COST 526

"Automatic Process Optimization in Materials Technology"

(APOMAT)

Half-Yearly Report

To be sent to **V.Tesch@access.rwth-aachen.de** until **August 27, 2004**

1. Reporting Period	**28.2.2004 – 27.08.2004**
Project title	Optimization of Fatigue Resistance of Cold Forging Tools by Considering Damage Mechanisms at Micro Scale
Project leader	Dr. Igor Gresovnik
Organization	C3M
Main collaborators involved	Faculty of Natural Sciences and Technology, University of Ljubljana, Slovenia.

2. Funding Situation	
Amount of money received specifically for COST	2.9 kEuros
Other resources partially used for the project	kEuros

3. International Collaboration

(mention group and type of work done in collaboration during the reporting period)

NTF, Ljubljana – specification of the test multi-scale solution procedure

LMT Cachan, preparation of the software background for the multi-scale example (implementation in FEAP, parallelization of micro-level simulations, setting up computational environment).

Participation in the Working Group Meeting in Angers + project progress report

- ❒ YES ➨
- ❒ NO

4. Industry participation

(mention name of companies and work done in collaboration during the whole project)

Iskra-Avtoelektrika. Analysis of service life of tooling systems

5. Meetings, visits, exchange of scientists, short-term scientific missions	**Location, date**
Project Meeting	Angers, 13. & 14. 5. 2004

6. Progress within the reporting period

(Not exceeding 3 pages, including tables and figures)

The optimization test case involving multiscale simulation approach has been treated. Response of a specimen made of inhomogeneous material to a prescribed loading is considered, with some details described in the previous report.

In the reported period, the parameterization of shape of inclusions in a periodic material structure has been worked out. We have chosen a parameterization model that relies on exact mesh representation at the microscopic level. By this approach, elements of the mesh can belong either entirely to inclusion or to matrix material and the mesh must be adjusted to fit the boundary between the two materials. In order to achieve meshing consistent with parameterization, the reference mesh for a periodic cell corresponding to circular inclusions was first generated. This mesh was then transformed by a parametric spatial map acting within a periodic cell, designed to transform the circular inclusion boundary to other shapes. In line with periodicity assumption, the mesh generated in such a way has been combined in a grid of cells in order to build a geometrical representation of a whole macroscopic element.

The following explicit form of the shape transform has been applied:

$$\mathbf{F}(r,\phi,\mathbf{p})=\begin{cases}\left(r\dfrac{r_p(\phi,\mathbf{p})}{r_{in}(\phi)},\phi\right) & ;\, r<r_{in}(\phi)\\[2ex] \left(r_{ext}(\phi)-\left(r_{ext}(\phi)-r\right)\dfrac{r_{ext}(\phi)-r_p(\phi,\mathbf{p})}{r_{ext}(\phi)-r_{in}(\phi)},\phi\right) & ;\, r\geq r_{in}(\phi)\end{cases},$$

where **p** are the design parameters, (r,ϕ) are co-ordinates of a material point expressed in the polar co-ordinate system with origin centered in the middle of the periodic cell, $r_{ext}(\phi)$ describes the external boundary of the cell and $r_{in}(\phi)=r_0=d/4$ specifies the reference shape of the inclusion-matrix boundary, d being the size of the periodic cell.

We considered simple three parametric description of inclusion boundary leading to elliptical shapes, which dictates the following expression for inclusion boundary at given design parameters:

$$r_p(\phi,a,b,\alpha)=\sqrt{\frac{1}{\dfrac{\cos^2(\phi-\alpha)}{a^2}+\dfrac{\sin^2(\phi-\alpha)}{b^2}}}\ .$$

The three parameters define two half-axes (a, b) and inclination angle α of the ellipse describing the inclusion shape (Figure 1).

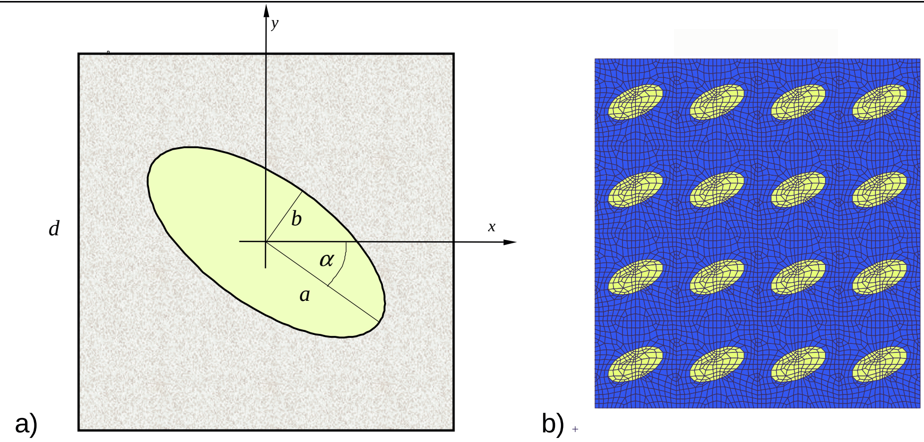

Figure 1: a) Scheme of parameterization of the inclusion shape and b) generated mesh for the microscopic finite element model.

Since we intend to use the described parameterization in an automatic optimization procedure, geometric feasibility of the produced inclusion shapes for any possible set of parameters is of primary concern. This has been ensured by limiting the range of achievable inclusion shapes by imposing a transform of the inclusion boundary of the form

$$\bar{r}_p(\phi,\mathbf{p}(\tilde{\mathbf{p}})) = f_l\left(r_p(\phi,\mathbf{p}(\tilde{\mathbf{p}})), r_{p\min}(\phi), r_{p\max}(\phi), d(\phi)\right) ,$$

where $f_l(x, \min, \max, d)$ represents a family of monotonous functions with a limited range in the first argument, and the rest of its arguments define the lower and upper range bound on f_l and the size of the transition area (Figure 2). An instance of the resulting finite element mesh used at the micro scale is shown in Figure 1 b.

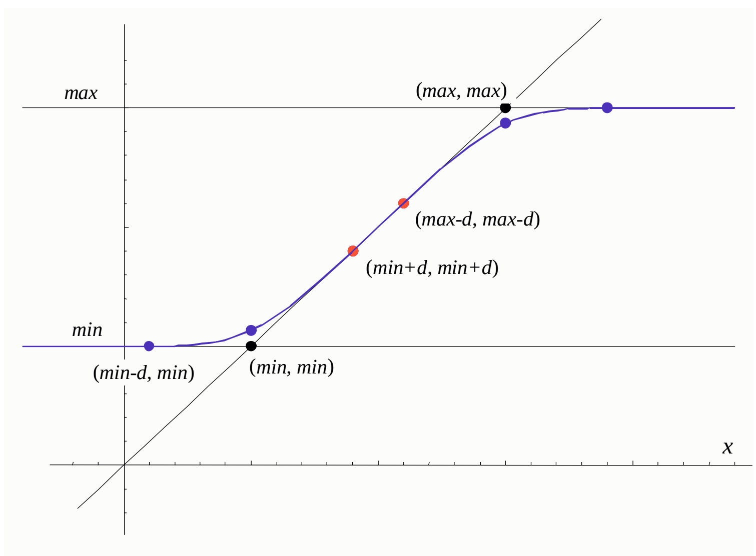

Figure 2: A representative of the family of limiting functions used to limit the range of inclusion boundary.

Optimization with respect to different goals was considered, from designing a material which will reduce as much as possible the damage in the given zone, thus increasing the durability of the structure, to designing a material which will maximize the damage in a given zone with the intention of concentrating energy dissipation in a structure. We have investigated the characteristics of the response functions that reflect these goals and observed performance of two different optimization algorithms, a non-gradient Nelder-Mead simplex and a gradient Sequential quadratic programming (SQP) algorithm.

The gradients necessary for the optimization algorithm were calculated numerically according to the forward difference scheme. The SQP turned superior in performance, taking on average about 60 evaluations of the objective and constraint functions to converge, compared to about 200 evaluations which were necessary for the simplex algorithm in order to converge within a similar tolerance. At each evaluation point, three additional evaluations were performed just to compute the gradient, which means that the SQP would typically require up to 20 evaluations if the gradients were calculated analytically. Although a good performance could be demonstrated, there were some concerns regarding the choice of the step for numerical differentiation and the tolerance for convergence check. Because of the numerical noise, the algorithm misbehaved if these were set too small. Making a good decision about the size of these parameters turns critical, and this could become much more worrying when solving more complex problems featuring a substantial amount of numerical noise or a large number of badly-scaled parameters.

For comparison, a sample convergnece paths in the parameter space are shown for the Simplex and for the SQP algorithm in the figure below.

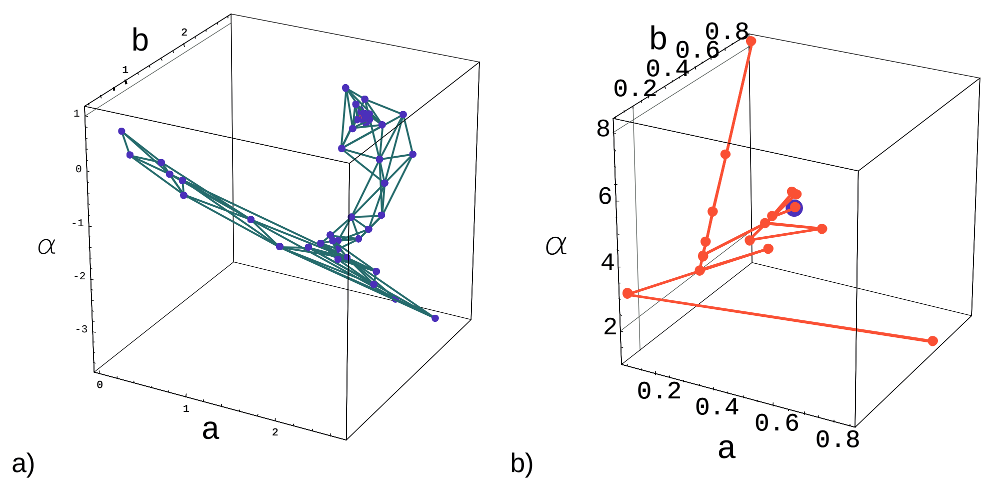

Figure 3: Convergence of a) simplex and b) SQP algorithm in the parameter space.

7. List of publications
a) Published

Grešovnik, Igor, Markovič, Damijan, Rodič, Tomaž, Ibrahimbegović, Adnan, "Optimization of Inclusion Shape in Inhomogeneous Structural Elements." In: Adnan Ibrahimbegović & Boštjan Brank (editors): Multi-physics and Multi-scale Computer Models in Non-linear Analysis and Optimal Design of

Engineering Structures under Extreme Conditions, NATO Advanced Research Workshop, Bled, Slovenia, p.p. 484-487, 2004.

b) Submitted for publications

c) In preparation

Adnan Ibrahimbegović, Igor Grešovnik, Damijan Markovič, Sergiy Melnyk and Tomaž Rodič: »Shape optimization of two-phase material with microstructure«, in preparation.