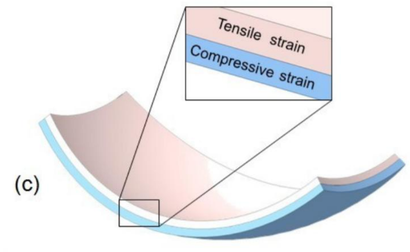
Effective two dimensional theories for multi-layered plates

Miguel de Benito Delgado

Fabrication of **3D micro- and nano-structures**

- Exploit mismatching energy wells



Bilayers

- Rolled structures for **intracellular microinjections**, **nanoreactors**, on-chip **capture and detection of micro-organisms**, ...
- Temperature driven **release of microparticles and cells**, **microfluidics devices**, ...

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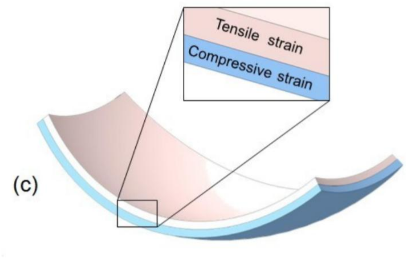

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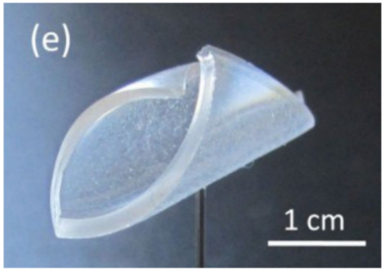

Large pre-strains

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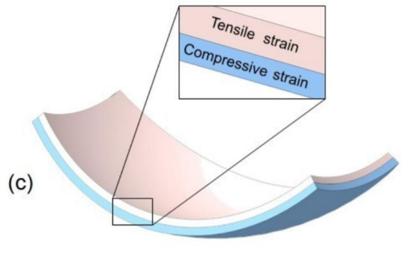

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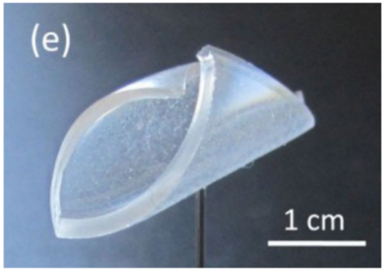

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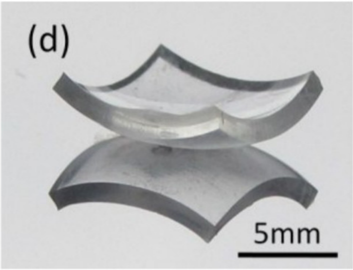

Thick samples

Egunov et al. 2015

- Rolled structures for **intracellular microinjections**, **nanoreactors**, on-chip **capture and detection of micro-organisms**, ...

- Temperature driven **release of microparticles and cells**, **microfluidics devices**, ...

Goals

multi-layered or pre-strained plates

effective, 2D theories

multiple scalings

minimisers

A hierarchy of plate models

- Reference *plate*:

$$\Omega_h = \omega \times (-h/2, h/2) \subset \mathbb{R}^3$$

  with *mid-plane* ω and **aspect ratio** $h/1 \ll 1$.

- Inhomogenous **energy density**

$$W_\alpha^h(x_3, F) = W_0(x_3, F\,(I + h^{\alpha-1}\,\theta^\lambda\,B^h(x_3))), \quad F \in \mathbb{R}^{3\times 3}.$$

  B^h models the **misfit**

- Minimise **scaled energy per unit volume** on **rescaled domain**

$$\mathcal{I}_\alpha^h(y) = \frac{1}{h^{2\alpha-2}} \int_{\Omega_1} W_\alpha^h(x_3, \nabla_h\, y(x))\,\mathrm{d}x, \quad \alpha \in [2, \infty).$$

- Take the Γ-limit as $h \to 0$ for $\alpha \in [2, \infty)$.

- Later: investigate minimisers.

Theorem 2.6: A hierarchy of models

- Let $X_\alpha := \begin{cases} W^{1,2}(\omega;\mathbb{R}) & \text{if} \quad \alpha \in (2,3), \\ W^{1,2}(\omega;\mathbb{R}^2) \times W^{1,2}(\omega;\mathbb{R}) & \text{if} \quad \alpha \geqslant 3. \end{cases}$
- Define $W^{1,2}(\Omega_1;\mathbb{R}^3) \ni \boldsymbol{y^h} \longrightarrow \boldsymbol{w} \in X_\alpha$ iff the averaged and scaled displacements

$$\begin{cases} u_\alpha^h(x') & := & \dfrac{1}{h^\gamma} \displaystyle\int_{-1/2}^{1/2} (y^{h\prime}(x', x_3) - x')\,\mathrm{d}x_3, \\ v_\alpha^h(x') & := & \dfrac{1}{h^{\alpha-2}} \displaystyle\int_{-1/2}^{1/2} y_3^h(x', x_3)\,\mathrm{d}x_3, \end{cases}$$

converge *weakly* in X_α to w.

- Then, under conditions on W_0, the scaled energies

$$\mathcal{I}_\alpha^h(y) = \frac{1}{h^{2\alpha-2}} \int_{\Omega_1} W_0(x_3, F\,(I + h^{\alpha-1}\,\theta^\lambda\,B^h(x_3)))\,\mathrm{d}x,$$

with $\alpha \in [2,\infty)$, Γ-converge to...

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  converge *weakly* in X_α to w. With "$|u| \sim \mathcal{O}(|v|/h)$"
- Then, under conditions on W_0, the scaled energies

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  with $\alpha \in [2,\infty)$, Γ-converge to…

Theorem 2.6: A hierarchy of models

If $\alpha = 2$: **non-linear Kirchhoff**, pure bending (Schmidt, 2007)

$$\mathcal{I}_{Ki}(v) := \begin{cases} \frac{1}{2}\int_\omega \overline{Q}_2^\dagger(\mathrm{II}_{(v)}(x'))\,\mathrm{d}x' & \text{if } v \in W^{2,2}(S) \cap \{\nabla v \in \mathbb{O}(2,3)\}, \\ \infty & \text{otherwise.} \end{cases}$$

If $\alpha \in (2,3)$: **Kirchhoff with linearised isometry constraint**, pure bending

$$\mathcal{I}_{lKi}(v) := \begin{cases} \frac{1}{2}\int_\omega \overline{Q}_2^\star(-\nabla^2 v(x'))\,\mathrm{d}x' & \text{if } v \in W^{2,2}(S) \cap \{\det \nabla^2 v = 0\}, \\ \infty & \text{otherwise.} \end{cases}$$

If $\alpha = 3$: **von Kármán type**, coupled bending and stretching in stress-strain

$$\mathcal{I}_{vK}^\theta(u,v) := \frac{1}{2}\int_\omega \overline{Q}_2\big(\sqrt{\theta}\,\big(\nabla_s u + \tfrac{1}{2}\nabla v \otimes \nabla v\big), -\nabla^2 v\big)\,\mathrm{d}x'.$$

If $\alpha > 3$: **linearised von Kármán**

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Theorem 2.6: A hierarchy of models

$\alpha \in (2,3)$ $\quad \mathcal{I}_\alpha^h \xrightarrow[h\downarrow 0]{\Gamma} \mathcal{I}_{lKi}$

$\alpha = 3$ $\quad \mathcal{I}_\alpha^h \xrightarrow[h\downarrow 0]{\Gamma} \mathcal{I}_{vK}^\theta$

$\alpha > 3$ $\quad \mathcal{I}_\alpha^h \xrightarrow[h\downarrow 0]{\Gamma} \mathcal{I}_{lvK}$

Goal: Let $y^h \to w \in X_\alpha$. Show:

$$\liminf_{h\to 0} \mathcal{I}_\alpha^h(y^h) \geqslant \mathcal{I}_{(\cdot)}(w).$$

- Note we have maps $R^h: \omega \to \mathrm{SO}(3)$ s.t.

$$\|\nabla_h y^h - R^h\|_{0,2,\Omega_1} \lesssim h^{\alpha-1}.$$

- Rewrite energy with $A^h = A^h(\nabla_h y^h, B^h, R^h)$:

$$W_h(x_3, \nabla_h y^h) = W_0(x_3, I + h^{\alpha-1} A^h)$$

- Use Taylor to lower bound and $\operatorname*{ess\,sup}_{-1/2<t<1/2} \sup_{|F|\leqslant s} |W_0(t, I+F) - \frac{1}{2} Q_3(t,F)| = o(s^2)$:

$$\begin{aligned}\liminf_{h\downarrow 0} \frac{1}{h^{2\alpha-2}} \int_{\Omega_1} W_0(x_3, I + h^{\alpha-1}\chi^h A^h) &\geqslant \liminf_{h\downarrow 0} \frac{1}{2}\int_{\Omega_1} Q_3(x_3, \chi^h A^h) + o(1) \\ &\geqslant \frac{1}{2}\int_{\Omega_1} Q_2\Big(x_3, \check{G} + \check{\check{B}}\Big).\end{aligned}$$

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- The limit strain $\check{G} + \check{\check{B}}$ can be identified for $\alpha \geqslant 3$:

$$\frac{1}{2}\int_{\Omega_1} Q_2\big(x_3, \check{G} + \check{\check{B}}\big) = \begin{cases} \frac{1}{2}\int_\omega \overline{Q}_2\big(\theta^{1/2}\big(\nabla_s u + \frac{1}{2}\nabla v \otimes \nabla v\big), -\nabla^2 v\big) & \text{if } \alpha = 3, \\ \frac{1}{2}\int_\omega \overline{Q}_2(\nabla_s u, -\nabla^2 v) & \text{if } \alpha > 3. \end{cases}$$

- If $\alpha \in (2,3)$, relax Q_2 to

$$\overline{Q}_2^\star(F) := \min_{E \in \mathbb{R}^{2\times 2}_{\mathrm{sym}}} \int_{-1/2}^{1/2} Q_2(t, E + t\,F + \check{B}(t))\,\mathrm{d}t$$

and conclude

$$\frac{1}{2}\int_{\Omega_1} Q_2\big(x_3, \check{G} + \check{\check{B}}\big)\,\mathrm{d}x \geqslant \frac{1}{2}\int_\omega \overline{Q}_2^\star(-\nabla^2 v)\,\mathrm{d}x'.$$

Upper bound for $\alpha \in (2,3)$, sketch

Goal: Let $v \in W^{1,2}$. Construct $y^h \to v$ s.t.

$$\operatorname*{lsup}_{h\to 0} \mathcal{I}_\alpha^h(y^h) \leqslant \frac{1}{2}\int_\omega \overline{Q}_2^\star(-\nabla^2 v) \text{ if } v \in W^{2,2}_{sh}(\omega),$$

or $< \infty$ otherwise.

Core ideas:

- Show density in $W^{2,2}_{sh}(\omega)$ of

$$\mathcal{V}_0 := \{v \in C^\infty(\overline{\omega}) \colon \exists \eta > 0 \text{ s.t. } \eta v = y_3 \text{ for some “special” isometry } y\}.$$

- $\mathcal{V}_0 \ni v \rightsquigarrow$ construct isometries [FJM06, Thm. 7].
- Had to relax Q_2 to $\overline{Q}_2^\star \rightsquigarrow$ need **representation theorem for symmetric tensors** to attain the minimum.

Upper bound for $\alpha \in (2,3)$, sketch

- Rec. sequence based on $\alpha = 2$ + terms to attain min in $\overline{Q}_2^\star$ + corrector terms

$$y^h(x', x_3) \;:=\; \bar{y}_\varepsilon(x') + h\,(x_3 - a(x'))\,b_\varepsilon(x') + h^{\alpha-1}\,(g(x'), 0) \\ + h^\alpha \int_0^{x_3} d(x', \xi)\,\mathrm{d}\xi + D^h(x', x_3).$$

- **Representation theorem** provides optimal tensor in $\overline{Q}_2^\star$ as $A = \nabla_s g + a\,\nabla^2 v$.
- Exploit **frame invariance** with rotations

$$R_\varepsilon := (\nabla \bar{y}_\varepsilon, b_\varepsilon) \qquad \text{and} \qquad \mathrm{e}^{-h\tilde{F}_a^h},$$

to obtain

$$W_0(x_3, \nabla_h y^h\,(I + h^{\alpha-1}\,B^h)) \overset{(\dots)}{=} W_0(x_3, I + h^{\alpha-1}\,(A^h + B^h) + o(h^{\alpha-1})),$$

where $A^h \to (a - x_3)\,\hat{\nabla}^2 v + \hat{\nabla} g + d \otimes e_3$.

- Choose d using the map $\mathcal{L}$ attaining the minimum in Q_2, substitute a_k, g_k for a, g.

$$\mathcal{I}_\alpha^h(y_k^h) \to \frac{1}{2}\int_\omega \overline{Q}_2^\star(-\nabla^2 v)\,\mathrm{d}x' + o(1)_{k\to\infty}.$$

Theorem 2.22. *Assume* $A \equiv 0$ *in a neighbourhood of* $\{\nabla^2 v = 0\}$*. There exist smooth maps* a, g_1, g_2 *such that* $a = g_i = 0$ *on* $\{\nabla^2 v = 0\}$ *and*

$$A = \nabla_s g + a \nabla^2 v.$$

Reduce to [Sch07b, Lemma 3.3]

The interpolating regime

$\alpha \in (2,3)$ $$\mathcal{I}_\alpha^h \xrightarrow[h\downarrow 0]{\Gamma} \mathcal{I}_{lKi}$$

$\alpha = 3$ $$\mathcal{I}_\alpha^h \xrightarrow[h\downarrow 0]{\Gamma} \mathcal{I}_{vK}^\theta$$

$\alpha > 3$ $$\mathcal{I}_\alpha^h \xrightarrow[h\downarrow 0]{\Gamma} \mathcal{I}_{lvK}$$

The interpolating regime

$$\alpha \in (2,3) \qquad \mathcal{I}^h_\alpha \xrightarrow[h\downarrow 0]{\Gamma} \mathcal{I}_{lKi}$$

$$\Gamma \Big\uparrow \theta\uparrow\infty$$

$$\alpha = 3 \qquad \mathcal{I}^h_\alpha \xrightarrow[h\downarrow 0]{\Gamma} \mathcal{I}^\theta_{vK}$$

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$$\Gamma \uparrow \; \theta\uparrow\infty$$

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$$\Gamma \downarrow \; \theta\downarrow 0$$

$$\alpha > 3 \qquad \mathcal{I}^h_\alpha \xrightarrow[h\downarrow 0]{\Gamma} \mathcal{I}_{lvK}$$

Theorem 2.7. *The following two Γ-limits hold:*

$$\mathcal{I}^{\theta}_{vK} \xrightarrow[\theta\uparrow\infty]{\Gamma} \mathcal{I}_{lKi}, \quad \textit{and} \quad \mathcal{I}^{\theta}_{vK} \xrightarrow[\theta\downarrow 0]{\Gamma} \mathcal{I}_{lvK}.$$

Theorem 2.14. *Let $(u_\theta, v_\theta)_{\theta>0}$ be a sequence in X_w with finite energy*

$$\sup_{\theta>0} \mathcal{I}^{\theta}_{vK}(u_\theta, v_\theta) \leqslant C.$$

Then:

1. *The sequence $(v_\theta)_{\theta\uparrow\infty}$ is weakly precompact in $W^{2,2}(\omega)$ and the weak limit is in $X_v \cap W^{2,2}_{sh}(\omega)$. Additionally $(u_\theta)_{\theta\uparrow\infty}$ is weakly precompact in $W^{1,2}(\omega;\mathbb{R}^2)$.*
2. *The sequence $(\theta^{1/2}\, u_\theta,\, v_\theta)_{\theta\downarrow 0}$ is weakly precompact in $W^{1,2}(\omega;\mathbb{R}^2) \times W^{2,2}(\omega)$ and the weak limit is in $X_u \times X_v$.*

The structure of minimisers

Theorem 3.1. *The minimisers of $\mathcal{I}_{lKi}$ are of the form*

$$v(x') = \frac{1}{2} x'^{\top} F x,$$

where

$$F \in \mathcal{N} := \operatorname{argmin} \{ Q_2^*(F - F_0) \colon F \in \mathbb{R}^{2\times 2}_{\text{sym}}, \det F = 0 \}$$

and Q_2^*, F_0 are explicitly computed from Q_2 and B.

v is unique up to the addition of an affine transformation.

Ideas: Compute $\overline{Q}_2^\star(F) = Q_2^*(F - F_0) + a_0$ using the moments of $M(t)$ in $Q_2(t, A) = a^\top M(t)\, a$.

Use local representation of $\nabla^2 v$. Show it is constant over ω.

$\rightsquigarrow$ minimisers are cylindrical

Theorem 3.2. *The minimisers of $\mathcal{I}_{lvK}$ are of the form*

$$u(x') = E_0\, x' \quad \text{and} \quad v(x') = \frac{1}{2} x'^{\top} F_0\, x',$$

where $E_0, F_0 \in \mathbb{R}^{2\times 2}_{\mathrm{sym}}$ are explicitly computed from Q_2 and B.

u is unique up to an infinitesimal rigid motion and v up to the addition of an affine transformation.

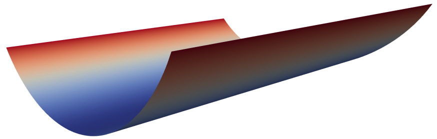
Idea: (Absorb the misfit) Compute constants $E_0, F_0 \in \mathbb{R}^{2\times 2}_{\mathrm{sym}}$ and $c_0 \in \mathbb{R}$ depending on B and Q_2, such that

$$\overline{Q}_2(E - E_0, F - F_0) = \int_{-1/2}^{1/2} Q_2(t, E + t\, F) + c_0.$$

Pick (u_0, v_0) such that $\nabla_s u_0 = -E_0$ and $\nabla^2 v_0 = F_0$. For any (u, v):

$$0 \leqslant \inf \mathcal{I}_{lvK}(u, v) = \tilde{c}_0 + \inf \mathcal{I}_{lvK}^{B\equiv 0}(u - u_0, v - v_0).$$

$\alpha \in (2,3)$ $\quad \mathcal{I}_\alpha^h \xrightarrow[h\downarrow 0]{\Gamma} \mathcal{I}_{lKi}$

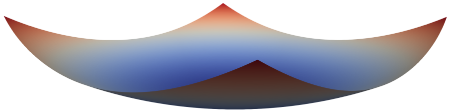


$\Gamma \uparrow \theta\uparrow\infty$

$\alpha = 3$ $\quad \mathcal{I}_\alpha^h \xrightarrow[h\downarrow 0]{\Gamma} \mathcal{I}_{vK}^\theta$

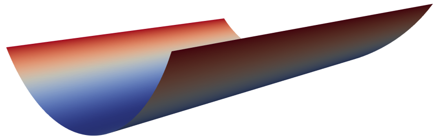
$\Gamma \downarrow \theta\downarrow 0$

$\alpha > 3$ $\quad \mathcal{I}_\alpha^h \xrightarrow[h\downarrow 0]{\Gamma} \mathcal{I}_{lvK}$



Minimisers for $\alpha = 3$

$\alpha \in (2,3)$ $\quad \mathcal{I}^h_\alpha \xrightarrow[h \downarrow 0]{\Gamma} \mathcal{I}_{lKi}$



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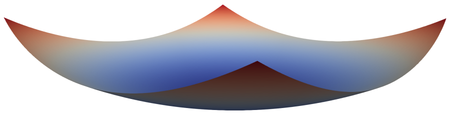
$\Gamma \downarrow \theta \downarrow 0$

$\alpha > 3$ $\quad \mathcal{I}^h_\alpha \xrightarrow[h \downarrow 0]{\Gamma} \mathcal{I}_{lvK}$



Minimisers for $\alpha = 3$

$$\mathcal{I}^{\theta}_{vK}(u,v) := \frac{1}{2}\int_{\omega} \overline{Q}_2\big(\sqrt{\theta}\,\big(\nabla_s u + \tfrac{1}{2}\nabla v \otimes \nabla v\big), -\nabla^2 v\big)\,\mathrm{d}x'$$

Conjecture. *There exists a critical value $\theta_c > 0$ such that minimisers of $\mathcal{I}^{\theta}_{vK}$ are (roughly):*

- *paraboloids for $\theta < \theta_c$,*
- *cylinders for $\theta > \theta_c$.*

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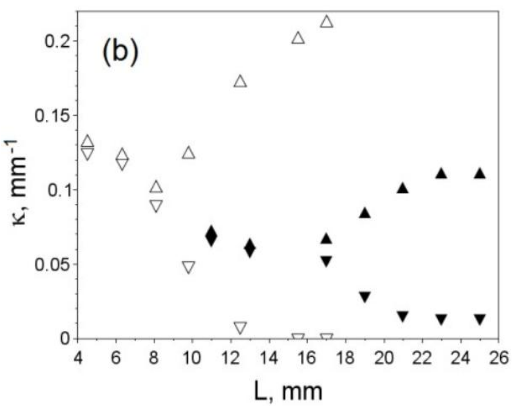
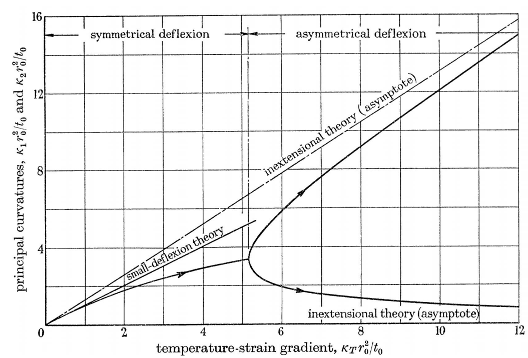


Maximum and minimum curvatures of two square bilayer films with layers in each of approximately equal thickness.

Open / filled triangles: $h = 0.8\,\mathrm{mm}$ / $1.3\,\mathrm{mm}$

Egunov et al. 2015

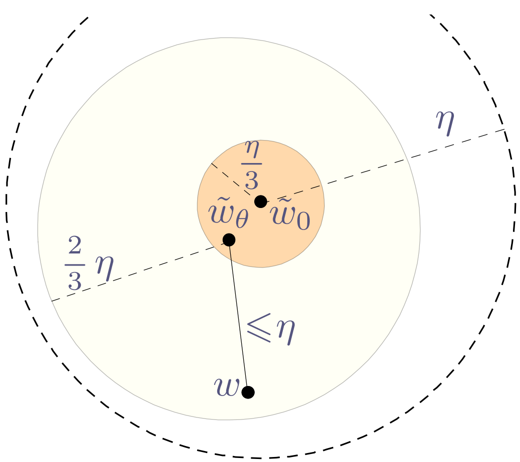


Variation of principal curvatures with temperature gradient through thickness for a lenticular disk.

Mansfield 1962

Theorem 3.10. *There exist* $(u_0, v_0) \in X$ *and a unique* $\phi\colon [0, \varepsilon) \to X$ *with* $\phi(0) = (u_0, v_0)$*, such that every* $\phi(\theta) \in X$ *is a critical point for* $\mathcal{I}^{\theta}_{vK}$ *and viceversa.*

Theorem 3.12. *There exists* $\theta_c > 0$ *such that for every* $\theta \in (0, \theta_c)$ *every critical point of* $\mathcal{I}^{\theta}_{vK}$ *is the global minimiser.*



Numerics

Goal: investigate minimisers of

$$\mathcal{I}^{\theta}_{vK}(u,v) = \frac{\theta}{2}\int_\omega Q_2\big(\nabla_s u + \tfrac{1}{2}\nabla v \otimes \nabla v\big) + \frac{1}{24}\int_\omega Q_2(\nabla^2 v - B).$$

Problem: Find minimisers of

$$J^{\theta}(u,z) = \frac{\theta}{2}\int_\omega Q_2\big(\nabla_s u + \tfrac{1}{2} z \otimes z\big) + \frac{1}{24}\int_\omega Q_2(\nabla z - B),$$

with $B \in \mathbb{R}^{2\times 2}_{\mathrm{sym}}, u, z \in W^{1,2}(\omega;\mathbb{R}^2)$ and

$$z \in Z := \{\zeta \in W^{1,2}(\omega;\mathbb{R}^2)\colon \operatorname{curl}\zeta = 0\}.$$

If $z \notin Z$, then $J^{\theta}(u,z) = +\infty$.

Discrete problem: Let $\mu_\varepsilon > 0$. Compute minimisers of the discrete energy

$$J_\varepsilon^\theta(u_\varepsilon, z_\varepsilon) = \frac{\theta}{2}\int_\omega Q_2^\varepsilon\big(\nabla_s u_\varepsilon + \tfrac{1}{2} z_\varepsilon \otimes z_\varepsilon\big) + \frac{1}{24}\int_\omega Q_2(\nabla z_\varepsilon - B) + \mu_\varepsilon \int_\omega |\operatorname{curl} z_\varepsilon|^2,$$

for $(u_\varepsilon, z_\varepsilon) \in V_\varepsilon^2$, with

$$V_\varepsilon := \{v_\varepsilon \in C(\overline{\omega}; \mathbb{R}^2) \colon v_{\varepsilon|T} \in P_1(T)^2 \text{ for all } T \in \mathcal{T}_\varepsilon\}.$$

- Discrete projected gradient flow: $w_\varepsilon^{j+1} := w_\varepsilon^j + \alpha_j \pi_{X_u}(d_\varepsilon^j)$ with $d_\varepsilon^j \in V_\varepsilon \times V_\varepsilon$ s.t.

$$(d_\varepsilon^j, \xi_\varepsilon) = -DJ_\varepsilon^\theta[w_\varepsilon^j](\xi_\varepsilon) \text{ for all } \xi_\varepsilon \in V_\varepsilon \times V_\varepsilon$$

Theorem 4.8. *Assume* $\mu_\varepsilon \to \infty$ *but* $\mu_\varepsilon = o(\varepsilon^{-2})$ *as* $\varepsilon \to 0$. *Then*

$$J_\varepsilon^\theta \xrightarrow{\Gamma} J^\theta$$

as $\varepsilon \longrightarrow 0$ *wrt. weak convergence in* $W^{1,2}$.

Theorem 4.9. *Let* $(u_\varepsilon, z_\varepsilon)_{\varepsilon>0}$ *be a sequence in* $(V_\varepsilon \cap X_u)^2$ *with bounded energy. Then there exist* $u \in W^{1,2}, z \in Z$ *such that* $u_\varepsilon \rightharpoonup u$ *and* $z_\varepsilon \rightharpoonup z$. *in* $W^{1,2}$.

Recall:

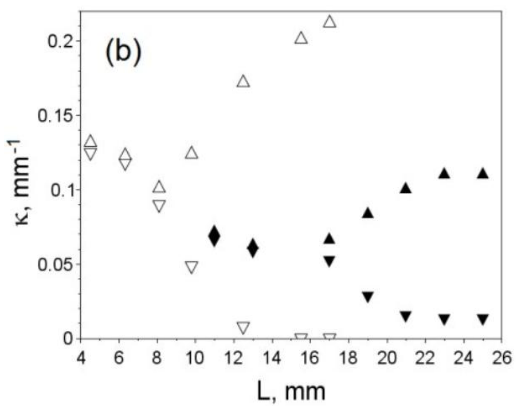
$$X_u := \left\{ u \in W^{1,2}(\omega; \mathbb{R}^2) \colon \int_\omega \nabla_a u = 0 \text{ and } \int_\omega u = 0 \right\}.$$

Results

Recall: conjecture

There exists a critical value $\theta_c > 0$ such that minimisers of $\mathcal{I}^{\theta}_{vK}$ are (roughly):

- paraboloids for $\theta < \theta_c$,
- cylinders for $\theta > \theta_c$.



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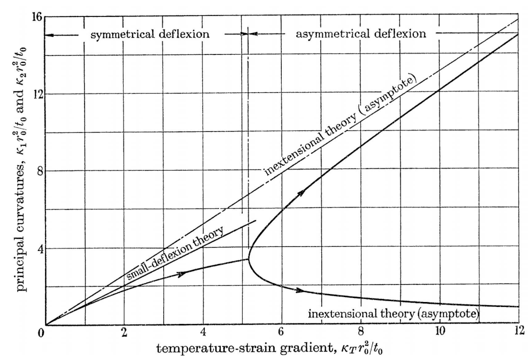

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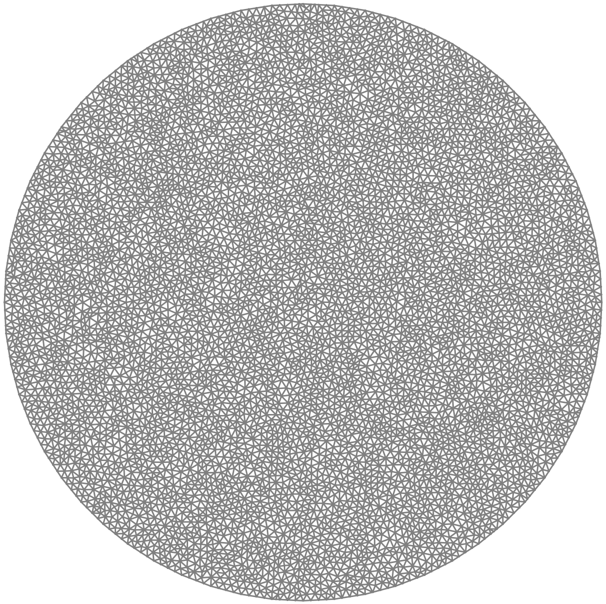
Mansfield 1962

A flat reference state



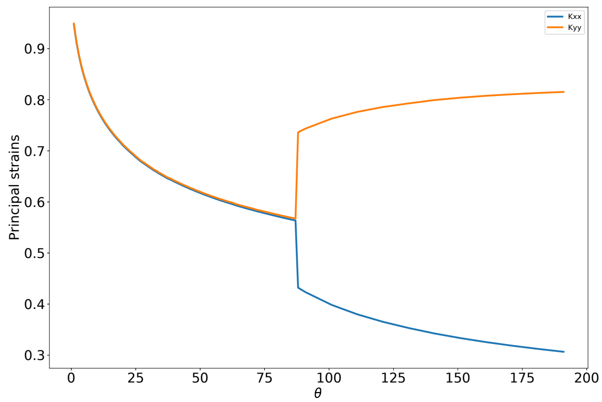
~ 7000 nodes

No initial deformation

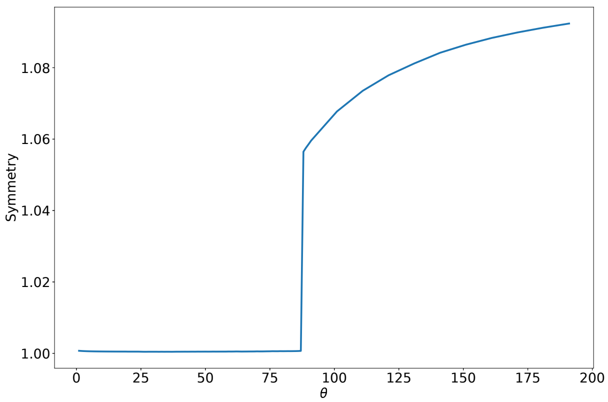
$B \equiv \mathrm{Id}$

Investigate principal bending strains as θ varies

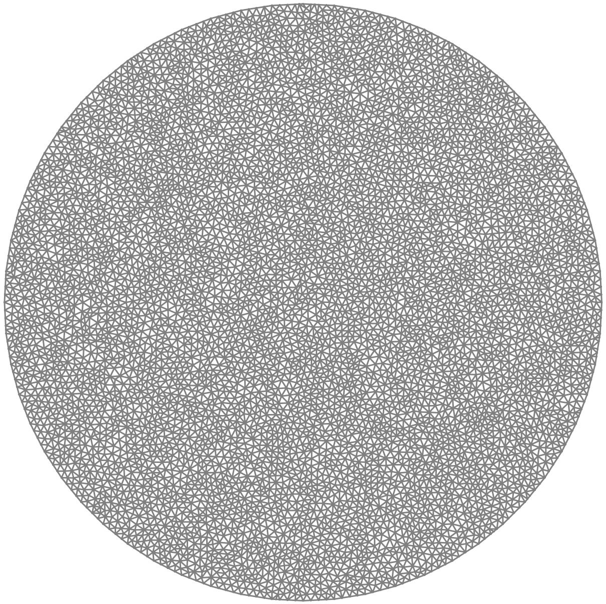
Mean principal strains



Symmetry



A pringle



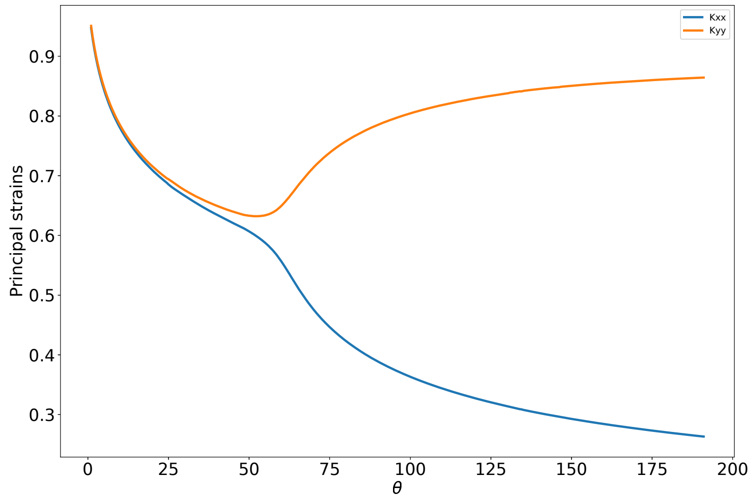
~ 7000 nodes

Anisotropic initial deformation

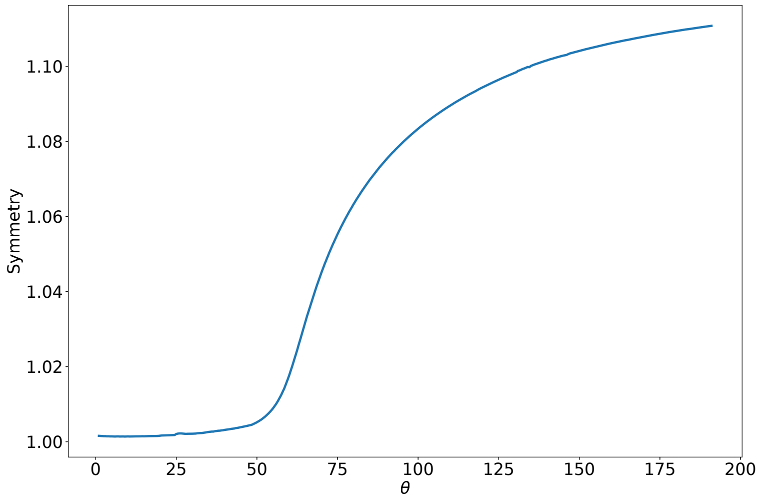
$B \equiv \mathrm{Id}$

Investigate principal bending strains as θ varies

Mean principal strains



Symmetry



Questions?