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Miniworkshop: Analytical and Numerical Treatment of Singularities in PDE

November 3rd – November 9th, 2002

This workshop was organized by Susanne C. Brenner (Columbia), Monique Dauge (Rennes) and Anna-Margarete Sändig (Stuttgart). The goal of the workshop was to bring together a group of experts interested in both the analytical and the numerical aspects of singularities in partial differential equations to discuss the latest developments in this area.

It is well-known that solutions of elliptic boundary value problems on smooth domains are smooth if the data of the problem (coefficients, source terms and boundary conditions) are smooth. However, singularities in the solutions of partial differential equations appear when the domains are non-smooth, when the coefficients of the equations are non-regular, or when the boundary conditions change type. Such singularities are observed in physical and engineering problems and they affect the effectiveness of numerical methods for partial differential equations. Problems where these singularities are present are among the most challenging ones in scientific computing today.

The participants of the workshop include mathematicians working in the theory of partial differential equations, numerical analysts and engineers. Survey talks were given on the structures of 3D singularities, interface singularities, singularities in electromagnetism, singularities in nonlinear problems, numerical treatment of singularities and engineering applications.

A book project which will include survey articles about the topics at this workshop with emphasis on 3D problems is underway. Further information about this workshop, including slides from the presentations can be found at http://www.math.sc.edu/~fem/ow02.html

Abstracts

Anisotropic Finite Elements: Results and Challenges

Thomas Apel

We consider partial differential equations in non-smooth three-dimensional domains. A finite element method with optimal convergence requires anisotropic mesh refinement towards edges with large internal angles. Such meshes contain elements with a small mesh size perpendicular to the edge (in the direction of the rapid variation of the solution) and a much larger mesh size in the direction of the edge. For a motivation we compare anisotropic and isotropic mesh refinement in selected examples and focus on a-priori error estimates. In the second part we suggest a multigrid scheme combining semi-coarsening and line smoothers to obtain a solver of optimal algorithmic complexity for anisotropic meshes along edges. Modern discretization methods do not work on one fixed mesh but adapt it iteratively to the solution. Besides reliable and efficient a-posteriori error estimators, further information like the desired stretching direction and the appropriate aspect ratio of the elements are necessary to obtain for the adaptive refinement. The optimal reconstruction of the mesh is one of the current challenges.

Multigrid Methods for Singular Solutions and Stress Intensity Factors

Susanne C. Brenner

It is well-known that solutions of two-dimensional elliptic boundary value problems suffer a loss of regularity near a point where there is a geometric singularity (e.g., a reentrant corner or a crack tip), an abrupt change in the boundary conditions (e.g., Dirichlet/Neumann), or a discontinuity of the coefficients of the differential operator (e.g., a cross point of an interface problem). This loss of regularity is detrimental to the convergence of standard finite element methods using low order elements and quasi-uniform grids. Traditional remedies include the p-version of the finite element method and local mesh-refinement.

In this talk we show that using a multilevel approach the optimal convergence rate for the P1 finite element method on quasi-uniform grids can be recovered at the presence of singular points, provided we combine the full multigrid methodology with the singular function representation of the solution of the boundary value problem and the extraction formulas that express the stress intensity factors in terms of the solution.

Algebraic Convergence for Edge Elements in Polyhedral Domains

Annalisa Buffa

We consider time harmonic Maxwell equations in a bounded Lipschitz polyhedron with perfectly conducting boundary. Among the available Galerkin methods, we choose the approximation obtained by edge elements. Due to the presence of singularities, the convergence of the scheme for uniform meshes is very poor. Given a $k \in \mathbb{N}$, we design a suitable refining technique ensuring the speed of convergence to be of order $N^{k/3}$, N being the total number of degrees of freedom.

Approximation of Maxwell Singularities by Higher Order Nodal Finite Elements

Martin Costabel

Near reentrant corners of a perfectly conducting boundary, electromagnetic fields have strong singularities that are not in H^1. The standard regularized variational formulation of the time-harmonic Maxwell equations, when discretized using nodal (C^0) finite elements, leads to non-convergent Galerkin methods. The weighted regularization method is a simple modification of the variational formulation that leads to convergent nodal finite element methods.

In its hp version, the WRM is particularly efficient. For 2D problems, exponential convergence can be shown. The method works well for 3D problems, too. In the talk, some points from the proof of exponential convergence in 2D will be presented.

The convergence behaviour will be illustrated by the the results of computations in 2D and in 3D. From the numerical computations in 3D, in particular for the "Fichera corner," we learn several interesting lessons:

• Polynomials of moderate degree (4, for example) are quite capable of approximating even very singular functions if the right variational formulation is used.

• It is advisable to use extremely strong refinements near the edges and corners, even though this leads to strongly anisotropic meshes.

Edge-Corner Interaction Inside Polyhedral Singularities

Monique Dauge

Elliptic boundary value problems in polyhedral domains have singular solutions along their edges and at their corners. The two end points of each edge are corners of the domain. Each corner is associated to the cone with which the domain coincides at its neighbourhood. This cone itself possesses edges.

These two interactions have their specific effects:

(i) The edge coefficients have special behaviours at the end points of the edge;

(ii) The spherical part of corner singularities has sub-singularities.

These two interactions will be clarified by the introduction and the comparison of two different expansions at a polyhedral corner.

As examples, we will consider the Laplace operator, electric potential transmission problems, the Maxwell system. We will mention the particular and important case of a domain defined by the three-dimensional region exterior to a plane polygonal surface (crack or screen problems).

Corner Singularities in 3D: Numerical Computation and Applications

Atanas Dmitrov

It is well known that the solution of an elliptic boundary value problem may contain gradient singularities in a non-smooth domain. In the case of cones or polyhedral corners in $\mathbb{R}^3$ the solution behaves in the vicinity of the singular point asymptotically like

$$\mathbf{u} = \sum_{\mathbf{i}} \sum_{\mathbf{k=0}}^{\mathbf{k_j}} \mathbf{K_{ik}} |\mathbf{x}|^{\lambda_\mathbf{i}} \ln^{\mathbf{k}}(|\mathbf{x}|) \mathbf{U_{ik}}(\mathbf{x}/|\mathbf{x}|), \tag{1}$$

where λ_i are the singularity exponents, $\mathbf{U}_{ik}$ the so called angular functions and K_{ij} the corner stress intensity factors (CSIFs). If one considers special geometries or material properties the series (1) can be constructed explicitly. However, for general three-dimensional problems some numerical methods are needed.

In this talk we present a general numerical procedure for the computation of corner singularities in $\mathbb{R}^3$ for compressible elasticity and Stokes flow problems. The method is based on a weak formulation and a Galerkin-Petrov nite-element approximation. In the case of Stokes ow problems (or incompressible elasticity) a mixed $\mathbf{u}, p$ formulation is used. In both cases an algebraic eigenvalue problem from type

$$(\mathbf{P} + \lambda \mathbf{Q} + \lambda^2 \mathbf{R})\mathbf{d} = \mathbf{0}, \tag{2}$$

is obtained, which depends only on $\mathbf{x}/|\mathbf{x}|$ and not on $|\mathbf{x}|$, due to a separation of variables. Thus only a part of the unit sphere should be discretized. For the numerical solution of (2) the iterative Arnoldi method is used and therefore only *one* direct matrix factorization as well as few matrix-vector products are needed to find *all* eigenvalues $\Re(\lambda) \in (-0.5, 1.0)$ as well as the corresponding eigenvectors simultaneously. In the case of elastic problems with homogeneous material properties also an adaptive remeshing technique based on *a-posteriori* error estimation is provided. Some benchmark test show that this method is robust and very accurate.

In the last part of the talk several numerical results are presented for illustrating the applicability to problems of practical interest. The results for the surface-breaking crack for instance are used to explain some 3D effects in crack propagation detected by many numerical and experimental findings in the framework of linear elastic fracture mechanics.

On Nonlinear Elastic Material Models of Power-law Type

Dorothee Knees

This talk deals with nonlinear elastic materials where the constitutive equations are of power-law type. In fracture mechanics one investigates for such materials the corresponding HRR-fields (Hutchinson/Rice/Rosengren) in order to describe the behaviour of cracks under loading. HRR-fields are derived by the assumption that solutions can be decomposed as in the case of linear elliptic equations into a singular and a more regular part: $u = u_{\text{sing}} + u_{\text{reg}} = r^\alpha v_s + u_{\text{reg}}$, where (α, v_s) is an eigenpair of a nonlinear eigenvalue problem. From the mathematical point of view it is an open problem whether or not variational solutions admit such an asymptotic expansion in the nonlinear case in general.

In the talk we briefly show existence of weak solutions. The main part deals with the discussion of local and global regularity results, which can be derived by difference quotient techniques.

One consequence of the results is that under the assumption that $u = r^\alpha v_s + u_{\text{reg}}$, the worst possible exponent α is exactly the exponent which is calculated in the HRR-theory.

Space-time Regularity of the Solution to Maxwell's Equations in Singular Domains

Simon Labrunie

I present various regularity results for the time-dependent Maxwell's equations. The general results, based on the standard semi-group and variational theories, are valid for any Lipschitz domain. They are optimal on the scales C^α (in time) and H^s (in space) for smooth or convex domains.

This is no longer the case for domains with singularities. In this case, one can apply the space decomposition principle, but this is of little practical use for a general three-dimensional domain, because the spaces of singularities lacks so far a practical description, even though some interesting characterisations of them are known.

On the other hand, when symmetry considerations allow to reduce the equations to two-dimensional problems, more precise results can be proven. They are also of the type $C^\alpha(0, T; H^s(\Omega))$, where the limiting exponents α and s are controlled by the geometry of the singularities. These developments rely on known explicit expression for the singular fields, and on the singularity theory of the scalar wave equation by Grisvard.

Singularities and Density Results in Electromagnetism

Stephanie Lohrengel

The propagation of electromagnetic waves in polyhedral domains is characterized by singularities at corners and edges. These singularities may induce a lack of density of the subspace of regular fields in the involved functional space. The aim of the talk is to give an overview of the different situations that may occur depending on the boundary condition (perfect conductor or impedance b.c.) and the material properties of the body (homogeneous or composite). We further discuss the consequences of these density or non-density results for a discretization by nodal finite elements.

PDEs on Multistructures and Applications

Serge Nicaise

The goal of my talk will be to give an overview of regularity results of solutions of PDE on 2d and 3d-multistructures, including the so-called interface problems. Some singular decompositions will be presented. Some lower bounds of the corner singular exponents will be given. The case of Signorini's boundary conditions will be considered. Finally some applications will be shortly described.

The Neumann Problem for Second Order Elliptic Systems in Polyhedral Domains

Jürgen Rossmann

The talk deals with the Neumann problem for elliptic systems of second order differential equations in a polyhedral cone. In particular, the Green matrix for this problem is studied. One of the main results are point estimates for the Green matrix and its derivatives. These estimates are used to prove

1. the solvability of the Neumann problem in weighted L_p Sobolev and Hölder spaces,
2. the existence of weak solutions in weighted L_p Sobolev spaces,
3. regularity assertions for the solutions.

As an example, the Neumann problem for the Lamé system is considered. A feature of this problem is that $\lambda = 1$ is always an eigenvalue of the operator pencils characterizing the singularities of the solutions near the edges. Therefore, an H^2 regularity result for the solutions is not obvious.

Weakly Nonlinear Boundary Value Problems in Non-smooth Domains

Anna-Margarete Sändig

In comparison with the linear case the theory of nonlinear problems in nonsmooth domains is much less developed. We distinguish between weakly and strongly nonlinear boundary value problems. The weakly nonlinear problems are characterized by the fact that a linearized problem dominates the singular behaviour of bounded small solutions. To this class belong semilinear equations (the principal part is linear) and a class of quasilinear equations where the coefficients satisfy certain growth conditions. Well know examples are the stationary Navier-Stokes system, where solutions near corner points or edges behave like solutions of the Stokes system or the von Karman plate equations, where the singular behaviour is dominated by the Kirchhoff plate model. The singularities of the second class, the strongly nonlinear problems, cannot be described by the singularities of a linearized problem. To this class belong the p-Laplacian, physically and geometrically nonlinear elastic materials and pseudo-plastic flows.

The main topic of this lecture is to give an overview on weakly nonlinear boundary value problems in domains with corners and edges. We start with semilinear systems and consider the stationary Navier-Stokes equations system. Then we investigate systems of quasilinear partial differential equations, performing the analysis in weighted Sobolev spaces with attached asymptotics. This attached asymptotics is generated by the singularities of the solutions of a linearized problem. Applying the Local Invertibility Theorem in these spaces we find growth conditions which imply small solutions of the nonlinear problem having the same asymptotic behaviour as the solutions of the linearized problem. The main tools are multiplication theorems and properties of composition (Nemytskij) operators in weighted Sobolev spaces. The general results are illustrated by examples.

Composite Finite Elements and Multigrid

Stefan Sauter

Composite Finite Elements allow the discretisation of elliptic PDEs on complicated domains, where the minimal number of unknowns is independent of the possibly very complicated shape of the domain. They can be used in the context of multigrid methods to solve high-dimensional finite element discretizations on very complicated domains. We will prove for some model problems that the convergence of the composite finite element multigrid method is robust with respect to the size and number of geometric details.

hp-approximation of Time Singularities in Evolution Problems

Christoph Schwab

We discuss analytic time-regularity of parabolic evolution problems. Boundary incompatibility of initial data and nonlinearity is well known to cause a loss of time analyticity.

We describe weighted Gevrey classes, the weight describing the loss of time-regularity.

Time semidiscretization by hp time-stepping is shown to give exponential rates of convergence.

We apply the results to the rapid solution of parabolic problems which march from $t = 0$ to $T > 0$ with N degrees of freedom in $O(N|logN|^a)$ work.

A Multigrid Method for Edge Singularities

Li-yeng Sung

We will discuss a multigrid method that can compute edge singularities efficiently using only low order finite elements on quasi-uniform grids (This is joint work with S.C. Brenner and S. Nicaise).

Singularities and Boundary Layers in Solid Mechanics: An Engineering Perspective

Barna Szabó

Singularities and boundary layers are of considerable interest in mathematical analysis because they characterize the regularity of the solution. The solutions in the neighbourhoods of singular points and generally at steep stress gradients are of great engineering interest also because failure events typically originate in those neighbourhoods. Most of the development work to date has been concerned with linear models.

The question of why and under what conditions is it possible to employ linear models for the prediction of failure in solid bodies, an essentially nonlinear phenomenon, is addressed. Engineering computations are usually performed with one of three objectives in mind: (a) Establishment of criteria for design; (b) design, and (c) certification of design.

Establishment of design criteria is a continuously evolving process. It involves the formulation of a hypothesis and experimental testing to determine whether to accept or reject the hypothesis. The ultimate goal is to validate a hypothesis for a widest possible range of conditions. Since the parameters postulated by the hypothesis are not observable directly, they must be determined by computation. The asymptotic expansions in linear models have been used very successfully for metallic bodies subjected to cyclic loading.

The investigation of design criteria for composite materials and metals at elevated temperatures is much more complicated and typically requires that non-linear behaviour be taken into account. This suggests the need for extending the investigation of critical regions to nonlinear models. Examples will be presented.

Potential in a Polygonal Body Coated with a Thin Dielectric Layer

Gregory Vial

Approximate boundary conditions appear in many applications in electromagnetism: anechoïd chambers, wave absorption by dielectric layers. In such situations, in order to determine the field, we need to solve a transmission problem in a domain - bounded or not - with a thin dielectric layer of thickness $\epsilon \ll 1$. For the numerical treatment, a fine mesh is needed, the elements being of size ϵ: the computation becomes very long and may not be accurate. That leads us to replace the thin layer by a boundary condition, called *approximate boundary condition* or *impedance condition*. In the new problem - which is close to the original one - the thin layer does not appear anymore and we can use a coarser mesh.

The derivation of such boundary conditions is well-known in the case of smooth domains: it is based on the construction of an asymptotic expansion of the solution as $\epsilon \to 0$, obtained via a dilation of the thin layer in the normal direction. We are here interested in a two-dimensional situation of a corner domain. Singularities appear near the corner and we cannot perform the same technique as in the smooth case.

Our method consists in a decomposition of the solution into regular and singular parts: the first one can be studied via the "smooth techniques". But the second one requires tools coming from the theory of singularities in corner domains (Mellin transforms). We introduce an auxiliary problem in an infinite sector, which allows the construction of *profiles* which are the bases of the structure of the expansion of the singular part near the corner. The complete expansion involves non-integer components of ϵ, depending on the opening of the corner. The impedance conditions are not as efficient as in the smooth case: the nearer the angle is from 2π, the less precise is the approximation of the thin layer by the impedance condition.

Numerical tests have been performed with the library MÉLINA. The illustration of the asymptotic expansion needs very accurate results, allowed by high order elements. The p-version is particularly adapted to our case because we can use anisotropic elements in the layer.

This is joint work with Gabriel Caloz and Monique Dauge.

Computing Singular Characteristics of the Elliptic 2-D and 3-D Problems Using p-FEM

Zohar Yosibash

As well known the solution of linear elliptic 2nd order PDEs describing heat transfer and elasticity problems, can be expressed by an asymptotic series in the vicinity of singular points in 2-D domains or edges/vertices in 3-D domains. It is typically characterized by a sequence of eigenpairs and their corresponding coefficients. The determination of these eigenpairs, and reliable computation of the coefficients of the asymptotic expansion will be addressed in this talk. These are of practical engineering importance because failure theories involve them.

Several methods for the computation of eigen-pairs (modified Steklov method, the determinant method, and others), and the determination of the coefficients of the asymptotic expansion for 2-D singularities (space enrichment, dual-singular integral also known as CIM, and complementary energy method) will be presented and discussed in terms of robustness, efficiency and ease of generalization. Some of the methods are implemented in a p-FEM code, and their performance will be illustrated (superconvergent rates of the computed data is demonstrated).

In 3-D domains, the singular asymptotic expansion is more complicated: it contains edge singularities, vertex singularities and vertex-edge singularities. The characteristics of vertex singularities can be computed as a straight forward extension of the methods encountered in 2-D domains, whereas edge-singularities have a special structure including so-called shade eigen-functions. The special representation of the edge singularities for the simplified Laplace operator will be presented, and methods for the computation of their characteristics will be demonstrated by numerical methods. Special methods for the computation of the edge flux intensity functions, developed by M. Costabel and M. Dauge are used in conjunction with the p-FEM and numerical examples are shown.

Edited by Susanne C. Brenner

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