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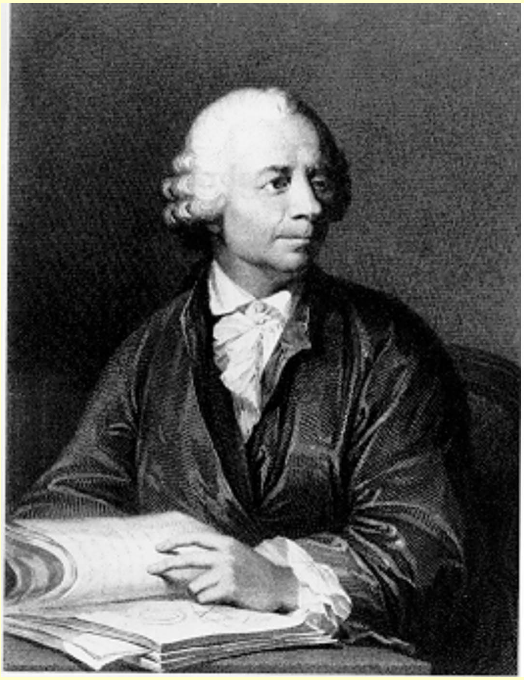
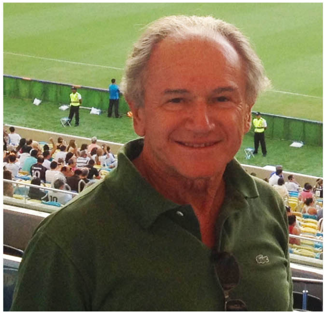
On Diffusion, Local and Not

Geometry and Mechanics
Celebrating Marcelo Epstein's 70th Birthday
The 53d Meeting of the Society for Natural Philosophy
Calgary, 20 Aug 2015

dedicated to M.E

In Crossfire





A quotation from CT's

"Six Lectures in Modern Natural Philosophy"

from the opening of Lecture VI,

Method and Taste in Natural Philosophy

"I am frequently asked to define rational mechanics or natural philosophy. The questioner usually wishes particularly to know what is excluded. Is everything else "irrational" or "unnatural"?

. . . the term "rational mechanics" indicates an interest *broader* than any of today's specialities, but no less precise . . .

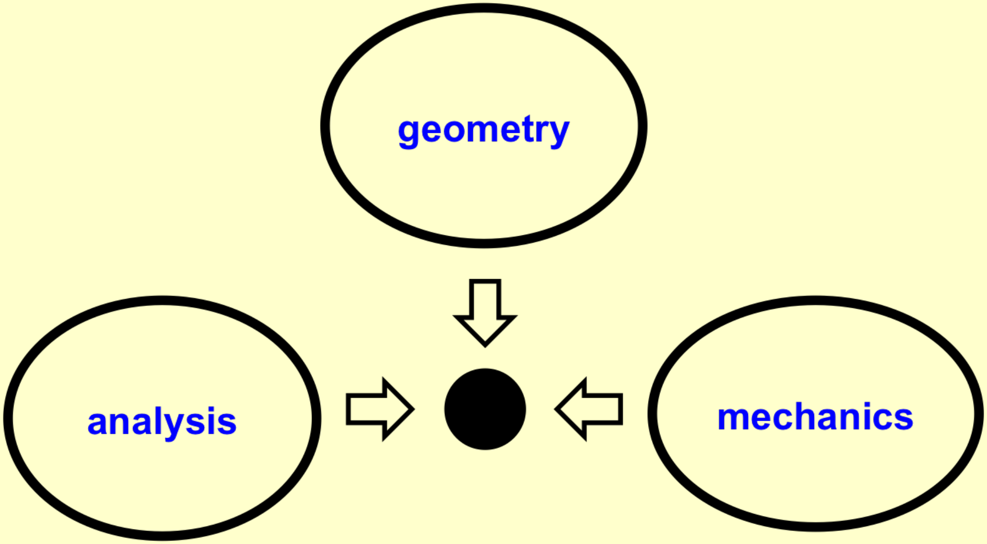
. . . a still broader term of equal age and standing was sought and found in "natural philosophy", which includes all the mathematical sciences of natural phenomena."

The Scarlet Letters we proudly wear

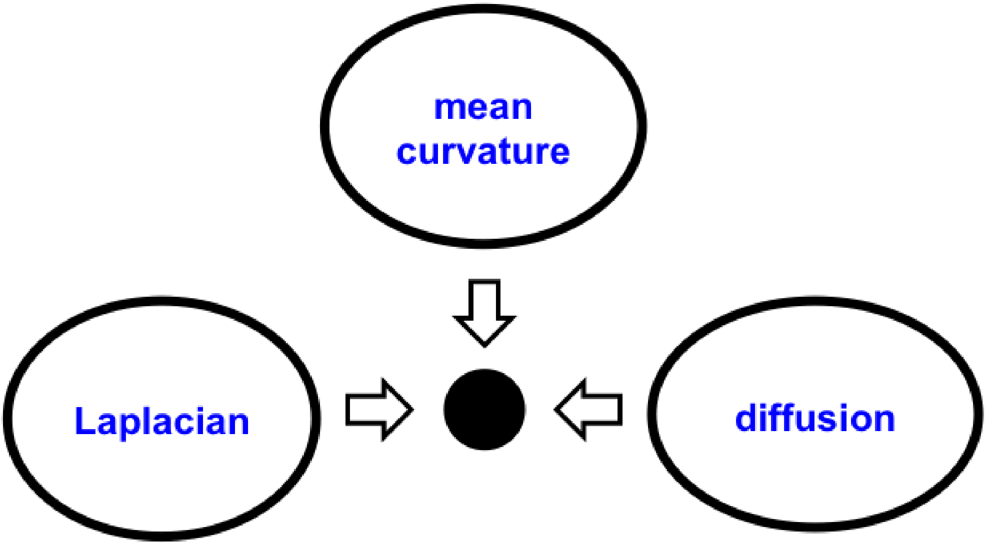
MNPh

1. Inspecting a Triple Point

A triple point of what?



What's in there



Taking a closer look

- ***Minimal surfaces*** $\equiv$ **the critical points of the minimum-area functional, surfaces with constant mean curvature.**

- ***Motion by mean curvature*** $\equiv$ **the motion of a material but massless surface, driven by surface tension ($\propto$ mean curvature H) and opposed by a dissipative force ($\propto$ normal velocity V):**

$$V = H\,.$$

- ***Heat-flow approximation of motion by mean curvature*** **(B. Merriman, J.K. Bence, and S. Osher, 1992)**

$$\partial_t u(x,t) = \Delta u(x,t), \quad u(x,0) = \widetilde{\chi}_E(x) := \chi_E(y) - \chi_{\mathcal{C}E}(y)\,;$$

approximating mean-curvature evolution by Fickian *diffusion* brings in the *Laplacian*.

2. Local Diffusion, Laplacian

Another quotation from CT’s “Six Lectures”

from the opening of Lecture V,

The ergodic problem in classical statistical mechanics

"I am often asked
why rational mechanics is necessarily continuum mechanics.

The answer is that it is not. The cultivators of rational mechanics try to maintain standards of two kinds:

1. **The model adopted should mirror nature.**
2. **The mathematics, besides being rigorous, should match the model generality.**

Both these standards are hard to reach in Statistical Mechanics. The subject is inherently more difficult than Continuum Mechanics."

Three more Scarlet Letters

R

C S

Diffusion in C and S Mechanics. 1/2

$$\partial_t c = d_o \, \Delta c \,,$$

$c \equiv$ ***concentration*** **of a tagged collection of particles diffusing in a bunch of untagged identical particles occupying a very large region** $E \subset \mathbb{R}^n$**.**

Our purpose is no different from Einstein's in 1905:
to achieve a SM interpretation of the CM self-diffusion coefficient d_o**.**

We envisage an evolution where:

- ***all tagged particles are injected at the initial time at one and the same internal point*; consequently, both concentration of tagged particles and their outflow get smaller and smaller all over the boundary of larger and larger balls.**

- **at each time** t**, we normalize** $\hat{c}(\cdot, t)$ **:** $\displaystyle\int_E \hat{c}(x,t) = 1$**, so as to regard concentration as a** ***probability measure*** **over** E**.**

Diffusion in C and S Mechanics. 2/2

- **Imitating Einstein, we introduce the integral**

$$\int_E \hat{c}(x,t)|\mathbf{x}|^2,$$

the *width of the concentration profile* of tagged particles at time t.

- **We multiply diffusion equation by $|\mathbf{x}|^2$, integrate over E, and use the boundary and normalization conditions to conclude that**

$$d_o = \frac{1}{2n}\,\partial_t\langle|\mathbf{x}|^2\rangle, \quad \langle|\mathbf{x}|^2\rangle := \int_E \hat{c}(x,t)|\mathbf{x}|^2\ :$$

the *CM self-diffusion coefficient* d_o is expressed in terms of the time rate of a SM *observable*, a microcanonical ensemble average that can be computed by post-processing the information gathered in a molecular-dynamics simulation.

Diffusion for the Analyst. 1/2

I here take freely from

L. Caffarelli, The mathematical idea of diffusion. Enrico Magenes Lecture, Pavia, March 2013.

$B_\varepsilon(x) \equiv$ **a ball of radius** ε **centered at** x, $u \equiv$ **a scalar field. In view of the Mean Value Thm, there is** $\bar{x} \in B_\varepsilon(x)$ **for which**

$$\Delta u(\bar{x}) = \fint_{B_\varepsilon(x)} \Delta u = \frac{1}{\textbf{\textit{vol}}\,(B_\varepsilon(x))} \int_{\partial B_\varepsilon(x)} \partial_{\mathbf{n}} u \,.$$

Given that

$$\lim_{\varepsilon \to 0} \Delta u(\bar{x}) = \Delta u(x) \quad \& \quad \lim_{\varepsilon \to 0} \Big(\frac{u(y) - u(x)}{\varepsilon} - \partial_{\mathbf{n}} u(y) \Big) = 0 \,,$$

we have that

$$\Delta u(x) = 3 \lim_{\varepsilon \to 0} \varepsilon^{-2} \Big(\fint_{\partial B_\varepsilon(x)} u \; - u(x) \Big) \,.$$

Diffusion for the Analyst. 2/2

Moreover, according to a stripped-to-the-bone evolution equation:

$$\partial_t u = \Delta u,$$

we see that, within the standard local descriptive framework, ***diffusion implies that asymptotically the field of interest takes at any given point the value of its average over the boundary of any of its neighbourhoods.***

A complementing quotation from LC's Magenes Lecture:

- **"...diffusion processes tend to flatten and regularize solutions, due to some tendency to average behaviors."**

3. Nonlocal Diffusion, s-Laplacian

Integral-diffusion processes

Caffarelli terms *"integral-diffusion" processes* the solutions of

$$\partial_t u(x,t) = L[u](x,t), \quad L[u](x,t) = \int [(u(y,t) - u(x,t)]\kappa(x,y)dy\,.$$

$u(x)$ **compares itself with** $u(y)$ **over a *fixed* region and weights the discrepancy with** κ**, a positive and symmetric *kernel*; the expected asymptotic behavior is similar to that induced by the Heat Equation.**

Caffarelli gives two examples:

- **the *geostrophic equation*, a model for the evolution of ocean temperature due to the ocean-atmosphere interaction;**
- **the *Levy-Kintchine equation***

$$\partial_t u(x,t) = \int [(u(x+y,t) + (u(x-y,t) - 2u(x,t)]dm(y),$$

(during a process, particles jump randomly in space and time, in a manner independent of their past path).

The s-Laplacian

The *s-Laplacian* (aka *fractional Laplacian*) is

$$(-\Delta)^s(u(x)) := c_{n,s}\, PV \int_{\mathrm{R}^n} \big(u(x) - u(y)\big)|x-y|^{-(n+2s)}dy, \qquad s \in (0,1),$$

where $PV \equiv$ principal value; the integral-diffusion format is recovered by setting

$$\kappa(x,y) = c_{n,s}\, |x-y|^{-(n+2s)}\,.$$

An essentially equivalent definition, which has the format of the Levy-Kintchine equation, is:

$$(-\Delta)^s(u(x)) := c_{n,s}\, PV \int_{\mathrm{R}^n} \big(u(x{+}y){+}u(x{-}y){-}2u(x)\big)|x{-}y|^{-(n+2s)}|dy\,.$$

Whatever the definition, *the limit for $s \to 1$ restitutes the local Laplacian*.

Sets of minimum s-perimeter, motions by s-nonlocal mean curvature, s-diffusion. 1/3

Here I take freely from N. Abatangelo & E. Valdinoci, 2014.

A recent generalization of the classic *minimal-surface problem*:

for a given set $U \subset \mathbb{R}^n$, to find a measurable set $E \subset \mathbb{R}^n$ such that

(i) $E \setminus U$ **is not modifiable (**U **plays a role of boundary datum, analogous to the role of the support curve for minimal surfaces);**

(ii) its s-perimeter is minimal, in the sense that E minimizes the *s-perimeter functional*

$$\mathbf{Per}_s(E, U) := \mathcal{F}(E \cap U, U \setminus E) + \mathcal{F}(E \cap U, \mathcal{C}U \cap \mathcal{C}E) + \mathcal{F}(E \setminus U, U \setminus E),$$

where

$$\mathcal{F}(A, B) := \frac{1}{\omega_{n-1}} \int_A dx \int_B dy \frac{1}{|y - x|^{n+2s}}, \quad s \in (0, 1/2),$$

mimics a *mutual distance interaction* between sets A and B.

Sets of minimum s-perimeter, motions by s-nonlocal mean curvature, s-diffusion. 2/3

- **the critical points of Per_s satisfy in a suitable weak sense the E-L equation:**

$$\int_{\mathrm{R}^n} \widetilde{\chi}_E(y)|x-y|^{-(n+2s)}dy = 0; \tag{1}$$

- **the classical setting is recovered in the following limit:**

$$\lim_{s\to 1/2}(1-2s)\mathbf{Per}_s(E,B_\rho) = \mathbf{Per}(E,B_\rho) \quad \textbf{for a.e. } \rho > 0;$$

- **the critical points of the minimum-area functional are surfaces with constant mean curvature.**

This justifies the idea of making use of the left side of equation (1) to introduce a s-dependent notion of *nonlocal mean curvature*.

Sets of minimum s-perimeter, motions by s-nonlocal mean curvature, s-diffusion. 3/3

Granted that

$$s{-}NMC \propto \int_{\mathrm{R}^n} \widetilde{\chi}_E(y)|x-y|^{-(n+2s)}dy,$$

it is 'natural' to study *motion by s-nonlocal mean curvature*,

- **as is;**
- **in its short-time approximation obtained by evolving the function $\widetilde{\chi}$ according to the s-Laplacian,**

that is, to approximate motions by s-nonlocal mean curvature by means of related *motions by s-diffusion*.

4. Curvatures: Mean and Gaussian, Local and not

Local notions. 1/2

In classical differential geometry of C^2-surfaces embedded in $\mathbb{R}^3$, for

$$\mathbb{R}^2 \ni (\zeta^1, \zeta^2) \leftrightarrow x = \widehat{x}(\zeta^1, \zeta^2)$$

the equation of an orientable and oriented surface S,

- **the unit *normal* at a typical point x is:**

$$\mathbf{n}(x) := \frac{\mathbf{e}_1(x) \times \mathbf{e}_2(x)}{|\mathbf{e}_1 \times \mathbf{e}_2|}, \quad \mathbf{e}_\alpha := \partial_{\zeta^\alpha} x \ \ (\alpha = 1, 2);$$

- **the *curvature tensor* K, a linear map of $\mathcal{T}_E(x)$ into itself, is:**

$$\mathbf{K}(x) := -{}^s\nabla \mathbf{n}(x) = -\mathbf{n}_{,\alpha}(x) \otimes \mathbf{e}^\alpha(x), \quad \mathbf{e}^\alpha := \partial_x \zeta^\alpha \ \ (\alpha = 1, 2);$$

- **the *mean curvature* H and the *Gaussian curvature* G are defined as follows in terms of the orthogonal invariants of K:**

$$H(x) := \frac{1}{2} tr \mathbf{K}(x), \quad G(x) := det\, \mathbf{K}(x).$$

Local notions. 2/2

The standard definitions of mean and Gaussian curvatures are *algebraic* in nature. They cannot be carried over to nonlocal situations.
Are there alternative 'transportable' definitions?

- **For** $\mathrm{e} \in \mathcal{T}_E(x)$**, the *directional curvature* of** S **in the direction** e **is:**

$$K_{\mathbf{e}}(x) := \mathbf{K}(x) \cdot \mathbf{e} \otimes \mathbf{e};$$

one finds that

$$⨍ K_{\mathbf{e}}(x) = \mathbf{K}(x) \cdot ⨍ \mathbf{e} \otimes \mathbf{e} = H(x);$$

- **moreover,**

$$det\, \mathbf{K}(x) = \widetilde{\mathbf{K}}(x)\mathbf{e}_\alpha \times \widetilde{\mathbf{K}}(x)\mathbf{e}_\beta \cdot \widetilde{\mathbf{K}}(x)\mathbf{n} = \mathbf{n},_\alpha \times \mathbf{n},_\beta \cdot \mathbf{n}\,, \quad \widetilde{\mathbf{K}} := \mathbf{K} + \mathbf{n} \otimes \mathbf{n}\,.$$

We now show that the following definitions are 'transportable':

$$\boxed{H := ⨍ (\mathbf{k}_{\mathbf{e}} \cdot \mathbf{e}), \quad G := \mathbf{k}_{\mathbf{e}_\alpha} \times \mathbf{k}_{\mathbf{e}_\beta} \cdot \mathbf{n}}\,, \quad \mathbf{k}_{\mathbf{e}} := \mathbf{K}\mathbf{e}\,.$$

Nonlocal notions. 1/4

Let $\pi(x, \mathbf{e}) := \{y \in \mathbb{R}^n \mid y = \rho\mathbf{e} + h\mathbf{n}(x), \;\; \rho > 0, \;\; h \in \mathbb{R}\}$ **denote the half-plane through** $x \in \partial E$ **defined by vectors** $\mathbf{e} \in \mathcal{T}_E(x)$ **and** $\mathbf{n}(x)$**.**

Abatangelo & Valdinoci define:

- **the *nonlocal directional curvature* (NDC) at** x **in the direction** $\mathbf{e}$**:**

$$K_{s,\mathbf{e}}(x) := \int_{\pi(x,\mathbf{e})} \frac{|y' - x'|^{n-2}\, \widetilde{\chi}_E(y)}{|x-y|^{n+2s}} dy, \quad y' = x + \rho\mathbf{e}, \; x' = x;$$

- **the *nonlocal mean curvature* (NMC) at** $x \in \partial E$**:**

$$H_s(x) := \frac{1}{\omega_{n-2}} \int_{\mathrm{R}^n} \widetilde{\chi}_E(y)|x-y|^{-(n+2s)} dy, \quad s \in (0, 1/2)$$

(in both cases, taking the principal value of the integral is implied; $\omega_{n-2} \equiv$ **Hausdorff measure of** S^{n-2} **unit sphere).**

Nonlocal notions. 2/4

Abatangelo & Valdinoci concentrate their attention on nonlocal directional and mean curvatures; they prove that

- **NDC and NMC tend to their local counterparts in the limit when $s \to 1/2$:**

$$\lim_{s\to 1/2}(1-2s)K_{s,\mathbf{e}} = K_{\mathbf{e}}, \quad \lim_{s\to 1/2}(1-2s)H_s = H\,;$$

- **the circular average of NDC is equal to NMC:**

$$H_s = \frac{1}{\omega^{n-2}}\int_{S^{n-2}} K_{s,\mathbf{e}}\, d\mathcal{H}^{n-2}$$

(recall that, in the local case, $H = \fint K_{\mathbf{e}}$).

What about nonlocal Gaussian curvature?

Nonlocal notions. 3/4

Observe that, for $g(y) = |y|^{-(3+2s)} \widetilde{\chi}_E(y)$**,**

$$PV \int_0^{+\infty} d\rho \int_{-\infty}^{+\infty} dh\, \rho\, g(\rho, h, \varphi) = \int_{S^1} d\varphi \lim_{\varepsilon\to 0} \int_{\pi(x,\mathbf{e})\setminus B_\varepsilon(x)} \big((y-x)\cdot \mathbf{e}\big)\, g(y)\, dy$$
$$= \int_{S^1} K_{s,\mathbf{e}}\, d\varphi\,.$$

Let

$$\boxed{\mathbf{k}_s(\mathbf{e}) := \lim_{\varepsilon\to 0} \int_{\pi(x,\mathbf{e})\setminus B_\varepsilon(x)} g(y)(y-x)\, dy}\,,$$

whence

$$\textbf{NDC}: \quad K_{s,\mathbf{e}} = \mathbf{k}_s(\mathbf{e})\cdot \mathbf{e} \quad \& \quad \textbf{NMC}: \quad H_s = ⨍ (\mathbf{k}_s(\mathbf{e})\cdot \mathbf{e})\,.$$

Nonlocal notions. 4/4

Once again: $$\boxed{\mathbf{k}_s(\mathbf{e}) := \lim_{\varepsilon\to 0}\int_{\pi(x,\mathbf{e})\setminus B_\varepsilon(x)} g(y)(y-x)\,dy}\,.$$

- **Recall that in the local case we set $\mathrm{k}_{\mathrm{e}} := \mathrm{K}\mathrm{e}$. I conjecture that**

$$\lim_{s\to 1/2}(1-2s)\mathbf{k}_s(\mathbf{e}) = \mathbf{k}_{\mathbf{e}}, \quad \forall\, \mathbf{e}\in\mathcal{T}_E(x)\,.$$

- **Recall our alternative definition of the *local Gaussian curvature*:**

$$G := \mathbf{k}_{\mathbf{e}_\alpha}\times\mathbf{k}_{\mathbf{e}_\beta}\cdot\mathbf{n}\,.$$

I propose the following definition of *nonlocal Gaussian curvature*:

$$\textbf{NMC}:\quad G_s := \mathbf{k}_s(\mathbf{e}_m)\times\mathbf{k}_s(\mathbf{e}_M)\cdot\mathbf{n}\,,$$

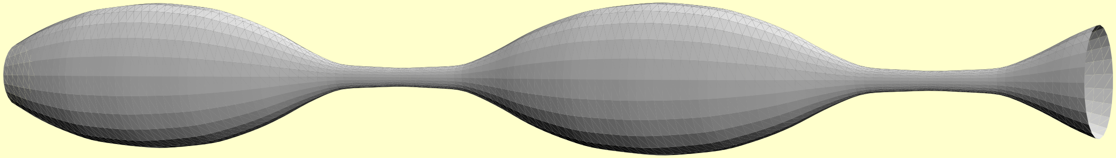
where e_m and e_M denote the unit vectors in $\mathcal{T}_E$ for which the NDC is, respectively, minimal and maximal.

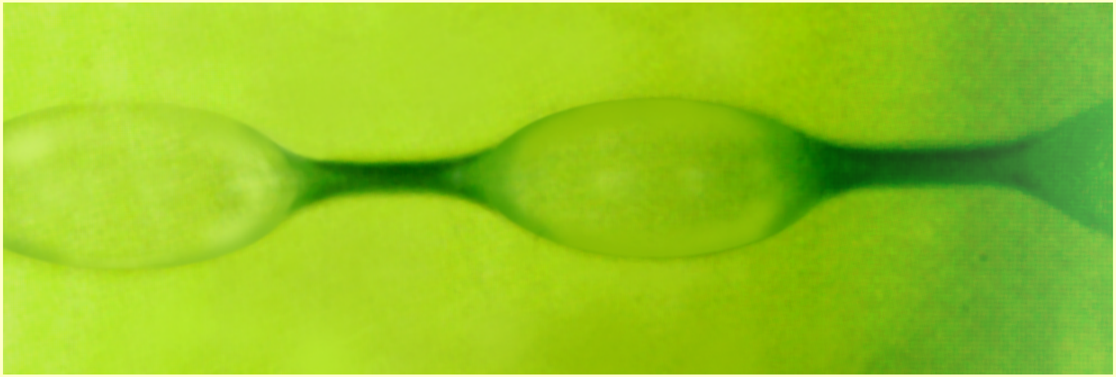
Recap

1. **Inspecting a Triple Point**
2. **Local Diffusion, Laplacian**
3. **Nonlocal Diffusion, s-Laplacian**
4. **Curvatures: Mean and Gaussian, Local and not**

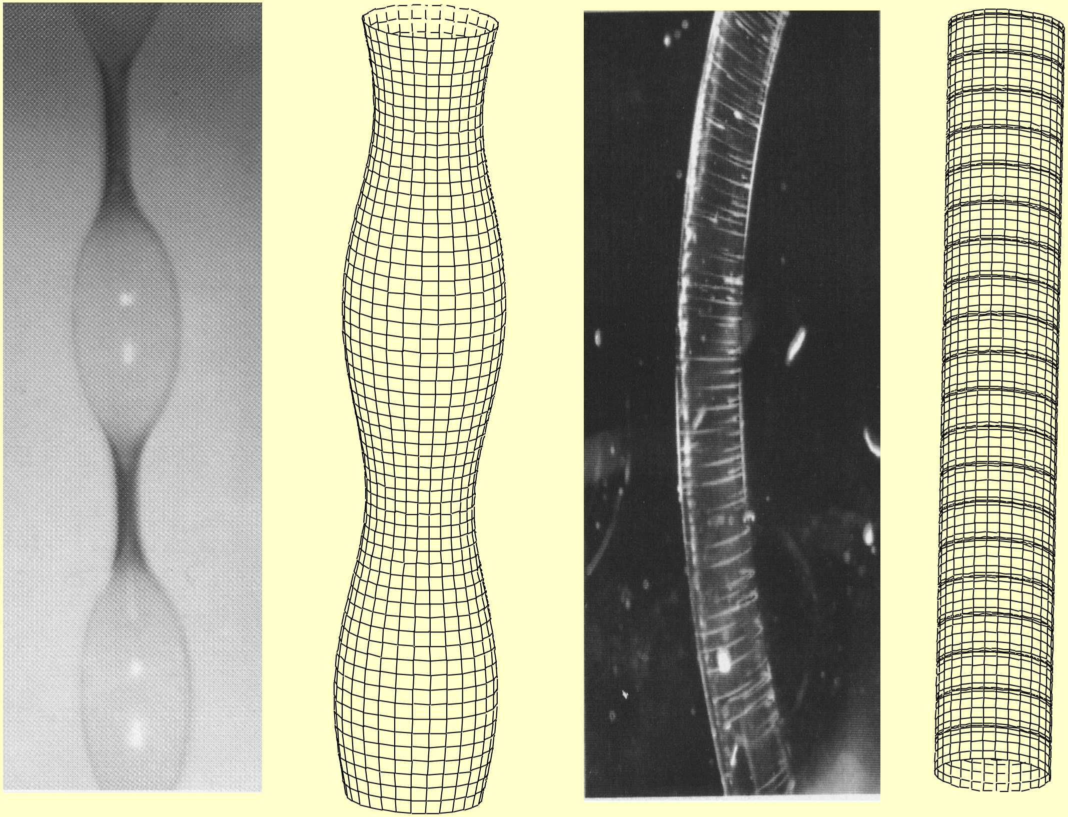
Bubble pattern of a shrinking gel

(courtesy of S. Chaieb, KAUST)





Bubble and bamboo patterns of a shrinking gel



(a) (b)

Thank you for your kind attention!

Ad multos annos, Marcelo!