Bartels, S.

Error Estimates for the Adaptive Computation of a Scalar Three Well Problem

We investigate the numerical approximation of Young measure solutions appearing as generalised solutions in scalar non-convex variational problems. A priori and a posteriori error estimates for a macroscopic quantity, i.e., the stress, are given. Numerical experiments for a scalar three well problem, occurring as a subproblem in the theory of phase transitions in crystalline solids, show that the computational effort can be significantly reduced using an adaptive mesh-refinement strategy combined with an active set technique by Carstensen and Roubíček.

1. Introduction

Non-convex variational problems occur in the theory of phase transitions in martensitic crystals, e.g., in shape memory alloys [2].

Infimising sequences for the corresponding typically non-convex energy functional show fast oscillations and this leads to the necessity of a natural extension of the problem. We use an extension that is constructed by means of Young measures.

A scalar subproblem of the mathematical model reads as follows.

$$(P) \qquad \begin{cases} \text{Minimise } I(u) := \int_\Omega W(\nabla u(x))\,dx - \int_\Omega f(x)u(x)\,dx \\ \text{subject to } u \in W^{1,2}(\Omega),\ u|_{\partial\Omega} = u_D|_{\partial\Omega}. \end{cases}$$

Here, $\Omega \subseteq \mathbb{R}^n$ is a bounded Lipschitz-domain, $W^{1,2}(\Omega)$ is the standard Sobolev space, $u_D \in W^{1,2}(\Omega)$ is some given boundary data, $f \in L^2(\Omega)$ is a given force, and $W : \mathbb{R}^n \to \mathbb{R}$ is a given continuous energy density satisfying $c|F|^2 - C \le W(F) \le C(1+|F|^2)$, $F \in \mathbb{R}^n$, for constants $c, C > 0$. Note that I is not weakly lower semi continuous if W is not convex so that we can, in general, not expect existence of solutions [2, 5]. If we consider a crystal in the austenite phase with three tetragonal variants then W can be modelled, with $F_1, F_2 \in \mathbb{R}^n$ given, by

$$W(F) = \min\{|F|^2, |F-F_1|^2, |F-F_2|^2\}, \quad F \in \mathbb{R}^n. \tag{1}$$

This specific energy density leads to a three well problem.

2. Relaxation of (P) and its Discretisation

Young measures are weakly measurable maps from Ω into the space of probability measures $PM(\mathbb{R}^n)$ on $\mathbb{R}^n$ and are denoted by $YM(\Omega;\mathbb{R}^n)$ [1, 5]. A relaxation of (P) reads as follows.

$$(GP) \qquad \begin{cases} \text{Minimise } \overline{I}(u,\nu) := \int_\Omega \int_{\mathbb{R}^n} W(F)\,d\nu_x(F)\,dx - \int_\Omega f(x)u(x)\,dx \\ \text{subject to } \nabla u(x) = \int_{\mathbb{R}^n} F\,d\nu_x(F) \quad \text{f.a.a. } x \in \Omega, \\ \qquad\qquad u \in W^{1,2}(\Omega),\ \nu \in YM(\Omega;\mathbb{R}^n),\ u|_{\partial\Omega} = u_D|_{\partial\Omega}. \end{cases}$$

Problem (GP) admits a solution which is the weak limit of an appropriate infimising sequence for (P). In [4, 5] the following discretisation of (GP) is proposed for a regular triangulation $\mathcal{T}$ of Ω and a uniform discretisation of $\mathbb{R}^n$ with mesh-size $d > 0$.

$$(GP_{d,h}) \qquad \begin{cases} \text{Minimise } \overline{I}(u_h,\nu_h) \text{ subject to } \nabla u_h(x) = \int_{\mathbb{R}^n} F\,d\nu_{h,x}(F) \quad \text{f.a.a. } x \in \Omega, \\ \quad u_h \in \mathcal{S} := \{v_h \in C(\overline{\Omega}) : \forall T \in \mathcal{T},\, v_h|_T \text{ affine}\}, \\ \quad \forall T \in \mathcal{T},\, \nu_h|_T = \sum \theta_i^T \delta_{S_i},\ \theta_i^T \in \mathbb{R}_{\ge 0},\ \sum \theta_i^T = 1,\ S_i \in d\mathbb{Z}^n,\ u|_{\partial\Omega} = u_{D,h}|_{\partial\Omega}. \end{cases}$$

The Dirac measure δ_{S_i} is for $S_i \in \mathbb{R}^n$ defined by $\int_{\mathbb{R}^n} W(F)\,\delta_{S_i}(F) = W(S_i)$. The pair (u_h, ν_h) is a solution of $(GP_{d,h})$ if and only if there exists a multiplier $\lambda_h \in L^\infty(\Omega;\mathbb{R}^n)$ elementwise constant such that [4, 5]

$$\max_{S \in d\mathbb{Z}^n} (\lambda_h(x)\cdot S - W(S)) = \int_{\mathbb{R}^n} (\lambda_h(x)\cdot F - W(F))\,d\nu_{h,x}(F) \quad \text{f.a.a. } x \in \Omega \tag{2}$$

$$\text{and} \quad \int_\Omega (\lambda_h(x)\cdot\nabla v_h(x)\,dx - f(x)v_h(x))\,dx = 0 \quad \text{for all } v_h \in \mathcal{S},\ v_h|_{\partial\Omega} = 0. \tag{3}$$

3. Error Estimates and Active Set Strategy

Based on the optimality conditions (2) and (3) we can derive the following error estimates for the stresses.

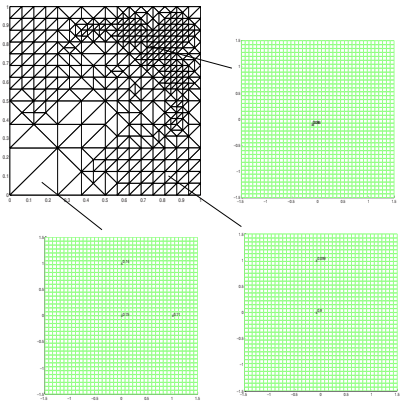
Theorem 1 ([3]). *Let (u_h, ν_h) be a solution of $(GP_{d,h})$ with multiplier λ_h. Let (u, ν) solve (GP), let W^{**} denote the convex hull of W, and let $\sigma := DW^{**}(\nabla u)$. Then, there holds*

$$\begin{aligned} \|\sigma - \lambda_h\|^2_{L^2(\Omega;\mathbb{R}^n)} &\leq c_1 \min_{v_h \in \mathcal{S}, v_h|_{\partial\Omega} = u_{D,h}} \|\nabla(u - v_h)\|^2_{L^2(\Omega)} + c_2 d, \qquad \text{and} \\ \|\sigma - \lambda_h\|^2_{L^2(\Omega;\mathbb{R}^n)} &\leq c_3 \Big(\sum_{T \in \mathcal{T}} h_T^2 \|\operatorname{div} \lambda_h + f\|^2_{L^2(T)} \Big)^{1/2} + c_4 \Big(\sum_{E \in \mathcal{E}} h_E \|[\lambda_h \cdot n_E]\|^2_{L^2(E)} \Big)^{1/2} + c_5 d. \end{aligned}$$

$\mathcal{E}$ denotes the set of faces of elements in $\mathcal{T}$, h_T and h_E the lengths of elements and faces, and $[\lambda_h \cdot n_E]$ the jump of λ_h in the normal component across an edge $E \in \mathcal{E}$.

The theorem proves convergence for the stresses but the convergence cannot be quantified. Note that we face a loss of efficiency due to degeneracy of the problem. The terms in the first two sums of the second estimate are well-known refinement indicators and allow an adaptive refinement of $\mathcal{T}$ [6]. The optimality conditions state that the discrete probability measure $\nu_h(x)$ is supported only in those atoms $S_i \in d\mathbb{Z}^n$ in which the maximum is attained. To reduce the numerical effort, Carstensen and Roubicek define in [4] an 'active set' A and compute a Young measure solution ν_h that is supported in A.

In a numerical experiment we solve $(GP_{d,h})$ with $\Omega = (0,1)^2$ and W as in (1) for $F_1 = (1,0)$ and $F_2 = (0,1)$. The right hand sides are piecewise polynomial and chosen such that the solution u_h is in a single variant in $(1/4,1)^2$ and a mixture of all three variants in $(0,1/4)^2$. In the remaining parts of Ω a mixture of two variants determines u_h. Our numerical example shows that the adaptive algorithm refines the mesh in the region where the stresses are large. Moreover, the active set strategy selects only those atoms which are needed to attain the minimum in $(GP_{d,h})$. The figure shows the adaptively refined mesh after five iterations and the support of the probability measure $\nu_h|_T$ for three different elements $T \in \mathcal{T}$. The implementation was performed in MATLAB and the large optimisation problem was solved with the interior-point linear program solver HOPDM.



Acknowledgements

The author thankfully acknowledges partial support by the German Research Foundation (DFG) within the Graduiertenkolleg 'Effiziente Algorithmen und Mehrskalenmethoden'.

4. References

1 Ball, J.M.: A version of the fundamental theorem for Young measures. In: Rascle, M.; Serre, D.; Slemrod, M. (eds.), PDEs and Continuum Models of Phase Transition. Lecture Notes in Physics **344** (1989), Springer, Berlin, pp. 207-215.
2 Ball, J.M.; James, R.D.: Fine phase mixtures as minimisers of energy. Arch. Rational Mech. Anal., 100:13-52 (1987).
3 Bartels, S.: Numerical analysis of a three well problem. In preparation (2001).
4 Carstensen, C.; Roubíček, T.: Numerical approximation of young measures in non-convex variational problems. Numer. Math. 84:395-415 (2000).
5 Roubíček, T.: *Relaxation in optimization theory and variational calculus.* W. de Gruyter (1998).
6 Verfürth, R.: *A review of a posteriori error estimation and adaptive mesh-refinement techniques.* Wiley-Teubner (1996).

Dipl.-Math. Sören Bartels, MSc, Mathematisches Seminar, Christian-Albrechts-Universität zu Kiel, Ludewig-Meyn-Str. 4, D-24098 Kiel, Germany.