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From phase transformation fronts to the growth of long bones

A Multiscale Approach to a Basic problem of Materials Mechanics (inert or living material)

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Various routes to the understanding of the propagation of phase-transition fronts in crystalline substances examined in the light of recent works. These include lattice dynamics, meso-scopic considerations, and the fully macroscopic thermomechanical approach on the material manifold that combines an engineering interest with an invariance-theoretical viewpoint.

How would these apply to a problem of **mechano-biology**: the growth of long bones?

Introduction

A full understanding of the phenomenon of the propagation of phase-transition fronts in deformable crystals - metals, alloys - is one of the essential problems of contemporary materials science and mechanics at both theoretical and application levels.

This unique problem can be examined at three different scales (cf. Figures 1-3)

(i) a *microscopic scale* (lattice dynamics) in the absence of thermodynamical irreversibility: inspired by the Landau-Ginzburg theory, although discrete to start with, deals with nonlinear localized waves (solitonic structures : solitary wave, soliton complexes) where nonlinearity and dispersion (discreteness) are the main ingredients.

(ii) a *mesoscopic scale* (exploitation of continuum thermomechanical equations in a structured front), (involves nonlinearity, dispersion *and* dissipation (viscosity)).

(iii) a *macroscopic scale*, that of engineering applications (the front is seen as an irreversibly driven singular surface and where macroscopic thermodynamics (theory of irreversible processes) and numerical methods such as finite-element and finite-volume methods are used in conjunction with a criterion of progress.

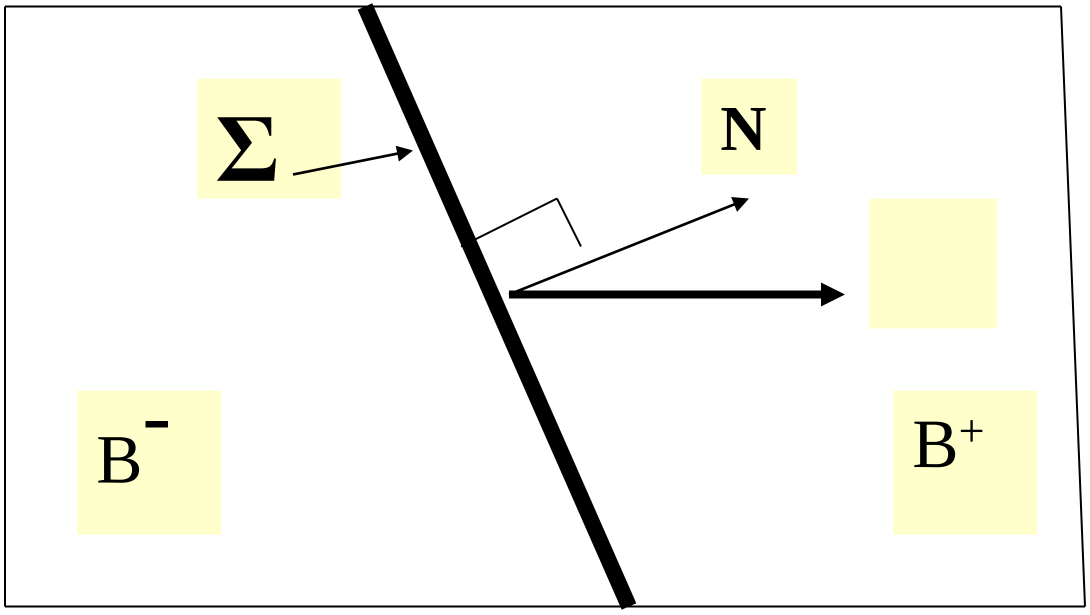

FIGURE 1

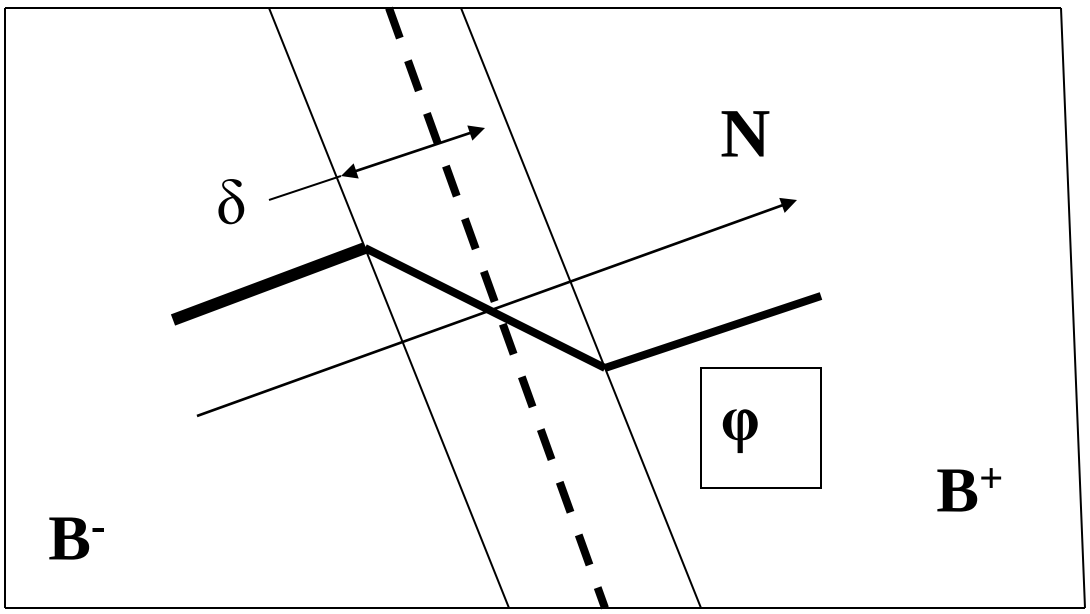

FIGURE 2

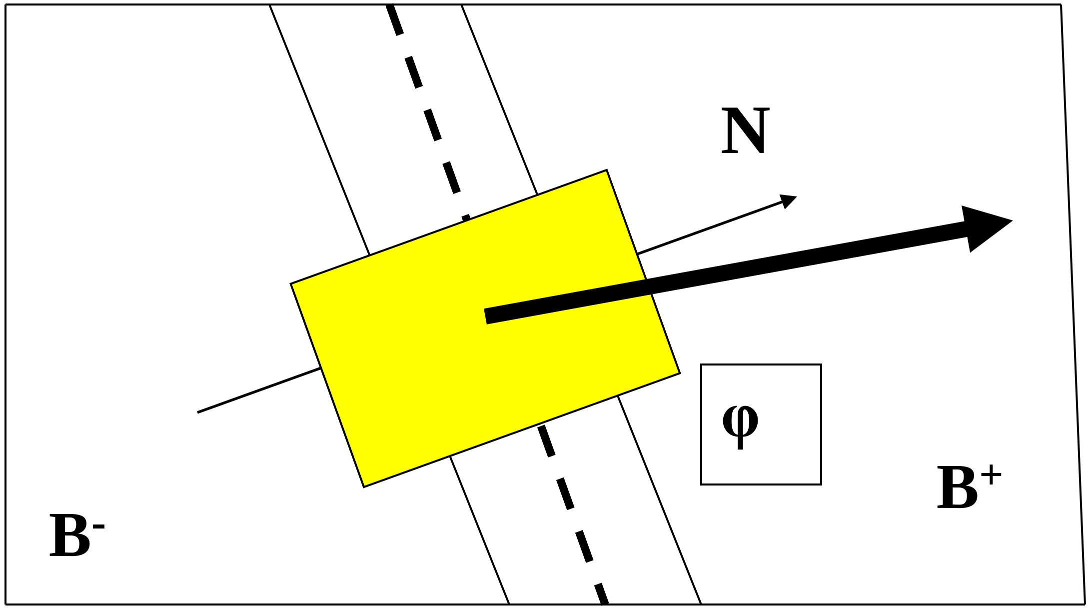

FIGURE 3

The three scales are reconciled by the fact that all solutions satisfy the same *Hugoniot conditions* sufficiently far away from the front, whether structured as a solitonic or dissipative structure, or without thickness such as a singular surface.

This multi-level, multi-physics approach gathers the view points of condensed-matter physicists (micro-scale) , applied mathematicians (meso-scale) and engineers (macro-scale), and even that of the theoretical physicist via the inclusive notion of quasi-particles and the underlying and pervasive invariant-theoretical framework.

Microscopic condensed-matter-physics approach : solitonics

The first approach considered is that dealing with the *micro scale* of lattice dynamics *in a perfect lattice*, so that there is no dissipation and effects of temperature are not involved, except perhaps in the phase-transition parameter (Falk, Pouget, Maugin and Cadet).

This allows one to readily obtain a dynamical representation of a phase boundary (here a kink) as a *solitonic structure* for a two-degrees of freedom, but essentially one-dimensional, system. The reason for this is that, unless one wants to study the *lateral stability of this system*, the « theorem of the flea» applies : the « flea » sees only the *first-order geometrical description* of the transition layer , hence essentially the normal direction to a layer of constant thickness.

Notice that the continuum model obtained in the *long-wave length limit* is that of a *nonlinear elastic body with first gradients of strains* taken into account but no dissipation.

This long-wave limit is admissible because the transition layer between two phases, although thin (perhaps a few lattice spacings), is nonetheless large enough.

Numerical simulations can be performed *directly* on the lattice. The elastic potential is non-convex in general. To exemplify this approach, we consider a one-dimensional (x), two-degrees of freedom, lattice with transverse (main effect) and longitudinal (secondary effect) displacements from the initial position.

In the so-called *long-wave limit* where the discrete dependent variables (strains) s_n and e_n vary slowly from one lattice site to the next and they can be expanded about the reference configuration (na,O), the discrete equations yield the following system of two (nondimensionalized) coupled partial - in (x,t) - differential equations (with an obvious notation for partial x and t derivatives)

$$s_{tt} - c_T^2 s_{xx} + \left(s^3 - s^5 + 2\gamma\, es + \alpha\, s_{xx}\right)_{xx} = 0,$$

$$e_{tt} - c_L^2 e_{xx} + \gamma\left(s^2\right)_{xx} = 0\,, \quad \alpha \equiv \beta - \left(c_T^2 / 2\right),$$

$$s \equiv v_x \ , e \equiv u_x \ .$$

where s and e are the shear and elongation strains, γ *is a coupling coefficient, and* α and β *are nonlocality parameters*. Parameters c_T and c_L are the characteristic speeds of the linear elastic system. This corresponds to stresses and energy density given by

$$\sigma_s = \bar{\sigma}_s - \frac{\partial}{\partial x} M = \frac{\delta}{\delta s}\psi \ , \sigma_e = \frac{\partial}{\partial e}\psi,$$

$$\bar{\sigma}_s = \frac{\partial}{\partial s}\psi \ , \ M = \frac{\partial}{\partial s_x}\psi \ ,$$

$$\psi(s,e,s_x) = \frac{1}{2}\left(c_T^2 s^2 - \frac{1}{2}s^4 + \frac{1}{3}s^6 + c_L^2 e^2 - 2\gamma s^2 e + \alpha(s_x)^2\right).$$

In other words, eqns.(1)$_{1\text{-}2}$ are none other than the *x*-derivatives of the balance of (physical) linear momentum for a continuum made of a nonlinear, homogeneous elastic material with strain gradients - with both nonlinearity and strain gradients relating only to the *shear* deformation.

Complicated as they look, eqns.(1)$_{1\text{-}2}$ still admit exact dynamical solutions of the *solitonic type*. A thorough discussion of the existence of such solutions connecting two different or equivalent minimizers (i.e., two phases) of the potential energy was given by Maugin and Cadet to whom we refer the reader.

The remarkable fact is that such complicated solutions are shown (by computation) to satisfy the following (temperature-independent) *HUGONIOT* condition between *states at infinity* :

$$\boxed{Hugo := \left[\overline{W}\left(s, e \text{ fixed} \right) - \langle \overline{\sigma}_s \rangle s \right] = 0,} \qquad (3)$$

where $\overline{\sigma}_s$ is the shear strain *without strain-gradient effect*, and $\overline{W}$ is the elastic energy with such effects similarly neglected.

Obviously, gradient effects play a significant role only within the rapid transition zone that the kink solution represents, while outside the state is practically spatially uniform, although different on both sides of the localized front. Here we have used the following definitions for the jump and mean value of any quantity *a*:

$$[a] := a(+\infty) - a(-\infty)\,,\ \langle a \rangle := \frac{1}{2}\big(a(+\infty) + a(-\infty)\big)\ . \quad (4)$$

Equation (3) is typical of the *absence of dissipation* during the transition, in general a working hypothesis that is *not* realistic. Furthermore, it can in fact be rewritten as the celebrated *Maxwell's rule of equal areas*.

Macroscopic engineering approach : singular surface and thermodynamic criterion

In this second approach the phase boundary is considered *locally* and *macroscopically* as a discontinuity front Σ in the first-order derivatives - hence, like a *shock wave*, a *singular surface* of the first order in Hadamard's classification - of the basic field (e.g., the physical placement $\mathbf{x} = \chi(\boldsymbol{X},t)$ of a « particle » $\boldsymbol{X}$) ; *Σ has no thickness. The « theorem of the flea» applies again : only the first-order geometrical description of the singular surface -its normal- is involved unless one introduces some kind of surface tension. But the front itself is not necessarily flat. It may curve and even form cusps in the worst situations.*

The local viewpoint refers to the fact that it is assumed at each instant of time that the thermoelastic solution is known by any means - analytical, but more than often, numerical - on both sides of Σ so that one can compute a *driving force* acting on Σ. Further progress of Σ must not contradict the second law of thermodynamics. The latter, therefore, governs the local evolution of Σ which is generally *dissipative* (although no microscopic details are made explicit to justify the proposed expressions).

The approach is *thermodynamical* and *incremental* (in total analogy with modern plasticity). All physical mechanisms responsible for the phase transformation are contained in the *phenomenological-macroscopic* relationship given by the *local criterion of progress* of Σ. Without entering details which can be found in papers (Maugin and Trimarco, 1995; Maugin, 1997) and considering from the outset the finite-strain framework.

We remind the reader that at any regular point in the body (i.e., on both side of Σ) we have the balance of (physical) linear momentum and the future heat equation written in the Piola-Kirchhoff form for a *heat-conducting thermoelastic material* ($W(\mathbf{F},\theta)$ in general is different on both sides of Σ, *and generally non-convex in its first argument and concave in the second one - the thermodynamical temperature* θ). But while each phase is materially homogeneous, the presence of *Σ is a patent mark of a loss of translational symmetry on the overall body, hence the consideration of a global material inhomogeneity.*

The field equation capturing this breaking of symmetry is the **jump relation associated** with the equation of momentum *on the material manifold*, i.e, what we called **the balance of pseudo-momentum**. This jump equation, together with that for entropy, governs the phase-transition phenomenon at Σ. These equations apriori read

$$\boxed{\begin{aligned} &\mathbf{N}.\left[\mathbf{b}+\overline{\mathbf{V}}\otimes P\right]+\mathbf{f}_{\Sigma}=\mathbf{0}\ , \\ &\mathbf{N}.\left[\overline{\mathbf{V}}S-\left(\mathbf{Q}/\theta\right)\right]=\sigma_{\Sigma}\geq 0\ , \end{aligned}} \qquad (5)$$

where the last inequality is a statement of the second law of thermodynamics at Σ.

$\mathbf{N}$ is the unit normal to Σ oriented from the *minus* to the *plus* side, and we defined the jumps and mean values at Σ by (compare to eqns.(4)) :

$$\boxed{[a] := a^{+} - a^{-} \ , \langle a \rangle := \frac{1}{2}\left(a^{+} + a^{-}\right),} \qquad (6)$$

where $a^{\pm}$ are the uniform limits of

a in approaching Σ on its two faces along $\mathbf{N}$. $\overline{\mathbf{V}}$ is the material velocity of Σ , S is the entropy density, θ is the thermodynamical temperature, and the material or *pseudo* momentum and the *Eshelby stress tensor* are defined by

$$\boxed{\begin{aligned} &P = -\rho_0 \mathbf{v}.\mathbf{F} \;,\; \mathbf{b} = -\left(L\mathbf{1}_R + \mathbf{T}.\mathbf{F} \right) \quad , \\ &L := \frac{1}{2}\rho_0 \mathbf{v}^2 - W(\mathbf{F},\theta) = \bar{L}(\mathbf{F},\theta,\mathbf{v}) \;, \end{aligned}} \tag{7}$$

and

$$\boxed{\begin{aligned} &\mathbf{v} = \left.\frac{\partial \chi}{\partial t}\right|_{\mathbf{X}} ,\; \mathbf{F} = \left.\frac{\partial \chi}{\partial \mathbf{X}}\right|_{t} \equiv \nabla_R \chi \;,\; \mathbf{v} = -\,\mathbf{F}.\mathbf{V}\,, \\ &W = W\left(\mathbf{F},\theta\right),\; \mathbf{T} = \partial W / \partial \mathbf{F}\,,\; S = -\partial W / \partial \theta . \end{aligned}} \tag{8}$$

The « force » $\mathbf{f}_\Sigma$, just like σ_Σ , is an unknown and like other thermodynamical material forces it acquires a physical meaning only in the computation of the power it expands here in the material velocity . $\overline{\mathbf{V}}$

On performing this computation (e.g., Maugin, 1997) in the case of a *coherent phase-transition front* Σ for which there holds the continuity conditions $[\mathbf{V}] = \mathbf{0}$ and $[\theta] = 0$ (no dislocations at Σ *that is also homothermal - the transition occurs at a temperature shared by the two phases), we obtain the compatibility condition between* $\boldsymbol{f}_\Sigma$ *and* σ_Σ:

$$\boxed{\mathbf{f}_\Sigma . \overline{\mathbf{V}} = f_\Sigma \overline{V}_N = \theta_\Sigma \sigma_\Sigma \geq 0,}$$

$$\boxed{f_\Sigma = -Hugo_{PT}\,,\; Hugo_{PT} := \mathbf{N}.\left[\mathbf{b}_S\right].\mathbf{N} = \left[W - \langle \mathbf{N}.\mathbf{T} \rangle . \mathbf{F}.\mathbf{N}\right],}$$

where $\mathbf{b}_S$ is the quasi-static part of $\mathbf{b}$ (although the computation is made without neglecting inertia).

If this inertia is really neglected, then we have following reduction :

$$\boxed{Hugo_{PT} = \left[W - tr\left(\langle \mathbf{T} \rangle . \mathbf{F}\right)\right].} \qquad (11)$$

In this canonical formalism the driving force $\mathbf{f}_{\Sigma}$ happens to be purely normal but it is constrained to satisfy, together with the propagation speed $\bar{V}_N$ the surface dissipation inequality indicated in the last of (9). In other words, any relationship between these two quantities must be such that the inequality (9) be verified. This is the basis of the formulation of a *thermodynamically admissible criterion of progress* for Σ. Indeed, we look for a relationship

$$\boxed{\bar{V}_N = g\left(f_{\Sigma}; \theta_{\Sigma}\ fixed\right)}$$

which satisfies the last of (9).

If we « force » the system evolution to be such that there is effective progress of the front at $\mathbf{X} \in \Sigma$ while there is *no dissipation*, then we must necessarily enforce the following condition

$$\boxed{f_\Sigma = 0 \;\; i.e., \; Hugo_{PT} \equiv \left[W - \langle \mathbf{N}.\mathbf{T} \rangle . \mathbf{F}.\mathbf{N} \right] = 0 \,.}$$

(12)

On account of the fact that temperature (θ_Σ) is fixed, and the thickness of the front is taken as zero, so that uniform states are reached immediately on both sides of Σ, eqn.(12) is none other than the condition of « Maxwell » (3) in the one-dimensional pure-shear case. Thus a macroscopic approach dear to the engineer has allowed us to obtain, in general, a more realistic (in general, dissipative) progress of the front.

The case of Section 2 appears then as a « *zoom* » - in the nondissipative case - on the situation described in the present section since the front acquires, through this zoom magnification (asymptotics), a definite, although small, thickness and a structure while rejecting the immediate vicinity of the zero-thickness front to infinities. The next approach allows one to introduce both a *thickness* and *dissipation*.

Mesoscopic applied-mathematics approach : structured front

Here the front of phase transformation is looked upon as a mixed « *viscous-dispersive* » structure at a « meso » scale. We refer to this as the *applied-mathematician approach*. This dialectical approach in which one applies macroscopic concepts at a smaller scale to obtain an improved phenomenological description is finally fruitful (cf. Truskinowsky;, 1994, to whom we refer

We therefore consider a one-dimensional model (along the normal to the structured front - « theorem of the flea ») and we envisage a *competition* between viscosity (i.e., a simple case of dissipation) and some *weak nonlocality* accounted for through a strain-gradient theory (compare Section 2). The critical nondimensional parameter which compares these two effects is defined by

$$\boxed{\omega = \eta / \sqrt{\varepsilon}\,.} \qquad (13)$$

where η is the viscosity and $\varepsilon \approx L^2$ is the nonlocality parameter (size effect).

Progressive-wave solutions $u = u(\xi = x - \bar{V}_N t)$ of the continuous system that relate two minimizers (uniform solutions at infinities that minimize $\overline{W}$) over a distance of the order of $\delta = \sqrt{\varepsilon}$ are discussed in terms of this parameter. The mathematical problem reduces to a *nonlinear eigenvalue problem* of which the specification of the points of the discrete spectrum constitutes the looked for *kinetic relation*

$\bar{V}_N = g(f;\varepsilon)$ where $f = \bar{\sigma} - \bar{\sigma}(+\infty)$ plays the role of *driving force*.

As a matter of fact the speed of propagation $\bar{V}_N$ satisfies the *Rankine-Hugoniot equation*

$$\bar{V}_N^{\,2} = [\bar{\sigma}] / [s]$$

where strain gradients and viscosity play no role and the jumps are taken between asymptotic values at infinity - cf. eqns.(4).

Theoretical-physics Approach : Quasi-particle and transient motion

The approach of section 3 simply accepts the value of $\overline{V}_N$, whatever its evolution, as it is computed from the full field solution at each instant of time and each material point $\mathbf{X} \in \Sigma$**.** In contrast, the approaches of Sections 2 and 4 provide *progressive-wave* solutions, i.e ., waves that are steady in the sense that the propagation speed, although a property of the solution (and not only of the material as in linear-wave propagation) does not vary in time along the propagation path. This is a type of *inertial motion.*

What about a *non-inertial motion* ?

To look at such a case, we envisage the problem in the following way. The localized -but with non-zero thickness- dynamical solutions of Section 2 are looked upon as global entities behaving like mass particles in motion in the appropriate *point mechanics*, i.e., as so-called *quasi-particles*.

All perturbing effects such as dissipation, inhomogeneities, etc, will then be treated as *perturbing forces* on the inertial motion that becomes thus *non-inertial*.

To understand this view point, it is sufficient to envisage the presence of a viscous (more generally, dissipative) contribution in the right-hand side of the classical balance of linear momentum . This results in the presence of an additional *material* force $\mathbf{f}_D^{inh} = -\mathbf{f}_D.\mathbf{F}$ in the right-hand side of the canonical momentum equation. The latter equation is used, after integration over the path of the wave, to treat the material force as a perturbation on the solution in the absence of $\mathbf{f}_D$.

The essential problem consists then in identifying the *point mechanics* that is associated with a particular system of partial-differential equations on account of some of its exact integrals. This point mechanics - that is, a coherent system of relations between mass, momentum and energy of a point particle - can be completely new and a priori unforeseeable.

For this viewpoint we refer the reader to published works by Christov and Maugin. In particular, a perturbative approach of the canonical, quasi-particle, type (19) was suggested by Fomethe and Maugin to study the varied motion of a phase-transition front under the action of a temperature gradient.

Some references

Maugin, G.A., (1999). ***Nonlinear Waves in Elastic Crystals,*** Oxford Mathematical Monographs, Oxford University Press, UK.

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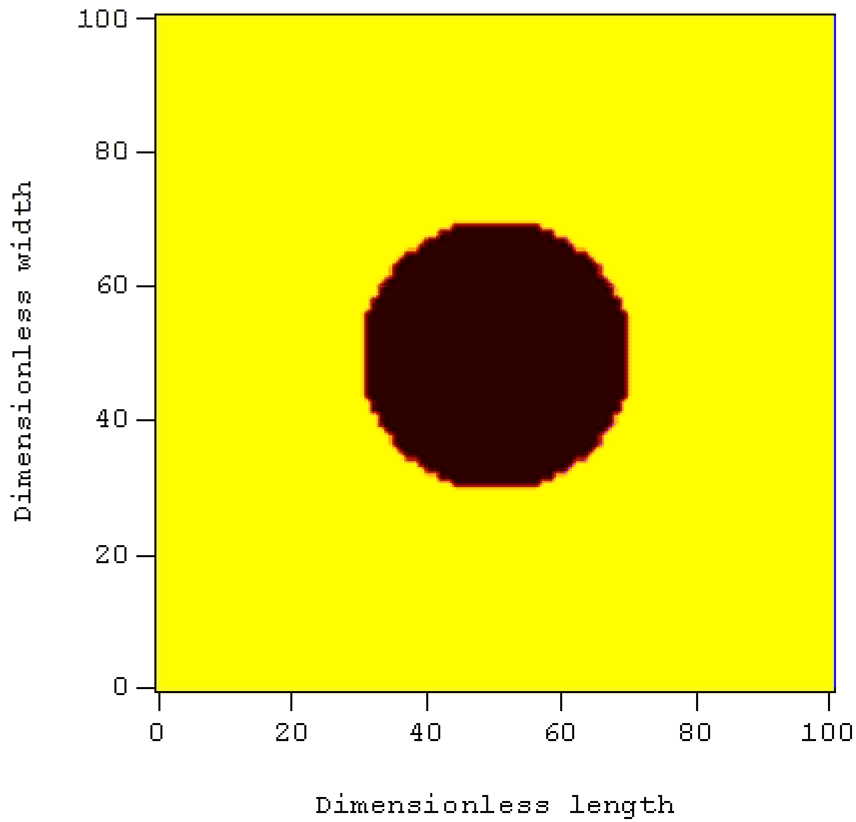
Maugin, G.A. , and Christov, C.I., (2002). Nonlinear Waves and Conservation Laws : Nonlinear Duality Between Elastic waves and Quasi-particles. In : ***Selected Topics in Nonlinear Wave Mechanics***, Eds. C.I.Christov and A.Guran, pp.117-160, Birkhauser, Boston. .

Berezovski A., Maugin G.A. and Engebrecht J., (2008), ***Numerical simulation of waves and fronts in Inhomogeneous solids***, World Scientific , New Jersey.



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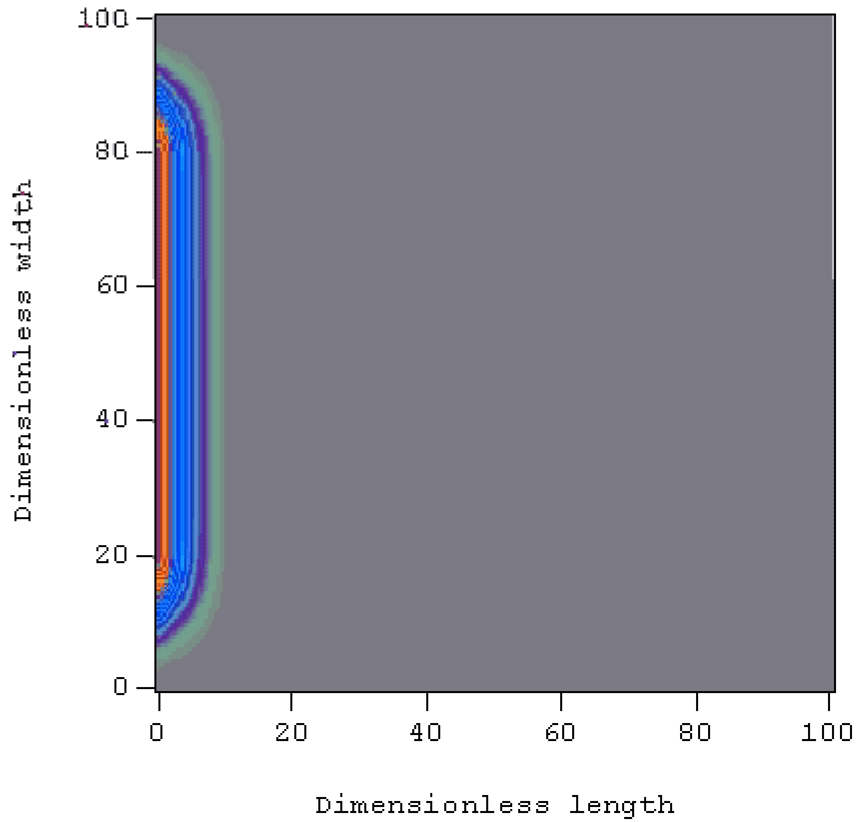

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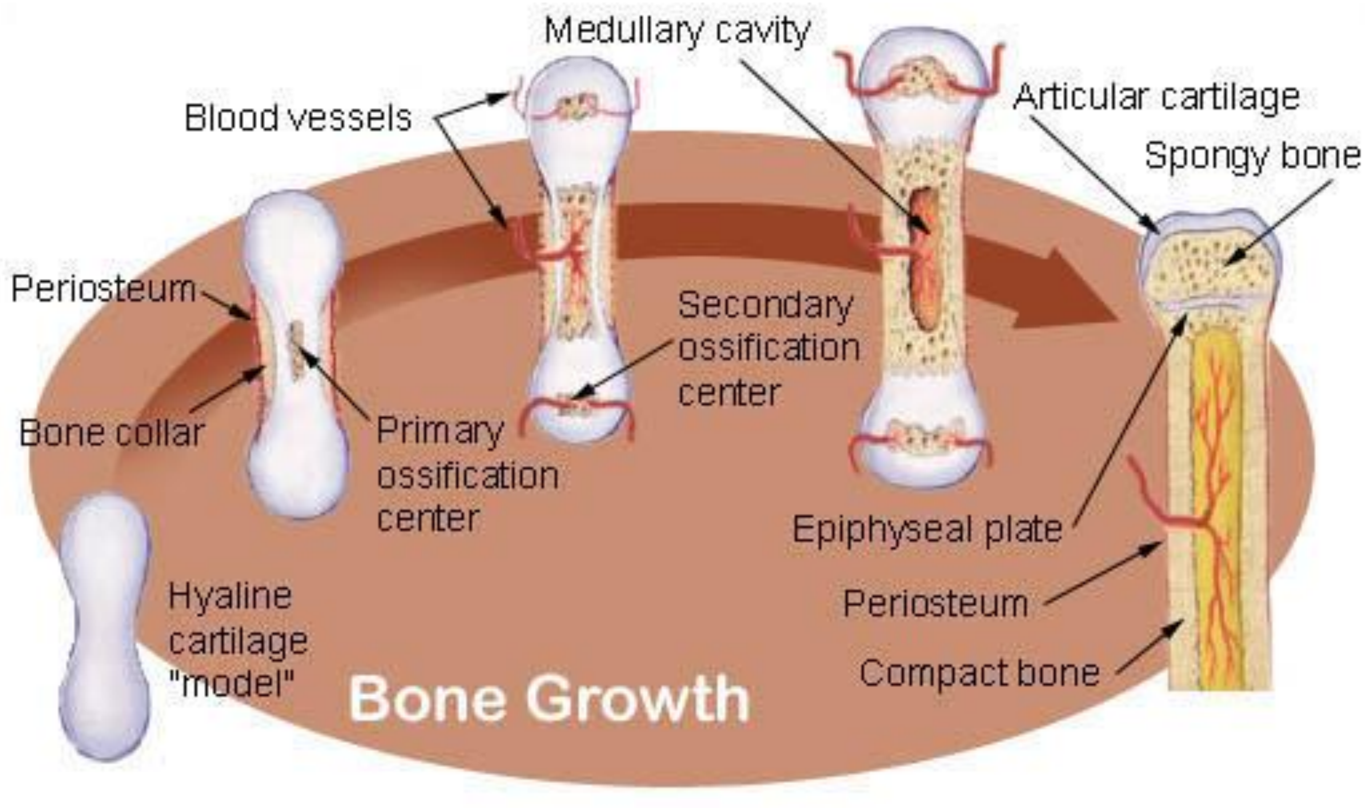
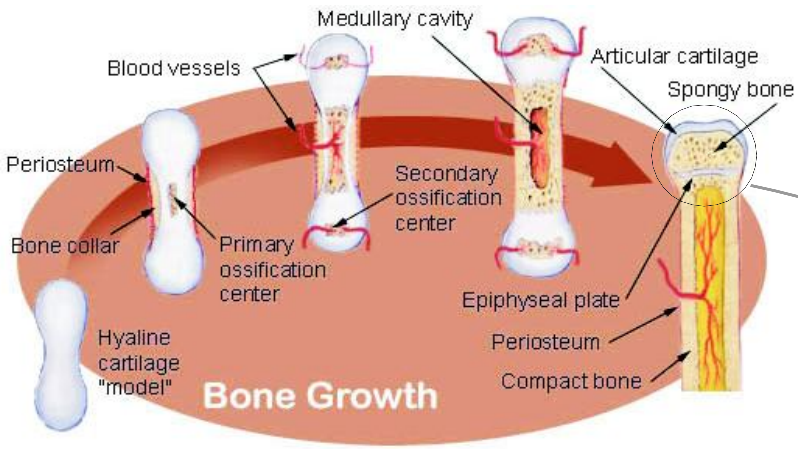
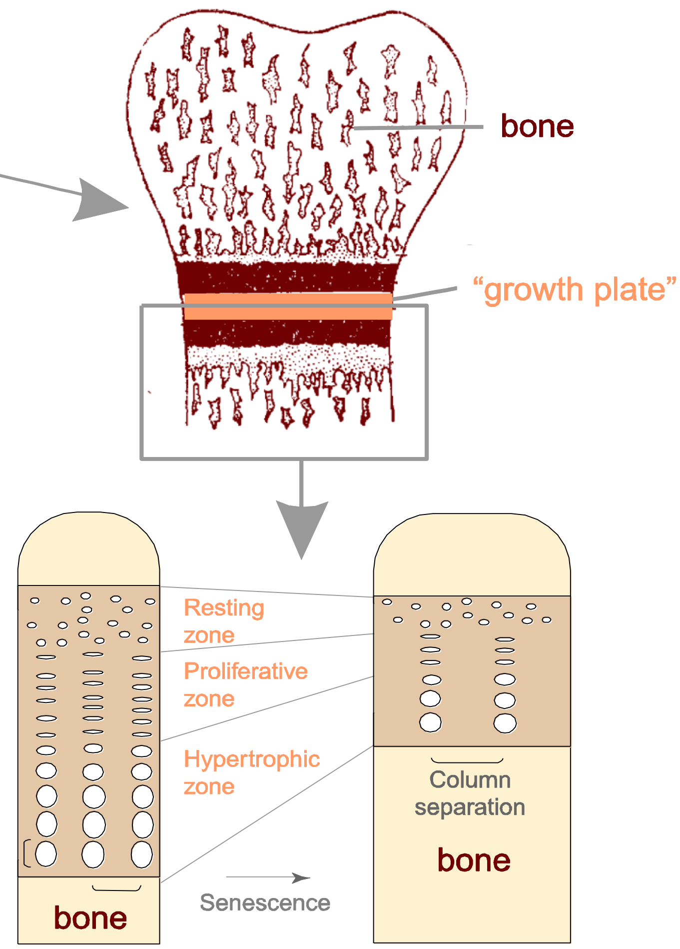
Endochondral ossification in long bones



Growth and ossification in “growth plate”



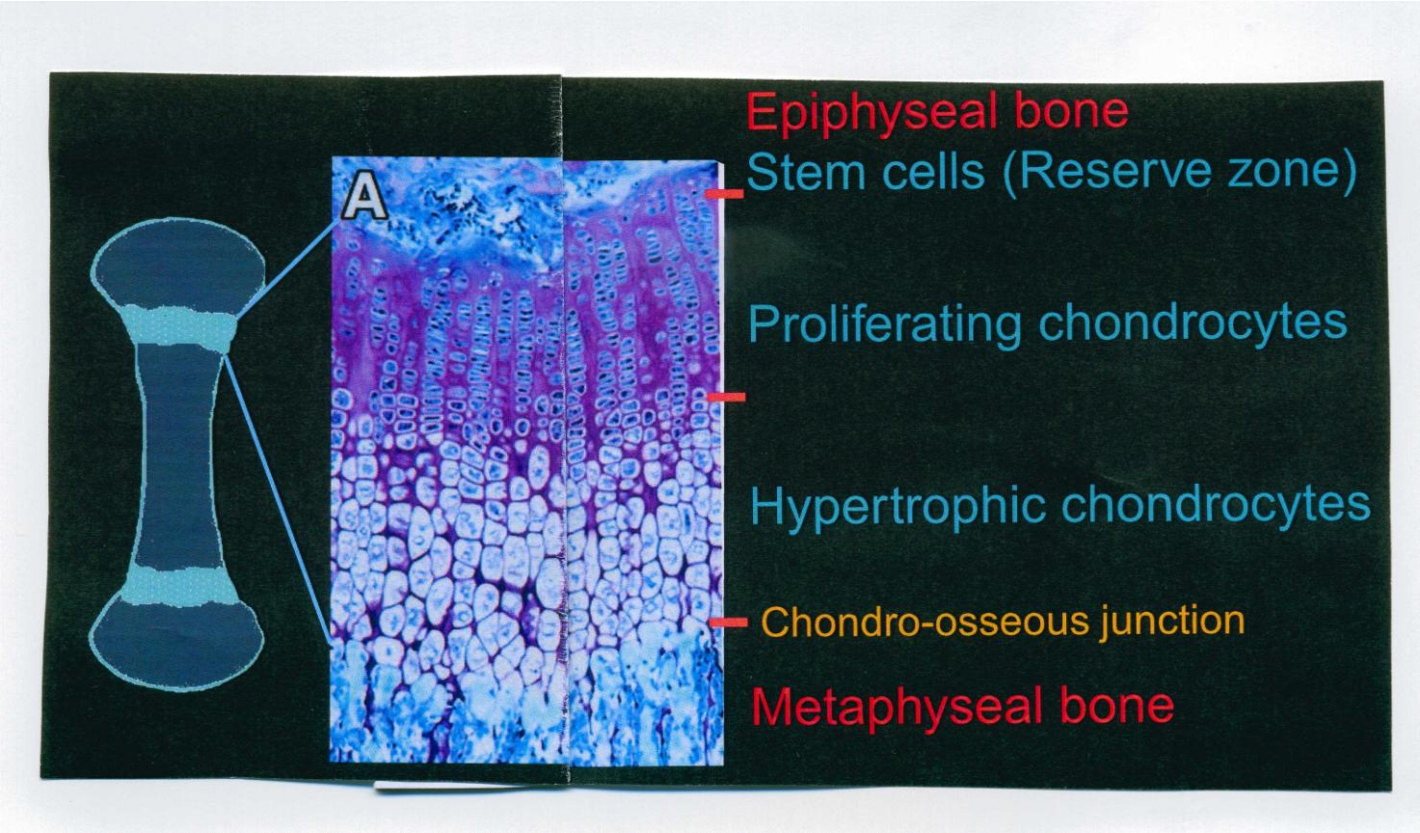


The modelling aims at explaining the various phases of the evolution until the end of growth (in the early twenties of most adult humans) in nonpathological situations as also with the possibility of some pathological development (instabilities, untimely arrest of growth).

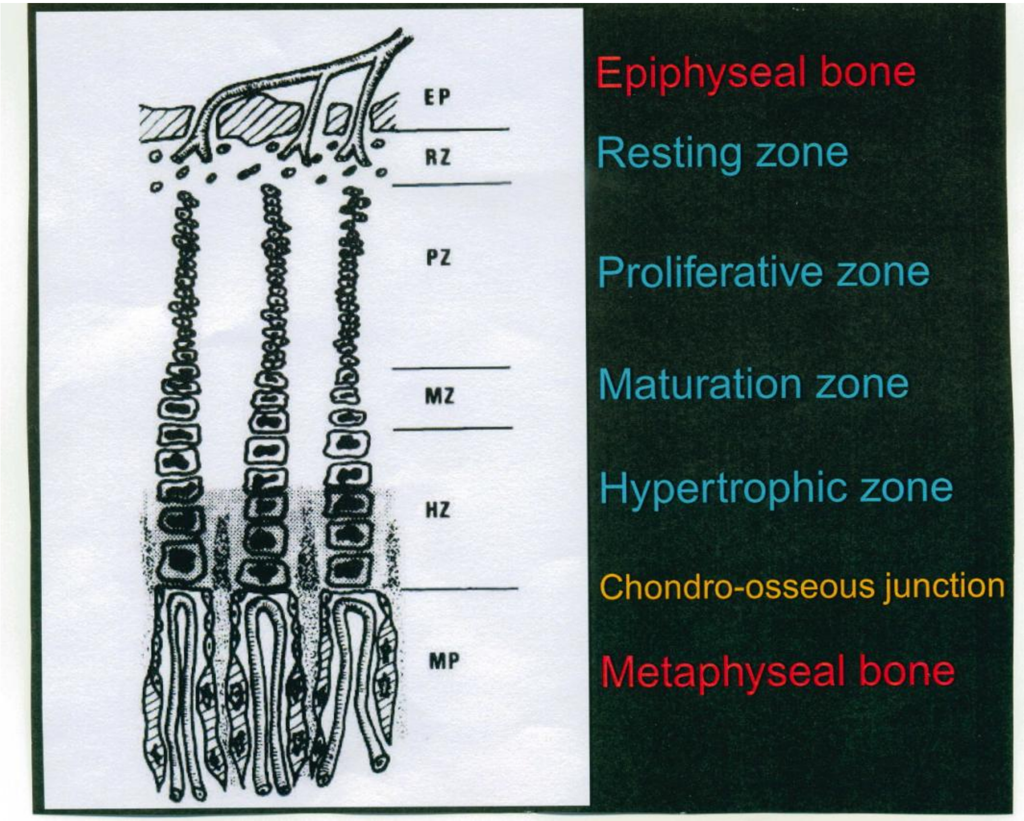
This problem represents, at the various degrees of description, a true benchmark for the evolution of such transition regions with resemblance and difference with what occurs in inanimate matter (crystals, alloys; see above).

Some pictures and data concerning the growth of long bones

(Figures)

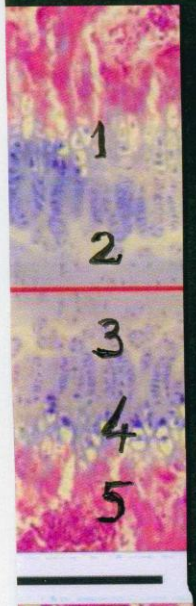


Structure of the growth plate



Structure of the growth plate (2)

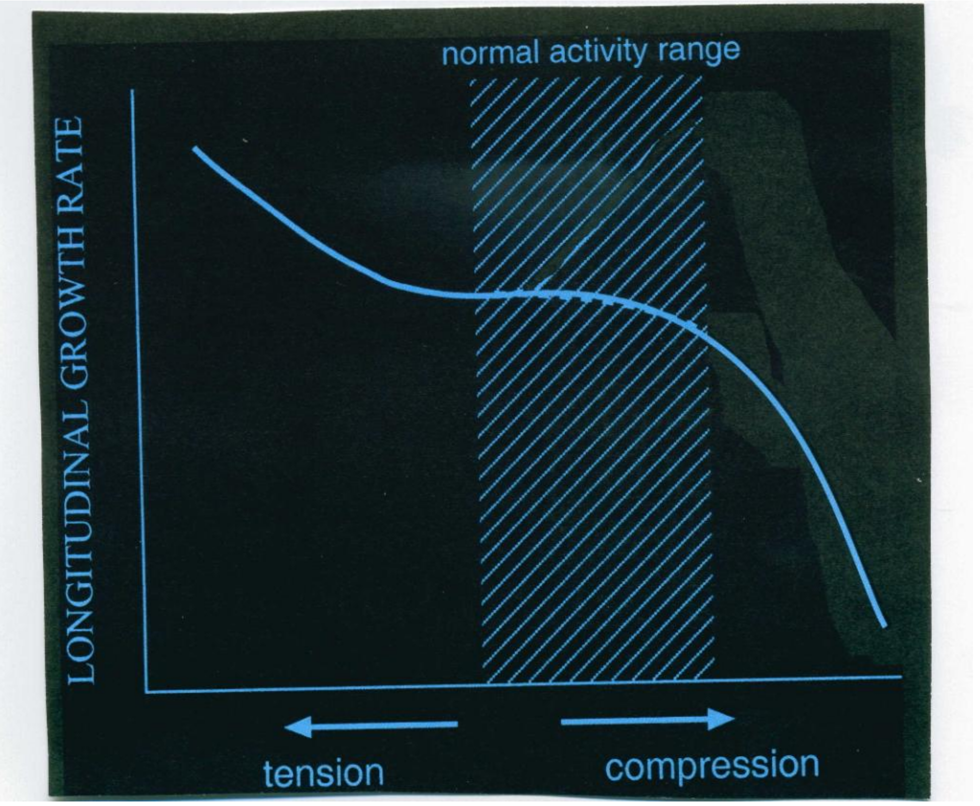
(Source: G.J.Breur *et al*, J.Orthopedic Res., 9, 348-359, 1991)



Rabbit	Zone 1	Zone 2	Zone 3	Zone 4	Zone 5
1	0.60	0.70	1.00	1.22	1.64
2	0.61	0.71	0.83	0.86	1.13
3	0.54	0.75	0.81	1.27	1.30
4	0.50	0.72	1.02	1.16	1.32
5	0.62	0.70	0.88	1.05	1.41
6	0.62	0.69	0.94	1.13	1.64
7	0.49	0.72	0.78	1.21	1.62
8	0.54	0.66	0.82	1.30	1.45
Mean	0.57	0.71	0.88	1.15	1.44
S.D.	0.05	0.03	0.09	0.14	0.19

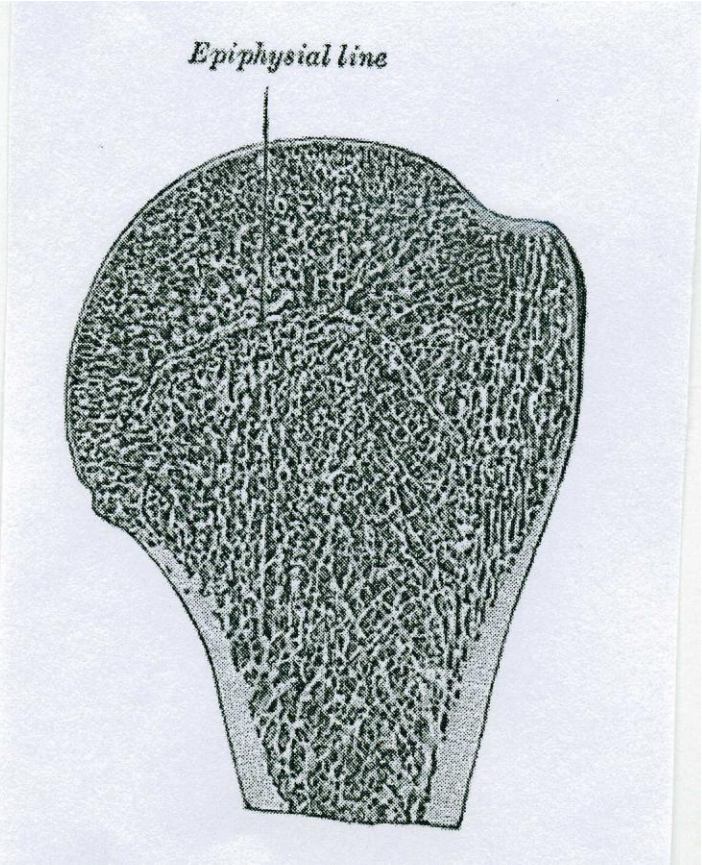
Gradient elasticity of the growth plate

(Source: P.Radhakrishnan *et al*, Annals of Biomed.Engng., 32/2, 284-291, 2004)

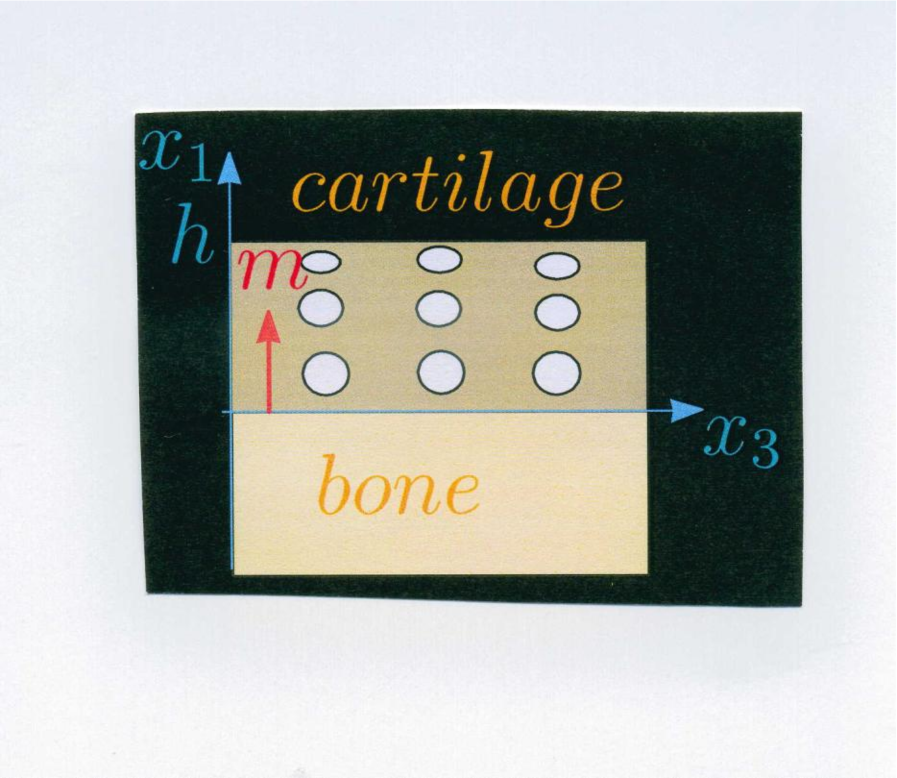


Influence of a mechanical loading

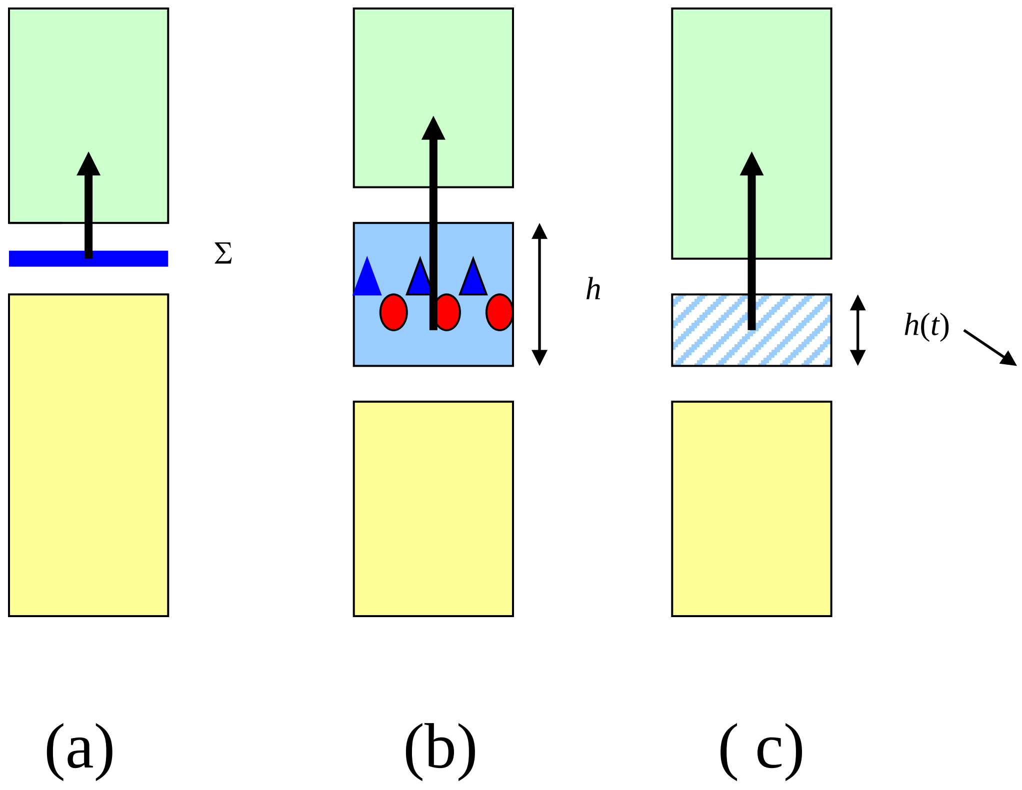
(afterH.M.Frost, Anat.Rec., 226, 423-432, 1990)



Practically closed plate



Structured transition zone



Three stages of modelling the evolution of the growth plate

(a) The first relatively simple model sees the growth plate as a practically zero-thickness transition zone moving steadily although slowly (here the time scale is in years) under the action of **a driving force** related to the mechanical environment (mechanical loading of the long bone). This exploits arguments from the theory of Eshelbian-(configurational) material forces as fruitfully developed in recent years by the author and co-workers.

An interesting question to be answered here is the **stability** of this evolution (i.e., the absence of pathological development; work in co-operation with A.B. Freidin's team in St Petersburg))

(b) The second modelling should see the growth plate as a transition zone with relatively smoothly varying properties through the small albeit finite thickness. The modelling inside this transition zone may rely on the **gradient theory of elasticity** or a refined microstructured theory such as that of so-called **Cosserat continua**.

(c) The third and final modelling views the growth plate as an evolving dissipative structure with thickness variation in time until final closing of the plate (end of growth). The last two modellings will bring into the picture the evolution of "**nonlinear (dissipative structures**" of varying complexity.

Closure of the growth plate

Ultimate behavior : possible fracture at the weak remnant growth (line)

That is all.

Thank you for your attention.

GAMM