STAND-ALONE PROJECT - FINAL REPORT

P21411-N13	**Project number**
Project title	Topologieoptimierung von Rissen
Project leader	KOVTUNENKO Victor
Project website	http://www.kfunigraz.ac.at/~kovtunen/project.html

Summary for public relations work

In a broad scope, the project addressed to the problem of structure design aiming at fracture resistance in the context of topology optimization. The specialty of the optimization problems was focused on singular geometric objects with emphasize on cracks. This specific task was motivated by cracking phenomena appearing in a wide range of real world applications. The conducted research involved proper modelling, theoretical analysis, and construction of computational tools for efficient solution of the underlying nonstandard problems. With the help of non-smooth optimization and topology sensitivity methods, the necessary mathematical description of singular geometric structures like cracks with respect to their topological properties was attained. In particular, the topology changes due to kink phenomenon, which of primary importance for fracture, were investigated. The theoretical results were supported by the corresponding numerical algorithms and codes suitable for computations on irregular domains. The results obtained under the project advance our understanding important for fracture mechanics, destructive testing, identification of defects, and the related engineering applications in geo-, bio-, and material sciences.

Im weiteren Sinne liegt das Projekt im Themenbereich Topologieoptimierung von Strukturen, welche aus Sicht von Bruchmechanismen bzw. Rissbeständigkeit wichtig sind. Die Motivation solcher physikalischer Modelle liegt in zahlreichen relevanten Rissphänomenen. Aus diesen Gründen fokussiert das Projekt auf die Topologieoptimierung des rissähnlichen geometrischen Objekts. Dieser Aspekt gehört auch in den Bereich der mathematischen Modellierung und des wissenschaftlichen Rechnens. Die notwendigen mathematischen Werkzeuge zur Beschreibung topologischer Eigenschaften von zugehörigen singulären Objekten sind erfolgreich durch eine nichtglatte Optimierung sowie die topologische Analyse konstruiert und weiter untersucht worden. Dies ist für Anwendungen bei relevanten Rissproblemen begründet, wobei Rissumleitung eine wichtige Rolle spielt. Numerische Experimente auf irregulären Gebieten unterstützen unsere theoretische Untersuchungen im Projekt. Diese Fortschritte erweitern unser Verständnis für die Probleme der Bruchmechanik, zerstörenden Prüfungen sowie Identifikation von Defekten, welche Anwendungen in den Bereichen Geo-, Bio-, und Materialwissenschaften haben.

2. Brief project report

2.1 Report on the scientific work

2.1.1 Information on the development of the research work

In a broad scope, the project addressed to the problem of structure optimization and identification of defects with emphasize on cracks. This task was motivated by cracking phenomena appearing in a wide range of real world applications. The research conducted under the project consisted of modelling, analysis, and computing of the optimization problems addressed. The necessary mathematical tools for description of singular geometric structures like cracks were derived with respect to their topological properties. The crucial point concerned topology changes of a structure produced by varying geometric object (voids, respectively, cracks) inside a domain. In the standard approach, the voids are generated typically by regular geometric objects with a boundary of co-dimension one. Opposite to regular objects, cracks appear as high, i.e., more than one, co-dimension sets which are due to the presence of the crack tip or crack branches. This fact results generally in a lack of smoothness of the solutions determined in singular domains, thus, distinguishes the principal mathematical difficulties for analysis. Consequently, the specialty of the topology optimization was focused on singular geometric objects. This is a challenging mathematical problem. In this respect, the following results were obtained in the project:

- The adequate kinematic description of singular geometric objects which represents the topology changes of bifurcation, kinking, and alike was derived.
- Topological sensitivity analysis of the energy-type objective functionals dependent on singular domains with cracks was justified.
- The shape and topology optimization procedure for structure design aiming at fracture resistance and identification of cracks was described.

These results were attained using the velocity method relaxed on non-smooth velocities, the Lagrange approach for analysis of the underlying non-smooth optimization problems, and the generalization of topology sensitivity methods for singular geometric objects. The theoretical investigations were supported by developing the corresponding numerical algorithms and codes for computations on irregular domains.

2.1.2 Most important results and brief description of their significance (main points) with regard to

A rigorous description of topological changes plays a crucial role in structure optimization. While the engineering and numerical applications are rather extensive, the difficulty of analysis of state systems when changing their topological properties is connected with the singular character of the problem. On the other hand, velocity based methods are well known as a very powerful tool meeting shape optimization goals, which is well established for variational problems. Moreover, level set (implicit surface) techniques can be naturally incorporated into the velocity context. However, the velocity is required to be smooth enough. This is not the case when topology changes occur. Relaxing on non-smooth velocities, we developed concepts adapting the velocity method to topological sensitivity analysis.

We investigated the ability of velocity methods to describe changes of topology by creating defects like voids or holes of arbitrary shape. Motivated by applications in mechanics, for the shape optimization energy-type objective functions were considered, which depended on the geometry by means of state variables. The state system was represented by abstract, quadratic, constrained minimization problems stated over domains with defects. The velocity method provided the shape derivative of the objective function due to finite variations of a defect. Sufficient conditions were derived which allowed us to pass the shape derivative to the limit with respect to diminishing defect, thus, to obtain the topological derivative of the objective function due to a topology change. Our generalization has a rather broad scope of generally non-smooth data subject to topological changes. An illustrative example was calculated analytically for a circular hole bored at the tip of a crack. More generally, the hole can be of arbitrary form, thus suitable to represent the topology changes of crack bifurcation like kinking as well as branching.

Appearing in a wide range of real world applications, the problem of crack kink including determining the direction in which an incipient crack will propagate is of the primary interest for fracture mechanics. We argued a kink of the crack path during its evolution as arrest of movement in the direction tangential to the previous smooth path and appearance of a new crack branch, thus presenting change of the topology class of the continuum. For a model linear elasticity problem, based on the refined method of matched asymptotic expansions we got an expansion of the objective function representing the potential energy with respect to the infinitesimal defect (micro-crack) at the tip of the macro-crack. As the consequence, the asymptotic model was derived in the terms of stress intensity factors. In particular, this generalizes the concept of topological derivatives of the first-order, which were out of the case of the smooth conception of topological derivatives.

As it shows experimental results, interaction phenomena between the crack faces are involved certainly in the processing of cracks. Even in a plane configuration, contact occurs due to twisting around the direction of propagation. Motivated by these physical observations, we proposed the anti-plane model of a solid subject to a non-penetration condition imposed at the kinked crack. This is reasonable for multi-material junctions, slanting cores, delamination of wedges, and alike. Using variational methods, we expanded the objective function of the potential energy with respect to the diminishing branch of the incipient crack. The topology sensitivity analysis was provided by a Saint-Venant principle and a local decomposition of the solution of the variational problem in the Fourier series. Examining between admissible geometries containing the crack before kink and the crack after kink, the energy release rate (implying a generalized topological derivative of the first-order) gave rise to criteria of kinking.

Another interesting application of the topology sensitivity methods was found for the problem of frictional interaction of the crack faces in contact. In fact, there was a long mathematical discussion known to us from 90^{th} on solvability of the problem under a nontrivial friction coefficient in the vicinity of crack. We studied a model of interfacial crack between two bonded dissimilar linearized elastic media under the Coulomb friction law and non-penetration condition assumed to hold on the whole crack surface. With the help of a Saint-Venant principle relevant to topology variation we stated the existence theorem of the weak solution. Further by means of Goursat-Kolosov-Muskhelishvili stress functions convergent expansions of the solution were derived near the crack tip. Moreover, a primal-dual formulation of the problem brought about primal-dual active set algorithms efficient for the numerical solution.

Cracks occur under destructive tests for materials by means of fracture resistance. We considered a class of crack problems based on the physical models of Cherepanov, Barenblatt, Dugdale, Leonov-Panasyuk, and Novozhilov, which describe quasi-brittle fracture. The principal feature is that these models admit contact with cohesion or plasticity between the crack faces. The cohesion phenomenon is relevant to a frictional interaction between the crack faces. We proposed to describe the cohesion problems by a hemi-variational inequality. To compute solutions of the hemi-variational inequality, a primal-dual active set algorithm was suggested, which obeyed global and monotone convergence properties and was incorporated into an adaptive finite-element method.

As the result of optimization, we computed numerical examples of the quasi-brittle fracture. Since the quasi-brittle model admits closing of the crack faces, the loading needs not be monotone in time. As the consequence, the processes of bonding (closing the crack) as well as de-bonding (opening the crack) along the interface were described similarly, regardless of the loading history. The active-set approach determined exactly the points of crack tip which separated the closed part of the interface from the open one (the crack) during the fracture process. In the numerical tests we observed the zone of plastic deformations where the normal stress attained the elastic limit, thus preventing the solution from infinite stresses at the interface. All these quasi-brittle features have advance in situations where the standard Griffiths model of brittle fracture is unacceptable.

In the context of non-destructive testing with acoustic waves, the inverse problem of identification of small sound-hard defects was investigated. This problem was treated within the topology optimization framework. Using topological sensitivity analysis and generalized methods of singular perturbations, a proper asymptotic model of the test object was justified rigorously. The underlying topology optimization problem was solved semi-analytically within the concept of equivalent ellipses and applying variational calculus. With the help of variational methods we described the geometry of defects of arbitrary shapes. In particular, crack shaped defects are well suitable for the identification problem.

2.1.3 Information on the running of the project, use of the available funding and where appropriate any changes to the original project plan relating to

The 36-month project period began on 1.02.2009 and finished on 31.01.2012 without changes to the original project plan. The FWF funding of the project leader as an independent scientist was used.

The costs of 2.468,13 Euro for the peer-reviewed publication in Journal de Mathematiques Pures et Appliquees by Elsevier were applied and granted by the FWF additionally in 2010.

As the scientific result of the research, we report on 8 main publications (List 1), participation in 8 scientific meetings (List 2), and organization of two ones (List 5). The proposed national and international cooperation (List 3) was supported with joint publications, mutual scientific visits, and related meetings reported in List 5 in the Attachments.

2.2. Personnel development – importance of the project for the scientific careers of those involved (including the project leader)

The FWF-funding of the scientific work was definitively successful for the scientific career of the project leader.

The project strengthened undoubtedly national and international cooperation (see List 3). We mark the interdisciplinary research on cracks as the pre-stage of tsunami continued with the Japanese scientists. Not marked in the list, we established new research interests with the Latin America Network in Applied Mathematics (especially, O.Vasilieva). There were also joint activities with O. Steinbach (Graz University of Technology), with M. Efendiyev (Helmholtz Centre Munich), with J. Haslinger (Charles University Prague), with Y. Spasov (BHYDRA Research), with V. Stamatov (Australian Institute of High Energetic Materials), and the others of low extent.

We emphasise the effective collaboration with members within the Institute for Mathematics and Scientific Computing led by K.Kunisch at the University of Graz, which mutual experience was much helpful for the project.

2.3 effects of the project outside the scientific field

In List 5 there is detailed our contribution to the organization of the International Conference on Applied Mathematics and Informatics (ICAMI) held in 2010 in Colombia. After its success, the conference series is planned to be continued in 2013.

The particular results relevant to the project were incorporated in the following seminars and lectures given at the University of Graz:

- Partial Differential Equations, seminar (SS08/09, SS09/10);
- Mathematical Modelling, seminar (SS09/10);
- Numerical Mathematics, lecture (SS10/11).

During the research carried out under the project we treated the problem of identification of unknown geometric objects with emphasize on cracks. The crack problems are inherent for fracture and have the principal difficulty in the static situation, due to the singular domain and thus singular solutions. A generic example of the identification problem associates to the Helmholtz equation, which has inherent difficulties due to wave phenomena (for instance, due to pollution effects, eigen-frequences, large wave numbers, scattering, etc.). These phenomena are outside of the project scope and need elaborating new theoretical concepts as well as numerical methods. For this separate investigation, we applied to the FWF with a new proposal presented in List 6 in the Attachments.

3. Information on project participants

not funded by the FWF			funded by the FWF (project)		
co-workers	**number**	**Person-months**	**co-workers**	**number**	**Person -months**
non-scientific co-workers			non-scientific co-workers		
diploma students			diploma students		
PhD students			PhD students		
post-doctoral co-workers			post-doctoral co-workers		
co-workers with “Habilitation” (professorial qualifications)			co-workers with “Habilitation” (professorial qualifications)		
professors			professors		

4. Attachments

List 1

1.a. Scientific publications

1.a.1. Peer-reviewed publications

1) I.I. Argatov and V.A. Kovtunenko, Generalization of the concept of the topological derivative for a kinking crack, in: Proc. 2009 ICCMME, Melbourne, Australia, P.228-233, Australian Inst. High Energetic Materials, 2010. (published)

2) I.I. Argatov and V.A. Kovtunenko, A kinking crack: generalization of the concept of the topological derivative, 2009 Ann. Bull. Australian Inst. High Energetic Materials, 1 (2010), 124-130. (published)

3) A.M. Khludnev, V.A. Kovtunenko and A. Tani, On the topological derivative due to kink of a crack with non-penetration. Anti-plane model, J. Math.Pures Appl. 94 (2010), 571-596. (published); PubMed 22163369 http://www.sciencedirect.com/science/article/pii/S0021782410000796

4) H. Itou, V.A. Kovtunenko and A. Tani, The interface crack with Coulomb friction between two bonded dissimilar elastic media, Appl. Math. 56 (2011), 1, 69-97. (published)

5) M. Hintermueller, V.A. Kovtunenko and K. Kunisch, Obstacle problems with cohesion: A hemi-variational inequality approach and its efficient numerical solution, SIAM J. Opt 21 (2011), 2, 491-516. (published)

6) V.A. Kovtunenko, A hemivariational inequality in crack problems, Optimization (2010) 60 (2011), 8-9, 1071-1089. (published)

7) M. Hintermueller and V.A. Kovtunenko, From shape variation to topology changes in constrained minimization: a velocity method based concept, Optimization Meth. Software 26 (2011), 4-5, 513-532. (published)

8) V.A. Kovtunenko, State-constrained optimization for identification of small inclusions, Proc. Appl. Math. Mech. 11 (2011), 1, 721-722. (published)

1.a.2. Non peer-reviewed publications

1) A.M. Khludnev, V.A. Kovtunenko and A. Tani, On the topological derivative due to kink of a crack with non-penetration, Research Report KSTS/RR-09/001, Math. Department, Keio University, 2009, 37pp. (published)

2) H. Itou, V.A. Kovtunenko and A. Tani, The interface crack with Coulomb friction between two bonded dissimilar elastic media, Research Report KSTS/RR-10/001, Math. Department, Keio University, 2010, 22pp. (published)

3) M. Hintermueller and V.A. Kovtunenko, From shape variation to topology changes in constrained minimization: a velocity method based concept, MATHEON Report 768, 826, DFG-Forschungszentrum, TU-Berlin, 2011, 26pp. (published)

List 2 Project-related participation in international scientific conferences

2.2. Conference participations - lectures

1) VIII Brazilian Workshop on Continuous Optimization celebrating A.Iusem's 60th birthday, Mambucaba-Rio de Janeiro, Brazil, 12-18.07.2009.
(lecture "Semismooth methods for a hemivariational inequality")

2) International Conference on Applied Mathematics and Informatics (ICAMI 2010), San Andres, Colombia, 28.11-3.12.2010.
(section chair, lecture "On topological methods in crack problems")

3) 82nd Annual Meeting of GAMM, Graz, Austria, 18-21.04.2011.
(section chair, lecture "On topological methods of optimization")

2.3. Conference participations - posters

1) Workshop on Wave Propagation and Scattering, Inverse Problems and Applications in Energy and the Environment during Special Semester on Multiscale Simulation & Analysis in Energy and the Environment, Radon Institute for Computational and Applied Mathematics (RICAM), Linz, Austria, 21-25.11.2011.
(poster "Variational methods for the identification of objects")

2.4. Conference participations - other

1) Interdisciplinary Conference on Chemical, Mechanical and Materials Engineering with Virtual Participation (2009 ICCMME), Melbourne, Australia, 7-20.12.2009.

2) Workshop on COMSOL Multiphysics, Trend Hotel Europe Graz, Austria, 4.05.2010.

3) Tag der Forschung, Karl-Franzens University of Graz, Austria, 15.11.2010.

4) International Workshop on Control and Optimization of PDES, Graz, Bildungshaus Mariatrost, Austria, 10-14.10.2011.

List 3 Development of collaborations

Indication of the most important collaborations (maximum 5), that took place (initiated or continued) in collaboration please give the name of the collaboration partner (name, title, institution) and a few words about the scientific content. Please also assign one of the following **categories** to each collaboration:

N			Nature	**N**	(national);
				E	(European);
				I	(other international cooperation)
	E		Extent	**E1**	**low** (e.g. no joint publications but mention in acknowledgements or similar);
				E2	**medium** (collaboration e.g. with occasional joint publications, exchange of materials or similar but no longer-term exchange of personnel);
				E3	**high** (extensive collaboration with mutual hosting of group members for research stays, regular joint publications etc.)
		D	Discipline	**D**	within the discipline
				T	transdisciplinary

N	E	D	Collaboration partner / content of the collaboration
I	E2	D	1) Name: Ivan I. Argatov Title: Dr. Institution: New Mexico State University, USA Content: topological derivatives for cracks
E	E3	D	2) Name: Michael Hintermüller Title: Prof. Institution: Humboldt-Universität Berlin, Germany Content: numerical methods for optimization problems
I	E3	D	3) Name: Hiromichi Itou Title: Dr. Institution: Gunma University, Kiryu, Japan Content: frictional problems for cracks
I	E3	D	4) Name: Alexander M. Khludnev Title: Prof. Institution: Lavrent'ev Institute of Hydrodynamics, Novosibirsk, Russia Content: asymptotic methods of topology sensitivity analysis
I	E3	T	5) Name: Atusi Tani Title: Prof. Institution: Keio University, Yokohama, Japan Content: cracks with kink

Note: general scientific contacts and occasional meetings should not be considered as collaborations in the above sense.

List 5 Effects of the project outside the scientific field

5.1. Organization of scientific events

5.1.1. Congresses, symposiums or workshops with participants from outside Austria

1) Program Committee of the International Conference on Applied Mathematics and Informatics (ICAMI 2010), San Andres, Colombia, 28.11-3.12.2010.

2) Organizer of Minisymposium on "Topological Methods of Optimization, Application to Cracks" (jointly with A.M. Khludnev) during ICAMI 2010.

5.1.2. Meetings relevant to the project (scientific visits to cooperation partners)

1) Mathematical Department at Keio University in Yokohama (A.Tani) and Graduate School of Engineering at Gunma University in Kiryu (H.Itou), Japan, 21.02-2.03.2010.

2) Lavrent'ev Institute of Hydrodynamics (A.M. Khludnev) of the Siberian Branch of the Russian Academy of Sciences, Novosibirsk, Russia,12.07-13.8.2010.

List 6 Applications for follow-up projects

6.1 Applications for follow-up projects (FWF projects)

1) A stand-alone project P24879-N25 “Object identification problems: numerical analysis” is submitted to FWF.

5. Zusammenarbeit mit dem FWF

Sie werden gebeten folgende Aspekte der Zusammenarbeit mit dem FWF zu bewerten. **Anmerkungen (Ausführungen)** unter Verweis auf den entsprechenden Referenzpunkt bitte auf Beiblatt.

Skala
-2 sehr unzufriedenstellend,
-1 unzufriedenstellend;
0 angemessen;
+1 zufriedenstellend;
+2 sehr zufriedenstellend.
X nicht beansprucht

Regelwerk
(Richtlinien für Programm, Antrag, Verwendung, Bericht) **Wertung**

Antragsrichtlinien	Umfang	**+2**
	Übersichtlichkeit	**+2**
	Verständlichkeit	**+2**

Verfahren (Einreichung, Begutachtung, Entscheidung)

	Beratung	**+2**
	Dauer des Verfahrens	**+2**
	Transparenz	**+2**

Projektbegleitung

Beratung	Verfügbarkeit	**+2**
	Ausführlichkeit	**+2**
	Verständlichkeit	**+2**

Durchführung Finanzverkehr (Überweisungen, Gerätebeschaffungen, Personalwesen)	**+2**

Berichtswesen/ Prüfung/ Verwertung

	Aufwand	**+2**
	Transparenz	**+2**
	Unterstützung bei Öffentlichkeitsarbeit/ Verwertung	**+2**

Anmerkungen zur Zusammenarbeit mit dem FWF:

Besten Dank für die beste Unterstützung!