Pavel Solin: Overview of Research

My current research interests lie in the development and numerical analysis of adaptive higher-order methods for nonlinear coupled problems (mainly finite element methods for PDEs but also higher-order Galerkin methods for integral equations). I am interested in coupled problems involving electromagnetic fields (such as electromagnetic-thermal, electromagnetic-fluid, electromagnetic-fluid-thermal processes) as well as in various other coupled problems in solid and fluid mechanics, such as thermoelastic deformations, phase changes, and others.

Numerical solution of coupled problems is more difficult than the solution of single PDEs – various physical fields exhibit important qualitative differences (some are smooth, some have singularities, others contain boundary layers, etc.), and often they interact on vastly different scales. Moreover, the variational formulations of coupled problems involve various scalar and vector-valued function spaces with different conformity requirements and interpolation and projection mechanisms. I am also very interested in questions related to compatibility of numerical approximations with the De Rham complex.

Many techniques that have been developed for standard PDEs do not work well in the context of coupled problems. As an example, let us mention error estimation: In most PDEs, it is sufficient to estimate the error in all elements, and refine those with the largest error contribution, to reduce the overall error. In a coupled problem, however, large error in quantity Q_1 and element K_1 of the domain can be due to a very small error in another quantity Q_2 and a different element K_2. Note: standard adaptivity mechanism will not mark the element K_2 for refinement, and thus the error in element K_1 will not be reduced. This is a fundamental open problem related to dependencies among physical fields in coupled problems, where standard sensitivity analysis does not provide an answer.

In coupled problems, stiffness matrices typically are indefinite and ill-conditioned, and therefore one has to use direct sparse solvers rather than the iterative ones. However, nowadays, sparse direct solvers still have problems with very large matrices. We have been successful in reducing the size of the discrete problems by employing adaptive higher-order methods. However, still we face problems related to finite computer accuracy, caused by multiple resolution scales. A last example of an exciting challenge in coupled problems is the modeling of uncertainty propagation – I am very interested in both interval and stochastic techniques.

In the past, I was involved in numerous interdisciplinary projects related to car industry (modeling of various parts of the car drive train), oil industry (modeling of automatic drilling devices based on electromagnetic sensing), electrical engineering (electromagnetic launchers, electromagnetic heating of metals, electromagnetic stirring of molten metals), mechanical engineering (flow past cascades of profiles and water separators in steam turbines), civil engineering (modeling of temperature and moisture transport in reactor walls), and ecology (modeling of air pollution in urban areas). Interdisciplinary collaborations have been the most rewarding and motivating experiences of my career, and I intend to continue doing that in the future.

Selected Results

- New adaptive algorithms for the *hp*-FEM, including a new algorithm for goal-oriented adaptivity (*P. Solin, L. Demkowicz: Goal-Oriented hp-Adaptivity for Elliptic Problems, Comput. Methods Appl. Mech. Engrg. 193 (2004), 449 - 468.*) and automatic adaptivity on meshes with arbitrary-level hanging nodes (*P. Solin, J. Cerveny, I. Dolezel: Arbitrary-Level Hanging Nodes and Automatic Adaptivity in the hp-FEM, MATCOM, in press, doi:10.1016/j.matcom.2007.02.011.*).

- New higher-order shape functions for the *hp*-FEM based on generalized eigenfunctions of the underlying partial differential operators. These shape functions exhibit a unique double-orthogonality property which yields outstanding conditioning of the corresponding discrete problems (*P. Solin, T. Vejchodsky: Higher-Order Finite Elements Based on Generalized Eigenfunctions of the Laplacian, Int. J. Numer. Methods Engrg, in press, doi:10.1002/nme.2129.* and *P. Solin, K. Segeth: Hierarchic Higher-Order Hermite Elements on Hybrid Triangular/Quadrilateral Meshes, MATCOM (76) 2007, pp. 198 - 204*). Extension to higher-order edge elements of electromagnetics is in progress.

- New adaptive multi-mesh *hp*-FEM for coupled problems where various physical fields are approximated on individual meshes, consisting of different types of finite elements and equipped with independent adaptivity mechanisms. Until now, we have applied this approach to thermally conductive incompressible flow (*P. Solin, J. Cerveny, L. Dubcova, I. Dolezel: Computer Simulation of a Flow-Thermal Coupled Problem, Research Report No. 2007-03, Department of Mathematical Sciences, UTEP*) and to linear thermoelasticity (*P. Solin, J. Cerveny, L. Dubcova: Adaptive Multi-Mesh hp-FEM for Linear Thermoelasticity, submitted to CMAME, November 2007.*). In both cases, the results exceeded our expectations. This is one of our most promising research directions for the near future.

- New methodology for the computation of eddy currents and consequent induction heating based on a reformulation of the Maxwell's equations into second-kind Fredholm integral equations. This technique can be applied to very complicated and moving arrangements due to the fact that the field is not solved in the air subdomain (important advantage vs. PDE models). The method was applied to a wide range of practical engineering problems and will appear in a new monograph *Integral Methods in Low-Frequency Electromagnetics* with J. Wiley & Sons in Fall 2008.

- New approach to the analysis of discrete maximum principles based on discrete Green's functions. Note that standard results on DMP for linear finite elements based on M-matrices cannot be extended to higher-order elements naturally. The new methodology was used to prove the first maximum principles for the *hp*-FEM. These results disproved a general expectation that higher-order finite elements do not satisfy DMP which was due to a negative result for quadratic finite elements by Höhn and Mittelmann from 1981. Our new results were published in a series of papers, see the list of publications.

- Proof of non-uniqueness of almost uni-directional inviscid compressible fluid flow (one-dimensional Euler equations with variable cross-section). The same effect was observed numerically in multiple convergent-divergent nozzles modeled by axisymmetric 3D Euler equations. The corresponding paper *P. Solin, K. Segeth: Non-Uniqueness of Almost-Unidirectionel Inviscid Compressible Flow, Appl. Math. 49, pp. 247 - 268, 2004* won the Best Paper Award in this journal in 2004.

- New model of the dynamics of polluted gas flow with application to water separators in steam turbines and air pollution in urban areas (*P. Solin: On a Model of Polluted Gas Flow, Acta Technica 45 (2000), No. 1, pp. 1 - 20*).

- Novel scheme for unstructured mesh generation based on analogy with electrostatics (*P. Solin: On a Mesh Generation Technique Based on a Special Smoothing Procedure for Uniform Inner Point Distribution, Acta Technica 45 (2000), No. 4, pp. 397 - 417*).

- Extension of the Osher-Solomon approximate Riemann solver from 2D to 3D (*J. Felcman, P. Solin: On the construction of the Osher-Solomon scheme for 3D Euler Equations, East-West J. Num. Math. (1998), pp. 43 - 64*).

Future Research

We intend to expand our research in the following areas:

- Adaptive multi-mesh FEM for coupled problems:
  - Extend the inf-sup condition for incompressible flow to the multi-mesh FEM (where velocity components and the pressure are approximated on geometrically independent meshes).
  - Develop new adaptive multi-mesh methods where some physical fields are approximated using finite elements and other by means of discontinuous Galerkin methods. Such approach should be advantageous for coupled problems involving flows.
  - Study error propagation in coupled problems. As mentioned above, this requires to develop a new approach to sensitivity analysis which will be able to model dependencies among various physical fields on the discrete level.
  - Study the propagation of uncertainty in coupled problems via interval and stochastic techniques. This is closely related to the sensitivity analysis mentioned in the previous point.

- Automatic adaptivity for time-dependent problems based on a combination of the multi-mesh FEM with the Rothe's method: The Rothe's method transforms the time-dependent PDE into a system of PDEs which do not depend on time. Each of them will be solved using automatic adaptivity in space, starting from some coarse mesh. As a result, the approximations on various time-levels will be defined on different meshes (i.e., mesh refinement and coarsening will be taken into account automatically). Our new multi-mesh FEM is able to handle this situation. Temporal adaptivity will be incorporated through a variation of the time step.

- We would like to continue research in the area of optimal higher-order shape functions for various differential operators, in the context of nonlinear coupled problems.
- We intend to analyze discrete maximum principles for 2D and 3D problems. The main complication here is that the discrete Green's functions are defined in $\mathbb{R}^4$ and $\mathbb{R}^6$, respectively.
- Recently, we have developed a new method for controlled image and data compression based on exponentially convergent adaptive higher-order finite element methods (*P. Solin, D. Andrs: New Image Compression Algorithm Based on Adaptive hp-FEM, Research Report No. 2007-07, Department of Mathematical Sciences, UTEP*). This method uses adaptivity mechanisms inherited from adaptive *hp*-FEM and works on the basis on orthogonal projections in Hilbert spaces. It provides a guaranteed compression error and is more efficient than standard techniques such as JPEG 2000. We need to extend the technique to three dimensions, where we expect even better results than in 2D. It is our ambition to change the way scientific data and images are compressed today.
- We intend to pursue a project on quantum-chemical analysis of fullerene molecules that we started recently. Fullerene molecules are composed entirely of carbon, in the form of hollow spheres, ellipsoids, or tubes. They have potential medicinal use, binding specific antibiotics to the structure of target resistant bacteria, and they can target certain cancer cells such as melanoma. On the mathematical side, this work involves the solution of eigenvalue problems in special Hilbert spaces, leading to orthonormal bases which are important to the chemists. This is complicated technically, since the corresponding Hilbert spaces extend over many-dimensional domains and the inner products come in the form of nontrivial integrals. We expect that the application of adaptive higher-order finite element methods could yields better results than standard approaches based mostly on finite differences.
- We would like to study genuine spacetime adaptivity for time-dependent problems (this means a four-dimensional setting for 3D problems). Besides the large size of these problems, the main difficulty is that the space-time variational forms lose certain good properties compared to a Cartesian variational setting. However, we did numerical experiments with the heat transfer equation using our 2D code (1D space and 1D time) and 3D code (2D space and 1D time), and in both cases the adaptive methods worked well. It is not clear whether this will work for more complicated problems such as fluid dynamics, but the potential benefit is so large that it is worth the risk.

Research Articles Co-Authored by Students

I am striving continuously to motivate the students to pursue their careers in the field of Computational Science. This effort includes offering them a possiblity to join my research group, and if they decide to do so, then I support them by all means, mentoring them, sending them to workshops and conferences, guiding them in research and helping them publish their first papers at a very high scientific level.

Examples of refereed papers accepted or published in impacted high-level international scientific journals co-authored with UTEP students are given in the following. The names of UTEP students are in bold face.

1. P. Solin, **J. Avila**: Equidistributed Error Mesh for Problems with Exponential Boundary Layers, JCAM, in press, doi:10.1016/j.cam.2007.04.048.
2. P. Solin, **J. Cerveny**, I. Dolezel: Arbitrary-Level Hanging Nodes and Automatic Adaptivity in the hp-FEM, MATCOM, in press, doi:10.1016/j.matcom.2007.02.011.
3. T. Vejchodsky, P. Solin, **M. Zitka**: Modular hp-FEM System HERMES and Its Application to the Maxwell's Equations, MATCOM, accepted, 2006.
4. P. Solin, T. Vejchodsky, **R. Araiza**: P. Solin, T. Vejchodsky, R. Araiza: Discrete Conservation of Nonnegativity for Elliptic Problems Solved by the hp-FEM, MATCOM, in press, doi:10.1016/j.matcom.2007.01.015.
5. **M. Zitka**, P. Solin, T. Vejchodsky, **F. Avila**: Imposing Orthogonality to Hierarchic Higher-Order Finite Elements, MATCOM, in press, doi:10.1016/j.matcom.2007.01.025.
6. I. Dolezel, P. Solin, **M. Zitka**, B. Ulrych: On Electromagnetic Stirring of Molten Metals, Acta Technica CSAV, 48 (2005), pp. 1 - 18.
7. **M. Zitka**, K. Segeth, P. Solin: Higher-order FEM for a system of nonlinear parabolic PDEs in 2D with a-posteriori error estimates. In: Numerical Methods and Advanced Applications. (Proceedings of ENUMATH 2003, Prague 2003.) M. Feistauer, V. Dolejsi, P. Knobloch, K. Najzar, eds. Berlin - Heidelberg - New York, Springer Verlag, ISBN 3-540-21460-7, 854 - 863, 2004.

Papers in refereed conference proceedings co-authored by UTEP students:

1. P. Solin, T. Vejchodsky, **M. Zitka**: Orthogonal hp-FEM for Elliptic Problems Based on a Non-Affine Concept. In: Numerical Mathematics and Advanced Applications (Proceedings of ENUMATH 2005; A. Bermudez, D. Gomez, P. Quintela, P. Salgado Eds.), Springer, 2006, pp. 683 - 690.
2. T. Vejchodsky, P. Solin, **M. Zitka**: On Some Aspects of the hp-FEM for Time-Harmonic Maxwell's Equations. In: Numerical Mathematics and Advanced Applications (Proceedings of ENUMATH 2005; A. Bermudez, D. Gomez, P. Quintela, P. Salgado Eds.), Springer, 2006, pp. 691 - 699.

3. P. Solin, **M. Zitka**, I. Dolezel: On hp-Finite Element Method for Singular Electro- and Magnetostatic Problems, In: Proceedings of ISEF, 15 - 17 September 2005, Baiona, Spain, ISBN 84-609-7057-4, 6 pages.
4. P. Solin, **M. Zitka**, K. Segeth: Singularities in Electro- and Magnetostatics and Their Efficient Resolution by hp-FEM, Seminar on the Occasion of the 100 Anniversary of Birth of Prof. Vycichlo, Czech Technical University, Prague, 26 - 27 April, 2005, 20 pages.
5. **M. Zitka**, P. Solin, K. Segeth: PARSYS_2D – a higher-order FE solver for systems of nonlinear elliptic and parabolic equations. In: ECCOMAS 2004 CD ROM Vol. 2. (Proc. of Congress, Jyvaskyla 2004.) Jyvaskyla, University of Jyvaskyla 2004, 15 pp.
6. **M. Zitka**, P. Solin, K. Segeth: The hp-FEM Solver PARSYS_2D and Applications in Electrostatics, IGTE Conference, September 2004, Graz, Austria. Publishing House Graz University of Technology, pp. 51 - 56.

Examples of Conferences Where My Students Presented Their Work

When I work with a student, as soon as he/she gets first results, I help her/him to finalize them and send her/him to a conference to present them. This has many positive effect on the students – they understand that I appreciate the work they do, that I trust their research skills, that I trust in their ability to present results on their own, and that I am serious about their support. After they go to a few conferences, typically I can see an improvement in their presentation skills, which is extremely valuable for future scientists. Here are a few examples of conferences where my students presented their work in person:

- Finite Element Rodeo, University of Houston, March 2 - 3, 2007.
- International Congress MAFELAP 2006, Brunel University, Uxbridge, England, June 13 - 16, 2006.
- Reliable Engineering Conference (REC 2006), Georgia Tech, Savannah, February 22 - 24, 2006.
- 28th Texas PDE conference, Edinburg, Texas, March 19 - 20, 2005.
- ENUMATH 2005, Santiago de Compostela, Spain, July 18 - 22, 2005.
- International Seminar of Applied Mathematics, Czech Technical University, Prague, September 12 - 16, 2005.
- Modelling 2005 – Third IMACS Conference on Mathematical Modelling and Computational Method, Pilsen, Czech Republic, July 4 - 8, 2005.

- International Congress ECCOMAS 2004, University of Jyvaskyla, Finland, July 24 - 28, 2004.
- International Conference IGTE 2004, Graz, Austria, September 13 - 15, 2004.

Awards Received by Students Supervised

Svatava Vyvialova's M.S. thesis (Spring 2006) was awarded an *Outstanding Thesis Award of the College of Science* in May 2006. Martin Zitka (M.S. Spring 2006) was awarded *Outstanding Student Award of the College of Science.*

Monograph *Higher-Order Finite Element Methods, 408 pages, Chapman & Hall/CRC Press, 2003*

This monograph presents cutting-edge results and methodologies for solving partial differential equations by means of higher-order finite element methods. It contains original results obtained by the author as well as references to results of other significant contemporary researchers. I spent two years working on the manuscript. The monograph became one of the main references in the field of higher-order finite element methods. For illustration of the contents and scope of this book, I present the preface of the book here.

Preface

The finite element method is one of the most popular tools for the numerical solution of engineering problems formulated in terms of partial differential equations. The latest developments in this field indicate that its future lies in adaptive higher-order methods, which successfully respond to the increasing complexity of engineering simulations and satisfy the overall trend of simultaneous resolution of phenomena with multiple scales.

Among various adaptive strategies for finite elements, the best results can be achieved using goal-oriented *hp*-adaptivity. Goal-oriented adaptivity is based on adaptation of the finite element mesh with the aim of improving the resolution of a specific quantity of interest (instead of minimizing the error of the approximation in some global norm), and *hp*-adaptivity is based on the combination of spatial refinements (h-adaptivity) with simultaneous variation of the polynomial order of approximation (p-adaptivity). There are nonacademic examples where the goal-oriented *hp*-adaptivity turned out to be the only way to resolve the problem on a required level of accuracy. Automatic *hp*-adaptivity belongs to the most advanced topics in the higher-order finite element technology and it is subject to active ongoing research. We refer the reader to works by Demkowicz et al. The goal of this book is more modest – we present the basic principles of higher-order finite element methods and the technology of conforming discretizations based on hierarchic elements in spaces H^1, $H(\mathrm{curl})$, and $H(\mathrm{div})$. An example of an efficient and robust strategy for automatic goal-oriented *hp*-adaptivity is given in Chapter 6.

In the introductory Chapter 1 we review the aforementioned function spaces and their basic properties, define unisolvency of finite elements, formulate conformity requirements for finite elements in these spaces, introduce the basic steps in the finite element procedure, and present several families of orthogonal polynomials. Section 1.3 is devoted to the solution of a one-dimensional model problem on a mesh consisting of elements of arbitrary polynomial order. The technical simplicity of the one-dimensional case gives the reader the opportunity to encounter all the important features of higher-order finite element discretization at the same time.

A database of scalar and vector-valued hierarchic master elements of arbitrary order on the most commonly used reference domains in 2D and 3D is provided in Chapter 2. This chapter contains many formulae of higher-order shape functions and is intended for reference rather than for systematic reading. Chapter 3 discusses the basic principles of higher-order finite element methods in two and three spatial dimensions that the reader was first exposed to in Section 1.3. We begin with generalizing the standard nodal interpolation to higher-order hierarchic elements, and describe the design of reference maps based on the transfinite interpolation technique as well as their polynomial isoparametric approximation. We discuss an approach to the treatment of constrained approximations (approximations comprising "hanging nodes") and mention selected software-technical aspects at the end of this chapter.

Chapter 4 is devoted to higher-order numerical quadrature in two and three spatial dimensions. Numerical quadrature lies at the heart of higher-order finite element codes and its proper implementation is crucial for their optimal performance. In particular the construction of integration points and weights for higher-order Gaussian numerical quadrature is not at all trivial, since they are not unique and the question of their optimal selection is extremely difficult. For illustration, each newly explored order of accuracy usually means a new paper in a journal of the numerical quadrature community. Tables of integration points and weights for all reference domains up to the order of accuracy $p = 20$ are available on the CD-ROM that accompanies this book.

Chapter 5 addresses the numerical solution of algebraic and ordinary differential equations resulting from the finite element discretization. We present an overview of contemporary direct and iterative methods for the solution of large systems of linear algebraic equations (such as matrix factorization, preconditioning by classical and block-iterative methods, multigrid techniques), and higher-order one-step and multistep schemes for evolutionary problems.

Chapter 6 presents several approaches to automatic mesh optimization and automatic h-, p- and hp-adaptivity based on the concept of *reference solutions*. Reference solutions are approximations of the exact solution that are substantially more accurate than the finite element approximation itself. We use reference solutions as robust error indicators to guide the adaptive strategies. We also find it useful to recall the basic principles of goal-oriented adaptivity and show the way goal-oriented adaptivity can be incorporated into standard adaptive schemes. The mathematical aspects are combined with intuitive explanation and illustrated with many examples and figures.

We assume that the reader has some experience with the finite element method – say that he/she can solve the Poisson equation ($-\triangle u = f$) in two spatial dimensions using piecewiselinear elements on a triangular mesh. Since it is our goal to make the book readable for both engineers and applied researchers, we attempt to avoid unnecessarily specific mathematical language whenever possible. Usually we prefer giving references to more difficult proofs rather than including them in the text. A somewhat deeper knowledge of mathematics (such as Sobolev spaces, embedding theorems, basic inequalities, etc.) is necessary to understand the theoretical results that accompany some of the finite element algorithms, but some of these can be skipped if the reader is interested only in implementation issues.