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Equilibrium and stability of mechanical structures: From fracture to multistable shells

par

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Foreword

The aim of this manuscript is to collect and synthetically present the results of the research activities that I developed after my Ph.D. degree. My Ph.D. thesis concerned the modeling of composite piezoelectric beams including electric circuits for vibration control applications. It was developed in the framework of a joint program between the La Sapienza and the University Pierre and Marie Curie, under the supervision of Francesco dell'Isola and Joël Pouget. The thesis, defended in 2005, followed my graduate studies in Mechanical Engineering at La Sapienza and Virginia Tech. During that period I had the opportunity to work with a group of talented young italian colleagues who were for me a great source of inspiration and motivation in the study of continuum mechanics and applied mathematics among them, in alphabetic order, Maurizio Porfiri (now Associate Professor at NYU), Giulio Sciarra (now Assistant Professor at La Sapienza), and Stefano Vidoli (now Associate Professor at La Sapienza). I joined the d'Alembert Institute at UPMC in 2005, first as Attaché Temporaire d'Enseignement et de Recherche (two-year contract with teaching and research duties) and then as *Maître de Conférences* (permanent position, from 2007). In this period, with Stefano Vidoli, I began to study geometrical nonlinear beams and shells for shape control applications. This was a natural extension of my previous works on beam modeling in the nonlinear realm, influenced also by the presence of other researchers at d'Alembert working on similar subjects: Basile Audoly, Amancio Fernandes, Joël Frelat, Sebastien Neukirch, and Angela Vincenti. At d'Alembert I had the opportunity to meet Jean-Jacques Marigo (now at Ecole Polytechnique), who introduced me to the world of damage and fracture mechanics. The further collaboration with Blaise Bourdin (Lousiana State University) on the associated numerical aspects had a fundamental influence on the evolution of my research.

My works can be broadly classified into two subjects: (i) damage and fracture mechanics, and (ii) shape-change and multi-stability of nonlinear rods, plates and shells. Accordingly, this manuscript is organized into two main chapters. Both of them begin with an overview of the subject and a general presentation of the adopted modeling framework. Then, I synthetically report my research works in the field, with minimal technical details. Each chapter includes a separate preamble, a list of my publications on the topics, and some external references (that are not pretended to be exhaustive). Concluding remarks and perspectives are drawn in a dedicated chapter at the end of the manuscript. Citations follow the alphabetic style. For convenience, my publications are distinguished from external references by specific prefixes: [J-] for journal papers and [C-] for conference proceedings. A full list of my publications is included at the end of this manuscript. An extended CV is attached as a separated document.

For the sake of conciseness and to preserve the continuity of the narrative, I choose to not report here the outcomes of few published works, including [J-MPV07] on the multi-parameter actuation of bistable beams, [J-Neu+12] on the vibration of buckled rods, and [J-Ann+12] on the modeling and identification of the anisotropic behavior of the skin. For the latter two publications this is partially justified by my relatively limited personal contribution to the research. The first work has been important in my personal evolution, but the main concepts and results, reported there for beams, are equally well represented in the works dealing with shells resumed in Chapter 2.

Chapter 1

Crack nucleation and complex fracture patterns

Preamble

I started working on damage and fracture mechanics after my Ph.D. thesis, when I met Jean-Jacques Marigo at d'Alembert. At that time, my knowledge on fracture mechanics was minimal and I naively regarded it as a tedious and obscure exercise on the calculation of stress intensity factors. However, I was profoundly interested by the variational vision of the problem proposed by Francfort and Marigo [FM98] and its deep links with applied mathematics, joining my primal interests in rational mechanics, as a student and researcher. I started by co-supervising with Jean-Jacques Marigo the Ph.D. thesis of Hanen Amor (2005-08) and Kim Pham (2007-2010). These works were essentially aimed at the study and the improvement of the gradient damage models that arise as variational regularizations of the brittle fracture model proposed by Bourdin et al. [BFM00]. Hence, I studied the application of the variational modeling framework to explain and predict complex fracture phenomena, including the morphogenesis and the propagation of complex crack patterns. Damage models are usually derived by the homogenization of elementary volume element with micro-cracks. These theories always puzzled me because they assume the pre-existence of structured crack patterns without justifying their presence. One of my aims was to reverse this viewpoint: instead of postulating the presence of micro-cracks with specific distributions and a brittle fracture model to describe their evolution, is it possible to use purely phenomenological damage models to explain the formation of structured crack patterns? In which situations do similar crack patterns arise? How do they evolve? In the attempt to answer these fundamental questions, I promoted several projects focused on carefully selected specific situations in which complex crack patterns are a known phenomenon and its prediction is important for applications: the thermal shock of brittle materials and thin film systems. In this context, I obtained some fundings (PICS CNRS 2008-2010, Emergence UPMC 2009-2013, ANR T-shock 2010-2013, Ph.D. thesis of A.A. León Baldelli) and I had the possibility of establishing enriching collaborations. In particular, I worked with Blaise Bourdin on a long-term common research plan on the numerical aspects of variational damage and fracture mechanics, including the joint supervision of students and the co-development of the numerical codes.

This Chapter is structured as follows. In a first part (Section 1.1), I give a general introduction to the variational models of brittle fracture, including the variational formulation of the Griffith model proposed in [FM98; BFM00] and the gradient damage models studied in [Pha10; PM10b; J-PMM11]. The presentation of this part is quite technical, in the sense that it does not avoid the use of equations. Its aim is to provide a minimal self-consistent reference for the rest of Chapter to the reader not familiar with the related concepts. It also include several comments that illustrate my personal viewpoint on some delicate issues. Then, I present the specific outcomes of my works avoiding the technical details, for which the reader can refer to the related publications. Section 1.2 deals with the analysis of the evolution problem for gradient damage models with stress-softening, resuming the results presented in [J-Pha+11] and [J-PMM11]. This theoretical part is essential to understand how damage models may be used in numerical applications to approximate brittle fracture. In this sense it completes the introductory section. Few comments on the numerical implementation are reported in Section 1.3. Section 1.4 reports on an attempt to improve the models to include unilateral contact effects at the crack lips [J-AMM09]. Hence I illustrate the results of my work on the morphogenesis and propagation of complex crack patterns in three different applications: thermal shock problems (Section 1.5, [J-Leo+14; J-Bou+14]), thin films (Section 1.6, [J-Leo+13; J-Leo+14]), and drying of capillary suspensions (Section 1.7, [J-Mau+13]).

All the works presented here been done in the framework of several collaborations. Besides B. Bourdin and J.-J. Marigo, they include applied mathematicians (J.-F. Babadjian and D. Henao), experimentalists (G. Gauthier and V. Lazarus), and Ph.D. students (H. Amor, A.A. León Baldelli, K. Pham, and P. Sicsic).

1.1 Variational approach to fracture and damage

1.1.1 Modeling failure of brittle solids: Griffith, damage, and phase-field models

Theoretical and computational approaches to model the fracture of solids at the macroscopic scale can be broadly classified in two categories [see e.g. dBor+04]: (i) discrete, or sharp, crack models with an explicit geometric modeling of cracks as surfaces of discontinuities and (ii) smeared crack models, approximating cracks with continuum fields having high gradients localized in thin bands. Sharp crack approaches include the Griffith model [Gri21] and more advanced cohesive zones models [XN94; CO96; OP99; MB02; MD07; RdBN08]. Their numerical implementation requires specific techniques to introduce discontinuous fields in the numerical model. The classical method consists in changing the mesh geometry by introducing new boundaries as the crack propagates together with adaptive remeshing [IS84]. Efficient alternatives are the extended finite element methods [MDB99], which enrich the finite element shape functions with discontinuous fields on the basis of a partition of unity concept [BM97], and inter-element crack methods [XN94; CO96], which constrain cracks to propagate along the element interfaces. Smeared crack (or continuum) approaches, include damage models [see e.g. Jir98; PB87; LA99; Com01] and diffuse interface (or phase-field) models [AKV00; HK09; MJ05]. In the comparative study of Song et al. [SWB08], these approaches are synthetically classified as *element deletion methods*. They are based on the use of phenomenological constitutive laws with strain-softening. It is well-known that they require to account for some kind of non-local effects and the introduction of an internal length to penalise extreme strain localization. The key advantage of smeared approaches over discrete ones is the ability to recover crack nucleation from sound materials and to elude the issues related to the computational modeling of strong discontinuities and crack sets with complex topologies. Although several works attempt to establish an equivalence between the sharp and the smeared approaches [MP96; Oli+02; MP03; dBor+04; Caz+09], the link between damage and fracture remains vague in most of the literature.

In this panorama, the variational approach to fracture proposed by Francfort and Marigo [FM98] has the merit to open the path for a deep-rooted mathematical theory. By reformulating fracture mechanics as an energy minimization problem, it associates a clear and general mathematical formulation with a consistent numerical solution strategy [BFM00] able to account for complex fracture phenomena in space (multi-cracking, crack branching and coalescence) and time (nucleation, brutal propagation). The use of the direct methods of the calculus of variations and the advanced theory of *free-discontinuity* problems allows for the establishment of precise results on the existence and regularity of the solutions. It suggests also efficient regularized models [MS89; AT92] ready for the numerical implementation [BFM00]. Remarkably, the regularization of the Griffith model introduced by [BFM00] may be regarded as a gradient damage model with internal length [FN96; LSB01; LB05; FBM08]. Gamma-Convergence results [Bra98; Cha04; Gia05] prove that when the internal length tends to zero, gradient damage models with specific constitutive properties converge towards a model of brittle fracture of the Griffith type. In this sense, the mathematical theory of free-discontinuity problems and Gamma-Convergence theorems give a precise sense to the intuitive idea of using smeared crack approaches to approximate brittle fracture [Bra98; LN07]. The energetic equivalence with the Griffith model, absent in other smeared approaches, is a fundamental property for the identification, verification, and validation of the regularized models used for the numerical simulation of the fracture phenomena. Nowadays, the community of computational mechanics [MWH10; Bor+12; VdB13] regards this approach as the most promising tool to solve complex crack nucleation and propagation problems, using the suggestive appellation of phase-field models.

In the following I will briefly introduce the variational approach to fracture and damage. Then, I will resume my personal work on the subject. Even if extension to dynamics are possible and already initiated by several authors [BLR11; Bor+12; HM13], I will focus here and henceforth only on quasi-static rate-independent evolution problems, according to the scope of my works.

1.1.2 Griffith model and its variational formulation

Pre-assigned path

Cracks in a body are surfaces where the displacements may jump. The celebrated Griffith model gives an energetic view of the fracture phenomena [Gri21]. As a main assumption it supposes that energy required to create a crack is directly proportional to its surface, through a constant, G_c , called fracture toughness. Hence, it states that a crack can propagate in an elastic solid only if the associated release of elastic energy can pay off the surface energy required for its creation. To fix the ideas, we will consider here and henceforth a body Ω , with imposed displacements U_t on $\partial_u \Omega$. Except if explicitly stated, we will assume that the rest of the boundary is free and that volume forces are absent.

If one supposes the crack path to be known in advance, the time-evolution of a single crack may be tracked by its length l, *i.e.* the curvilinear abscissa locating the crack tip. For smooth (in space and in time) evolutions, the law for crack propagation can be written as follows:

$$\dot{l}(t) \ge 0, \qquad P'_t(l(t)) + G_c \ge 0, \quad (P'_t(l(t)) + G_c)\dot{l}(t) = 0.$$
 (1.1)

where *t* is the loading parameter (or time) and $P_t(l)$ the potential energy of the structure for a given crack length. The prime denotes a derivative of a function with respect to its argument, the dot the derivative with respect to the time *t*. In (1.1), the first condition imposes the *irreversibility* of the crack set, in order to rule out self-healing. The second condition states that the energy release rate G(l) := -P'(l) cannot exceed the threshold G_c . It can be interpreted as the first order optimality condition for the minimality of the total energy $E_t(l) = P_t(l) + G_c l$. As such, in the framework of an energetic approach, this second condition may be regarded as a necessary condition for the stability of the state l(t) at the load loading *t*. The third conditions in (1.1) says that the crack may propagate only if the energy release rate *G* equals the critical value G_c . Also this condition, usually known as *consistency condition*, has an energetic interpretation. It is equivalent to an energy balance for regular-in-time evolutions, stating that the time variation of the total energy *E* must be balanced by the work of the external loads. In summary, the evolution law (1.1) may be restated in terms of three requirements: (ir) irreversibility, (st) stability, and (eb) energy balance. These three items are at the basis of the variational formulation of the quasi-static evolution problem of rate independent systems [Mie05].

The numerical solution of the problem usually implies the time-discretization in N steps $\{t_i\}_{i=1}^N$. In this setting, the crack length $l_i = l(t_i)$ at time t_i can be found by solving the following time-discrete version of (1.1):

$$l_i - l_{i-1} \ge 0, \qquad P'_{t_i}(l_i) + G_c \ge 0, \quad (P'_{t_i}(l_i) + G_c)(l_i - l_{i-1}) = 0.$$
 (1.2)

Interesting enough, (1.2) are the first-order necessary optimality conditions of the following boundconstrained minimization problem:

$$l_i = \underset{l \ge l_{i-1}}{\operatorname{argmin}} P(l). \tag{1.3}$$

Equation (1.3) gives the *time-discrete variational formulation* of the quasi-static evolution problem.

The formulations above can be generalized to the case of elastic bodies with several crack tips with known crack paths, and used to state bifurcation and stability conditions of a system of interacting cracks [see Ngu87; SV98]. Many of the numerical and theoretical works on fracture mechanics in the last decades focused on the calculation of the energy release rate G(l) = -P'(l), either analytically, for several geometric configurations and load cases, or numerically, by appropriate discretization methods and post-processing utilities. This effort produced fundamental results and constitutes now the basic knowledge at the disposal of structural engineers. However, I believe that nowadays the most fundamental theoretical problems for the advance of the field are of different nature. For example: How to track crack propagation along complex unknown paths, including crack branching and merging? How to deal with discontinuous in time (brutal) propagations? How to explain crack nucleation? The variational formulation proposed by Francfort and Marigo [FM98] furnishes a sound theoretical framework to generalize the classical models and tackle some of these challenging problems.

Arbitrary path: Griffith revisited by Francfort and Marigo

Francfort and Marigo [FM98] generalized the Griffith model considering an arbitrary crack set $\Gamma \subset \Omega$ and possibly non-smooth evolutions. They considered for simplicity linearised elasticity with isotropic and homogeneous fracture energy of the Griffith type. In this framework, denoting by *u* the vector-valued displacement field, $\varepsilon(u) = (\nabla u + \nabla u^T)/2$ the linearised strain tensor, and by A_0 the fourth order elastic stiffness tensor, the potential energy of the cracked body $\Omega \subset \mathbb{R}^n$ reads as

$$E(u,\Gamma) = \frac{1}{2} \int_{\Omega \setminus \Gamma} A_0 \varepsilon(u) \cdot \varepsilon(u) \, dx + G_c \, \mathcal{H}^{n-1}(\Gamma) \tag{1.4}$$

where $\mathcal{H}^{n-1}(\Gamma)$ denotes the Hausdorff measure of the crack set, corresponding to the number of cracks for n = 1, to the crack length for n = 2, or to the crack surface for n = 3.

Consider an initial state (u_0, Γ_t) and the loading given by an imposed displacement U_t on a part of the boundary $\partial_u \Omega$. A *quasi-static rate-independent evolution* is a one-parameter family of displacement fields and crack set (u_t, Γ_t) indexed by the time t that verifies the following requirements at each time t > 0:

- (ir) *Irreversibility*: $\forall \tau \in [0,t)$: $\Gamma_{\tau} \subseteq \Gamma_{t}$
- (gst) Unilateral global stability:

$$E(u_t, \Gamma_t) \le E(\hat{u}, \hat{\Gamma}), \quad \forall (\hat{u}, \hat{\Gamma}) \text{ such that } \hat{\Gamma} \supseteq \Gamma_t, \quad \hat{u} \in \mathcal{C}_t(\hat{\Gamma}), \quad (1.5)$$

where $C_t(\Gamma) \equiv \{u \in H^1(\Omega \setminus \Gamma), u = \overline{U}_t \text{ on } \partial_u \Omega\}, H^1$ denoting the standard Sobolev space.

(eb) Energy balance:

$$E(u_t, \Gamma_t) = E(u_0, \Gamma_0) + \int_0^t \left(\int_{\partial \Omega \setminus \Gamma(\tau)} (\sigma_\tau \mathbf{v}) \cdot \dot{U}_\tau \, d\mathcal{H}^{n-1} \right) d\tau \tag{1.6}$$

where $\sigma_{\tau} = A_0 \varepsilon(u_{\tau})$ is the stress tensor and v the outer normal to $\partial \Omega$.

In this formulation, the crack path is treated as a genuine unknown. It determines the zones where the displacements field may jump.

The *time-discrete variational formulation* of the evolution reduces to the solution of the following unilateral minimization problem at each time step:

$$(u_i, \Gamma_i) = \underset{u \in \mathcal{C}_t(\Gamma_i), \Gamma \supseteq \Gamma_{i-1}}{\operatorname{argmin}} E(u, \Gamma),$$
(1.7)

where the crack set should verify the irreversibility with respect to the crack set Γ_{i-1} at the previous time-step. The time-discrete version of the evolution problem is the starting point for most of the mathematical studies on the evolution problem. Francfort and Larsen [FL03] prove its convergence toward the time-continuous version, as the time step tends to zero.

The arbitrariness of the crack set, where the displacement field may jump, renders the problem extremely complex from the theoretical and numerical standpoints. This is called a *free discontinuity problem*, for which a wealth of mathematical literature is now available [AFP00]. An efficient method for its numerical solution, initially introduced in analogue problems of image segmentation [MS89; AT92], is the use of regularized formulations where the sharp discontinuities are smeared across bands of non-vanishing width [Bra98]. Especially, Bourdin et al. [BFM00] applied the Ambrosio-Tortorelli regularized formulation to the fracture mechanics problem. This approach introduces a smooth scalar field α and the regularized energy functional

$$\mathcal{E}(u,\alpha) = \int_{\Omega} \frac{1}{2} ((1-\alpha)^2 + k_\ell) A_0 \varepsilon(u) \cdot \varepsilon(u) dx + G_c \int_{\Omega} \left(\frac{\alpha^2}{4\ell} + \ell \nabla \alpha \cdot \nabla \alpha \right) dx, \qquad (1.8)$$

where $k_{\ell} = o(\ell)$, and ℓ is a scalar regularizing parameter. Studies based on the direct methods of the calculus of variations and asymptotic analysis show that, for $\ell \to 0$, *global* minimizers of the regularised energy (1.8) tend toward *global* minimizers of the Griffith energy (1.4). In particular, Giacomini [Gia05] shows that the solutions of the quasi-static evolution problem (1.7) may be approximated by solving at each time step the following minimization problem:

$$(u_i, \Gamma_i) = \operatorname*{argmin}_{u \in \mathcal{C}_t, \alpha \in \mathcal{D}(\alpha_{i-1})} \mathcal{E}(u, \alpha)$$
(1.9)

where

$$\mathcal{C}_t \equiv \{ u \in H^1(\Omega), \, u = U_t \text{ on } \partial_u \Omega \}, \quad \mathcal{D}(\beta) \equiv \{ \alpha \in H^1(\Omega), \alpha \ge \beta, \, \alpha = 0 \text{ on } \partial_\alpha \Omega \},$$

imposing the damage field to be null where Dirichlet boundary conditions on the displacement are imposed (*i.e.* $\partial_{\alpha}\Omega \equiv \partial_{u}\Omega$). The crack irreversibility requires a *unilateral minimization* on the damage field.

Comments

The variational approach applied to the Griffith theory of fracture provides a first self-consistent mathematical model for describing crack evolutions without *a priori* hypotheses on the crack path. This was a major contribution that paved the path for the development of a large research stream at the boundary between theoretical mechanics and applied mathematics on the mathematical analysis of the fracture mechanics problem. However, as underlined by Francfort and Marigo [FM98] in their original paper and largely discussed in [FBM08], the Griffith model and the quasi-static setting may fail to reproduce the evolution of real physical systems for the following two main reasons:

• The requirement of *global minimality* is fundamental to retrieve crack initiation within the Griffith model and it is also necessary for the mathematical analysis based on the direct methods of the calculus of variations. However, global minimization is physically debatable as a stability criterion. This is one of the key motivations to enrich the Griffith model either by more complex surface energies (cohesive models) or by considering regularised approaches including bulk dissipation and additional material parameters (damage models).

• The energy balance is here written in an integral form (in time), so as to allow for evolutions with *jumps in time* in the framework of the theory of rate-independent processes [Mie05]. However, also in this respect, the model is questionable on the physical basis, because the pertinence of a rate-independent quasi-static model for time-discontinuous evolutions is far to be clear.

Keeping these *caveats* in mind, the model should not be rejected or considered useless. Indeed, it provides a first framework to mathematically describe the evolution of cracks in a solid without hypotheses on the crack path and the time history, most probably the simplest¹ that one can formulate. Although being a relatively rough model on the physical basis, its main merit is to be mathematically self-consistent and to constitute a solid departure point for a deep mathematical analysis.

1.1.3 Gradient damage models

Related publications [J-PMM11]

The energy functional (1.9) may be interpreted as the total energy of a gradient damage model [FN96; LA99; BM07; PM10a; PM10b], where α is regarded as a scalar *damage field* and the "small" parameter ℓ as a material parameter, the *internal length*. In the framework of the Ph.D. theses of Hanen Amor [Amo08] and Kim Pham [Pha10], we studied with Jean-Jacques Marigo the properties of a general family of gradient damage models characterized by a strain energy density in the form

$$W(\varepsilon, \alpha, \nabla \alpha) = \frac{1}{2}a(\alpha)A_0\varepsilon \cdot \varepsilon + w_1\left(w(\alpha) + \frac{\ell^2}{2}\nabla\alpha \cdot \nabla\alpha\right), \qquad (1.10)$$

where the first term stands for the elastic energy density, whilst the second represents an energy dissipation, including a local term, $w(\alpha)$, and a gradient contribution. The function $a(\alpha)$ models the isotropic modulation of the elastic stiffness through the damage field. It is natural to suppose that *a* is a monotonically decreasing function of α (the damage reduces the stiffness) and that *w* is monotonically increasing with α (positive dissipation). The thermodynamics of these models can be justified in the framework of the formalism of *generalized standard materials* [HN75].Considering a structure Ω loaded by the applied displacement U_t on $\partial_u \Omega$, the total energy reads as

$$\mathcal{E}_t(u,\alpha) = \int_{\Omega} W(\varepsilon(u),\alpha,\nabla\alpha) \,\mathrm{d}x. \tag{1.11}$$

Hence, following the variational rate-independent formulation proposed in [PM10b; J-PMM11], we define the admissible quasi-static evolutions of the damage model as the one-parameter pairs of displacement and damage fields (u_t , α_t) that respect the following conditions:

- (ir) *Irreversibility*: α_t is a non-decreasing function of time,
- (uls) Unilateral local stability:

$$\forall (v, \beta) \in \mathcal{C}_t \times \mathcal{D}(\alpha_t), \quad \exists \bar{h} \ge 0: \quad \forall h \le \bar{h}$$
(1.12a)

$$\mathcal{E}_t(u_t + h(v - u_t), \alpha_t + h(\beta - \alpha_t)) \ge \mathcal{E}_t(u_t, \alpha_t),$$
(1.12b)

¹Using appropriate non-dimensional variables, one can show that the energy functional (1.4) of the Griffith model is characterised by a single non-dimensional parameter: the Poisson ratio. In particular it does not contain any intrinsic length-scale.

(eb) Energy balance:

$$\mathcal{E}_t(u_t, \alpha_t) - \mathcal{E}_0(u_0, \alpha_0) = \int_0^t \left(\int_{\partial \Omega} (\sigma_\tau \mathbf{v}) \cdot \dot{U}_\tau \, \mathrm{d}s \right) \, \mathrm{d}\tau \tag{1.12c}$$

where $\sigma_t = \frac{\partial W}{\partial \varepsilon} = a(\alpha_t)A_0\varepsilon(u_t)$ is the stress tensor.

For regular (in space and time) evolutions, the irreversibility reads as $\dot{\alpha}_t(x) \ge 0$. Moreover, the stability and energy balance are equivalent to the following local conditions, where *n* denotes the external normal to $\partial \Omega$:

(eq) The equilibrium equations

div $\sigma_t = 0$ in Ω , $\sigma_t n = 0$ on $\partial \Omega \setminus \partial_u \Omega$, (1.13a)

(dc) The damage criterion defined by the Kuhn-Tucker conditions

$$\dot{\alpha}_t \ge 0, \quad g(\varepsilon(u_t), \alpha_t, \nabla^2 \alpha_t) \ge 0, \quad g(\varepsilon(u_t), \alpha, \nabla^2 \alpha_t) \dot{\alpha}_t = 0, \quad \text{in} \quad \Omega,$$
 (1.13b)

$$\dot{\alpha}_t \ge 0, \ \frac{\partial \alpha_t}{\partial n} \ge 0, \ \frac{\partial \alpha_t}{\partial n} \dot{\alpha}_t = 0, \quad \text{on} \quad \partial \Omega \setminus \partial_\alpha \Omega, \qquad (1.13c)$$

where
$$g(\varepsilon, \alpha, \nabla^2 \alpha) = \frac{a'(\alpha)}{2} A_0 \varepsilon \cdot \varepsilon + (w'(\alpha) - \ell^2 \nabla^2 \alpha) w_1$$

A fundamental question is to understand how the properties of the constitutive functions a and w affect the solutions of an evolution problem. A first step in this direction is to analyze the solutions with *homogenous damage*, which is tantamount to the analysis of the response of a material point. Following [J-PMM11], a first important distinction is between materials showing a finite or infinite dissipation at complete failure, denoted as *strongly brittle* or *weakly brittle* materials, respectively. In *strongly brittle* materials, one can renormalize the damage variable in the interval [0,1] and assume that a(0) = 1, a(1) = 1, w(0) = 0, w(1) = 1. In this case, the constant w_1 in (1.10) can be interpreted as the energy required to fully damage a volume element, commonly denoted as *specific fracture energy* [CP01]. Moreover, for homogeneous solutions, the damage criterion and the stress-strain relationship imply that the domains of admissible strains and stresses are given by:

$$\mathcal{A}_{\varepsilon}(\alpha) = \left\{ \varepsilon : \quad A_0 \varepsilon \cdot \varepsilon \leq -\frac{2w_1 w'(\alpha)}{a'(\alpha)} \right\}, \qquad \mathcal{A}_{\sigma}(\alpha) = \left\{ \sigma : \quad A_0^{-1} \sigma \cdot \sigma \leq \frac{2w_1 w'(\alpha)}{s'(\alpha)} \right\},$$

where $s := a^{-1}$ is the modulation of the elastic compliance. The material is said to be with

- strain hardening (resp. softening) if A_{ε} is increasing (resp. decreasing) with α , *i.e.* if $w'(\alpha)/a'(\alpha)$ is increasing (resp. decreasing),
- stress hardening (resp. softening) if A_{σ} is increasing (resp. decreasing) with α , *i.e.* if $-w'(\alpha)/s'(\alpha)$ is increasing (resp. decreasing).

In can be also show that these properties are equivalent to convexity conditions of the energy density and its Legendre transform [see PM10a]. In [J-PMM11] and [J-Pha+11], we show that to recover an energetic equivalence with Griffith brittle fracture, it is essential to use a *strongly brittle* material with *stress-softening* (see also the following Section). The first requirement is necessary to obtain damage localizations with a well-defined fracture energy, assimilable to a fracture toughness. Stress-softening is at the origin of all the interesting phenomena (and difficulties): multiple solutions, bifurcations, loss of stability. For strain-hardening materials the energy (1.11) is strictly convex and the solution of the evolution problem is unique.

The energy functional (1.11) includes as a special case the Ambrosio-Tortorellli functional (1.8) used in [BFM00] to approximate the evolutions of the Griffith model (1.4). However here the *global* minimality requirement is replaced here by a *local* one. A *meta-stable* state, obtained as unilateral local minimum of the energy is accepted as stable state during an evolution. This implies that, even if global minimizers of the energy of damage models converge towards global minimizers of the Griffith energy functional (1.4), the evolutions obtained by the damage model (local minimization) and the Griffith model (global minimization) presented above may be very different. As effectively resumed by [LR09], while the original formulation of [BFM00] assumes that brittle fracture is *the model* and uses the Ambrosio-Tortorelli regularisation (1.8) as *the approximation*, in the damage model formulation one reverses the viewpoint: the gradient damage model is *the model* and brittle fracture à *la* Griffith is *the approximation*.

1.2 Traction of a stress-softening bar: one-dimensional analysis

Related publications [J-Pha+11; J-PMM11].

The study of the apparently trivial case of the traction of a one-dimensional bar discloses most of the properties of the damage models, including their ability to recover crack nucleation and their link with brittle fracture à *la* Griffith. In [J-Pha+11; J-PMM11], we report analytical results about the solution of the evolution problem for a bar under imposed end-displacements. We considered the competition of the two fundamentally different damaging modes: (i) solutions with damage *homogenous* in space, and (ii) solutions with *localized* damage. In both cases, the mechanical equilibrium imposes the stress to be constant throughout the bar. The key results are briefly resumed below.

Gradient damage model for a one-dimensional bar model. For a bar of length L with imposed end-displacements u(0) = 0 and $u(L) = U_t$, the energy (1.11) reads as

$$\mathcal{E}(u,\alpha) = \int_0^L a(\alpha) E_0 \frac{u'(x)^2}{2} + w_1 \left(w(\alpha) + \frac{\ell^2}{2} \alpha'(x)^2 \right) dx, \tag{1.14}$$

where E_0 is the undamaged Young modulus of the material. The stress is given by $\sigma = a(\alpha)E_0u'(x)$. The equilibrium equation implies that the stress is a constant throughout the bar. The damage criterion is in the form (1.13b). Introducing the compliance modulation function $s = a^{-1}$ and writing the deformation u' as a function of the stress σ , the function g defining the damage criterion in (1.13b) may be written in the form

$$g(\varepsilon, \alpha, \alpha'') = -\frac{s'(\alpha)}{2E_0}\sigma^2 + (w'(\alpha) - \ell^2 \alpha'')w_1.$$



Figure 1.1: Response and stability of the homogenous solutions of the one-dimensional traction problem with two variants of the gradient damage model (1.14), see [J-Pha+11].

Homogeneous solutions and their stability. Considering an evolution problem for an initially undamaged bar ($\alpha = 0$), the solution remains purely elastic until the stress reaches the *elastic limit*:

$$\sigma_c = \sqrt{w_1 E_0} \sqrt{\frac{2w'(0)}{s'(0)}}.$$
(1.15)

Indeed, for smaller loading the damage criterion is verified as a strict inequality and the energy balance imposes the variations of α to be null. For bars made of *stress-softening* materials, σ_c is also the maximum allowable strain, in the sense that solutions with $\sigma > \sigma_c$ do not exist. After the elastic limit is reached, the stress decreases with the loading. The response depends on the material model, *i.e.* on the choice of the two constitutive functions $w(\alpha)$ and $a(\alpha)$. Figures 1.1(a) and 1.1(b) report the homogenous response obtained for two models used in numerical applications:

- (AT1): $w(\alpha) = \alpha/2$, $a(\alpha) = (1 \alpha)^2$,
- (AT2): $w(\alpha) = \alpha^2/8$, $a(\alpha) = (1 \alpha)^2$.

The model (AT2) is particularly interesting because corresponds to the energy (1.8) of the regularized approximation of Griffith proposed by [Amb90] and used in [BFM00]. In this case, being w'(0) = 0, the elastic limit is null and the homogeneous response is with non-null damage for any non-null loading, being characterized by a stress-hardening phase, followed by stress-softening. The model (AT1) has a non-null elastic limit given by $\sigma_c = \sqrt{w_1 E_0}$.



Figure 1.2: Localised solution with the AT1 model: damage field along the bar.

The homogenous response gives a solution to the evolution problem respecting the first order conditions (1.13). Its knowledge is important to characterize the material behavior. However the actual structural response can be different because this solution may be unstable. We analyzed point in dept in [J-PMM11], testing second order stability conditions, by studying for a general class of models the sign of second derivative of the energy around the homogenous state along all admissible perturbations non-decreasing the damage. It is possible to obtain analytical expressions of the stability limits. The results for the (AT1) and (AT2) are reported in Figures 1.1(c)-1.1(d). The stability diagrams highlight a scale effect: the stability limit for the homogenous solution depends on the ratio between the bar length L and the internal length ℓ . For short bars with $(L \ll \ell)$ the homogenous solution may be stable also in the stress-softening regime, whilst for long bars $(L \gg \ell)$, it becomes unstable immediately after leaving either the elastic (AT1) or the stress-hardening (AT2) phase. Moreover, distinction should be made between the condition of stability and of (local) uniqueness of the solution, as well known in plasticity and other irreversible phenomena [Hut74; Pot82; Ngu87; Ngu94]. It may be shown that the homogeneous solution (fundamental branch) may show a continuous family of bifurcated branches before its loss of stability, as it happens for the classical plastic Shanley column [Hut74; Ba 88]. Formally, one should differentiate a stability and a non-bifurcation condition, depending if one takes into account or not the irreversibility constraints in the test of the sign of the second derivative in the energy. The bifurcation and stability analysis of the homogenous solution is reported in [J-PMM11].

Localised solutions. Localized solutions can be constructed by assuming that the damage evolves $(\dot{\alpha} \neq 0)$ only in a segment of the bar. Because of the energy balance (eb), in this segment the damage criterion must be verified as an equality. In the one-dimensional case, the associated equation has a first integral and, assuming that the rest of the bar in undamaged, it reduces to the solution of

$$-\frac{\sigma^2}{2E_0w_1}(s(\alpha)-1) + w(\alpha) + \frac{\ell^2}{2}\alpha'^2 = 0$$

in a segment of unknown length with $\alpha = \alpha' = 0$ on the boundary. The solution of this nonlinear boundary value problem gives the damage profile and the length of the damaging zone for each level of stress. The case of vanishing stress is particularly important: it is the regularized representation of a crack. For $\sigma \to 0$, the length of the localization zone, say *D*, and the energy dissipated in this solution, say G_c , are given by

$$D = c_{1/w}\ell, \qquad G_c = c_w w_1 \ell.$$
 (1.16)

where $c_{1/w} = \sqrt{2} \int_0^1 \sqrt{1/w(\alpha)} d\alpha$ and $c_w = 2\sqrt{2} \int_0^1 \sqrt{w(\alpha)} d\alpha$ are two dimensionless constants. Figure 1.2 reports the fully localized damage profile for the model AT1, for which $c_{1/w} = 4$ and $c_w = 4/3$.



Figure 1.3: Numerical simulation of the traction test using the AT1 model ($E_0 = 1., G_c = 1., \ell = .1$) for a bar of length L = 1. and width W = .1. The vertical gridlines denote the analytically calculated elastic limit $U_e = L\sqrt{3G_c/8E_0\ell} = \sigma_c L/E_0$ and critical Griffith loading $U_G = \sqrt{2G_c L/E_0}$; the horizontal gridline is the dissipated energy for a transverse crack according to the Griffith model.

Conclusions and comparisons to Griffith. Brittle fracture may be phenomenologically described by two key material parameters: the fracture toughness G_c , which is the energy dissipates in a crack of unit length, and the limit stress σ_c , defined as the stress level at failure in an uniaxial traction test. Our analysis concludes that the gradient damage models introduced in Section 1.1.3 are good candidates to model brittle fracture if they respect two fundamental conditions: (i) they should be with *stress softening* and (ii) *strongly brittle*, in the sense of the definitions given at the end of Section 1.1.3. The existence of a non-null elastic limit (w'(0) > 0) is desirable for physical and computational reasons. In this sense, the model (AT1) is preferable over the model (AT2) used in [BFM00]. A large class of models shows a similar behavior for *brittle structures* that are long enough with respect to the internal length. Their response is mainly characterized by the two material parameters G_c and σ_c . For *strongly brittle materials*, the link with Griffith's fracture model may be emphasized by replacing the volume dissipation constant w_1 with the dissipation in a localized solution G_c and rewrite the energy density (1.10) in the form:

$$W(\varepsilon, \alpha, \nabla \alpha) = \frac{1}{2}a(\alpha)A_0\varepsilon \cdot \varepsilon + \frac{G_c}{c_w}\left(\frac{w(\alpha)}{\ell} + \frac{\ell}{2}\nabla\alpha \cdot \nabla\alpha\right)$$
(1.17)

where the internal length should be chosen so as to recover the correct limit stress, i.e. using (1.15) and (1.16),

$$\ell = \frac{2w'(0)}{s'(0)c_w} \frac{G_c E_0}{\sigma_c^2}.$$
(1.18)

For numerical applications, we choose to retain the model (AT1). Indeed, it combines the simplicity of its numerical implementation with the good constitutive properties: it has an energy density quadratic with respect to α , it is strongly brittle, it has a finite elastic limit, and it shows stress-softening.

Figure 1.3 reports the numerical solution for a two-dimensional version of the traction test obtained through a finite element code implementing the AT1 model (see Section 1.3). The time history can be deduced from Figure 1.3(a), which shows the time evolution of the elastic and dissipated energy. In agreement with the analytical predictions, the solution is homogenous and elastic for $U_t < U_e$. At $U_t = U_e$ the homogenous solution becomes unstable and the numerical algorithm finds a new minimum of the energy corresponding to the solution with one localization (a transverse crack). For $U_t < U_e$ the elastic energy is a quadratic function the applied displacement (linear elasticity) and the dissipated energy is null. For $U_t > U_e$ the elastic energy is null and the dissipated energy is equal to G_c times the width of the bar W, as in a Griffith model. The localization profile of Figure 1.3(b) coincides with the one reported in Figure 1.2. This example is particularly useful to show that although this kind of gradient damage models are energetically equivalent to Griffith, the evolution they predict may be different from the one given by the Griffith model. The Griffith model requires to accept global minimization as evolution law to retrieve crack nucleation. According to the global minimization criterion, the crack would appear as soon the cracked solution is energetically cheaper than the elastic solution, *i.e.* at $U_G = \sqrt{2G_c L/E_0}$ (see Figure 1.3(a)). The result given by the gradient model on nucleation appears physically more acceptable because it implies the presence of limit stresses in the material. Moreover it introduces a size effect depending on the ratio between the structural size L and the internal length ℓ , which is coherent with the experimental observations.

1.3 Numerical implementation

Related publications: [J-AMM09; J-Bou+14], [Mau14]

In the regularized approach, the numerical solution of the quasi-static fracture/damage problem is obtained by looking for the solution of the minimization problem (1.9). This is done by an iterative method introduced in [BFM00], based on the alternate minimization of the energy functional with respect to displacement, at blocked damage field, and with respect to the damage field, at blocked displacement, until convergence. The first sub-problem is a standard elastic problem, with the stiffness modulated by the damage field. The second sub-problem involves the minimization of a convex functional under box-constraints (the irreversibility condition on the damage field). For space-discretization, we employ standard finite elements with linear basis functions and uniform isotropic meshes with typical mesh size $h \sim \ell/5$. This implies the recourse to parallel computing for full-scale simulations. Further details can be found in [FBM08; Bou07; J-AMM09].

My implication in the numerical developments, started with the co-supervision of the thesis of Hanen Amor in 2007, increased progressively. Our first implementation [J-AMM09] was done in Matlab/C and introduced few modifications with respect to the original work of Bourdin [BFM00]. They concerned mainly the method to impose the boundary conditions on the displacement field and to account for the irreversibility conditions on the damage field. While the original implementation of Bourdin was aimed at reproducing the evolution of the Griffith model through the global minimisation of the Ambrosio-Tortorelli functional, our goal was to follow the local minima of the energy of the damage model. Solvers for bound-constrained problems were used to exactly respect the irreversibility condition on the damage field, whilst the initial approach in [BFM00] allows for the decrease of the damage for α smaller than 1 and imposes Dirichlet boundary conditions on the damage where α is sufficiently close to one. The use of solvers for variational inequalities is necessary also for using models different from the standard Ambrosio-Tortorelli regularization, like the AT1 model presented in Section 1.2. Several cooperation projects with Blaise Bourdin allowed mutual visits and the establishment of a long-term collaboration. In this framework, I was introduced to the modern tools of parallel computing and with Blaise Bourdin we started to re-implement a code (MEF90) in Fortran 90 merging our mutual developments, further expanded in the framework of the Ph.D. thesis of Andrés León Baldelli and Paul Sicsic to solve thin film and thermal crack problems. This code is now mainly maintained and developed by Blaise Bourdin. Currently, I develop a finite element code (varfrac_fenics) based on the use of the FEniCS finite element library, that allows us to perform large-scale parallel computations through a simplified python interface. The main advantage of this approach is the availability of a high-level interface easily accessible to students and extremely useful for rapid prototyping and development. The use of automatic code generation in C++, just-in-time compilation, and a high-performance linear algebra library (PETSc) allows for efficient parallel computations. Demo code distributed at the CISM-IUTAM Summer School on "Variational Approaches to Damage in Continua and Interfaces" (Udine, June 2013) are available at https://bitbucket.org/cmaurini/varfrac_for_cism. The interface to variational inequality solvers introduced in FEniCS to solve the damage problem and the application to fracture mechanics were presented at the latest FEniCS'14 workshop [Mau14].

1.4 Unilateral effects

Related publication: [J-AMM09]

One of the main limitation of the original Francfort-Marigo model and its regularization presented is Section 1.1 is to provide a symmetric response in traction and in compression. For example, reversing the sign of the loading in the traction test of Figure 1.3 would lead to the same crack evolution, but with displacements of opposite signs and the unphysical interpenetration of the crack lips. This renders the model physically admissible only for traction-cracks. We propose a possible solution to this issue in [J-AMM09]. To introduce an asymmetry in the behavior in traction and compression, we decompose the elastic energy density in the spheric and deviatoric parts. Hence, depending on the sign of spheric part, we let the damage affect only the deviatoric, or both the deviatoric and the spheric part. This translates into the use of a damage model characterized by the following energy density:

$$W(\varepsilon, \alpha, \nabla \alpha) = \kappa_0 \frac{\operatorname{tr}^-(\varepsilon)^2}{2} + (a(\alpha) + k_\ell) \left(\kappa_0 \frac{\operatorname{tr}^+(\varepsilon)^2}{2} + \mu \varepsilon_D \cdot \varepsilon_D \right) + w_1 \left(w(\alpha) + \frac{\ell^2}{2} \nabla \alpha \cdot \nabla \alpha \right)$$
(1.19)

where $\operatorname{tr}^{\pm}(\varepsilon)$ stands for the positive/negative part of the trace of the strain tensor and ε_D for its deviatoric component, κ_0 and μ being the compressibility and the shear moduli of the undamaged material, and k_ℓ a small residual stiffness. This approach extends a model for shear fracture proposed by Lancioni and Royer-Carfagni [LR09] and is for many aspects similar to the one proposed



Figure 1.4: Numerical simulation of a holed plate with the model (1.19) presented in [J-AMM09]. The hole is blocked and a vertical displacement is applied on the top side with free sliding. The top and bottom rows of images report the results for traction (t > 0) and compression (t < 0) loading, showing the asymmetric behavior of the proposed model. The standard model would give the same crack pattern in traction and in compression.

by Comi [Com01] and Comi and Perego [CP01] in the framework of non-local damage models. The different behavior in traction and compression is highlighted in the numerical results reported in Figure 1.4. Our conjecture, still unproven but supported by numerical results, is that this model converges toward a Griffith model with a geometrically linearised non-interpretation condition on the crack lips. The same model has been successively used in [MHW10; Bor+12] and further extended by introducing a more complex decomposition of the strain energy in positive and negative parts on the basis of the sign of principal strains. Notwithstanding, we think that our model and those presented in the literature are still unsatisfactory for many aspects: (i) The geometrical linearised unilateral contact condition applied on the Griffith model may lead to existence issues [see the counterexample J-AMM09, Sec. 3.1]; (ii) It lacks any form of cohesion and/or friction on the lips of compressive cracks; (iii) The numerical results are unsatisfactory, showing convergence issues and poor quality, probably because of numerical locking issues and the bad conditioning of the elastic problem when compressive cracks are present [as suggested in J-AMM09, Sec. 6.1]. We partially address these issues in ongoing works in the framework of Ph.D. thesis of N. Traore. An interesting viewpoint is also that of non-linear elasticity, introducing the non interpenetration condition in the geometrically non-linear context [see DLM07].

1.5 Thermal shock of a brittle slab

Related publications: [J-SMM14; J-Bou+14]

The shrinkage of materials, induced by cooling or drying, may lead to arrays of regularly spaced cracks. Similar phenomena appearing at very different length-scales have always intrigued

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researchers and common people: drying of concrete, the exposure of glass or ceramics to a thermal shock, the drying of soils, or the cooling of lava fronts with the formation of columnar joints. The understanding and the predictive simulation of the morphogenesis and propagation of similar complex crack patterns is a major issue for classical fracture mechanics, which usually studies the propagation of a single preexisting crack. Yet similar problems may be naturally tackled, theoretically and numerically, in the framework of the variational approach to damage and fracture mechanics. These motivations led me to initiate a research project focused on these problem, in collaboration with Blaise Bourdin and Jean-Jacques Marigo. The main outcomes are published in [J-SMM14; J-Bou+14].



Figure 1.5: Full scale numerical simulation of a ceramic slab submitted to a thermal shock. (a) Damage field from the numerical simulation (blue $\alpha = 0$, red $\alpha = 1$). (b) Experimental results from [Sha+11, Fig. 5(d)]. (c) Average crack spacing *d* as a function of their depth *a* for (a) and (b). The solid line is an approximate scaling law obtained in [Bah+10] by imposing a period doubling condition on a Griffith model. Here $\ell = 46 \,\mu\text{m}$ is the material internal length, $\ell_0 = G_c / (Ea^2 \Delta T^2) = 14 \,\mu\text{m}$ the Griffith length (loading parameter), $2L = 9.8 \,\text{mm}$ the total depth of the slab.

As a model problem, we focused on the thermal shock of a brittle slab, for which experimental results are available in [BFW86; Sha+10; GN82]. The specimen is a thin slab, free at the boundary, composed of a homogeneous material without prestress in its initial configuration. In experiments, several slabs are stacked together, uniformly heated at temperature T_0 and then quenched in a cold bath inducing a temperature drop ΔT on the lateral surfaces. To include the material shrinkage induced by the thermal effects in the damage model, we consider the following energy functional (1.11):

$$\mathcal{E}(u,\alpha) = \int_{\Omega} \left(\frac{1}{2} (1-\alpha)^2 A_0(\varepsilon - \varepsilon_0) \cdot (\varepsilon - \varepsilon_0) + G_c \frac{3}{8} \left(\frac{\alpha}{\ell} + \ell \,\nabla \alpha \cdot \nabla \alpha \right) \right) \,\mathrm{d}x. \tag{1.20}$$

where $\varepsilon_0 = \beta(T_t - T_0)$ is the thermally induced inelastic deformation, β being the thermal expansion coefficient and T_t the temperature field at time t. As a first approximation, T_t is calculated as the solution of thermal evolution problem on the homogenous undamaged solid by solving the transient heat equation. Taking a uniform temperature field T_0 as initial condition, a temperature drop ΔT is imposed on the boundary exposed to thermal shock. The quasi-static evolution problem is then formulated on the basis of the principle of irreversibility, local stability, and energy balance as in Section 1.1.3. The dimensional analysis of the energy (1.20) highlights three characteristic lengths: the size of the domain L, the internal length ℓ , and the Griffith length $\ell_0 = G_c / (E\beta^2 \Delta T^2)$. Using the material's internal length as the reference unit, the problem can be reformulated in terms of two dimensionless parameters, the size of the structure L/ℓ (a geometric parameter) and the intensity of the thermal shock ℓ_0/ℓ (a loading parameter). This is a significant departure from the classical Griffith setting where the only relevant parameter is L/ℓ_0 [Jag02; Jen05; Bah+10].

The time-discrete quasi-static evolution problem is solved numerically with the technique detailed in Section 1.3. Figure 1.5 shows the crack pattern at the end of the cooling process, comparing the numerical results with the experimental findings¹. The central part of the specimen, where the temperature field only depends on the distance from the wet surface, presents an array of parallel cracks. Some of these cracks stop earlier during the penetration and the spacing of the crack increases with the depth. The most intriguing phenomena are the period doubling in the crack spacing during the propagation inside the body and the crack initiation. The numerical simulation of Figure 1.5a is the result of a full-scale computation performed on one half of the slab. For the slab of width L = 1cm, the internal length ℓ is set to $0.46\mu m$, a value identified using equation (1.18) and the material parameters communicated by [Jia+12]. The temperature drop at the exposed surfaces is $\Delta T = 380^{\circ}C$.

In [J-SMM14], we studied in depth the problem of crack nucleation showing that the morphogenesis of the periodic crack pattern may be explained through a bifurcation analysis of the underlying damage model. As shown in Figure 1.6a for the idealized case of a semi-infinite slab, the damage field is initially non-null only in a band close to the surface and varies only with the depth variable. At a critical time t^* , when the band has penetrated for a length D^* , we observe periodic oscillations of the damage field with a wavelength λ^* , that may further develop into fully formed cracks as those visible in Figure 1.5a. The results of the semi-analytical bifurcation analysis are shown in Figure 1.6b and compared with the outcomes of the direct numerical simulations showing an excellent agreement. The semi-analytic results are obtained by a bifurcation and stability analysis of the fundamental solution through a partial Fourier expansion in the direction parallel to the surface of the thermal shock. Hence, we solve numerically a linear eigenvalue problem in one dimension (the depth) through a finite element discretization and establish critical bifurcation times and wavelength. The behaviour sketched in Figure 1.6a is observed for severe enough thermal shocks $(\ell_0/\ell < 3/8)$. For milder shocks $(\ell_0/\ell > 3/8)$ the damage criterion is never attained and the solution remains purely elastic without damage for any time t. For extremely severe shocks ($\ell_0 \ll \ell$), the results of Figure 1.6b disclose a well-definite asymptotic behaviour with $\lambda^* \sim \sqrt{\ell_0 \ell}, D^* \sim \ell$, and $t^* \sim \ell_0 \ell$.

¹ We had access to the unprocessed experimental data of [Jia+12] thanks to a collaboration established in the framework of a international French-Chinese ANR project (ANR T-shock).



Figure 1.6: Crack nucleation. (a) Damage field close to the surface before (left) and after (right) the bifurcation time t^* for $\ell_0/\ell = 0.107$ showing the bifurcation of a horizontally homogeneous damage band of depth D^* toward a periodic solution with wavelength λ^* . (b) The wavelength, time, and damage penetration detected from the numerical simulations for several intensities of the thermal shock ℓ_0/ℓ (dots) are verified against the results of semi-analytical bifurcation analysis [J-SMM14] (solid lines). For $\ell_0/\ell > 8/3$ the response is purely elastic without damage.

One of the key advantages of the variational formulation and the associated numerical solution strategy is that it extends seamlessly in a three-dimensional setting, which poses formidable difficulties for the classical numerical methods of fracture mechanics. The price to pay is that of the computational resources. With the spreading of massively parallel architectures and dedicated numerical tools developed as open-source libraries, this point does not constitute anymore a true bottleneck. Thanks to the collaboration with Blaise Bourdin, we get access to the several supercomputers of the US network and we were able to perform fully three-dimensional simulations. Figure 1.7 shows a three-dimensional analogue of the simulation of Figure 1.5. During the simulation, a disordered pattern of small cells nucleates in the first time steps and propagates quasi-statically inside the domain with a selection mechanism that lets a more and more regular honeycomb pattern with cells of increasing diameter emerge. To get a scaling law for the diameters of the cells isolated by the cracks as a function of the depth, we performed a series of computations varying the domain size and the internal length. The result, obtained through an automatic postprocessing, is reported in Figure 1.8. All the results collapse with a reasonable accuracy on the approximate scaling law obtained by Bahr and collaborators for a two-dimensional case [Bah+10], showing that three-dimensional effects do not play a crucial role in the scale selection mechanism.

The result obtained for the thermal shock problem furnishes a nice illustration of how the analysis of the damage model reported in Section 1.2 for the apparently trivial 1D setting extends to the complex 2D and 3D cracking problems. In particular, we prove the ability of the present approach to retrieve a regularized representation of cracks propagating according to the Griffith criterion and to obtain crack nucleation from a homogenous undamaged material through bifurcation and loss of stability of fundamental states. The bifurcation mechanism leading to the creation of the periodic array is expected to be generic and the associated ideas and techniques for the analysis to be directly transposable to many other applicative contexts.



Figure 1.7: Complex fracture pattern for $\ell_0 = G_c / (EG_c \beta^2 \Delta T^2) = 0.05 \ell$ in a domain of size $150\ell \times 150\ell \times 20\ell$. The simulation includes 44×10^6 elements with an approximate mesh size $h = \ell/5$. To help the visualization, the crack surfaces are colored with the distance from the bottom edge, where the thermal shock is applied.



Figure 1.8: Cross sectional diameter of the fracture delimited cells as a function of the distance to the exposed face in cubic domains with edge length *L* ranging from 2 mm to 2 m compared with the two-dimensional scaling law from [Bah+10] (solid line). All the simulations are with $\ell_0 = 14 \,\mu\text{m}$ and $\ell = L/40$. Inset: top view to the crack patterns for (a) $L = 2 \,\text{mm}$; (b) $L = 63.2 \,\text{mm}$; (c) $L = 2 \,\text{m}$.

1.6 Thin films

Related publications: [J-Leo+13; J-Leo+14].

Cracking of thin films systems is common in everyday life and technologic applications. Many examples are found in surface coatings for functional or aesthetic purposes including paintings, muds, thermal barriers for gas turbine blades, surface treatments for glasses, or electronic devices. In systems composed of a thin film bonded on a substrate, fractures are induced by the differential spontaneous deformations of the substrate and the film when submitted to external loadings such as moisture, heat, electric voltages, phase transformations, or material growth. The problem of predicting the conditions of nucleation and the properties of the crack patterns has an obvious industrial interest, not only to prevent failure, but also to generate specific microstructures through controlled crack networks. For this reasons the problem has been the object of a deep interest from researchers in mechanics, mathematics, physics, and material science. Milestone works include those from Hutchinson and Suo [HS91] and Xia and Hutchinson [XH00]. Because of the thinness of the film, full three-dimensional models are not adequate. Moreover, in many situations experimental results clearly show the emergence of two-dimensional fracture patterns. Hence, the problem clearly demands a reduced two-dimensional model.

In the framework of the León Baldelli's Ph.D. thesis, we aimed at developing a rigorous approach to thin film fracture and debonding problem, including: (i) the derivation of a two dimensional model from the 3D description through asymptotic methods, (ii) an analytical analysis of the problem in a 1D context, (iii) the development of numerical methods and effective finite element codes to solve complex multi-cracking and debonding problems. I briefly resume below the main results that we have obtained on each of these items.

Consider a thin film bonded on a substrate and submitted to tensile loadings. The loading is exerted by inelastic strains ε_0 in the film or the stretching of the substrate u_0 . The inelastic strain can model the effect of the mismatch between the thermal expansion coefficients of the substrate and the film when temperature change. Failure phenomena may include cracks in the films, debonding between the film and the substrate and cracks in the substrate. Excluding the case of substrate failure, and assuming a brittle behavior, a natural model is that of brittle membrane resting on an elastic foundation, that can eventually break. In a variational modeling framework, this translates in a two-dimensional flat surface ω characterized by in-plane displacement u, stretches ε , and an elastic energy given by

$$\mathcal{P}(u,\Gamma,\Delta) = \underbrace{\int_{\omega \setminus \Gamma} \frac{1}{2} A(\varepsilon(u) - \varepsilon_0) \cdot (\varepsilon(u) - \varepsilon_0) \, d\omega}_{\text{Film strain energy}} + \underbrace{\int_{\omega \setminus \Delta} \frac{1}{2} K(u - u_0) \cdot (u - u_0) \, d\omega}_{\text{Film/Substrate strain energy}}, \quad (1.21)$$

where A is the membrane stiffness of the film, K the stiffness of the elastic foundation, Γ is the unknown set representing the cracks in the film, and Δ the unknown region where the film is debonded. When adopting a Griffith model, the energy S required to create the cracks is supposed to be proportional to the measure of the crack set. In this case

$$S(\Gamma, \Delta) = \underbrace{G_{eq} \operatorname{length}(\Gamma)}_{\operatorname{Transverse cracks}} + \underbrace{D_{eq} \operatorname{surface}(\Delta)}_{\operatorname{Debonding}},$$
(1.22)



sequence)

Figure 1.9: Brittle thin film Ω_f bonded on a substrate Ω_s trough a brittle bonding layer Ω_b : (a) Three-dimensional model and its two-dimensional limit; (b) The recovery sequence used in the Gamma-convergence giving an optimal through-the-thickness distribution of the displacement field at points in bonded (x_1) and debonded (x_2) regions. The loading is given by inelastic strains ε_0 in the film. In the two-dimensional model, the cracks represent either transverse crack in the film Γ , which are one-dimensional sets, or two-dimensional debonded regions Δ .

where G_{eq} and D_{eq} are equivalent toughnesses for transverse cracks and debonding, respectively. Hence, the fracture mechanics problem can be formulated as a unilateral energy minimization problem for the total energy

$$\mathcal{E}(u,\Gamma,\Delta) = \mathcal{P}(u,\Gamma,\Delta) + \mathcal{S}(\Gamma,\Delta) \tag{1.23}$$

under the irreversibility condition on the crack sets. Thin film models using an equivalent elastic foundation to account for the effect of the substrate are widely adopted in the literature, starting from the work of Xia and Hutchinson [XH00]. However, at the best of our knowledge, their clear justification from a three-dimensional description is missing, even in the purely elastic case without fracture. From the practical point of view, it is not entirely clear what the elastic foundation equivalent stiffness is intended to represent, under which hypotheses the model holds, and how to identify the material constants of the reduced model from the three-dimensional geometry and material constants. In collaboration with two applied mathematicians, Duvan Henao and Jean-Francois Babadjian, we studied the dimensional reduction problem using asymptotic analysis. We established a rigorous results of Gamma-convergence for the thin film system of Figure 1.9 com-

posed of a brittle thin film bonded on a stiff substrate through a brittle thin elastic layer [see the Appendix of J-Leo+14]. We showed that a limit energy in the form of equations (1.21)-(1.23) emerges when the thicknesses of the film and the bonding layer go to zero and the bonding layer is much more compliant than the film. There is a competition between transverse fracture and debonding only if the toughness of the bonding layer is much smaller than the toughness of the film. The asymptotic result explicitly includes the possible presence of cracks with unknown shape and location. Figure 1.9(b) sketches the displacement distribution and crack orientation obtained in the limit model. The energy minimality requires that for thin systems the crack in the film are necessarily oriented along the thickness and that the crack in the bonding layer are necessary with an in-plane orientation. Moreover, one finds that the debonding condition results in a simple displacement-threshold criterion [J-Leo+14].

We performed a detailed analysis of the one-dimensional version of the minimization problem on the energy (1.23) to determine reference analytical solutions and disclose the key properties of the system in a simplified setting [J-Leo+13]. We proved that the crack patterns in the films are periodic and partition the bar in segments of equal length, a result usually postulated in the literature. Many transverse crack may appear suddenly at critical loads, that may be determined analytically. The debonding always starts at the end of each segment and evolves smoothy. The general evolution of the crack pattern depends on two key parameters, the relative stiffness and the relative toughness between the film and the substratum. The analytical results have been derived using the *global* energy minimization principle and the Griffith model. As commented in Section 1.1.2, the resulting time-evolution should be interpreted with caution: we supposed that the system is able to reach always the state of absolute minimal energy, but a physical system can be trapped in local minima of the energy, which are still (locally) stable states. Keeping this in mind, the Griffith model based on global minimization is still extremely useful because it allows for an analytical treatment and to highlight the key qualitative properties of the solutions. This system constitutes also a useful model problem for studying the emergence of structured crack patterns. Even in the one-dimensional case, the presence of the substrate and the competition between transverse cracking and debonding let non-trivial crack patterns emerge.



Figure 1.10: Combined fracture and debonding of a thin film/substrate system modelled by (1.23) and loaded by uniform isotropic inelastic strains ε_0 . Dark areas identify debonded regions, whose first onset is at the boundaries of the largest cells. At large loading all cells undergo debonding.

We conducted numerical experiments extending the classical regularization approach to the limit two-dimensional brittle model including the presence of the substrate as an elastic foundation. The analysis of the problem shows that the regularization is required only for the transverse cracks, whilst the debonded domain (of geometric dimension 2 in a 2D domain) can be described by a simple characteristic function. After a verification against the 1D analytical solutions, we performed several 2D tests. The numerical results capture complex evolving patterns, including hexagonal crack networks with transverse fracture and debonding (see Figure 1.10 and [J-Leo+14] for further details).

1.7 Directional drying of capillary suspensions

Related publication: [J-Mau+13]

Veronique Lazarus and George Gauthier (FAST, Paris 11) revisited an interesting experiment of Allain and Limat [AL95] producing periodic crack arrays during the directional drying of capillary suspensions in Hale-Shaw cells. They performed directional drying experiments on capillary tubes with different cross-sectional shapes, showing the formation of structured crack patterns (see Figure 1.11). I collaborated with them and Blaise Bourdin in order to explain this phenomenon using the variational fracture model. In this case the evolution problem is clearly three-dimensional, potentially coupling several phases and multi-physical phenomena. However experimental results show the establishment of stationary cross-sectional crack shapes, evolving in the axial direction with the drying front (see Figure 1.11). Hence, we adopted a over-simplified two-dimensional plane-strain model, looking for the optimal crack shapes in the cross-section as a function of the drying intensity, which is modeled by a uniform inelastic strain ε_0 , as in (1.20). The results resumed in Figure 1.12 show a remarkably good agreement of the results of the direct numerical simulations with the semi-analytical and experimental results, providing the verification and validation of our model and approach. This work does not include the solution of an evolution problem, but only the research of the optimal cross-sectional crack patterns at a given loading. We applied a *global* minimisation criterion to select the best crack shapes and a numerical procedure based on the progressive refinement of the internal length ℓ [see J-Mau+13] to reach low-energy crack patterns at each loading level. Our experimental and numerical results seem to confirm that the cross-sectional crack shape in the steady-state regime is the one associated with the global minimum of the energy. This state is reached in the three-dimensional evolution after an initial transient with disordered cracks.



Figure 1.11: A glass capillary tube oriented vertically is filled with a colloidal suspension; the opened bottom edge allows for evaporation of the water in an environment maintained at a constant relative humidity and temperature. The cross-sectional shape of the cracks depend on the tube shape and size and on the drying conditions. Left: Experimental setup and sketch of the self-organized star-shaped cracks. Right: Pictures of some cross section cuts (the tonality depends on the light used).



Figure 1.12: Cross-sectional crack shapes in directional drying of capillary suspensions in circular tubes. The diagram compares the crack shapes determined by semi-analytical (top), numerical (middle), and experimential (bottom) methods, as a function of the drying intensity (a non-dimensional parameter), without any fitting parameters.

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In the electronic version, click on Link to PDF to obtain the pdf file of the article.

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Chapter 2

Shape-change and multistability of slender elastic structures

Preamble

Immediately after my Ph.D. thesis I started studying geometrical nonlinear effects in beams and plates with embedded active materials, having in mind shape-control applications. This research subject was partially inspired by my Ph.D. work, dealing with linear piezoelectric beams with embedded electric circuits and vibration control applications. Chronologically, my first work dealing with nonlinear problems and shape control concerned the multi-parametric actuation of bistable buckled beams [J-MPV07]. Hence, with Stefano Vidoli (La Sapienza and long term visitor at d'Alembert), we studied the analog problem for plate and shells [J-FMV10; J-VM08]. This subject gave me the opportunity to collaborate with the group of Simon Guest and Keith Seffen at Cambridge (UK) in the framework of a joint research project on multistable shells financed by the CNRS and the Royal Society. The results of this collaboration were partially reported in [J-SM13], where we study the shape control of a disk through embedded membrane or bending actuation.

My work in the area of nonlinear beams and shells naturally led me to develop several interactions with the other researchers at d'Alembert interested on similar subjects. Informal daily discussions led to formal publications and financed research projects: on the vibrations of inextensible post-buckled beam with Joël Frelat and Sebastien Neukirch ([J-Neu+12] also with Alain Goriely, Oxford); on the large deformations induced by capillary effects of a soft beam embedded in a fluid with Basile Audoly ([J-Mor+13] also with Serge Mora, Montpellier, and Yves Pomeau, French Academy of Sciences); on multistable composite plates and shells with Angela Vincenti with the SLENDER project recently financed by the ANR).

My choice here is to report an overview of our approach and results on the multistability of plates and shallow shells (Section 2.1). This subject has been developed over the years as a structured project and better fits the format of a straight exposition. Hence, I will resume in Section 2.2 the work on soft hyperelastic beams immersed in a fluid [J-Mor+13], dealing with large shape-changes induced by capillary effects. I will not report on the works dealing with multiparameter actuation of a bistable buckled beam [J-MPV07] and on the vibration of inextensible post-buckled rods [J-Neu+12]. For them I refer the reader to the journal publications.

2.1 Multistable plates and shells

Slender structures may experience large global changes of their shape with small local deformations of the material. An explicit illustrative example is given by an initially straight beam of length L and thickness t bent in the shape of a circular arch of curvature k: a beam with an aspect ratio L/t = 100, made of a material having an elastic limit strain $\varepsilon_c \sim 10^{-2} \div 10^{-3}$ (e.g. aluminium) can experience transverse deflections of almost of the order of the length without any plastic deformation¹. In these situations, geometrical nonlinear effects may strongly influence the response, whilst the material behaviour can remain approximately elastic and reversible.

Most of the engineering applications exploit beams, arches, plates, and shells only in the linear regime and perform a nonlinear structural analysis only to estimate the limit of applicability of the linearised models. An emerging community of researchers proposes to benefit from geometrical nonlinearities to conceive structures able to hold multiple configurations of largely different shapes, each one associated to a specific functional regime. Similar systems are currently denoted as *morphing*, or *shape-changing*, structures. Their careful design can exploit geometric nonlinear effects to obtain great changes in shape through active materials with limited actuation power. Potential applications encompass aeronautics (shape-changing aerodynamic panels for flow control), energy (flexible and deployable solar cells), electronics (flexible and folding electronic devices), civil engineering (adaptive architecture including morphing functional elements), optics (shapechanging mirrors for active focusing), and microelectromechanical systems (micro-switches, mechanical memory cells, valves, micro-pumps).

The design of morphing multistable structures with embedded actuation is a challenging problem from the theoretical and technologic point of view. It demands to face two main difficulties: (i) taking into account nonlinear effects to design a structure with a set of assigned stable equilibrium configurations; (ii) conceiving efficient actuation techniques to control the transition among different equilibria. The starting point to tackle these issues is a careful study and a synoptic representation of the nonlinear static behavior of the considered class of structures as a function of several design parameters modeling initial shape, geometry, material, or actuation. This may be obtained only on the basis of simplified low-dimensional models, resuming the foremost qualitative properties of the system. Finite element numerical studies may constitute a validation tool in a second step of the analysis, keeping in mind that the numerical analysis of nonlinear systems with multiple stable equilibria remains a difficult task.

Thin structures as plates and shells appear as good candidates for shape-changing applications. In plate and shells, multistability is a consequence of the geometrical coupling between the Gaussian curvature and the membrane stretching. In a series of works [J-VM08; J-FMV10; J-SM13], we studied the possible stable equilibrium shapes with almost uniform curvature of free-standing linear elastic orthotropic plates or shallow shells submitted to membrane and bending inelastic strains. In absence of imposed displacements and external forces, our aim was to understand how the number and type of possible stable equilibria depend on the material properties, the initial shape and the prescribed inelastic strains. Our analysis can help designing of multistable structures

¹Approximating the arc of a circle with a parabola the transverse deflection w is of the order of kL^2 , whilst, assuming a through-the-thickness linear distribution for the strains in bending, the maximum deformation is $\varepsilon_{\max} \sim kt$. Hence the material stays in the elastic regime for transverse deflection up to $w/t \sim \varepsilon_c (L/t)^2$.

and understanding how the structural shape can be controlled through multiparameter embedded actuation. I give below a general overview of our simplified modeling approach for plate and shallow shells, before reporting some examples and the results obtained in this framework.

2.1.1 Uniform curvature model of orthotropic shallow shells with inelastic strains

The study of the nonlinear response of elastic surfaces is the object of a large number of recent research works ranging from the analysis of biological systems [For+05; LM11; AMT12; Arm+11] to the design of shape-changing, or morphing, engineering structures [KGP04; GP06; NSG08b; Sef07; Por+08; NSG08a]. Differently from the classical literature on the subject, many of these recent works identify several interesting nonlinear phenomena concerning *free-standing structures*, *i.e.* without boundary constraints and applied forces. The loading is exerted through prescribed *inelastic strains* that can model material growth in biological systems, thermal or hygroscopic strains, plastic deformations, or the action of active materials controlled through multiphysical couplings. The raising research activity in this context led to a revival of the study of nonlinear theories of shells and plates in order to assess the effect of the inelastic strains on the two-dimensional model [DCB09; ESK09] and the consistency of the different nonlinear plate and shell models [LMP11; LMP14], extending the works of Ciarlet and coworkers [CP86; CG06; Cia05].

In our work we applied an extremely simplified finite-dimensional model, based on the following key hypotheses:

- (i) a *shallow shell* approximation with von Karman kinematics, which assumes moderate rotations on the shell mid-plane normal;
- (ii) a *linear elastic* behavior with small deformations;
- (iii) a *uniform curvature* approximation, i.e. that the initial and the equilibrium shapes have almost uniform curvature in space.

The last hypothesis restricts the applicability of the model mainly to the case of *free-standing* shells, i.e. free at the boundaries and without any applied force. In what follows the loading is exerted through the imposed *inelastic strains* capable of modeling the large set of physical phenomena described above.

Extended Marguerre-von Karman model

The deformations of a two-dimensional surface embedded in the three-dimensional Euclidean space can be mathematically modelled by two 2×2 symmetric tensors, the extension (or metric) tensor *e*, and the curvature tensor *k*. A shear-indeformable linear elastic model for plates or shells is then based on the assumption that the elastic energy is a quadratic function of the strain measures (e, k), taking the following form:

$$W(e,k) = \frac{1}{2}A(e-e_I) \cdot (e-e_I) + B(k-k_I) \cdot (e-e_I) + \frac{1}{2}D(k-k_I) \cdot (k-k_I), \quad (2.1)$$

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Figure 2.1: Kinematical description of the shallow shell initial shape and equilibrium configuration taking the planform of the initial shape as reference configuration.

where e_I and k_I are the so-called *inelastic*, or *target*, deformations and *A*, *B*, and *D* are fourth-order tensors representing the membrane stiffness, the bending-to-extension coupling, and the bending stiffness. Hence, it is possible to introduce the membrane stress and the bending moment tensors defined by

$$N = \frac{\partial W}{\partial e} = A(e - e_I) + B(k - k_I)$$
(2.2a)

$$M = \frac{\partial W}{\partial k} = B^T (e - e_I) + D(k - k_I)$$
(2.2b)

The expressions above assume a linear elastic, possibly anisotropic, material behavior, which is valid only if $||e - e_I||$ and $||k - k_I||$ are small. To simplify the representation of the constitutive tensor, it is customary to adopt a Voigt representation of the tensorial quantities, so that (n,m,e,k,e_I,k_I) and A,B,D become three-component pseudo-vector and 3×3 pseudo-matrices, respectively. Here and henceforth we will assume this abridged notation.

We focus on shallow surfaces relatively close to a flat configuration. Hence, we distinguish the shell initial shape S_0 , its planform *S*, and the shell current equilibrium configuration according to the following definitions (see Figure 2.1):

Planform :
$$S \subset \mathbb{R}^2$$
 (2.3)

Initial shape :
$$\mathcal{S}_0 \equiv \{(x, y, w_0(x, y)) \in \mathbb{R}^3, (x, y) \in S\}$$
 (2.4)

Current configuration :
$$S \equiv \{(x+u_x(x,y), y+u_y(x,y), w(x,y)) \in \mathbb{R}^3, (x,y) \in S\}$$
 (2.5)

As sketched in Figure 2.1, the displacement field is decomposed in the in-plane component $u = (u_x, u_y)$ and in the out-of-plane component w, with respect to the planform S. In the hypothesis of moderate slopes of the tangent plane of the deformed configuration, the deformations may be expressed in terms of the displacement fields through the following expressions¹ [see e.g. Man89]

$$e(u,w) = \frac{1}{2}(\nabla u + \nabla u^T) + \frac{1}{2}\nabla w \otimes \nabla w - \frac{1}{2}\nabla w_0 \otimes \nabla w_0, \qquad k(w) = \nabla^2 w$$
(2.6)

¹The symbol \otimes denotes the usual tensor product. In component notation for two vectors $a, b: (a \otimes b)_{ij} = a_i b_j$

which are approximated so as to introduce the lowest order nonlinear contributions, by assuming that, up to a rigid motion:

$$u/L \sim (w/L)^2 \ll 1.$$
 (2.7)

where *L* is the diameter of *S*. This is the so-called *von Karman* kinematics. Denoting by $k_0 = k(w_0)$ the curvature of the initial configuration, it can be easily verified that, within the von Karman kinematics (2.6), the membrane and bending deformations verify the following compatibility conditions

$$\mathcal{L}(e) = \det k - \det k_0, \tag{2.8}$$

where det $k = k_x k_y - k_{xy}^2$ and det $k_0 = k_{0x} k_{0y} - k_{0xy}^2$ are the Gaussian curvatures of the deformed and initial configuration, respectively, while $\mathcal{L}(e)$ is a linear second order differential operator defined by

$$\mathcal{L}(e) := \operatorname{curl}\operatorname{curl} e = \frac{\partial^2 e_y}{\partial x^2} + \frac{\partial^2 e_x}{\partial y^2} - 2\frac{\partial^2 e_{xy}}{\partial x \partial y}.$$
(2.9)

Equation (2.8) is the moderate rotation version of the celebrated Gauss Theorema Egregium of surface theory [see Cia05]. Together with the following linearised version of the Codazzi-Mainardi equations

$$\frac{\partial k_x}{\partial y} - \frac{\partial k_{xy}}{\partial x} = 0, \qquad \frac{\partial k_y}{\partial x} - \frac{\partial k_{xy}}{\partial y} = 0, \qquad (2.10)$$

it gives the necessary and sufficient compatibility conditions on the deformation fields (e,k) for the existence of a displacement field (u,w) that verifies (2.6). The Gauss equation (2.8) synthetically resumes the fundamental coupling due to geometrical nonlinearities between the in-plane deformation and the bending curvature of a surface: the gaussian curvature is geometrically tied to at least quadratic variations of the membrane deformation.

The elastic energy of a free-standing shallow shell with the inelastic deformations (e_I, k_I) is given by

$$\mathcal{U}(u,w) = \int_{S} W(e(u,w),k(w)) \, dx dy. \tag{2.11}$$

Assuming the absence of other types of external loadings and the shell to be free on its boundary (*free-standing* shell), the stable equilibrium configurations are obtained by solving the following minimization problem

$$\min\{U(u,w), \quad u \in \mathcal{H}^1(S,\mathbb{R}^2), w \in \mathcal{H}_2(S,\mathbb{R})\}$$
(2.12)

where \mathcal{H}^1 and \mathcal{H}^2 are standard Sobolev function spaces. Assuming that the boundary and the material parameters are smooth, the stationarity conditions with respect to *u* and *w* give the equilibrium conditions for the membrane and bending sub-problems, respectively. In the case of vanishing inelastic deformations, the model above reduces to the *Marguerre-von Karman* model of shallow shells studied by Ciarlet and Paumier [CP86] and Ciarlet and Gratie [CG06]. Recently, Marta Lewicka and co-workers [LMP11; LM11; LMP14] addressed through rigorous mathematical analysis the problem of establishing precise results on the appropriateness of this kind of models in several regimes and their relation to three-dimensional elasticity. In particular, Lewicka et al. [LMP14] discuss in detail their asymptotic derivation from three-dimensional elasticity with incompatible strains.

The fundamental property of the von Karman model is that the energy (2.11) is globally nonconvex, but separately quadratic with respect to u and fourth-order in w. Hence the minimum with respect to u of $U(\cdot, w)$ at fixed w is unique. Indeed, the stationarity condition with respect to ugives the following equilibrium equation for the membrane stress N, where n is the outer normal of S:

$$\operatorname{div} N = 0 \text{ in } S, \quad Nn = 0 \text{ on } \partial S \tag{2.13}$$

which together with the linear constitutive equation (2.2) and the compatibility conditions (2.8) gives a linear problem with a unique solution¹ for (u, N) as a function of w. This in-plane problem may be solved in different ways, by either using the displacement or the stress as main unknown. The traditional formulation introduces a scalar Airy stress function ϕ and leads to two scalar non-linear partial differential equations for the scalar variables (w, ϕ) [see e.g. AP10]. This system is still of difficult solution in the general case, even if analytical solutions are possible in some situations [see for example DB08; AP10].

Uniform curvature approximation

We studied the possible stable equilibrium shapes when the initial curvature k_0 , the inelastic curvature k_I , and all material properties are uniform throughout *S*, except the inelastic membrane strain that may vary quadratically so as to keep constant $\mathcal{L}(e_I)$. Using what can be regarded as a Galerkin approximation, we look for the local minima of the energy among the class of *uniform curvature* shapes with transverse displacement in the form

$$w(x,y) = \frac{L^2}{R} \left(K_x \frac{x^2}{2L^2} + K_y \frac{y^2}{2L^2} + K_{xy} \frac{xy}{L^2} \right)$$
(2.14)

where (K_x, K_y, K_{xy}) are unknown non-dimensional curvatures independent of (x, y), *R* is a scaling radius of curvature and *L* the typical size of *S*. No restrictions are introduced on the membrane deformations *e*. Under this hypothesis, the Codazzi-Mainardi compatibility condition (2.10) is trivially satisfied. Using the constitutive equations (2.2a), and the fact that the curvature and the material properties are uniform, the Gauss compatibility condition (2.8) gives

$$\mathcal{L}(A^{-1}N) = \frac{(\det K - g_T)}{R^2}, \quad g_T = \det K_0 - R^2 \mathcal{L}(e_I).$$
(2.15)

where g_T can be defined as the non-dimensional *target gaussian curvature*. Equation (2.15) and the membrane equilibrium (2.2) give a system of linear differential equations to determine the membrane stress and strain (N, e). The misfit of the gaussian curvature in the r.h.s. of (2.15) is the only forcing term in this linear system, and within our hypotheses is independent of (x, y). Hence the solution for the membrane stress is in the form

$$N(x,y) = (\det K - g_T) N^{(1)}(x,y)$$
(2.16)

where $N^{(1)}(x, y)$ is the solution for $(\det K - g_T) = 1$. Analytical solutions for this membrane problem are possible for the case of orthotropic shells with an elliptical planform [Sef07]. For a general shape the solution can be obtained by solving it numerically once for all for a unit loading

¹Up to rigid motions.

[J-FMV10]. Plugging this solution and the uniform curvature hypothesis into (2.11) and setting an appropriate scaling radius R, the potential energy takes the following non-dimensional form

$$U(K) = \underbrace{\frac{1}{2}\tilde{D}(K - K_T) \cdot (K - K_T)}_{\text{bending energy}} + \underbrace{\frac{1}{2}(\det K - g_T)^2}_{\text{membrane energy}}$$
(2.17)

where

$$K_T = K_0 + K_I, \quad \tilde{D} = \frac{(D - B^T A^{-1} B)}{(D - B^T A^{-1} B)_{xx}} = \begin{bmatrix} 1 & v & 0 \\ v & \beta & 0 \\ 0 & 0 & \rho \left(1 - \frac{v^2}{\beta}\right) \end{bmatrix}$$

are the *target curvature* and the non-dimensional bending stiffness, where appearing the equivalent Poisson ratio v, Young modulus ratio β , and the shear stiffness ρ appear. To obtain the energy in the form (2.17) the curvatures should be scaled with a characteristic radius in the form

$$R = c_R \frac{L^2}{t} \tag{2.18}$$

where c_R is a dimensionless constant depending of the solution of the linear membrane problem, where *t* is the thickness and *L* the diameter of the planform. For an isotropic disk one gets $c_R = \frac{1-v^2}{16}$. A similar analytical calculation is possible for an orthotropic homogenous shell with elliptic planform [Sef07], whilst for a general shape (e.g. square) the pre-factor c_R must by evaluated numerically by solving, once for all, the linear membrane problem for unit loading [J-FMV10].

The uniform curvature estimation of the equilibria is obtained by solving the following nonlinear system of three algebraic equations imposing the gradient of the energy to be null:

$$G(K;K_T,g_T) := \frac{\partial U}{\partial K} = 0.$$
(2.19)

Moreover, the stability of the equilibria can be assessed by studying the sign of the 3×3 hessian matrix

$$H(K;K_T,g_T) := \frac{\partial^2 U}{\partial K^2}.$$
(2.20)

Despite its simplicity, the model above is rich and may incorporate disparate physical phenomena. Its consistency with a fully-nonlinear shell model with varying curvature is limited by the uniform curvature and moderate curvature assumptions. However, it condenses in a compact form many key qualitative properties of the problem under consideration, which are listed below.

• The energy is the sum of a quadratic term (bending energy) and a fourth-order term (membrane energy). For small curvatures the fourth-order term can be neglected with respect to the quadratic one, recovering the linear plate/shell model, which admits a single stable equilibrium $K = K_T$. For large curvatures, the fourth-order term becomes predominant, and the minimizers of the energy tend to respect the *inextensibility* constraint det $K = g_T$. In this regime, approximate solutions can be obtained by considering an *inextensible model*, *i.e.* looking for minimizers respecting exactly det $K = g_T$. Interestingly enough, although derived under the moderate curvature assumptions, the solutions obtained by this model in the large curvature regime are in good agreement with the almost uniform equilibria obtaining with a fully nonlinear finite element simulation [J-SM13; MVV10].

- In general, the membrane and bending inelastic strains (e_I, K_I) do not respect any compatibility constraint $(\mathcal{L}(e_I) \neq \det K_I)$ and the shell does not have a natural "zero-energy" configuration. If the inelastic deformations are compatible $(\mathcal{L}(e_I) = \det K_I)$, the configuration with $K = K_I$ and $e = e_I$ is a stable equilibrium without residual stresses and attains the global minimum of the energy.
- The target gaussian curvature g_T may differ from the determinant of the target curvature K_T for two reasons: (1) the presence of an inelastic curvature K_I and (2) the presence of non-uniform inelastic membrane strain e_I .
- One can consider without loosing the generality the case $\beta = 1$: the solutions for $\beta \neq 1$ can be obtained from the solutions for $\beta = 1$ by a linear anisotropic rescaling of the curvature [see J-FMV10].

In the following, I report the results obtained with this reduced model in the framework of different applications for several combinations of inelastic strains, initial shapes and material properties. These results were obtained progressively and published in several papers.

2.1.2 Tristable shallow shells

Related publication: [J-VM08]



Figure 2.2: Tristable shells. (a) Phase diagram obtained with the extensible uniform curvature model as a function of the initial curvatures $K_{0x} - K_{0y}$ for $K_{0xy} = 0$ ($\beta = 0.977$, $\nu = 0.766$, $\rho = 1.965$) where dark grey tristability regions, light grey bistability, and white monostability. (b) Energy and equilibria of the extensible model for the four initial curvatures (A, B, C, D), where the white points denote the minima, the white-black point denotes the natural configuration and the initial curvature.

In [J-VM08], we considered the problem of finding the possible stable equilibria of shallow shells without inelastic deformations as a function of their initial shape and the material anisotropy. Referring to equations (2.17)-(2.1.1) this situation corresponds to the case $K_I = e_I = 0$, for which the energy (2.17) takes the form:

$$U(K) = \frac{1}{2}\tilde{D}(K - K_0) \cdot (K - K_0) + \frac{1}{2}(\det K - \det K_0)^2$$
(2.21)

Our interest in this problem was inspired by the works of Guest and Pellegrino [GP06] and Seffen [Sef07]. Seffen [Sef07] exhibits analytical solutions for isotropic shells for a specific class of initial curvatures. He showed that, depending on the initial curvature, the shell can have up to two stable equilibrium shapes with (almost) uniform curvature. Studying the number of local minima of (2.21) as a function of the initial curvature in the coordinate direction K_{0x} and K_{0y} (see Figure 2.2(a)) we showed that an orthotropic shell may exhibit up to three stable equilibria, as represented in Figure 2.2(b). Further insight can be obtained considering the large curvature limit. Using an inextensible model, where the bending energy of the shell is tristable over the curvature manifold respecting the inextensibility constraint det $K = \det K_0$, we studied how the regions of tristability depend on the initial curvature and the material parameters. The analytical results conclude that the range of initial curvature leading to tristability may be enlarged by conceiving orthotropic shells, where the Young moduli ratio β and the Poisson ratio v approach the degeneracy condition $\beta = v^2$, provided that the shear modulus ρ is large enough to prevent twisting instabilities. In collaboration with Angela Vincenti [MVV10], we showed that this kind of effective material properties may be obtained considering a suitable stack of fibre-composite laminae. Our work attracted the interest of several other groups. Notably, Keith Seffen in Cambridge and Paul Weaver and co-workers in Bristol [Cob+13] were able to confirm our theoretical prediction showing experimental prototypes of tristable shells (see Figure 2.3). Some of our results were further exploited by Giomi and Mahadevan [GM12] to study the interesting case of anisotropic elastic strips.

2.1.3 Actuation of multistable plates with inelastic curvatures

Related publication: [J-FMV10]

In initially flat multilayered plates, the mismatch of the inelastic strains at different layers may induce residual stresses responsible for bifurcation phenomena and multiple stable equilibrium positions. Similar effects are well documented, being encountered in various applicative contexts, including unsymmetric composite laminates [Hye81a; Hye81b; Mat+07; GWP04], thinfilm/substrate systems extensively used in microelectronic applications, MEMS, thin-film coatings [FS96; Fre00; ZD04], biological systems [For+05; DB08]. In composite structures, a classical example of bistability is an asymmetric [0/90] laminate, made of two fibre-reinforced layers (carbon fibres in an epoxy matrix) oriented in orthogonal directions. During the curing process, the two layers are pressed together at high temperature. The cooling to the room temperature induces antagonistic contractions that can be modelled as opposite inelastic curvatures in the two coordinate directions [Hye81b] and cause bistability.

The uniform curvature model may account for similar phenomena in plates by setting in equation (2.17) $K_0 = 0$ (a plate is a flat shell) and $e_I = 0$ (no membrane inelastic deformations). In this



Figure 2.3: Experimental prototypes of tristable shells obtained confirming our theoretical prediction presented in [J-VM08]. The main technical difficulty is to fabricate the curved shell with the "limit" orthotropic material properties according to the design rules we obtained analytically. Left: Tristable shell obtained using waived tissues, courtesy of Keith Seffen and Evros Loukaides (Cambridge University). Right: tristable shell obtained using laminate composites, courtesy of Paul Weaver and co-workers (Bristol University) [Cob+13].



Figure 2.4: Number of stable equilibrium of a flat plate with inelastic curvature $K_{Ix} - K_{Iy}$, assuming $K_{Ixy} = 0$. The plot is for a plate with the stacking sequence in Figure 2.6, giving a relatively low shear stiffness. Right: general diagram showing the different behaviour for positive and negative Gaussian curvatures. Left: zoom for negative Gaussian curvature and two-parameter actuating path for passing from equilibrium configuration to the other without dynamic snap through.

case the equilibrium equations (2.19) read as:

$$K_x - K_{Ix} + \mu(K_y - K_{Iy}) + K_y \det K = 0, \qquad (2.22a)$$

$$K_y - K_{Iy} + \mu(K_x - K_{Ix}) + K_x \det K = 0,$$
 (2.22b)

$$2K_{xy}(\det K - 2\rho(1 - \nu^2)^2) = 0.$$
 (2.22c)

Figure 2.4 reports a phase diagram with the number of stable equilibria obtained for each combination of inelastic curvatures $K_{Ix} - K_{Iy}$, assuming $K_{0xy} = 0$ (untwisted inelastic deformations). The boundaries between the mono- and bi-stable regions are critical points where one stable equilibrium becomes unstable, or vice versa. These critical points are characterised by giving at least one vanishing eigenvalue of the Hessian matrix H defined in (2.20). Hence, they verify simultaneously the equilibrium equations (2.19) and the criticality condition det(H) = 0. The associated system of equations, can be solved analytically, locating the stability margins and the points Q and P^{\pm} in Figure 2.4. Looking at the null-space of the Hessian matrix, it is possible to show that the parabolae having the points Q as vertices are associated to twist instabilities, whilst the cusps with the vertices P^{\pm} correspond to an instability in the plane $K_x - K_y$, without twist. The distance between the points P^+ and Q depends on the shear stiffness and the two points coincide in the isotropic case. Analytical expressions for the curvature at the equilibrium can be obtained for the case of equal $(K_{Ix} = K_{Iy} = h)$ or opposite $K_{Ix} = -K_{Iy} = h$ inelastic curvatures, corresponding to the bisectors of the phase diagram in Figure 2.4. The results are graphically reported in Figure 2.5, showing two different types of bifurcations: without twist for plates with negative gaussian curvatures and with twist for plates with positive gaussian curvature. The case of opposite curvature of Figure 2.5b coincide with the asymmetric [0/90] laminate described above and studied by several authors through simplified models and finite element computations. Our analysis gives a more complete and global understanding of the behaviour of the system for arbitrary inelastic curvatures and material parameters. In light of this global phase portrait, we study in [J-FMV10] possible actuation techniques for controlling the transition of the plate between its two stable configurations. The effect of the active layers can be assimilated to added stiffness and added inelastic curvatures, the latter begin controlled by the applied electric voltages. We considered the applicative case of a laminated plate with the stacking sequence at the top of Figure 2.6, including two Macro-Fibre-Composite (MFC) piezoelectric layers with unidirectional actuation. The thermally induced inelastic curvature after curing is given by the point A in Figure 2.4b, at which the plate is bistable. We show that with a suitable two-parameter actuation (path ACDE in Figure 2.4b), it is possible to get a controlled quasi-static transition between the two stable equilibria, avoiding any instability phenomenon. Numerical simulations on a realistic case study support the technological feasibility of the proposed actuation technique and the agreement of finite element simulations and the results of the simplified uniform curvature model (see Figure 2.6). The use of a multiparameter actuation may open interesting perspectives in the shape control of nonlinear structures through embedded actuation.



Figure 2.5: Curvatures at the equilibrium as a function of the inelastic curvature for opposite-sense (reft, $K_{Ix} = -K_{Iy}$) and equal-sense (right, $K_{Ix} = K_{Iy}$) actuation. The bifurcation is without twist ($K_{xy} = 0$) in the first case and with twist ($K_{xy} \neq 0$) in the second.



Figure 2.6: Two-parameter actuation of a bistable plate. Left: stacking sequence including active piezoelectric layers with directional actuation (MFC). Right: curvature at the equilibrium when varying the inelastic curvature along the path on Figure 2.4 through piezoelectric actuation. Continuous line: result of the uniform curvature model; Dashed lines: result of fully nonlinear finite element simulations (Abaqus) with different type of imperfections.



Figure 2.7: Comparison of the largest out-of-plane displacements, d, on the edge of a circular disk subjected to bending (left) and extensional (right) growth. The disk has radius a = 0.1 m, thickness t = 0.001 m, and the material is isotropic with Poisson ratio v = 0.3. Solid lines are theoretical predictions from the uniform curvature model [J-SM13] while the dots are results extracted from a nonlinear finite element analysis (FEA).

2.1.4 Growth and shape control of disks by bending and extension

Related publication: [J-SM13]

Bending actuation produced in layered plates by mismatches of the inelastic strain of different layers is the classical technique used in engineering to generate out-of-plane distortions of an initially flat surface. However, the complex and beautiful three-dimensional shapes of many thin natural systems, as plant leaves or organs, can be explained by differential *membrane growth* [KES07; DB08]. In [J-SM13] we compare this two different actuating techniques by considering the case a initial flat disk with bending (K_I) and membrane (e_I) inelastic deformations, representing the two possible actuating modes. To compare the two actuation – or growth – modes one can consider an homogeneous disk with the following three dimensional distribution of inelastic deformations

bending actuation:
$$e_I^{3D}(x, y, z) = 2\frac{z\bar{\varepsilon}}{t} \Rightarrow K_{Tx} = K_{Ty} = \frac{2\bar{\varepsilon}}{t} g_T = 0,$$
 (2.23)

extensional actuation:
$$e_I^{3D}(x,y,z) = -\bar{\varepsilon} \frac{x^2 + y^2}{a^2} \Rightarrow K_{Tx} = K_{Ty} = 0, \ g_T = \frac{4\bar{\varepsilon}a^2}{t^2}, \ (2.24)$$

where z denotes the distance from the mid-plane. In both cases $\bar{\epsilon}$ represents the maximum actuation strain. A comparison of the maximum of out-of-plane displacements obtained with the two actuation modes is reported in Figure 2.7. These results clearly show the different shape induced in the two cases: cylindrical for bending growth and with non-zero gaussian curvature for extensional growth. They also show the very good, and somehow unexpected, agreement between the finite element results (Abaqus geometrically nonlinear shell model) and our extremely simplified model, assuming uniform curvature and von Karman kinematics. Our theoretical and numerical analysis concludes that there is a definite regime for which the extensional actuation can produce larger displacements than bending actuation with the same maximum actuation strain $\bar{\epsilon}$. It also points out the possible advantages of combining the two actuation modes [see J-SM13].



Figure 2.8: Shortening of an initially circular cylinder made of agar gel when immersed in toluene. Experimental observations are compared with theoretical predictions when varying the initial radius ρ_0 in the range 0.45 to 2mm, for different values of the shear modulus μ .



Figure 2.9: Rounding of the edges of an initially square based prism made of polyacrylamid gel, immersed in silicone oil. Experimental data are compared to results of finite element numerical simulations.

2.2 Capillary shaping of soft beams

Related publication: [J-Mor+13]

Serge Mora performs in Montpellier (Laboratoire Coulomb) interesting experiments using extremely soft hyperelastic gels to study the effect of capillarity in solids, a subject that received increasing attention in the last years. With Basile Audoly, we collaborated with him and Yves Pomeau to study the change in shape of soft rods immersed in a liquid through experimental, theoretical, and numerical techniques [J-Mor+13]. When the solid is sufficiently soft, capillary effects may be sufficiently strong to generate visible deformations at the macroscopic scale. Hence, they can be used to effectively shape, or actuate, mechanical structures.

Preliminary observations show that rods with circular cross-sections made of Agar gels (almost incompressible, shear module $\mu \sim 50 \div 500$ Pa) significantly shorten when immersed in a liquid



Figure 2.10: Bending of a triangular prism immersed in a fluid. The uniform surface stress induces a non-zero bending moment because the centroid H of the cross-section is distinct from the centroid G of its boundary (a). The results of nonlinear finite element simulations are compared with the experimental observations and the results of a linearised model (b,c).

(toluene or silicon oil). The phenomenon can be explained by using a hyperelastic material model including a surface energy to account for the effect of capillarity at the interface between the fluid and the solid. Hence, adopting a Neo-Hookean incompressible model and a Lagrangian approach, equilibrium shapes of a solid occupying the domain Ω in its natural reference configuration can be obtained by studying the minimisers of the following energy functional

$$\mathcal{E}(u) = \underbrace{\int_{\Omega} \frac{\mu}{2} (\operatorname{tr}(F^{T}F) - 3) dx}_{\text{Bulk energy}} + \underbrace{\gamma \int_{\partial \Omega} \left\| \det(F) F^{-T} n \right\| ds}_{\text{Surface energy}},$$
(2.25)

where $F = I + \nabla u$ is the gradient of the transformation and *n* is the normal to the boundary $\partial \Omega$ of the reference configuration. This simple model introduces only two material parameters, the shear modulus μ and the surface energy density γ , that define an intrinsic length scale in the nonlinear regime, the *elasto-capillary length* γ/μ . Note that, differently from Griffith models of fracture, here the surface energy is proportional to the area of the *deformed* boundary. For rods of circular cross-section it is possible to solve the problem analytically, neglecting boundary effects. Figure 2.8 reports a comparison between the experimental and theoretical findings when varying the radius and the shear modulus μ .

To solve the problem for more complex geometries we developed a finite element code on the basis of the FEniCS library¹. For rods with square cross-sections, in addition to the axial shortening, one observes an interesting change in shape of the cross-section, with rounding of the corners. Adopting a global measure of the sectional change in shape, we obtained a very good agreement between experimental results and three-dimensional finite element simulations (see Figure 2.9). Further numerical investigations disclosed also a new phenomenon that was successively verified experimentally: when the cross-section of the rods has fewer symmetries the capillary forces may generate bending. Figure 2.10 reports the corresponding results for the

¹To bypass the well-known locking problem encountered in the finite element simulations of incompressible solids, the numerical work is based on a mixed formulation and an almost incompressible model.

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case of a triangular cross-section. I refer the reader to [J-Mor+13] and its supplementary material (including the code used for the simulations) for further details on this subject.

Publications

In the electronic version, click on Link to PDF to obtain the pdf file of the article.

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Shape-change and multistability of slender elastic structures

Chapter 3

Conclusions and perspectives

3.1 Summary and comments

The works presented in this manuscript deal with two main subjects: damage and fracture of brittle solids and multistability of shallow plates and shells.

In fracture, I studied a general class of damage models with gradient on the damage variable. These models generalize the variational regularization of the Griffith model proposed by Bourdin et al. [BFM00] and give to it a precise mechanical interpretation. The bifurcation and stability analysis of their quasi-static rate-independent evolution problem allow us to explain and quantitatively predict their main properties and the influence of the constitutive assumptions [PMM11]. Models with stress-softening exhibit a limit stress, at which homogenous solutions bifurcate toward localized solutions. If the local dissipation at complete failure is finite, each localization implies a well-defined dissipated energy, which can be identified to the fracture toughness of the material. In this sense, strongly brittle gradient-damage models with stress-softening can be regarded as energetically equivalent to the Griffith model. Damage irreversibility plays an important role in the formulation and the analysis. Being essential to preserve thermodynamical consistency and to account for the energy dissipation, it implies a formulation based on variational inequalities that naturally leads to the establishment of the damage criterion in the form of Kuhn-Tucker conditions. The one-dimensional analysis allows us to improve the classical Ambrosio-Tortorelli functional used in regularized models of fracture. We establish a precise link between the internal length introduced in the damage models and the critical stress of the material, providing useful criteria for the identification of the material constants [Pha+11]. These fundamental studies in a one-dimensional setting were performed in the framework of the theses of Kim Pham and Hanen Amor, that I co-supervised with Jean-Jacques Marigo. At the same time, I worked on the extension of the available numerical implementations to efficiently apply the new models in two- and threedimensional contexts, including the effects of unilateral contact at the lips of cracks subjected to compressive stress [AMM09]. I promoted several research projected (CNRS/PICS exchange program, Emergences-UPMC, ANR T-shock) aimed at the understanding of the morphogenesis and the propagation of complex, almost periodic crack patterns. Being among the most fascinating manifestations of fracture phenomena in everyday life, similar problems constitute also an ideal framework to exploit the advantages of the variational approaches to the prediction of crack nucleation and the description of complex crack topologies. I focused my attention on two spe-

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cific situations, which are relevant for applications: thin film fracture and thermal-shock cracks. Thin film fracture was the object of the Ph.D. thesis of Andrés A. Léon Baldelli. In collaboration with applied mathematicians, we were able to derive from three-dimensional brittle fracture a two-dimensional membrane model including transverse fracture of the film and debonding from a substrate. We also proposed efficient numerical solution strategies [Leo+14] and derived analytical solutions in a simplified one-dimensional setting [Leo+13]. In the thermal shock problem we disclosed a generic mechanism leading to the formation of periodic crack patterns through a bifurcation analysis of the gradient damage models [SMM14]. We obtained a good qualitative and quantitative agreement between numerical results, semi-analytical studies, and experimental evidences, providing a verification and validation of the proposed modeling approach and hopefully contributing to the understanding of this complex physical problem [Bou+14]. These works, including important numerical development and large-scale numerical simulations, were performed in the framework of a long-term collaboration with Blaise Bourdin.

In my works on multistable structures, I studied problems related to shape control and multiparameter actuation of geometrically nonlinear bucked beams, and prestressed orthotropic plates and shells. These works are mainly based on extremely simplified models allowing for a full analytical treatment. In particular, in collaboration with Stefano Vidoli (La Sapienza), we proved that orthotropic shells may show up to three stable equilibrium positions with almost uniform curvature [VM08]. More in general, we showed how prestress, initial curvature and material parameters influence the number and type of stable equilibrium configurations. With Amancio Fernandes (d'Alembert), we investigated the application of this approach to the multiparametric actuation of composite bistable plates through active piezoelectric layers [FMV10], extending the results of a preliminary study on buckled beams [MPV07]. With Keith Seffen (University of Cambridge, UK), we investigated how the shape of an initially flat disk can be controlled through extensional or flexural actuation [SM13]. Our results show that in some regimes the extensional actuation mode, at the origin of the complex shapes of many biological thin systems, may be competitive with respect to bending actuation, commonly used in engineering structures. The analytical results obtained by extremely simplified discrete models are shown to be in a good agreement with fully nonlinear finite element simulations for a surprising large range of curvatures [FMV10; SM13].

At d'Alembert I had the chance to constantly interact with several collogues working on the stability of nonlinear slender structures. With Sebastien Neukirch and Joël Frelat, we studied the vibrations of post-buckled rods, emphasizing steep variations of the natural frequencies in the almost inextensible limit [Neu+12]. More recently, with Basile Audoly, Serge Mora, and Yves Pomeau, we studied the capillary deformations of soft hyperelastic rods immersed in a fluid. With theoretical, experimental, and numerical analysis we show that, depending of the cross-sectional shape, surface stresses can induce macroscopic axial stretching, rounding of sharp edges, and bending [Mor+13].

Almost all the works presented in this manuscript are based on models formulated through a variational energetic approach. Although this approach can involve some limitations and should not be regarded as an universal paradigm, it remains my preferred tool and my natural way of thinking when dealing with a new problem. First, it allows for a concise presentation of the mathematical model and to clearly identify the underlying modeling assumptions. Moreover, it constitutes the ideal departure point for the mathematical analysis of the problem and the develop-

ment of numerical solvers or simplified models. Finally, the energetic formulation is also a very effective means to understand the qualitative properties of the system. Namely, the formal use of the direct method of the calculus of variations provides an invaluable tool for an easy identification of asymptotic regimes, competing phenomena, and possible mathematical issues of the model. The case of fracture mechanics is exemplar, showing that the variational approach constitutes also a bridge between the communities of theoretical mechanics, computational physics, and applied mathematics.

Computational aspects progressively took an increasing important role in my research. The initial motivation came from fracture mechanics, where the simultaneous development of theoretical and numerical aspects is of great importance for the understanding of complex phenomena and the establishment of effective models. Progressively, I passed from the use of commercial finite element packages or simple numerical codes in Matlab or Mathematica to the development of customized high-performance parallel finite element codes based on advanced open-source computational tools. A similar passage demands a substantial investment of time and energies, which is only partially valorized in academic publications. However, I regard it as important for several reasons. The most obvious advantages are to gain a complete control on the computational toolchain, to be able to implement customized models performing more efficiently more complex computations, and to free oneself by commercial license restrictions and the relative costs. In my experience, additional significant benefits include also the possibility to diffuse the outcome of the research through open-source software and to interact with the open and multidisciplinary community of scientists in applied mathematics, physics, and computational science that contributes to open-source libraries for scientific computing.

3.2 Perspectives

After my Ph.D. thesis I radically changed my research topics to respond to a personal need for studying diverse physical problems with new approaches, methods, and techniques. I do not feel the same need for a sharp discontinuity at this moment of my career. My aim is to gradually enrich my current research activities in the broad realm of nonlinear solid mechanics and computational mechanics. I present below some perspective on variational models of fractures and on multistable structures, proposing few specific topics that I would like to develop in the next years.

3.2.1 Fracture and damage mechanics

Nowadays, models coming from variational regularizations, commonly denoted as phase-field models, are widely regarded as one of the most promising approaches for the effective simulation of complex fracture phenomena. They are the object of several plenary talks and specific sessions in the main international conferences on fracture and computational mechanics, with an increasing number of researchers contributing to their development.

Variational approaches represent a genuine advance in the field of computational and theoretical fracture mechanics, and open the possibility to revisit many classical problems of fracture for which classical approaches show clear limitations. The works on thermal shock and fracture of thin films presented in this manuscript furnish an example of my efforts in this direction. Further

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interesting open problems include fracture in anisotropic materials and fracture in heterogeneous structures. Some preliminary works have been published very recently, see [Li+14] and [Hos+14], but are far from being exhaustive. The investigation of the dynamic fracture, including crack branching and multiple wave reflections, is another extremely interesting potential application. The numerical developments required to include inertial effects in the simulations are straightforward and several published works include them in the presented numerical results [Bor+12; HM13]. However, dynamics introduces formidable difficulties from the theoretical point of view and the available models are neither validated against experimental data nor verified against theoretical predictions. Extending the models to include the effect of *multi-physical couplings* (e.g. electromechanical) or *geometrical nonlinearities* is quite simple from the point of view of the formulation and the development of the associated numerical codes [DLM07; AA12]. However, the theoretical analysis, verification, and validation in these complex contexts is much more difficult. In my opinion, the relative ease of the use of the variational regularizations to include new complex physical effects is at the same time a feature and a potential hazard. The risk is to neglect theoretical investigation, mathematical analysis, and verification of the numerical results and consequently miss the peculiarities at the origin of the success of this approach.

The available models are still unsatisfactory for many aspects and fundamental efforts should certainly be directed to their improvement. The ability to correctly model the failure of solids submitted to *compressive stresses* is one of the fundamental limitations. The approach that we proposed [AMM09] and the others available in the literature [FR10; LR09; DLM07] are able to introduce an asymmetric behavior in traction and in compression and avoid the interpenetration of the crack lips. However, they are affected by some numerical pathologies and none of them is able to quantitatively reproduce the behavior of real materials. For example, they do not reproduce the large difference between the strength in traction and in compressive stresses. I am currently working on these issues, by improving the numerical implementations and adding cohesive effects through damage-controlled plasticity. Further improvements may consider the introduction of separate damage variables for cracks in traction and in compression, as in [Com01]. The appropriate modeling of *brutal propagations* is another open issue. The introduction of dynamical and viscous effects appears as the natural solution. However, dynamics introduces new difficulties and its effect is far to be clear, as discussed in the previous paragraph.

The ideas presented above constitute interesting and challenging subjects for future works that fit in the spectrum of my research plans for the next years. In general, my aim is to maintain an equilibrated balance between theoretical and numerical developments, promoting the interactions with the community of applied mathematics. I would like to support, whenever possible, complex numerical simulations by careful theoretical studies in a simplified setting, as done in the works on the stability and bifurcation analysis of damage models, on thin film fracture, or on the multistability of plates and shells. I think that this approach is essential to understand the properties of highly nonlinear systems, select useful models, and provide a reference for the verification of the numerical codes. I report below a list of selected specific topics on which I am currently working or constitute my next priorities. Cohesive models. The variational approach to fracture proposed by Francfort and Marigo and the other phase-field models proposed by physicists regard the Griffith model of fracture as the reference model and adopt regularizations techniques to solve it numerically. The corresponding regularized models can be interpreted as gradient damage models that turn out to be richer than the Griffith model and more adequate to model the real behavior of brittle solids. In particular, they naturally include an internal length, they correctly account for the fact that the maximum allowable stresses in the material are finite, and they are able to reproduce crack nucleation in a solid without initial cracks or defects (the three properties are correlated). For this reason, we currently regard the damage model as the *model* and the Griffith model as the *approximation*, to use the words of [FR10]. A possible alternative to recover the key qualitative features of crack nucleation is to enrich the Griffith model by considering more complex surface energies including cohesive effects. Nonetheless, the numerical implementation of cohesive models for arbitrary crack paths is far from be straightforward. Variational regularisations of cohesive models are then attractive on the numerical point of view. Few recent works deals with this topic, namely [LCK12; VdB13] in computational mechanics and [DI13; Iur12] in applied mathematics. The works [DI13; Iur12] are particularly interesting. Studying the asymptotic behavior of gradient damage models with several small parameters, for example a residual stiffness and an internal length, they show that several models can be obtained in the limit when varying the asymptotic ratio between the different parameters. The limit models include the Griffith model, cohesive models, or perfect plasticity. I think that it would be extremely interesting to further analyze this works from a mechanical perspective and compare them to the those proposed in [LCK12] and [PMM11]. That can be done first by semi-analytical studies in a one-dimensional setting and then through numerical investigations in two dimensional situations, including smooth crack propagation and crack nucleation from a wedge.

Coupled damage and plasticity. The work presented here on the variational approach to fracture are limited to the brittle case and do not consider the effect of plasticity. It is well known that plasticity admits a similar variational formulation [Suq81; DDM06]. Recently, a coupled damage-plasticity model have been proposed and analyzed in a one-dimensional context by Alessi et al. [AMV14]. I am currently collaborating with Roberto Alessi to extend the current numerical formulation for damage to include the effect of plasticity and perform relevant tests in the two-dimensional context. The aim to understand the interplay between the two phenomena and the effect of multi-axial stresses in classical tests.

Fracture of tempered glass and laminated plates. Tempered glass plates are used for their increased strength and for breaking in smaller, less dangerous, fragments than standard glass. This behavior is obtained by inducing high compressive stresses in the external surfaces by suitable thermal or chemical treatments. Besides the classical application in architectures, this procedure was recently the subject of active applied research to obtain extremely thin glass plates with exceptional fracture properties to be used in portable electronic devices. The fabrication is mainly based on empirical experimental data. The scientific literature on the the theoretical and numerical aspects seems to be surprising limited [Le 14]. With Blaise Bourdin, we plan to extend our previous works on thin film fracture and thermal shock cracking to this interesting application. The phenomenology is for many aspect similar to our previous works on thin films, including a multilayered thin structure with a brittle layer (the central region submitted to traction stress)

constrained to a tough layer providing a high residual stiffness (the external highly compressed skin). I plan to study this applicative problem through a brittle plate model with inelastic strain. The preliminary idea is to investigate the qualitative behavior obtainable with phenomenological models adopting equivalent-single-layer or more complex layer-wise plate kinematics, which is extended so as to include global or layer-wise damage variables. As done in the case of thin films, I think that interesting indications on the possible qualitative behaviors can be obtained through a semi-analytical study considering only membrane mode and a one-dimensional problem. This can allow the selection of meaningful models and their successive application to two dimensional contexts. One important goal would be to derive informations on the proserties of the fragmentation process, including the dependence of the critical stress on the prestress level, and the average fragment size. The further application of a similar modeling approach to the fracture of (isotropic) laminated plates can constitute a natural extension of great applicative interest. As done for the thin film problem, it would be interesting to attempt at the rigorous derivation of the relevant limit two-dimensional brittle models through asymptotic techniques. Extension to dynamical fracture to further investigate the fragmentation process would be particularly interesting.

Fracture of heterogenous media. With Laurent Ponson and Angela Vincenti (d'Alembert), we recently obtained the funding from the *Ville de Paris* of a four-year project on the fracture of heterogenous media. Laurent is an expert of the theoretical and experimental aspects of this topics while Angela focuses on composite structures and optimization. The fundamental aim is to investigate the role of heterogeneities in crack propagation and nucleation and conceive meta-material with enhanced fracture properties. To achieve this ambitious goal we plan to perform coupled numerical and experimental analysis on materials with controlled microstructures, that can now be easily fabricated using rapid prototyping techniques (3D printing and laser-cutting). For the numerical analysis, we plan to perform two-dimensional simulations using the gradient damage models presented in Chapter 1. A subtle issue in this framework is the correct modeling of the energy dissipation of the complex time-evolution encountered in heterogenous structures, which include crack arrest and and re-initiation. It may be pertinent to start the analysis in a simplified one-dimensional context, like the tearing adhesive strip with toughness or stiffness heterogeneities.

3.2.2 Morphing structures

Independently of the specific class of system under consideration (beams, strips, plates, shells or more complex structures), the design of multistable structures implies two key difficulties. The first is of theoretical/numerical nature: to perform the global stability analysis of nonlinear structures as a function of several parameters. The second is of practical order: to obtain structures with the desired material properties and actuation capabilities. I present below two aspects on which I plan to work that can partially address these issues. Part of these research plans are financed by the ANR project SLENDER (2014-1018). In this framework, I will supervise a Ph.D thesis (Mehdi Tha) starting in october 2014. In addition, with Basile Audoly, we are also aiming at studying singularities in thin shells and strips, a fundamental phenomenon that is still poorly understood. The numerical developments proposed below will provide useful tools to guide analytical investigations based on asymptotic techniques and simplified models.

Numerical developments. My former works on multistable structures are mainly based on the analytical study of extremely simplified models. For validation purposes I performed several simulations with commercial finite element packages (Abaqus) including supposedly reliable nonlinear shells models. The use of commercial software presents several limitations including the lack of control on the technical aspects of the implementation of the models and the solvers, the difficulty to implement novel models or solution approaches, the lack of the access to the source codes, the licence issues to run the code on several multiprocessor machines and to distribute the results of the research to external academic and industrial partners. I would like to benefit from the experience in computational methods acquired in my works on damage and fracture to develop finite element codes for the multiparametric equilibrium and stability analysis of geometrically nonlinear plates and shells. Reliable finite element formulations of shell models exist in the literature [CK03], however there are not available in reliable open-source high-performance scientific library. The main technical difficulties consist in managing the differential geometry of shells and obtaining convergence rates independent of the shell thickness by avoiding locking issues. With Jack Hale (University of Luxemburg), we are starting a project to implement MITC [CK03] elements in FEniCS. Our aim is to progressive obtain reliable implementation for linear plates, von Karman plates and nonlinear shells. This will allow us to fully control the numerical aspects of the study equilibrium and stability of plate and shells and further develop path-following techniques to define stability margins of equilibria as a function of more than one parameters. To this end I plan to use the approaches proposed in [Bag01; LC02], that solve augmented systems composed of the equilibrium equations and the critical conditions on the determinant of the Hessian matrix for the change of stability. I am also starting a collaboration with Patrick Farrell (University of Oxford) to apply to multistable structure a deflation technique he is developing to find multiple equilibria of a nonlinear system. I think that these developments can furnish useful tools for the analysis of nonlinear shells and the dependence of their multiple stable equilibrium solutions on several parameters.



Figure 3.1: Dimpled shell (courtesy of Keith Seffen, University of Cambridge). Each dimple is generated by plastic indentation and has two stable states, up and down. Different up/down patterns give different macroscopic properties and stable shapes. Vice versa, the state of the dimples evolves with the macroscopic loading, as in phase-transformations.

Phase transformations in geometrically nonlinear meta-materials. Seffen [Sef06] studied experimentally and numerically dimpled shells where the global properties, as the number and types of equilibria, are tailored by selecting appropriate patterns of the up/down states of the locally bistable dimples (see Figure 3.2.2); vice versa, loading the shells by boundary moments results in a series of local snapping of the bistable dimples. This system provides a particularly interesting example of a meta-material coupling non-linear phenomena and multistability at two different scales. It shows a macroscopic behavior assimilable to that of a material undergoing phase-transformations, where each material point has two (or more) stable states. As in shape memory alloys, several microstructural patterns can produce different macroscopic properties and, vice versa, macroscopic loading can induce microstructural phase transformations. I plan to systematically study similar systems in the framework of the thesis of Mehdi Tha (starting in october 2014) with the aid of simple discrete models, numerical simulations, and experimental prototyping. A simplified one-dimensional analogous of the dimpled shell is the chain of bistable springs studied by Puglisi and Truskinovsky [PT00]. The approaches and results furnished in [PT00] can furnish a first guide in our study, that can be gradually extended to the two dimensional case. Ideally, we will be able to use nonlinear homogenization techniques to obtain macroscopic models of phase transformations from the analysis of the discrete system formed by the chain, or network, of bistable elements. It can be interesting also to quantitatively correlate the dissipation in the macroscopic rate-independent model with the viscous dissipation associated to the local microscopic snaps. In collaboration with Arnaud Lazarus (d'Alembert), we plan to realize also prototypes of systems with periodic multistable microstructures with the aid of the rapid experimental prototyping tools available in our laboratory (laser cutter and 3D printers). We hope that this kind of studies can provide further theoretical insights on phase-transformation phenomena and useful tools to design surfaces with an interesting macroscopic behavior.

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