P 4 Identification of parametric energy functionals from linearly constrained evolutions of critical points (K. Bredies, M. Fornasier) → AO, NS, IS

This doctoral project aims at the identification of the energies governing certain time-dependent phenomena from data collected by observing the evolution of their critical points driven by time dependent linear constraints. We are particularly focusing on energies in continuum mechanics modeling fracture initiation and evolution.

State of the art. In the IGDK project "P 4: Lagrangian methods for constrained nonconvex minimizations and applications in fracture mechanics", we investigated robust and efficient numerical simulations of fracture evolution in brittle materials. The evolution is driven by the realization of the Griffith principle of energy balance between elastic energy and a fictitious crack energy under time dependent forcing conditions

$$u(t) \in \arg \min_{\substack{z \in SBV(\Omega), \\ z|_{\Omega_D} = g(t)|_{\Omega_D}}} \int_{\Omega \setminus S_z} |\nabla z|^2 dx + \kappa \mathcal{H}^{N-1}(S_z), \tag{1}$$

where $\Omega_D \subset \Omega$ is the domain of the force g, κ a suitable constant, and S_u is the *jump set* of the function $u \in BV(\Omega)$, modeling the fracture region, see [1] for an introduction to such free-discontinuity problems. The main advantage of this model proposed by Francfort and Marigo in [11] is that the functional setting in SBV does not require a pre-defined crack path. However, the minimization of the nonconvex and nonsmooth functional involving unknown functions and sets makes the numerical realization of (1) very challenging. A smooth phase field Γ-approximation of the energy functional is given by the Ambrosio and Tortorelli functional

$$J_\varepsilon(u, v) = \int_\Omega (v^2 + \eta)|\nabla u|^2 dx + \kappa \int_\Omega \left[\frac{1}{4\varepsilon}(1 - v)^2 + \varepsilon |\nabla v|^2 \right] dx. \tag{2}$$

for $0 < \eta \ll \varepsilon \ll 1$. The near-zero set of the minimizing function $v \in H^1(\Omega)$ can be interpreted as an approximation to the jump set S_u. The minimization of the approximating functional (2) can be realized now by an alternating minimization. Bourdin, Francfort, and Marigo showed in [7] that the discretization of such an alternating minimization can produce reliable fracture simulation only by using very fine grids, with consequent very large computational time, or meshes designed according to the expected crack evolution. Indeed any discretization is likely to produce a bias towards a proper fracture propagation. More recently Burke, Ortner, and Süli [8] proposed a fully adaptive scheme based on isotropic mesh refinements, leading though to the generation of extremely fine adapted meshes as reported in their paper. The results we obtained in the first phase of the IGDK, and included in the papers [2, 3, 4], are building upon the work [8], but using adaptive anisotropic *remeshing*. Relevant features of the adaptive anisotropic remeshing method are: 1. The number of degrees of freedom and the computational times are dramatically reduced, despite the remeshing; 2. The remeshing does not alter the energy profile evolution; 3. On the crack tip the automatically generated mesh is nearly isotropic and does not constitute an artificial bias for the crack evolution. As a consequence of 2. and 3. we obtain always physically acceptable crack evolutions beyond state of the art simulations. It remains still open to provide rigorous

proofs for the improved complexity 1. as well as for the more fundamental properties 2. and 3. In [9] the approximation (2) has been extended

$$J_{A,F,G}(u,v) = \int_\Omega (F(v)+\eta)A(\nabla u)dx + \int_\Omega (\varepsilon^{-1}G(v) + \varepsilon|\nabla v|^2)dx. \tag{3}$$

to include more general (possibly nonlinear) elastic tensors A, a smooth increasing function F with $F(0) = 0$ and $F(1) = 1$, and a smooth nonnegative function G such that $G(z) = 0$ if and only if $z = 1$. This new parametric energy is modeling different nonlinear elastic properties of a material as well as its fracture potential.

Thesis project to be supervised by Massimo Fornasier. Accurate simulations of fracture initiation and evolution need to have at disposal a reliable physical model. Despite the many attempts of deriving reasonable mathematical descriptions of fracture evolution (see [10] and references therein), the problem of validating the model with data from real-life evolutions remains a crucial step for future reliable simulations. In this project we build upon our robust numerical approach based on anisotropic mesh refinements [2, 3, 4] towards the identifications of the function parameters A, F, G appearing in (3). After discretization we can describe the problem of recovering A, F, G as follows. First of all we need to define a proper notion of evolution of critical points. Given two Euclidean spaces $\mathcal{E} \simeq \mathbb{R}^n$, $\mathcal{F} \simeq \mathbb{R}^m$ for $m \leq n$, and an energy function $J : \mathcal{E} \to [0, +\infty)$, we define a linear operator $A : \mathcal{E} \to \mathcal{F}$, and an absolutely continuous function $f : [0, T] \to \mathcal{F}$. A linearly constrained evolution of critical points relative to the energy function J and the linear constraint pair (A, f) is a bounded measurable time-dependent map $u : [0, T] \to \mathcal{E}$, with the following properties

- $Au(t) = f(t), \quad \text{range}(A^*) \cap \partial J(u(t)) \neq 0, \text{ for a.e. } t \in [0, T],$
- there exists a bounded measurable function $q : [0, T] \to \mathcal{F}$ such that $A^*q(t) \in \partial J(u(t))$,
- and the energy inequality

$$J(u(t)) \leq J(u(0)) + \int_0^t \langle q(s), \dot{f}(s)\rangle ds, \text{ for almost every } t \in [0, T],$$

holds. See [5, Section 4.3] for instances of such evolutions.

Let us now assume that the energy $J = J[a]$ depends on a *unknown parameter function* $a : \mathbb{R}^d \to \mathbb{R}$ (d can just 1 or be also very large as for (3) where a is modeling A, F, G) and we are allowed to observe evolutions of critical points of $J[a]$ relative to a linear constraint pair (A, f) where $f : [0, T] \to \mathcal{F}$ might also be unknown.
In this project we want to study the properties of the following *adaptive algorithm* to recover the function parameter a. Given an evolution of critical points $u(t) := u[a](t)$, compute for $\Lambda^n \subset \Lambda^{n+1}$ (approximating subspaces for the solution space of a)

$$a^\ell \quad = \quad \arg\min_{a \in \Lambda^\ell} \int_0^T \text{dist}(\text{range}(A^*), \partial J[a](u(t)))^2 dt, \quad \ell = n, n+1.$$

Then we retain from Λ^{n+1} only those degrees of freedom $\lambda \in \Lambda^{n+1} \setminus \Lambda^n$ such that

$$\|a^{n+1}_\lambda - a^n_\lambda\| \geq \varepsilon > 0.$$

This method gets inspiration from the work [6] by Binev, Cohen, Dahmen, and DeVore on adaptive methods for approximating nonlinear regression functions with underlying probability distributions on the data. Notice the following properties:

- This adaptive refinement $\Lambda^n \to \Lambda^{n+1}$ works as a *regularization* method towards the identification of a, see [12] for more about regularization by discretization;
- The discretization is *adapted* both to the amount of information on the parameter a extracted along the trajectory $t \to u[a](t)$ and to the *smoothness* of a.

There are plenty of issues to be addressed: For a given initial condition $u(0)$ of the evolution of critical points, how much information can be captured and recovered by the adaptive algorithm on the unknown function a? If we are allowed to pick initial conditions at random or according to a best strategy, how is our recovery of a improving? How the initial discretization of the problem to reduce it to a finite dimensional evolution of critical points does affect the approximation of a?

Further topics. Beside the identification of energies (3) in fracture mechanics, such a method finds additional potential applications also in

- Magnetic resonance fingerprinting ($\Rightarrow$ Kristian Bredies);
- Optical flow in video processing: in this case the time-dependent *force field* f transporting an image snapshot to the next needs to be determined;
- Social dynamics: the energy J represents social interaction potentials and a the "social forces" to be identified from observation of group dynamics;
- Optimal control: the parameters a or f are used as a control for the evolution of critical points.

We used this technique already for the identification of *social interactions* in multiagent systems, with exceptionally robust results.

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