Multi-scale Dynamics in Microstructures

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Summary. We consider a singularly perturbed, non-convex variational problem describing microstructures in one space dimension. The minimizers of the functional exhibit a complicated multi-scale behavior. We propose a dynamical systems approach to analyse the critical points of the functional by applying methods from geometric singular perturbation theory to the corresponding Euler-Lagrange equations. We prove the existence of periodic solutions which explain the observed multi-scale structures. Numerical computations based on AUTO (a software package for continuation and bifurcation problems in ODEs [3]) are performed in order to study quantitative properties and bifurcations of solutions as key parameters vary.

Geometric approach to a variational problem

The appearence of microstructures in special classes of materials (e.g, shape memory alloys) is the key to understand their properties. Most of the existing mathematical models aim at describing microstructures as minimizers of certain energy functionals. Our starting point is a singularly perturbed non-convex variational model in one space dimension studied by Müller [1], which describes the occurrence of simple laminates microstructures. These are particular structures where two phases of the same material (e.g., austenite/martensite) simultaneously appear in an alternating pattern (Fig. 1). Such models are however quite hard to analyze by variational techniques even in simple settings. We propose to use a dynamical systems approach based on geometric singular perturbation theory with the goal to obtain further insight, e.g. on critical points (not just the minimizers) of the functional. The asymptotic formula presented in [1] for the period of minimizing solutions is then confirmed by our analysis.

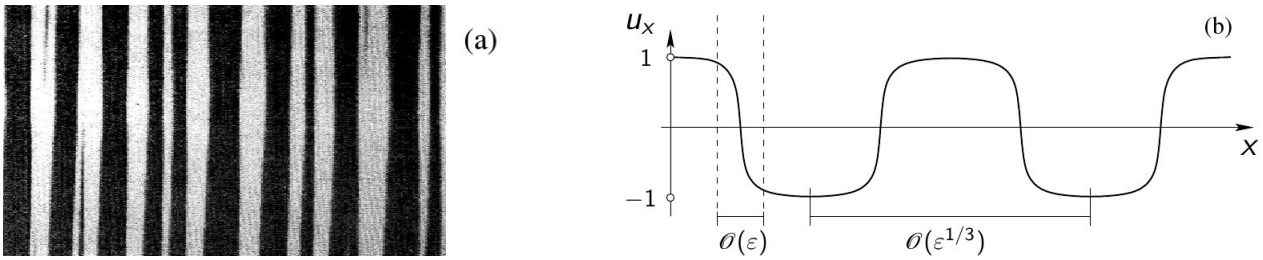

Figure 1: Simple laminates microstructures: (a) Microstructures in a Cu-Al-Ni single crystal: the main dynamics occur along one dimension. (b) Schematic representation as periodic solutions: u_x oscillates between ± 1, values representing the two different phases of the material.

Analysis of periodic orbits

The Euler-Lagrange equation associated to the energy functional is a necessary condition that critical points of the functional have to satisfy. Introducing new variables allows us to rewrite it as a 4-dimensional singularly perturbed Hamiltonian system of ODEs depending on a small parameter $0 < \varepsilon \ll 1$ with 2 slow and 2 fast variables. Microstructures can hence be interpreted as periodic solutions of this system. The existence of a family of periodic orbits $\{\gamma_\varepsilon^\mu\}$ parametrized by the value μ of the Hamiltonian for ε small can be proved as follows. First, a slow-fast analysis allows us to construct singular orbits ($\varepsilon = 0$) for every fixed value of the Hamiltonian. Then, using an argument based on [2], such orbits are proved to persist also for $\varepsilon \neq 0$.

Numerical continuation

Our analytical results are confirmed by numerical computations based on AUTO (a software package for continuation and bifurcation problems in ODEs [3]). In particular, we perform numerical continuation on the family of periodic orbits $\{\gamma_\varepsilon^\mu\}$ with respect to both parameters ε and μ (Fig. 2). The approach based on slow-fast systems allows us to geometrically identify certain classes of periodic orbits, which are needed as starting solutions for numerical continuation. Our results are in good agreement with Müller's [1] and show new, interesting patterns which require further investigations.

Conclusion and future work

Analytical and numerical study of a multi-scale model describing microstructures in one-space dimension is performed, with the aim of obtaining more insight on the rich structure of the minimizers. In future work, we aim to apply the techniques presented here to more general energy functionals.

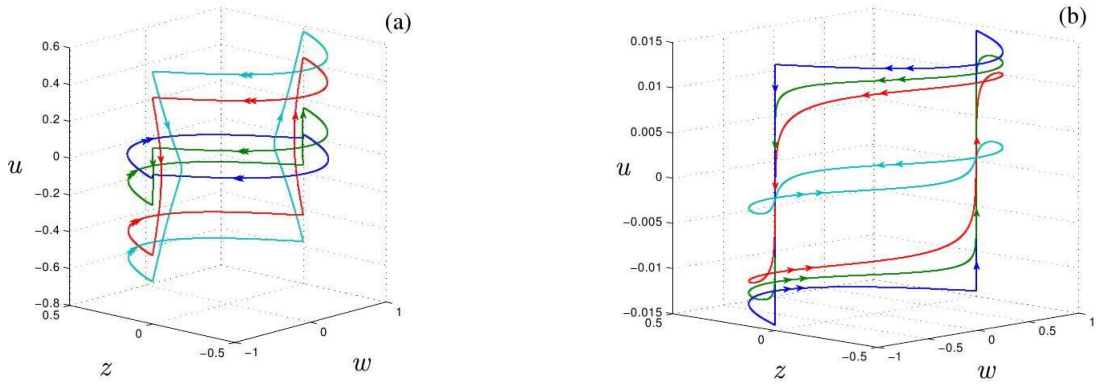

Figure 2: Numerical continuation with AUTO: (a) Continuation in μ ($\varepsilon = 0.001$) with decreasing values (from turquoise to blue): as μ decreases, the pattern becomes finer and finer, up to the limit $\mu = -\frac{1}{8}$, where the slow portions of the orbit reduce to two points. (b) Continuation in ε ($\mu \simeq -1/8$) (again decreasing values from turquoise to blue): as $\varepsilon \to 0$, the singular structure of the orbit becomes more and more evident.

References

[1] Müller S. (1993) Singular perturbations as a selection criterion for periodic minimizing sequences. *Calc. Var. Partial Differential Equations* **1**:169-204.

[2] Soto-Treviño C.(2001) A geometric method for periodic orbits in singularly-perturbed systems. *Multiple-time-scale dynamical systems* **122**:141-202.

[3] Doedel E. (1981) AUTO: a program for the automatic bifurcation analysis of autonomous systems. *Proceedings of the Tenth Manitoba Conference on Numerical Mathematics and Computing* **30**: 265-284.