial\kappa}{\partial a_{lk}} + a_{jl}\left(M_{lk} + \frac{\partial\kappa}{\partial a_{lk}}\right)\right]\\
&= 2\epsilon_{ijk}a_{jl}M_{lk}
\end{aligned}$$

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Field Torque

$$\chi(\mathbf{a}) = -\frac{1}{2}\varepsilon \boldsymbol{E} \cdot \mathbf{a}\boldsymbol{E}, \qquad \frac{\partial \chi}{\partial \mathbf{a}} = -\frac{1}{2}\varepsilon\, \overline{\boldsymbol{E} \otimes \boldsymbol{E}}$$

$$\boxed{\rho \boldsymbol{k} = \varepsilon \boldsymbol{E} \times \mathbf{a}\boldsymbol{E}}$$

Whenever the field $\boldsymbol{E}$ is an eigenvector of the alignment tensor $\mathbf{a}$ it exerts no torque, but $\dfrac{\partial \chi}{\partial \mathbf{a}}$ still contributes to $\dot{\mathbf{a}}$.