0.0.1 Lagrangian Methods for Constrained Nonconvex Minimizations and Applications in Fracture Mechanics (M. Fornasier and K. Kunisch,) $\rightarrow$ AO, NS, IS

In this project we are concerned with two fundamental and interrelated topics:

Augmented Lagrangian Methods for linearly constrained *nonconvex* optimization;

Adaptive numerical methods for applications in fracture mechanics.

State-of-the-art. Minimizers of integrals in calculus of variations typically possess singularities. For problems arising from mechanics, such singularities may represent physically interesting instabilities [1]. Singular minimizers exist that model aspects, for instance, of solid phase transformations and certain modes of fracture. In most of the models encountered in the literature in elasticity theory the energy functionals to be minimized are *nonconvex* [1]. Convexification usually is applied in order either to show existence of global minimizers or to have numerically stable techniques to approximate them. Lagrangian methods have been extensively studied for the solution of constrained *convex* variational problems as well as control problems [15]. In fact, usually, the given problems have additional conditions, for instance boundary conditions, to be taken into account, which can be included in augmented Lagrangian. However, in nature, local minimizers play a pivotal role, as often evolution of physical phenomena proceeds along energy local minimizers. Hence, also the appropriate solution of genuinely constrained nonconvex problems is of the highest interest as well as the accurate numerical treatment of the singularities which are expected to characterize the minimizers.

In this project, we shall investigate specifically stable numerical methods for the simulation of brittle fractures, following the variational model proposed by Francfort and Marigo [13, 14]. This model is intimately related to the Mumford and Shah functional, proposed for image segmentation [1, 16]. One of the most popular methods to address the numerical minimization of such nonconvex functionals involving volume (bulk) and surface energies is by Γ-approximation with functionals where the surface energy is more easily handled in terms of a smooth indicator function of the discontinuity set of minimal solutions, as proposed in the Ambrosio and Tortorelli approximation [2]. However, very recent adaptive numerical implementations of this approximating model for fracture simulation [4] showed that such relaxation is highly unstable with respect to the approximation parameters, as it very likely creates several spurious local minimizers, resulting in unreliable simulations, unless the resolution of the adaptive finite element discretization is extremely fine. In these implementations, one discretizes and adaptively approximates by the finite element method the Euler-Lagrange equations of the Ambrosio and Tortorelli approximation. An alternative technique of approximation stems from discretizing directly the original functional. This leads to a different Γ-approximation (discrete to continuous) of the problem, as investigated by Chambolle et al. [3, 5, 6, 7]. However, except for very special situations, as for univariate problems [6], there are so far no polynomial complexity algorithms solving the nonconvex minimization for such discrete problems. In the recent paper [12] an algorithm has been proposed, which, for a fixed discretization, computes local minimizers in polynomial time, and it has the potential of being extended to multivariate problems. For such an extension one has to take into account that the nonconvex minimization has to be constrained to vectors representing derivatives, i.e., curl-free vectors. In fact the idea of the method is to transform the original discrete minimizing body displacement problem into an equivalent problem exclusively based on the minimization of the discrete derivative of the body displacement. The original body displacement solution is recovered from the computed derivatives by a suitable integration process, eventually based on the solution of a second order partial differential equation. The proposed algorithm produces iteratively by sharp *thresholding* a sequence of derivatives which are separated in two groups, one indicating jump discontinuities and the other indicating the smooth part of the solution. For a fixed mesh, one of the feature of this algorithm is to indicate in a finite number of iterations which discrete derivatives are associated to discontinuities, allowing for a very precise criterion for adaptive mesh refinement around the discrete discontinuity set.

The proposed adaptive algorithm is based on *sharp* iterative thresholding operations which identify the discontinuity of the fracture on the given mesh, potentially with better precision than the approximation by Ambrosio and Tortorelli. The hope is that the overall algorithm can perform more stably than the solution proposed in [4], producing more reliable fracture simulations. To investigate this strategy for an effective fracture simulation, we propose two theses, one developed in the first period of the IGDK and the other addressed by a student of the second generation of the IGDK.

First thesis project to be supervised by Massimo Fornasier.

In this part of the project we shall formulate a general augmented Lagrangian method for linearly constrained nonconvex minimization, as a generalization of similar algorithms for convex problems [9, 15]. We shall investigate its convergence properties to local minimizers of Lipschitz nonconvex objective functions under the given linear constraint. For discretizations of classical free-discontinuity models, such as the Mumford and Shah functional for image segmentation, it will be necessary to generalize the iterative thresholding algorithm [12] for working on general anisotropic meshes and on multivariate domains, by applying the results of the first part of the thesis. The analysis of the resulting algorithm in terms of its convergence to local minimizers, detection at fixed mesh size and at finite number of iterations of the free-discontinuity, possibly convergence rates will constitute the fundamental building blocks for the development of a fully adaptive finite element method which will be addressed in the second thesis. In order to perform large scale simulations a generalization of domain decomposition methods for convex optimizations as in [8, 10, 11] has to be addressed, both to handle the nonconvexity of the problem and the possible additional linear constraints.

Second thesis project to be supervised by Massimo Fornasier.

In this second part of the project, we will strongly rely on the analysis of the algorithms proposed in the first thesis, in order to define robust criteria, based both on a posteriori free-discontinuity detection and error indicators, for refining the mesh. On the basis of such indicators, we shall investigate the formulation of a fully adaptive algorithm and its convergence to local minimizers of the given problem, by means of Γ-convergence techniques, similarly to the approach in [3, 7]. The numerical implementation for fracture simulation and the assessment of the stability properties of the given algorithm, in comparison with the existing results [4], will be a crucial step of the thesis. In order to consider problems of realistic size, we shall combine adaptive refinements and domain decomposition methods, by taking advantages of the results of the first thesis.

Added value: The first thesis addresses problems of optimization, and it can rely on the expertise of both the supervisors M. Fornasier at the Technical University of Munich and K. Kunisch at the University of Graz. The subject of the second thesis started as a matter of joint investigation of M. Fornasier with Endre Süli at the University of Oxford, distinguished expert in numerical methods for partial differential equations, who will also contribute to the work. The analysis of the convergence of the adaptive algorithm requires clarifying which is the Γ-limit optimization problem eventually solved by the adaptive algorithm; this part will be developed in cooperation with Francesco Solombrino, PostDoc, expert in calculus of variations and geometric measure theory at the Johann Radon Institute of Computational and Applied Mathematics of the Austrian Academy of Sciences. The numerical implementation and the assessment of the results in fracture simulation, will be a fundamental part of the thesis work, which will surely take advantage of the long experience of E. Süli and other faculty members of the IGDK, in particular Boris Vexler and Barbara Wohlmuth.

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