TECHNISCHE UNIVERSITÄT
CHEMNITZ

Fakultät für Mathematik

Chemnitz FEM-Symposium 2014

Chemnitz
FEM
Symposium

Programme

Collection of abstracts

List of participants

Chemnitz, September 22 - 24, 2014

Scientific topics:

The symposium is devoted to all aspects of finite elements and wavelet methods in partial differential equations.

The topics include (but are not limited to)

- adaptive methods,
- parallel implementation,
- high order methods.

This year we particularly encourage talks on

- Computational Mechanics / Plasticity
- Finite Elements and Uncertainty Quantification
- Eigenvalue Problems
- Exascale Computing

Invited Speakers:

Stefan Hartmann (TU Clausthal)

Raúl Tempone (KAUST Thuwal)

Daniel Kressner (EPF Lausanne)

Peter Arbenz (ETH Zürich)

Scientific Committee:

Th. Apel (München), S. Beuchler (Bonn), O. Ernst (Chemnitz), G. Haase (Graz),
H. Harbrecht (Basel), R. Herzog (Chemnitz), M. Jung (Dresden), U. Langer (Linz),
A. Meyer (Chemnitz), A. Rösch (Duisburg), O. Steinbach (Graz)

Organising Committee:

S. Mach, I. Riedel, H. Schmidt, R. Springer, R. Schneider, M. Pester, K. Seidel, A.-K. Glanzberg

http://www.tu-chemnitz.de/mathematik/fem-symposium/

Programme

Programme for Monday, September 22, 2014

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11:40	**Gerd Wachsmuth** . . . . . 12 Optimal Convergence Order for Control Constrained Optimal Control Problems.
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Collection of abstracts

Low-Rank Tensor Methods for High-Dimensional Eigenvalue Problems

Daniel Kressner[1]

We consider PDE eigenvalue problems on a tensorized domain, discretized such that the resulting matrix eigenvalue problem exhibits Kronecker product structure. In particular, we are concerned with the case of high dimensions, where standard approaches to the solution of matrix eigenvalue problems fail due to the exponentially growing degrees of freedom. Recent work shows that this curse of dimensionality can in many cases be addressed by approximating the desired solution vector in a low-rank tensor format. In this talk, we survey recent developments in this direction. Particular emphasis is placed on a priori approximation results and the use of preconditioners. Based on joint work with Michael Steinlechner, Christine Tobler, and Andre Uschmajew.

References:

[1] D. Kressner and A. Uschmajew. On low-rank approximability of solutions to high-dimensional operator equations and eigenvalue problems. Technical report, June 2014.
[2] D. Kressner, M. Steinlechner, and A. Uschmajew. Low-rank tensor methods with subspace correction for symmetric eigenvalue problems. Technical report, December 2013. To appear in SIAM J. Sci. Comput.
[3] D. Kressner and C. Tobler. Preconditioned low-rank methods for high-dimensional elliptic PDE eigenvalue problems. CMAM, 11(3):363–381, 2011.

[1] ANCHP, MATHICSE, EPFL, CH-1005 Lausanne,
daniel.kressner@epfl.ch

On the Convergence of a Preconditioned Gradient Subspace Eigensolver with Rayleigh Ritz Acceleration

Ming Zhou[1]

The topic of this talk is the convergence analysis of a preconditioned subspace eigensolver for the FE discretizations of self-adjoint and elliptic partial differential operators. This eigensolver aims at the computation of a few of the smallest eigenvalues and the associated invariant subspace. The Rayleigh Ritz procedure is applied on a subspace spanned by the current subspace iterate and its preconditioned residual to accelerate the convergence. The convergence analysis is based on the analysis of the associated vectorial eigensolver and uses the Sion's minimax theorem.

The efficiency of this eigensolver is demonstrated by solving an eigenvalue problem with more than 50 millions degrees of freedom within our AMPE (Adaptive Multigrid Preconditioned Eigensolver) software.

References:

[1] Klaus Neymeyr and Ming Zhou, The block preconditioned steepest descent iteration for elliptic operator eigenvalue problems. Electron. Trans. Numer. Anal. 41, 93-108, 2014.

[1] Universität Rostock, Institut für Mathematik, Rostock, Germany,
ming.zhou@uni-rostock.de

Model Order Reduction for an Acoustic Eigenvalue Problem

Antti Hannukainen[1] Jarmo Malinen[2] Antti Ojalammi[3]

We study a quadratic eigenvalue problem related to the modeling of human speech production: Find $(\lambda, u) \in (\mathbb{C}, V)$ such that

$$c^2(\nabla u, \nabla v)_{L^2(\Omega)} + \lambda c(u,v)_{L^2(\Gamma)} + \lambda^2(u,v)_{L^2(\Omega)} = 0,$$

in which $\Omega \subset \mathbb{R}^3$ is the computational domain, $\Gamma \subset \partial\Omega$ and c is the speed of sound. The finite element method is used for the spatial discretization, so that the finite-dimensional space V is a subset of $H^1(\Omega)$ with appropriate boundary conditions built in. For more details on this model, see [1].

Our interest is in the formants, that is, in the resonant frequencies of the vocal tract. We are especially interested in the effect of surgery or anatomical abnormalities to these resonances. As surgery changes the geometry of the vocal tract, assessing the effect requires solving several eigenvalue problems in different domains Ω.

Vocal tract resonances and corresponding geometries were simultaneously measured in [2] using an MRI machine and a special microphone setup. The authors performed an eigenvalue analysis using the geometries extracted from the MRI measurements and a Dirichlet boundary condition placed at the mouth. However, when compared to the measured formants, the computed ones exhibit a large error for certain cases. Based on our numerical experiments, this error is due to the truncation of the computational domain with a Dirichlet boundary condition at the mouth. That is, the effect of the exterior space is not taken into account.

Taking the exterior space into account increases the size of the system considerably, which is not desired. Since the geometry of the MRI-coil remains unchanged throughout the computations, we can reduce the size of the system by using model order reduction techniques in the exterior part of the domain. In this talk, we describe a technique for reducing the size of the system via computing a special basis for the exterior domain. We study the effect of this approach on the accuracy of the computed eigenvalues both numerically and analytically.

References:

[1] A. Hannukainen, T. Lukkari, J. Malinen, and P. Palo: Vowel formants from the wave equation. JASA-EL, 122(1), 2007, EL1-EL7.
[2] D. Aalto, O. Aaltonen, R.-P. Happonen, P. Jääsaari, A. Kivelä, J. Kuortti, J.-M. Luukinen, J. Malinen, T. Murtola, R. Parkkola, J. Saunavaara, and M. Vainio: Large scale data acquisition of simultaneous MRI and speech, Appl. Acoust., 83(1), 2014, 64-75.

[1] Aalto University School of Science, Department of Mathematics and Systems Analysis, Aalto, Finland, antti.hannukainen@aalto.fi

[2] Aalto University School of Science, Department of Mathematics and Systems Analysis, jarmo.malinen@aalto.fi

[3] Aalto University School of Science, Department of Mathematics and Systems Analysis, antti.ojalammi@aalto.fi

Hierarchical FEM for Anisotropic Adaptive Mesh Refinement

Rene Schneider[1]

In many practical PDE problems the solutions have a singularity component. Adaptive FEM is established as a convenient and efficient tool to get accurate approximations of the solution in this setting. Often the singularity components are anisotropic, e.g. layer phenomena or domains with re-entrant edges. If this anisotropic structure is exploited utilising suitable anisotropic meshes, significant savings in computational cost are possible. Yet, the majority of adaptive FEM approaches consider only isotropic refinement, thus neglecting potential savings.

We discus a new approach to anisotropic adaptive FEM based on hierarchical error estimation driving anisotropic subdivision of simplex elements. Examples will demonstrate the utility of the approach.

[1] TU Chemnitz, Fakultät für Mathematik, Chemnitz, Germany,
`rene.schneider@mathematik.tu-chemnitz.de`

Optimal Convergence Order for Control Constrained Optimal Control Problems

Gerd Wachsmuth[1] René Schneider[2]

In this talk we consider the numerical solution of control constrained optimal control problems. We are interested in obtaining the optimal convergence rate for the L^2-error w.r.t. the number of degrees of freedom. Due to the control constraint, the optimal control possesses a kink at the interface between the active and inactive set w.r.t. the control constraint. This kink limits the convergence order of a uniform discretization to $h^{-3/2}$.

We compare some approaches from the literature. Moreover, we provide a new, efficient and robust error estimator which is used for an adaptive refinement of the mesh.

We also present a new method for solving control constrained problems. In this method, we move the nodes of the mesh at the interface between the active and inactive set. This yields optimal order of convergence.

[1] TU Chemnitz, Faculty of mathematics, Chemnitz, Germany,
gerd.wachsmuth@mathematik.tu-chemnitz.de

[2] TU Chemnitz, Faculty of mathematics,
rene.schneider@mathematik.tu-chemnitz.de

A Posteriori Error Analysis for a Predictor Corrector Hp-Finite Element Method for Poisson's Equation in Polygonal Domains

Boniface Nkemzi[1] Stephane Sonkoue[2]

Solutions of elliptic boundary value problems in domains with corners, edges, cracks, conic vertices, etc. usually entail singularities which may severely reduce the accuracy of standard numerical schemes, such as the finite element, boundary element, finite difference methods. We present a new predictor-corrector hp-finite element algorithm for computing the coefficients of the singularities and the solution of boundary value problems for the Poisson equation in domains $\Omega \subset \mathbf{R}^2$ with corners and smooth data. The method makes use of the splitting $u = w + s$ of the solution into a regular part $w \in H^k(\Omega)$ and a singular part s with lower regularity and the explicit representation formulas for the coefficients of the singularities in terms of the right hand side function, the solution and a suitable smooth cut-off function. An initial finite element approximation of the solution and the coefficients of the singularities (predictors) are computed. Using the computed coefficients and an hp-finite element strategy, the regular part of the solution is computed and from which corrected finite element approximations of the coefficients and solution are obtained. A posteriori error estimates show that the algorithm yields very good convergence rates in various norms. A comparison with other methods shows that our method is more efficient.

[1] University of Buea, Mathematics, Buea, Cameroon,
nkemzi@yahoo.com

[2] University of Buea,

Sparsity Optimized High Order Finite Element Functions on Simplices

Sven Beuchler[1]

This talk reports several results on sparsity optimized basis functions for hp-FEM on triangular and tetrahedral finite element meshes. We give an overview on the sparsity pattern for mass and stiffness matrix in the space $L2$, $H1$, $H(div)$ and $H(curl)$. The construction relies on a tensor-product based construction with properly weighted Jacobi polynomials. In the last part of the talk, an recursive algorithm in order to compute the nonzero entries of the stiffness matrix is presented. The talk is the result of collaborations with V. Pillwein (Linz), S. Welter (Bonn) and S. Zaglmayr (Darmstadt).

[1] Uni Bonn, INS, Bonn, D,
beuchler@ins.uni-bonn.de

Space-Time Discretization in Computational Inelasticity

Stefan Hartmann[1]

Frequently, the inelastic material behavior is modeled using ordinary differential equations of first order (ODE). If the balance equations of thermo-mechanics (balance of linear momentum, balance of energy), which represent – in the context of the method of vertical lines – algebraic equations or ODEs itself, are coupled with these evolution equations, a system of differential-algebraic equations (DAEs) is obtained. In this lecture we start with some historical remarks of this procedure. First, diagonally-implicit Runge-Kutta methods are applied offering three aspects, classical approaches in finite elements as particular sub-problems, high-order integration in time, and time-adaptivity using embedded schemes. Second, other time-integration schemes such as Rosenbrock-type methods or half-explicit Runge-Kutta schemes are applied, where advantages and disadvantages are investigated. Some additional applications are discussed such as the combination to high-order finite elements, thermo-mechanical coupling, as well as some drawbacks with order-reduction for particular problems.

[1] Institute of Applied Mechanics, Clausthal University of Technology, Adolph-Roemer-Str. 2a, 38678 Clausthal-Zellerfeld, Germany,
stefan.hartmann@tu-clausthal.de

The Applicability of Plate Problem Preconditioners for the Laminated Plate Problem

Michael Weise[1] Arnd Meyer[2]

Laminated plates, i. e. plates composed of several material layers, are often used in lightweight construction. Since fibre-reinforced composites are only strong in fibre direction, multiple layers with different fibre directions are combined into a laminate to account for different load cases. Our goal is to simulate such structures with FEM.

The Kirchhoff plate model with constant materials over the thickness leads to the classical plate equation, which is decoupled from the in-plane deformation of the mid-surface. In the given problem this decoupling only holds true for a symmetric laminate sequence over the thickness but not in the general asymmetric case. Here in-plane deformations can cause out-of-plane deformations and vice versa.

The resulting FE system matrix comprises membrane, plate and couple parts. A preconditioner for the conjugate gradient method is needed in order to solve the system efficiently. One simple appproach for a preconditioner is to neglect the couple terms and to combine existing preconditioners for the membrane and plate problems. Our talk examines the effectiveness of this approach by the means of a spectral equivalence estimate.

[1] Technische Universität Chemnitz, Faculty of Mathematics, Chemnitz, Germany,
michael.weise@mathematik.tu-chemnitz.de

[2] Technische Universität Chemnitz, Faculty of Mathematics, Chemnitz, Germany,
arnd.meyer@mathematik.tu-chemnitz.de

Viscoelasticity at Large Strain Deformations

Hansjörg Schmidt[1] Arnd Meyer[2]

Injection moulding is a widely used process for mass production. But the geometry of the produced part matches not exactly the mould, due to shrinkage and warpage. This warpage originates from the cooling process from melting temperature to room temperature. Furthermore, thermoplastics exhibit viscoelastic behaviour between the melting temperature and the glass transition temperature. Additionally, viscoelastic materials reduce residual stresses over time. Thus, we have to consider a viscoelastic material model for the computation of residual stresses and the resulting warpage. Moreover, we want to include this computation in an optimisation procedure of the moulds.

We present a theory of viscoelasticity at large strain deformations. Starting from a non-linear weak formulation, we examine the viscoelastic stress-strain relation and the linearised system of equations.

[1] Technische Universität Chemnitz, Faculty of Mathematics, Chemnitz, Germany,
hanss@hrz.tu-chemnitz.de

[2] Technische Universität Chemnitz, Faculty of Mathematics, Chemnitz, Germany,
a.meyer@mathematik.tu-chemnitz.de

A Multigrid Approach to Obstacle Problems and to Optimal Control of Obstacle Problems

Michelle Vallejos[1] Roland Herzog[2]

An optimal control problem governed by an elliptic variational inequality is considered. We focus on the optimal control of the obstacle problem, which is a prototypical example of variational inequalities of the first kind. A robust multigrid strategy for solving obstacle problems will be presented. This algorithm is then extended in order to apply the same strategy for solving optimal control of obstacle problems. A collective smoothing multigrid is utilized since it belongs to the family of multigrid strategies which perform well in solving optimal control problems with PDE constraints. The algorithmic concept will be discussed and numerical examples will be presented to illustrate the efficiency of the proposed methods.

[1] TU Chemnitz, Reichenhainer Str. 41, 09107 Chemnitz,
mival@hrz.tu-chemnitz.de

[2] TU Chemnitz,
roland.herzog@mathematik.tu-chemnitz.de

Numerical Computation of Effective Properties for Heterogeneous Materials in Linear Elasticity and Fluid Dynamics

Felix Ospald[1] Matti Schneider[2]

For the simulation of materials and fluids involving several constitutes at the microscopic level, homogenization methods are usually applied to obtain a homogeneous effective material. We investigate an approach based on the Lippmann-Schwinger equation to compute the effective stiffness of short-fiber reinforced materials as well as the effective viscosity of fiber suspensions in a Stokesian flow regime. The equations are solved within a representative volume element (RVE) with periodic boundary conditions using a non-conforming (Fourier-)Galerkin method, originally proposed by Moulinec and Suquet [1]. The numerical results are compared to existing analytical solutions. Problems with infinite contrast require regularization, which is discussed in terms of a numerical convergence study. Further we discuss some aspects of the implementation, parallelization and scalability of the method.

References:

[1] H. Moulinec and P. Suquet: *A numerical method for computing the overall response of nonlinear composites with complex microstructure.* Comp. Meth. Appl. Mech. Engng., 157 (1998) 69-94.

[1] TU Chemnitz, Reichenhainer Str. 41, 09107 Chemnitz,
feo@tu-chemnitz.eu

[2] TU Chemnitz,
matti.schneider@mb.tu-chemnitz.de

Numerical Study of the Angular Vibrations of Rotating in a Vertical Plane System in the Field of Matlab/Simulink

Peter Pavlov[1] Svetlana Lilkova-Markova[2] Simona Doneva[3]

The paper presents a study of the dynamic behavior of the vibrating system in the vertical plane, by various capabilities of the software package Matlab/Simulink. The system consists of a vertical joint supported rod, concentrated masses and elastic-viscous horizontal sets, located along the height of the rod. A program for direct integration of the differential equation of vibrations of the system is composed in the field of Matlab. A simulation model for study of the same vibrations is drawn by the basic toolbox for symbolic modeling - Simulink. Based on the capabilities of the latest version of Matlab, a animated model of the vibrations is made too. Finally, a graphical user interface of the motion is created, by graphical environment Matlab/guide. The models allow to study the free vibrations for the given initial rotation of the rod and forced vibrations of kinematic interferences - most often with zero initial conditions. The survey is a stages of a wider study of the dynamics of the vibrations of a rotary body, including analytical, numerical - in the field of Matlab/Simulink, numerical based on FEM in the field of Ansys and finally - experimental study. The numerical study in the field of Matlab/Simulink, object of investigation in the report, serves to refining of the parameters of the designed stand for testing vertical angular vibrations of body. All of the surveys - analytical, numerical and experimental are related to development of part of the components of a new dynamic lab that will be opened in the fall in the oldest technical university in Bulgaria.

References:

[1] Pavlov, P., S. Lilkova-Markova, B. Nakov, J. Dancheva. Application of the new Achievements in the Simulating and Measuring Apparatus for the Construction of a Stand for Study Vibrations of a particle. Proceedings of Faculty of Architecture and Construction of the University of Nis, issue. 26, 2011, p 81-89.
[2] Pavlov, P., S. Lilkova-Markova, B. Nakov, J. Kehajova. A geometric oriented approach in drawing the simulation model of the small angular vibrations of a body. Miskolc Mathematical Notes,Vol. 14 (2013), No. 2, pp. 679–684

[1] University of Architecture, Civil Engineering and Geodesy (UACEG), Bulgaria, Sofia 1046, 1 Hr. Smirnenski Blvd, UACEG, dep. Technical Mechanics,
pdp_mech_fhe@uacg.bg

[2] University of Architecture, Civil Engineering and Geodesy (UACEG),
lilkova_fhe@uacg.bg

[3] University of Architecture, Civil Engineering and Geodesy (UACEG),
simona_doneva@mail.bg

Study, Based on FEM, of the Angular Vibrations of a Rotating in the Vertical Plane System of Rod and Concentrated Masses

Svetlana Lilkova-Markova[1] Peter Pavlov[2] Daniel Evlogiev[3]

The paper presents a study of the dynamic behavior of the vibrating in the vertical plane system, on the base of FEM. The system consists of a vertical joint supported rod, concentrated masses and elastic-viscous horizontal sets, located along the height of the rod. The composed, in the program environment Ansys, dynamic model allows to study the main types of vibrations - free and forced damped or undamped. Vertical rod is modeled by a variable number of frame type elements BEAM3, and concentrated masses are entered in the nodes of the rod by elements type MASS21. Elastic-viscous properties are defined by the parameters of elements type COMBIN14. By the model are studied the free vibrations for the given initial rotation of the rod and forced vibrations of kinematic interferences - most often with zero initial conditions. Thy survey is a stages of a wider study of the dynamics of the vibrations of a rotary body, including analytical, numerical - in the field of Matlab/Simulink, numerical based on FEM in the field of Ansys and finally - experimental study. The numerical study on the base of FEM, object of investigation in the report, serves to refining of the parameters of the designed stand for testing vertical angular vibrations of body. All of the surveys - analytical, numerical and experimental are related to development of part of the components of a new dynamic lab that will be opened in the fall in the oldest technical university in Bulgaria.

References:

[1] Pavlov, P., S. Lilkova-Markova, B. Nakov, J. Dancheva. Application of the new Achievements in the Simulating and Measuring Apparatus for the Construction of a Stand for Study Vibrations of a particle. Proceedings of Faculty of Architecture and Construction of the University of Nis, issue. 26, 2011, p 81-89.
[2] Pavlov, P., S. Lilkova-Markova, B. Nakov, J. Kehajova. A geometric oriented approach in drawing the simulation model of the small angular vibrations of a body. Miskolc Mathematical Notes,Vol. 14 (2013), No. 2, pp. 679–684

[1] University of Architecture, Civil Engineering and Geodesy (UACEG), Bulgaria, Sofia 1046, 1 Hr. Smirnenski Blvd, UACEG, dep. Technical Mechanics,
lilkova_fhe@uacg.bg

[2] University of Architecture, Civil Engineering and Geodesy (UACEG),
pdp_mech_fhe@uacg.bg

[3] University of Architecture, Civil Engineering and Geodesy (UACEG),
daniel_evlogiev@abv.bg

Efficient Simulation of Short Fibre Reinforced Composites

Rolf Springer[1] Arnd Meyer[2]

Lightweight structures became more and more important over the last years. In the development of these structures, fibre reinforced materials play an important role. One special class of fibre reinforced components, are short fibre reinforced composites, produced by injection moulding.
To avoid expensive experiments for testing the behaviour of these materials under several loads, an effective simulation is necessary. Therefore, material models are needed, which describe the specific behaviour.

In this talk, we will present how the material properties of short fibre reinforced composites and the arising stresses within can be described in the case of linear thermoelasticy. For this, we use the stress-strain-relation

$$\sigma = \mathfrak{C} : (\varepsilon - (\theta - \theta_0)\mathbf{T}),$$

with a fourth order material tensor $\mathfrak{C}$, a second order thermal expansion tensor $\mathbf{T}$, the temperature difference $(\theta - \theta_0)$, and the second order linearised strain tensor ε.
For the description of these properties, we start with the expressions for transversely isotropic material, where the tensors $\mathfrak{C}$, $\mathbf{T}$, and, thereby, σ depend on a function $p(x)$, with

$$p : \Omega \to \{y \in \mathbb{R}^3 \mid \|y\|_2 = 1\}.$$

Here Ω is the domain, where our computation is done. Therefore, $p(x)$ can be understood as the direction of a fibre inserted in point x of a mechanical component, which is described by Ω. So, a transversely isotropic component can be understood as a fibre reinforced structure the fibres of which are perfectly aligned along the given direction $p(x)$.

Now, in the case of short fibre reinforced composites the function $p(x)$ is not longer known exactly. Therefore, it has to be supposed as random. The only given information are the first moments of the distribution of $p(x)$, obtained by a simulation of the injection moulding process of this component. So, we show how the material properties and the arising stresses can be generalised from the transversely isotropic case using these moments.

[1] Technische Universität Chemnitz, Faculty of Mathematics, Chemnitz, Germany,
Rolf.Springer@mathematik.tu-chemnitz.de

[2] Technische Universität Chemnitz, Faculty of Mathematics, Chemnitz, Germany,
arnd.meyer@mathematik.tu-chemnitz.de

Multi-Index Monte Carlo: When Sparsity Meets Sampling

Raúl Tempone[1]

I will present our Multi Index Monte Carlo (MIMC) method. We propose and analyze a novel Multi-Index Monte Carlo (MIMC) method for weak approximation of stochastic models that are described in terms of differential equations either driven by random measures or with random coefficients. The MIMC method is both a stochastic version of the combination technique introduced by Zenger, Griebel and collaborators and an extension of the Multilevel Monte Carlo (MLMC) method first described by Heinrich and Giles. Inspired by Giles's seminal work, instead of using first-order differences as in MLMC, we use in MIMC high-order mixed differences to reduce the variance of the hierarchical differences dramatically. This in turn gives a new improved complexity result that increases the domain of the problem parameters for which the method achieves the optimal convergence rate, $\mathcal{O}(\mathrm{TOL}^{-2})$. Using optimal index sets that we determined, MIMC achieves a better rate for the computational complexity does not depend on the dimensionality of the underlying problem, up to logarithmic factors. We present numerical results related to a three dimensional PDE with random coefficients to substantiate some of the derived computational complexity rates. Finally, using the Lindeberg-Feller theorem, we also show the asymptotic normality of the statistical error in the MIMC estimator and justify in this way our error estimate that allows prescribing both the required accuracy and confidence in the final result.

References:

[1] Abdul-Lateef Haji-Ali, Fabio Nobile, and Raul Tempone. "Multi-Index Monte Carlo: When Sparsity Meets Sampling.", arXiv preprint arXiv:1405.3757 (2014)

[1] King Abdullah University of Science and Technology, Applied Mathematics and Computational Science, Thuwal, Saudi Arabia,
Raul.Tempone@kaust.edu.sa

Hierarchical Tensors Approximation for Uncertainty Quantification

Reinhold Schneider[1]

Hierarchical Tucker tensor format (HT - Hackbusch tensors) and Tensor Trains (TT- Tyrtyshnikov tensors, I.Oseledets) have been introduced recently for low rank tensor product approximation. Hierarchical tensor decompositions are based on sub space approximation by extending the Tucker decomposition into a multi-level framework. Therefore they inherit favorable properties of Tucker tensors, e.g they offer a stable and robust approximation, but still enabling low order scaling with respect to the dimensions. For many high dimensional problems, hard to be handled so far, this approach may offer a novel strategy to circumvent the curse of dimensionality.

For uncertainty quantification we cast the original boundary value problem, with uncertain coefficients problem into a high dimensional parametric boundary value problem, discretized by Galerkin method. The high dimensional problem is cast into an optimization problems, constraint by the restriction to tensors of prescribed ranks $\mathbf{r}$. This problem could be solved by optimization on manifolds, or more simply by alternating least squares. Since the norm of the underlying energy-space is a cross norm preconditioning is required only for the spatial part and e.g. performed by standard multi grid approaches, e.g BPX. Of Importance is, that this leads to a modification of the orthogonality of the used component tensors.

[1] TU Berlin, Institut für Mathematik, Germany,
schneidr@math.tu-berlin.de

Multilevel Quadrature Methods for Stochastic PDEs with Lognormal Diffusion Coefficients

Markus Siebenmorgen[1]

This talk is dedicated to multilevel quadrature methods for the rapid solution of stochastic partial differential equations with a log-normal distributed diffusion coefficient. The key idea of these approaches is a sparse grid approximation of the occurring product space between the stochastic and the spatial variable. We develop the mathematical theory and present error estimates for the computation of the solution's statistical moments with focus on the mean and variance. Especially, the present framework covers the multilevel Monte Carlo method and the multilevel quasi Monte Carlo method as special cases. We show that the quasi Monte Carlo method based on a Halton sequence is applicable in arbitrary high stochastic dimension provided that the diffusion coefficient complies certain regularity assumptions. The theoretical findings are supplementedby numerical experiments.

[1] Universität Basel, Mathematik und Informatik, Basel, Switzerland,
markus.siebenmorgen@unibas.ch

Numerical Solution of Elliptic Diffusion Problems on Random Domains

Michael Peters[1] Helmut Harbrecht[2] Markus Siebenmorgen[3]

In this talk, we provide regularity results for the solution to elliptic diffusion problems on random domains. Especially, based on the decay of the Karhunen-Loève expansion of the domain perturbation field, we establish rates of decay which imply the tractability of the Quasi-Monte Carlo method. By taking into account only univariate derivatives, the regularity results can considerably be sharpened in order to show also the applicability of the stochastic collocation method and related rates of convergence. We moreover employ parametric finite elements to compute the solution of the diffusion problem on each particular realization of the domain generated by the perturbation field. This simplifies the implementation and yields a non-intrusive approach. The theoretical findings are complemented by numerical examples.

[1] Universitaet Basel, Mathematik und Informatik, Basel, Switzerland,
michael.peters@unibas.ch

[2] Universitaet Basel,
helmut.harbrecht@unibas.ch

[3] Universitaet Basel,
markus.siebenmorgen@unibas.ch

A Robust Petrov-Galerkin Discretisation of Convection-Diffusion Equations

Dirk Broersen[1] Rob Stevenson[2]

A Petrov-Galerkin finite element discretization is presented of an ultra-weak variational formulation of the convection-diffusion equation in mixed form. Here, an optimal test space is introduced to get the best approximation to the solution from the trial space.

To arrive at an implementable method, the truly optimal test space has to be replaced by its projection onto a

finite dimensional test search space. To prevent that this latter space has to be taken increasingly large for vanishing diffusion, a formulation is constructed that is well-posed in the limit case of a pure transport problem.

Numerical experiments show approximations that are very close to the best approximations, uniformly in the size of the diffusion term.

[1] University of Amsterdam, KdVI, Amsterdam, The Netherlands,
d.broersen@uva.nl

[2] University of Amsterdam, KdVI, Amsterdam, The Netherlands,
r.p.stevenson@uva.nl

On the Numerical Analysis of the Oseen Equations

Katharina Höhne[1] Sebastian Franz[2]

Let us consider the stationary Oseen-equations

$$\begin{aligned} -\varepsilon\Delta\mathbf{v} + (\mathbf{b}\cdot\nabla)\mathbf{v} + c\mathbf{v} + \nabla p = f, &\quad \text{in } \Omega \subset \mathbb{R}^2 \\ \text{div}\,\mathbf{v} = 0, &\quad \text{in } \Omega \\ \mathbf{v} = 0, &\quad \text{on } \partial\Omega \end{aligned}$$

with $0 < \varepsilon \ll 1$ and a vector field $\mathbf{b}$.

Here the components of the velocity $\mathbf{v}$ are coupled via the additional pressure term and the divergence condition. These equations are simplifications of the non-linear Navier-Stokes system and can occur when discretising them.

While the structure of solutions of singularly perturbed convection-diffusion problems is well understood and the kind of layers is known, there is still not enough information known in the case of systems like the Oseen equations. Similarly to the convection-diffusion problems, they contain a small parameter that determines strongly the behaviour of its solution near the boundaries.

In this talk we will give some information on the layer structure of the solution $\mathbf{v}$ near the boundaries. We will make use of the stream-function formulation of the Oseen-equations that transform the problem for $\mathbf{v}$ and p into a fourth-order scalar PDE for ψ where $\mathbf{v} = (\psi_y, -\psi_x)$.

[1] TU Dresden, Institute for Numerical Mathematics, Dresden, Germany,
katharina.hoehne1@tu-dresden.de

[2] TU Dresden, Institute for Numerical Mathematics, Dresden, Germany,
sebastian.franz@tu-dresden.de

Discontinuous Galerkin Methods Applied to Convection-Diffusion Problems in Time-Dependent Domains

Khalid Adrigal[1] Gunar Matthies[2]

We consider convection-diffusion equations in time-dependent domains where the movement of the domain boundary is presribed. The time change of the domain is handled by the arbitrary Lagrangian-Eulerian (ALE) formulation. It prevents strong mesh distortions which may occur for pure Lagragian formulations since the given velocity of the domain boundary is extended to the mesh velocity inside domain in such a way that the mesh quality is preserved.

We will present conservative and non-conservative formulations of time-dependent convection-diffusion equations in time-dependent domains where special attention is paid to the time derivative and the mesh velocity.

To discretise in time, the discontinuous Galerkin methods (dG) as higher order variational time discretisation schemes is applied. We will present stability and error estimates for the semi-discretisation in time and the fully discrete problem.

[1] Universität Kassel, FB 10, Institut für Mathematik, Kassel, Germany,
adrigal@mathematik.uni-kassel.de

[2] Universität Kassel, FB 10, Institut für Mathematik, Kassel, Germany,
matthies@mathematik.uni-kassel.de

Bone Structure Analysis on Multiple GPGPUs

Peter Arbenz[1]

Osteoporosis is a disease that affects a growing number of people by increasing the fragility of their bones. The lifetime risk for osteoporotic fractures in women is estimated close to 40%, for men risk is 13%. Since global parameters like bone density do not admit to predict the fracture risk, patients have to be treated in a more individual way.

Today's approach consists of combining 3D high-resolution CT scans of individual bones with a micro-finite element analysis. To improve the understanding of bone, large scale computer simulations are applied. In recent years we have developed a fast, scalable and memory efficient solver for such problems called ParOSol. The equations of linear elasticity in pure displacement formulation are discretized by the finite element method. The resulting linear system of equations is solved by the conjugate gradient algorithm with a multigrid preconditioner. The solver is matrix free on all grid levels. Note that the principle obstacle in this problem is the very complicated computational domain entailed by osteoporotic bones. We have ported the solver to GPGPUs to profit from their exorbitant compute capabilities. We discuss how we modified the CPU code to run successfully on multi-GPGPUs. We present the implementation of ParOSol on Tödi (todi.cscs.ch), a machine at the Swiss Supercomputing Centre CSCS.

The code shows perfect weak scaling up to 256 GPGPUs. The largest problem solved on the machine contained about 8 billion voxel elements corresponding to about 25 billion degrees of freedom. Compared to the pure MPI code run on the 16-core nodes of Tödi we observe speedups of the MPI-Cuda code beyond five.

[1] ETH Zürich, Dep. Informatik, Switzerland,
arbenz@inf.ethz.ch

Simulating Lithium-Ion Batteries with Finite Elements

Markus Maier[1]

In this talk we present the numerical treatment of a micro-scale model for Lithium-ion batteries.

The battery is partitioned into $\Omega = \Omega_{\mathrm{an}} \cup \Omega_{\mathrm{e}} \cup \Omega_{\mathrm{ca}}$. The subdomains are representing the anode electrode, the electrolyte and the cathode electrode respectively. The conservation equation for Lithium $\partial_t c = -\nabla \cdot \vec{N}$ and the equation for local charge neutrality $0 = \nabla \cdot \vec{j}$ are decoupled in the electrodes but due to the existence of positively charged Ions in the electrolyte those equations are coupled in this region.

The Li-concentration c and the electrical Potential Φ may have jumps over the interfaces separating electrodes from electrolyte but they are coupled via highly nonlinear Neumann conditions. Additionally suitable boundary conditions are imposed in order to model the discharge of the battery at a constant macroscopic current.

A discretization by implicit Euler in time and H^1-conforming finite elements on triangular meshes in space is presented. Especially the treatment of the nonlinear terms is discussed. The performance of the `Matlab` implementation is demonstrated.

Finally we present how we are planning to integrate other physical effects like two-phase particles, intercalation-induced stress and Joule-heating into the numerical simulation.

References:

[1] A. Latz, J. Zausch, and O. Iliev. Modeling of species and charge transport in li-ion batteries based on non-equilibrium thermodynamics. Technical Report 190, Fraunhofer (ITWM), 2010
[2] J. Newman and K. E. Thomas-Alyea. Electrochemical Systems. Wiley, 2004

[1] Karlsruhe Institute of Technology, Institute for Applied and Numerical Mathematics, Karlsruhe, Karlsruhe, markus.maier@kit.edu

A Study on the Conditioning of Finite Element Equations with General (Anisotropic) Meshes via a Density Function Approach

Lennard Kamenski[1] Weizhang Huang[2]

The conditioning of the finite element stiffness matrix and the Jacobi preconditioned stiffness matrix is investigated using a density function approach proposed by Fried in 1973. It is shown that the approach can be used to develop bounds on the smallest eigenvalue and the condition number that are sharper than existing estimates in one and two dimensions and comparable in three and higher dimensions. The new results reveal that the mesh concentration near the boundary has less influence on the condition number than the mesh concentration in the interior of the domain. This is especially true for the Jacobi preconditioned system where the former has little or almost no influence on the condition number. Numerical examples are presented.

References:

[1] L. Kamenski and W. Huang. A study on the conditioning of finite element equations with arbitrary anisotropic meshes via a density function approach. J. Math. Study, 47(2):151–172, 2014.

[1] Weierstrass Institute, Numerical Mathematics and Scientific Computing, Berlin, Germany,
kamenski@wias-berlin.de

[2] The University of Kansas,
whuang@ku.edu

A Posteriori Error Control in Stochastic FEM and MLMC

Martin Eigel[1]

While a posteriori error estimation is a mature field in computational PDE, in particular FEM, there are only few adaptive methods for PDE with stochastic data as yet. We consider an elliptic model problem with dependence on a countable infinite set of independent uniform random variables. It is reformulated as parametric problem and discretised with the Stochastic Galerkin FEM in Legendre polynomial chaos. The introduction of a residual based reliable error estimator enables the formulation of an adaptive algorithm. The splitting into approximation and stochastic tail residuals leads to a refinement of the physical FEM space and of the anisotropic polynomial chaos simultaneously. In particular, the number of stochastic dimensions is adjusted in a problem-dependent way. Moreover, the algorithm can be shown to result in a convergent series of Galerkin discretisations. An extension of recent higher-order equilibration techniques facilitates the computation of guaranteed error estimators which do not involve unknown constants. Several benchmark problems illustrate the performance of the devised adaptive algorithm. Additionally, we give an outlook on how goal-oriented a posteriori error estimation can be included in FE-MLMC computations.

[1] Weierstrass Institute, Nonlinear Optimisation and Inverse Problems, Berlin, Germany,
eigel@wias-berlin.de

Continuous Galerkin-Petrov Methods in Time Combined with Stabilised Finite Element Methods in Space Applied to Time-Dependent Convection-Diffusion Problems

Gunar Matthies[1] Friedhelm Schieweck[2]

We consider the numerical solution of time-dependent convection-diffusion problems by combining continuous Galerkin-Petrov methods (cGP) in time with stabilised finite element methods in space. We will concentrate on symmetric spatial stabilisations like continuous interior penalty methods (CIP) or the local projection stabilisation (LPS).

As main result, error estimates for the fully discrete solution will be given in different norms. One main ingredient of the proofs is a lifting operator which maps the continuous solution trajectory of cGP into a trajectory which is continuously differentiable. This lifting is obtained on each sub interval in time by a post-processing of the cGP solution.

We present error estimates for the post-processed solution of order $\mathcal{O}(\tau^{k+2} + h^{r+1/2})$ for the $L^\infty(L^2)$-norm and the $L^2(L^2)$. Here, h is the spatial discretisation parameter, τ the temporal one, k the polynomial order in time, and r the ansatz order in space.

The theoretical predictions will be confirmed by numerical experiments.

[1] Universität Kassel, FB 10, Institut für Mathematik, Kassel, Germany,
matthies@mathematik.uni-kassel.de

[2] Otto-von-Guericke-Universität Magdeburg, Institut für Analysis und Numerik,
schiewec@ovgu.de

Guaranteed Energy Error Estimators for a Modified Crouzeix-Raviart Stokes Element

Alexander Linke[1] Christian Merdon[2]

This paper provides guaranteed upper energy error bounds for a modified lowest-order nonconforming Crouzeix-Raviart finite element method for the Stokes equations. The modification delivers a more robust Crouzeix-Raviart finite element method, that allows an optimal pressure-independent energy error estimate. In case of a right-hand side with large irrotational component in the sense of the Helmholtz decomposition, the modified element can lead to errors that are smaller by several magnitudes. Former guaranteed upper bounds for the unmodified Crouzeix-Raviart element are still applicable with small modifications, but result sometimes in a huge overestimation. To be efficient with respect to the modified solution, guaranteed upper bounds must approximate the divergence-free part of the Helmholtz decomposition of the right-hand side. Some designs are compared and verified by numerical benchmark examples. They show that guaranteed error control for the modified element is possible and almost as sharp as for the unmodified element.

[1] Weierstrass Institute, Numerical Analysis and Scientific Computing, Berlin, Germany,
alexander.linke@wias-berlin.de

[2] Weierstrass Institute,
christian.merdon@wias-berlin.de

Time-Adaptive Methods for the Incompressible Navier-Stokes Equations with High Order Accuracy in the Pressure Component

Joachim Rang[1]

Several classes of time stepping schemes are available for the simulation of incompressible fluids. In this talk we concentrate on implicit and linear-implicit Runge–Kutta methods since these methods allow an easy implementation of adaptive timestep control and allow higher order approximations.

Onestep methods have usually order reduction if they are applied on stiff ODEs. In the simulation of the incompressible Navier–Stokes equations this effect can usually observed in the pressure component. One well-known example of a stiff ODE is the example of Prothero and Robinson. We apply Rosenbrock-Wanner (ROW) methods on this problem and obain new order conditions which help us to improve the numerical order of convergence.

In comparison to DIRK and ROW methods a high dimensional nonlinear system of equations has to be solved in the case of the fully implicit Radau-IIA methods. This system can be transformed into smaller ones if the simplified Newton method is used. Then the solution of the linear systems can be computed in parallel with the help of the Component Template Library. The benefit of these Radau methods is the high order of convergence.

[1] TU Braunschweig, Institut fuer Wissenschaftliches Rechnen, Braunschweig, Deutschland, `j.rang@tu-bs.de`

Computing Resonances of Elastic Waveguide Problems with Hardy Space Infinite Elements

Martin Halla[1] Lothar Nannen[2]

Waveguide problems bear the difficulties of an unbounded domain. Instead of a boundary condition a radiation condition has to be fullfilled in the infinite direction, ensuring that waves are physically correct. A numerically problematic phenomen arising in elastic waveguides is the possibility of waves with different signs of phase and group velocity, often referred as backward propagating waves. Standard numerical methods like complex scaling (also known as PML) fail in such cases or become nonlinear in the frequency.

We introduce a transparent boundary condition based on a new variant of the pole condition and Hardy space infinite elements for its discretization. This method stays linear in the square of the frequency and thus resonance problems lead to linear eigenvalue problems. Numerical experiments exhibit super-algebraic convergence.

References:

[1] M. Halla, T. Hohage, L. Nannen, J. Schöberl, *Hardy Space Infinite Elements for Time-Harmonic Wave Equations with Phase Velocities of Different Signs*, ASC Report No. 18/2014, TU Wien, 2014.
[2] T. Hohage, L. Nannen, *Convergence of infinite element methods for scalar waveguide problems*, ASC Report No. 31/2013, TU Wien, 2013.

[1] Vienna University of Technology, Institute for Analysis and Scientific Computing, Vienna, Austria, martin.halla@tuwien.ac.at

[2] Vienna UT, lothar.nannen@asc.tuwien.ac.at

List of Participants

Surname, first name	Abstr.	**from**		**e-mail**
Adrigal, Khalid	[29]	Kassel	Germany	adrigal@mathematik.uni-kassel.de
Alkämper, Martin		Stuttgart	Germany	alkaemper@mathematik.uni-stuttgart.de
Arbenz, Peter	[30]	Zürich	Switzerland	arbenz@inf.ethz.ch
Beuchler, Sven	[14]	Bonn	Germany	beuchler@ins.uni-bonn.de
Broersen, Dirk	[27]	Amsterdam	The Netherlands	d.broersen@uva.nl
Busch, Ingolf		Chemnitz	Germany	ingolf.busch@mathematik.tu-chemnitz.de
Eigel, Martin	[33]	Berlin	Germany	martin.eigel@wias-berlin.de
Ernst, Oliver		Chemnitz	Germany	oliver.ernst@mathematik.tu-chemnitz.de
Garanza, Andrej		Siegen	Germany	garanza@mathematik.uni-siegen.de
Glänzel, Janine		Chemnitz	Germany	janine.glaenzel@iwu.fraunhofer.de
Haase, Gundolf		Graz	Austria	gundolf.haase@uni-graz.at
Halla, Martin	[37]	Vienna	Austria	martin.halla@tuwien.ac.at
Hannukainen, Antti	[10]	Aalto	Finland	antti.hannukainen@aalto.fi
Hartmann, Stefan	[10]	Clausthal	Germany	stefan.hartmann@tu-clausthal.de
Herzog, Roland		Chemnitz	Germany	roland.herzog@mathematik.tu-chemnitz.de
Höhne, Katharina	[28]	Dresden	Germany	katharina.hoehne1@tu-dresden.de
Jung, Michael		Dresden	Germany	mjung@informatik.htw-dresden.de
Kamenski, Lennard	[32]	Berlin	Germany	kamenski@wias-berlin.de
Krämer, Ulf		Darmstadt	Germany	ulf.kraemer@cst.de
Kressner, Daniel	[8]	Lausanne	Switzerland	daniel.kressner@epfl.ch
Licht, Martin		Oslo	Norway	martinwl@math.uio.no
Lilkova-Markova, Svetlana	[21]	Sofia	Bulgaria	lilkova_fhe@uacg.bg
Linke, Alexander	[35]	Berlin	Germany	alexander.linke@wias-berlin.de
Linß, Torsten		Hagen	Germany	torsten.linss@fernuni-hagen.de
Mach, Susann		Chemnitz	Germany	susann.mach@mathematik.tu-chemnitz.de
Maier, Markus	[31]	Karlsruhe	Germany	markus.maier@kit.edu
Matthies, Gunar	[34]	Kassel	Germany	matthies@mathematik.uni-kassel.de
Meyer, Arnd		Chemnitz	Germany	a.meyer@mathematik.tu-chemnitz.de

Surname, first name	Abstr.	**from**		**e-mail**
Nestler, Peter		Berlin	Germany	nestler@math.tu-berlin.de
Nkemzi, Boniface	[13]	Buea	Cameroon	nkemzi@yahoo.com
Ospald, Felix	[19]	Chemnitz	Germany	feo@tu-chemnitz.eu
Pavlov, Peter	[20]	Sofia	Bulgaria	pdp_mech_fhe@uacg.bg
Pester, Matthias		Chemnitz	Germany	pester@mathematik.tu-chemnitz.de
Peters, Michael	[26]	Basel	Switzerland	michael.peters@unibas.ch
Rang, Joachim	[36]	Braunschweig	Germany	j.rang@tu-bs.de
Riedel, Ilka		Chemnitz	Germany	ilka.riedel@mathematik.tu-chemnitz.de
Rösch, Arnd		Essen	Germany	arnd.roesch@uni-due.de
Schmidt, Hansjörg	[17]	Chemnitz	Germany	hanss@hrz.tu-chemnitz.de
Schneider, Reinhold	[24]	Berlin	Germany	schneidr@math.tu-berlin.de
Schneider, Rene	[11]	Chemnitz	Germany	rene.schneider@mathematik.tu-chemnitz.de
Seidel, Jens		Chemnitz	Germany	jens.seidel@mathematik.tu-chemnitz.de
Siebenmorgen, Markus	[25]	Basel	Switzerland	markus.siebenmorgen@unibas.ch
Springer, Rolf	[22]	Chemnitz	Germany	Rolf.Springer@mathematik.tu-chemnitz.de
Sprungk, Björn		Chemnitz	Germany	bjoern.sprungk@mathematik.tu-chemnitz.de
Tempone, Raùl	[23]	Thuwal	Saudi Arabia	raul.tempone@kaust.edu.sa
Unger, Roman		Chemnitz	Germany	roman.unger@mathematik.tu-chemnitz.de
Vallejos, Michelle	[18]	Chemnitz	Germany	mival@hrz.tu-chemnitz.de
Wachsmuth, Gerd	[12]	Chemnitz	Germany	gerd.wachsmuth@mathematik.tu-chemnitz.de
Weise, Michael	[16]	Chemnitz	Germany	michael.weise@mathematik.tu-chemnitz.de
Zhou, Ming	[9]	Rostock	Germany	ming.zhou@uni-rostock.de

Internet access:

The hotel offers free internet access. Wireless LAN is available in all rooms. Access details can be obtained from the hotel reception.

Food:

Breakfast: Buffet from 7:00.

Lunch: There is a lunch buffet each day.

The conference fee includes:

- Lunch on all three days of the symposium (one soft drink included)
- Tea, coffee, soft drinks and snacks during breaks.
- The conference dinner on Monday.

Recreation:

The hotel offers sauna for free.

Public transport:

Hotel guests may use their room identity-card ("Hotel-Ausweis") free of charge as travel ticket for all city's public transport in Chemnitz.
This is useful for our excursion on Tuesday (see below).

Excursion

Please mind the following hints for the excursion:

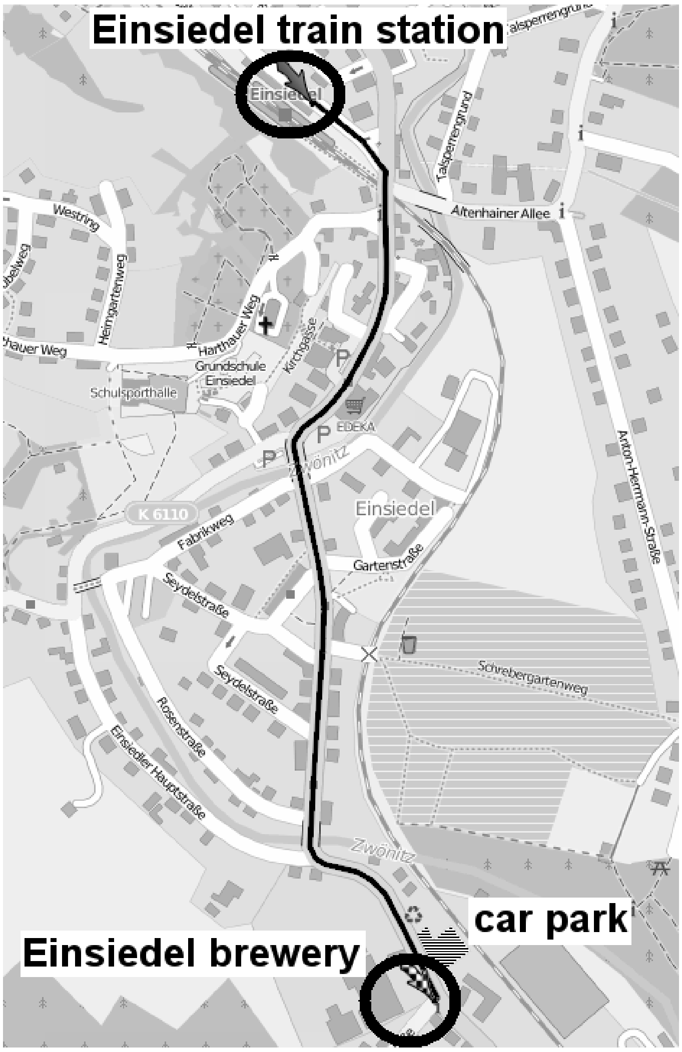
- **For those who spend the night in the hotel:**
  If you want to participate in the excursion please don't forget that you can use your room identity-card as ticket. This ticket is necessary for the train ride.
- **For those who don't spend the night in the hotel:**
  If you want to participate in the excursion please say if you need a ticket for the train until Tuesday 11:30 to one of the organizers.

Details for the excursion

The excursion will take place on Tuesday, 23 of September. We will go to the Einsiedel brewery for a guided tour through the production process, with a beer tasting.
Therefore, we will meet at 13:50 in front of the hotel "Chemnitzer Hof". We will go to Chemnitz main station and take the train to Chemnitz Erfenschlag at 14:10. (The train starts from platform 14.)

The first part of the excursion is to walk from there to the Einsiedel brewery. The distance is approximately 5 km. After the arrival at the brewery the second part starts at 15:45 with the guided tour.

For those who do not want to join the first part of the excursion (or miss the train) but want to participate in the brewery tour, there exist two ways to reach the brewery on their own.



taken from Openstreetmap

You can use the train from Chemnitz main station to Einsiedel train station and walk from there to the brewery. The train leaves at 15:10, platform 14 at the main station and will reach the station **"Einsiedel"** at 15:24 (**Note: not the station** "Einsiedel Hp Gymnasium"!). For the way from the train station to the brewery see the map on the left side. The distance is approximately 1 km. The guided brewery tour starts at 15:45.

If you want to go by car, there is a car park opposite the brewery.

The address of the brewery is:

Einsiedler Hauptstraße 144
09123 Chemnitz.

Chemnitz FEM Symposium

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TECHNISCHE UNIVERSITÄT CHEMNITZ

Technische Universität Chemnitz
09107 Chemnitz
www.tu-chemnitz.de