

Welcome

Dear participants,

welcome to the workshop on “Recent and Future Development with and of deal.II” at the University of Heidelberg. We are very glad that many people from different countries contribute to this workshop. The aim of this workshop is to bring together experts, researchers and students using deal.II.

This workshop is a platform for making contact and exchanging ideas in the field of scientific computing with deal.II. This software library has been developed a lot over the last few years. The meeting gives the opportunity to sustain this development. You can learn about new features of the library and you can present your own progress with and of deal.II.

Beside the interesting program on various topics, we hope that you will find enough time to discuss and exchange new ideas with your colleagues and friends during the breaks.

This booklet contains information on time schedules and locations. Moreover, you will find information about how to access the wireless network. At the end of this booklet you will find a list of all the participants of this workshop.

We hope you will enjoy the scientific and social program of this deal.II workshop and you are going to have as much fun here in Heidelberg as we had while preparing the workshop!

The Organizing Committee:

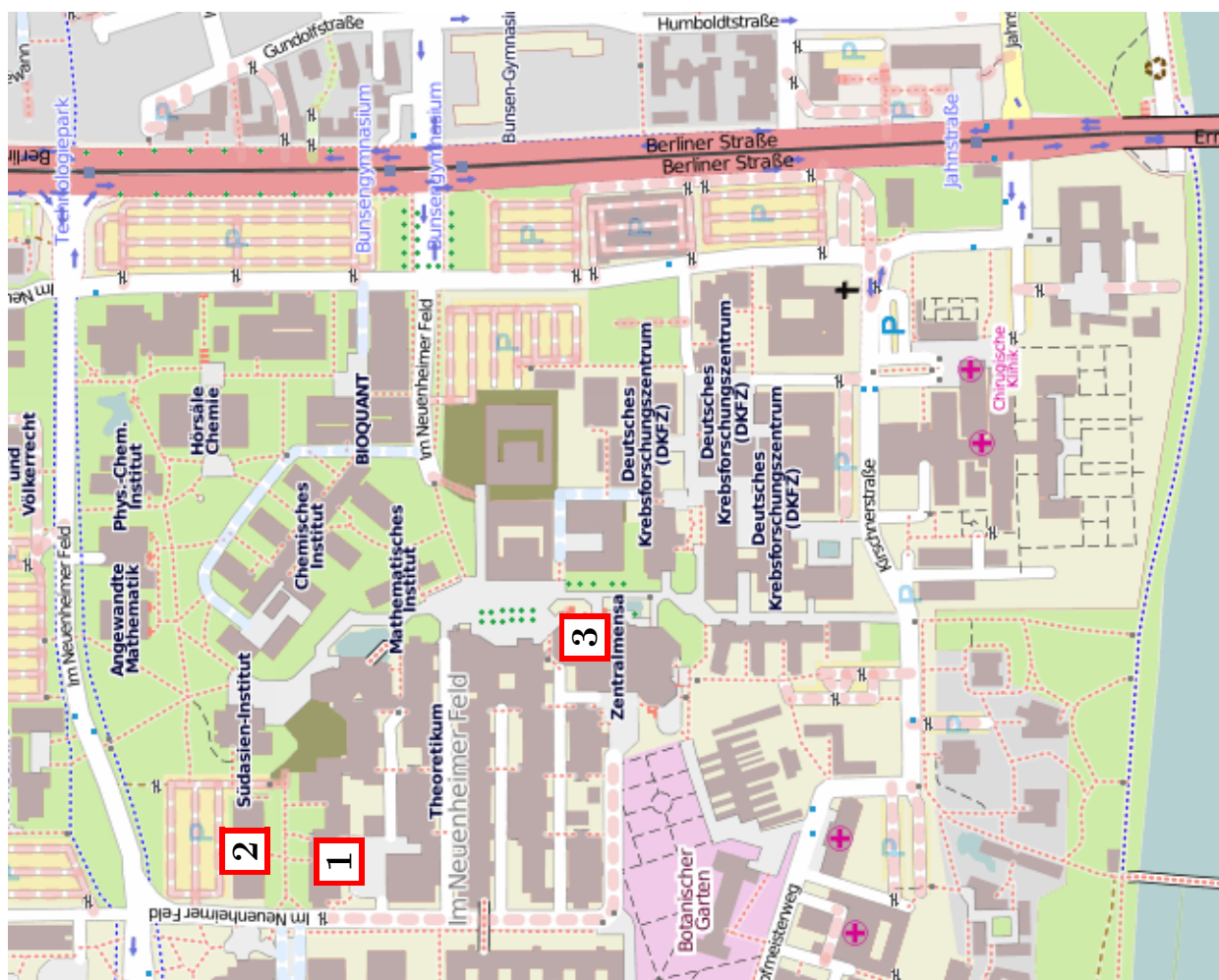


Thomas, Martin, Bärbel, Timo



Locations:

1. Conference location (IWR, Building 368, Room 432)
2. Computer room (OMZ, Building 350, Room U011/U012)
3. Cafeteria (Mensa)
4. Train station
5. Hotel Ibis (Willy Brandt Platz 3)
6. Dinner (Das Bootshaus, Schurmanstr. 2)
7. Hotel Kohler (Goethestraße 2)
8. Schloss



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Time table

	Monday	Tuesday	Wednesday	Thursday	Friday
09:15-09:45	Registration	W. Bangerth [6]	G. Kanschat [12]	Code jam	
09:45-10:15	Opening and history of deal.II				
10:15-10:30		Coffee break			
10:30-10:45	Coffee break				
10:45-11:15		M. Kronbichler [7]	A. McBride [13]		
11:15-11:45	R. Hartmann [1]	T. Heister [8]	M. Steigemann [14]		
11:45-12:15		B. Janssen [9]	T. Young [15]		
12:15-13:30	Lunch break				
13:30-14:00	M. Bürg [2]	A. Große-Wöhrmann [10]	T. Carraro [16]	Code jam	
14:00-14:30	C. Weiler [3]	M. Geiger [11]	J. M. Linhart [17]		
14:30-15:00	Coffee break				
15:00-16:00	W. Wollner and T. Wick [4]	Ideas for the future			
16:00-16:30	L. Heltai [5]	(Ideas for the future)			
16:30-18:00	Schloßbegehung				
from 19:00		Dinner			

Organization of “Ideas for the future”

This session is planned as a moderated discussion in the conference room. Everyone is open to suggest topics or questions about the future development of deal.II. A suggestion should consist of a title, your name and optionally a few more words as an explanation. We will hand out forms for that on Monday that you can hand back to us until the end of that day.

For the session we are going to prepare slides to the topics and ask the suggester to explain it to the audience in a few words. We then hope for interesting ideas and discussions to happen. Maybe we can even stimulate groups to work on some of those suggestions during the code jam or otherwise after the conference?

As we are not sure how this is going to turn out and how much interest there is, we might extend it to after the coffee break at 16:30 on Tuesday. Keep in mind that we need to judge if a suggestion is appropriate or that we might not find the time to include everything. To help you understand what kind of ideas we are thinking of, here are a few examples:

1. Bärbel Janssen: Offering Newton’s method and timestepping schemes as well as error estimators like DWR.
2. Martin Kronbichler: Size of the compiled library (> 2 GB) – can we reduce this by using less instantiations, making some functions with templates inline, introducing modules, etc.?
3. Thomas Wick: Discussion on efficient linear solvers for large coupled problems (at least in 3D) with more than two principal unknowns. For instance, parallel direct solver, explicit coupling via subiterations, or implicit solution approach, etc.?
4. Timo Heister: Multithreading in linear algebra (PETSc and Trilinos do not support multithreading, are there alternatives or do we need to write a replacement using TBB?).

Please help us to make this session great by suggesting topics and by discussing other ideas!

Organization of the “Code jam”

Even though the official part of the workshop ends on Wednesday, we decided to host the so called code jam on Thursday and Friday for interested participants of the workshop. The idea is pretty simple: We offer rooms (the computer pool) and you are doing the rest!

We would like to give you the opportunity to collaborate, write code together, sketch out new ideas, ask questions, discuss, present your ideas, look over the shoulders on how others work, or just chat with like-minded others.

Everyone is welcome to join us!



Abstracts

The talks are listed in session order and the numbers correspond to the numbers in the schedule.

1. Aerodynamic flow simulations based on `deal.II`

Ralf Hartmann, Institute of Aerodynamics and Flow Technology, German Aerospace Center (DLR), Braunschweig

Monday, August 23, 11:15–12:15

In this talk we present higher order and adaptive discontinuous Galerkin methods for an efficient and reliable prediction of aerodynamic force coefficients for aerodynamic flows. These methods are implemented in the discontinuous Galerkin flow solver PADGE [5] which is based on a modified version of the `deal.II` library [1, 2].

Aerodynamic force coefficients like the drag, lift and moment coefficients are important quantities in aerodynamic flow simulations. In addition to the exact approximation of these quantities it is of increasing importance, in particular in the field of uncertainty quantification, to estimate the error in the computed quantities. We demonstrate reliable adjoint-based error estimation and goal-oriented mesh refinement that targets at the accurate approximation of single as well as of multiple force coefficients (see [3]). Furthermore, the adjoint-based mesh refinement is combined with anisotropic mesh refinement (see [7, 8]) and with *hp*-refinement (see [9]).

In the PADGE code these techniques are implemented for 2d and 3d laminar and turbulent compressible flows as governed by the compressible Navier–Stokes equations and the Reynolds-averaged Navier–Stokes (RANS) and $k - \omega$ turbulence equations (see [6, 4]). The error estimation and adaptation algorithms is applied to aerodynamic test cases including a turbulent flow around a three-element high lift configuration and a turbulent flow around a wing-body configuration.

References:

- [1] W. Bangerth, R. Hartmann, and G. Kanschat. `deal.II` – A general purpose object oriented finite element library. *ACM Transactions on Mathematical Software*, 33(4), 2007.
- [2] W. Bangerth, R. Hartmann, and G. Kanschat. `deal.II Differential Equations Analysis Library, Technical Reference`. <http://www.dealii.org/>, 6.2 edition, 2009. First edition 1999.
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- [4] R. Hartmann, J. Held, and T. Leicht. Adjoint-based error estimation and adaptive mesh refinement for the RANS and k - ω turbulence model equations. *J. Comput. Phys.*, 2010. To appear.

- [5] R. Hartmann, J. Held, T. Leicht, and F. Prill. Discontinuous Galerkin methods for computational aerodynamics – 3D adaptive flow simulation with the DLR PADGE code. *Aerospace Science and Technology*, 2010.
<http://dx.doi.org/10.1016/j.ast.2010.04.002>.
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- [7] T. Leicht and R. Hartmann. Anisotropic mesh refinement for discontinuous Galerkin methods in two-dimensional aerodynamic flow simulations. *Int. J. Numer. Meth. Fluids*, 56(11):2111–2138, April 2008.
- [8] T. Leicht and R. Hartmann. Error estimation and anisotropic mesh refinement for 3d laminar aerodynamic flow simulations. *J. Comput. Phys.*, 2010. To appear.
- [9] T. Leicht and R. Hartmann. Error estimation and hp -adaptive mesh refinement for discontinuous Galerkin methods. In Z.J. Wang, editor, *Adaptive High-Order Methods in Computational Fluid Dynamics - with applications in aerospace engineering*. World Science Books, 2010. In review.

2. Higher-Order Nédélec Elements

Markus Bürg, Institut für Angewandte und Numerische Mathematik, Karlsruhe Institut für Technologie (KIT)

Monday, August 23, 13:30–14:00

In recent years a broad interest in considering electromagnetic phenomena numerically has come up. Usually the natural function space for such problems is the space $H(\text{curl})$ – the space of all square-integrable functions for which only some combinations of first derivatives, namely the components in the curl of the function, are square-integrable. The most common choice of finite elements representing the space $H(\text{curl})$ are the so called Nédélec elements, which were introduced by J.C. Nédélec in 1980. As for most finite elements the accuracy of approximation can be improved by increasing the polynomial degree of the element, if the solution of the corresponding problem is smooth.

In this talk we want to consider the mathematical theory of these elements in detail and present their implementation for arbitrary polynomial degree.

3. Nonlinear biharmonic equation and very weak Laplace problem

Christoph Weiler, Institut für Angewandte Mathematik, Universität Heidelberg

Monday, August 23, 14:00–14:30

In this talk we will be dealing with scalar nonlinear biharmonic equations. As an example we present the stream function formulation of the instationary Navier-Stokes equations. Solving a biharmonic equation requires C^1 -elements to get a conforming

finite element space. We discuss problems that arise when using these elements in deal.II.

This leads us to solve the Laplace problem in a very weak form. Sometimes one does not even have H^1 -regularity for the solution of the Laplace problem, which is eventually caused by reentrant corners. The very weak formulation of the problem, involving L^2 -projection of the boundary function, is of avail.

4. DOpE: deal.II Optimization Environment

Thomas Wick and Winnifried Wollner, Institut für Angewandte Mathematik, Universität Heidelberg

Monday, August 23, 15:00–15:45

We present a new software library based on deal.II. We discuss the aims of the project together with some numerical examples. We conclude by outlining future directions.

The goal of DOpE is to combine the advantages of deal.II, like various finite elements, different linear solvers, etc., with modular high level routines, like nonlinear solvers and optimization routines. That is, solution algorithms for nonlinear and linear stationary PDE problems as well as for PDE-constrained optimization problems are provided to the user. In addition, time dependent PDE problems can be solved with schemes like implicit and explicit Euler, Crank–Nicolson, and Fractional-Step-Theta.

In order to allow transparent switching of algorithms a unified interface is used to describe the problem under consideration. From this information the program assembles the information required by the algorithm without further interaction with the user.

This approach features simple interface for the implementation of different PDE and optimization problems. In addition, the modular framework enables us to test different algorithms and to compare them, e.g., switch between different time stepping schemes, without the need to rewrite (or copy) large amounts of code fragments thereby reducing the potential errors introduced by switching of algorithms.

The outlined programming framework will be substantiated with some numerical examples including stationary PDE-constrained optimization problems as well as stationary and nonstationary PDE problems.

5. The codimension one capabilities of Deal.II

Luca Heltai, International School of Advanced Studies, SISSA

Monday, August 23, 16:00–16:30

Since version 6.2, deal.II supports problems defined on manifolds of dimension one less than the space dimension.

In this talk we will present what has been introduced and how this structure can be used to solve, for example, Boundary Element Methods (BEMs), as in `step-34`, or interactions between PDEs defined on different dimensions, such as in Fluid Structure Interaction (FSI) between membranes and fluids, as in Immersed Boundary Methods (IBMs).

6. Using multiple cores on a single machine

Wolfgang Bangerth, Department of Mathematics, Texas A&M University

Tuesday, August 24, 9:15–10:15

Every laptop today has at least 2 processor cores; workstations often have 16 or more cores that can all access the same memory, and it is clear that both numbers will continue to grow in the foreseeable future. At the same time, each core runs at approximately the same speed as they did some 5 years ago. Consequently, to make programs faster, they have to use parallelism.

Starting with release 6.3, `deal.II` has incorporated the Threading Building Blocks (TBB), a generic library originally written by Intel. I will give an overview of the philosophy behind this library and how it is used in `deal.II`. I will also show ways how user programs can make use of the concepts introduced by the TBB. I will close with a number of observations and open problems.

7. Generic and efficient solvers for coupled flow/transport problems

Martin Kronbichler, Department of Information Technology, Uppsala University

Tuesday, August 24, 10:45–11:15

In many applications of computational fluid dynamics, the flow equations (described by the Stokes or Navier–Stokes equations) are coupled to the evolution of additional quantities. A simple model exhibiting this structure is the coupling to a scalar quantity driven by transport (advection) or advection–diffusion, with applications in the simulation of fluid flow driven by buoyancy, and the simulation of the two-phase flow with the level set model, with the interface separating the two fluids represented by a scalar level set function. The scalar quantity (temperature/level set function) induces a force in the momentum equation. In this talk, I will give an overview of programming techniques to solve such problems, which is also the topic of the `deal.II` example programs `step-31` and `step-32` with serial and parallel implementations. For time-dependent flows, it is convenient to use time-lag schemes that perform the fluid solution and the scalar evolution equation in two steps. This allows to implement the fluid solver separately from solver for the scalar transport. The force and boundary conditions to the flow solver are set in the implementation of the scalar evolution equation. Different models can then be implemented easily on top of a fixed fluid solver, or different fluid solvers can be compared for the same problem setting, allowing to reuse large fractions of the program.

8. Massive Parallel Computations with deal.II

Timo Heister, Institut für Numerische und Angewandte Mathematik, Universität Göttingen

Tuesday, August 24, 11:15–11:45

I present our recent work to enable deal.II to scale on high performance clusters with thousands and more CPUs. The trend in computing goes to larger problems that need to be solved in shorter time frames. Fortunately HPC cluster are becoming widely available. We had to change several aspects of deal.II in order to leverage this computing power: fully distributed mesh handling with all consequences in different parts of the library, new algorithms for degree of freedom distribution, efficient indexing, ghost values in the linear algebra, to name the most important parts.

We see promising scalability in our numerical results that confirm our research. The code is hopefully merged into the deal.II project soon, so that it is available for every user. It allows parallel implementations with only few changes compared to the old MPI model.

References:

- [1] W. Bangerth, C. Burstedde, T. Heister, and M. Kronbichler. Algorithms and Data Structures for Massively Parallel Generic Finite Element Codes. *In preparation*.
- [2] T. Heister, M. Kronbichler, and W. Bangerth. Generic finite element programming for massively parallel flow simulations. *Eccomas 2010 Proceedings*, 2010.

9. Multilevel Methods with Local Smoothing

Bärbel Janssen, Institut für Angewandte Mathematik, Universität Heidelberg

Tuesday, August 24, 11:45–12:15

So far Multilevel Methods implemented in deal.II have been working only for global refinement on continuous finite elements. In this talk, we derive a consistent multilevel method for discretizations on meshes with hanging nodes. The implementation for continuous finite elements of arbitrary order is discussed.

Our design goals for such a method are

- convergence rates may not be significantly lower than on regular meshes without local refinement
- each step should be performed with optimal computational complexity
- the matrix structures involved must be easy to obtain in a finite element code and may not severely increase memory requirements
- smoothing should only happen on subgrids without hanging nodes to simplify cell-based smoothers

- the scheme should be able to use the continuity conditions across faces for any finite element

We confirm the efficiency of the resulting method with numerical experiments. Results for computations in two and three dimensions for finite elements up to order three are presented.

10. A posteriori control of modelling and discretization errors in thermoelasticity

André Große-Wöhrmann, Heribert Blum, and Marcus Stiemer, Institut für Angewandte Mathematik, Technische Universität Dortmund

Tuesday, August 24, 13:30–14:00

The concept of adaptive error control for finite element Galerkin discretizations has more recently been extended from the pure treatment of the discretization errors [1], [2] also to the control of modelling errors [4, 5]. These techniques can be employed for a rigorous justification of the local choice of the model out of a given hierarchy with increasing complexity. In the present talk the concept is exemplified by a hierarchy of models arising out of the scope of thermoelasticity [6]. Significant reduction of the computational complexity can be achieved by a proper choice of the model in different subdomains, automatically chosen by the error estimators. Several error indicators are investigated in the context of goal oriented error estimation. Their efficiency is compared by means of finite element simulations [3].

Acknowledgements:

This project is supported by the Deutsche Forschungsgemeinschaft (DFG) under grant SFB-TR 73 “Sheet-Bulk Metal Forming” (<https://www.tr-73.de>).

References:

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- [2] R. Becker, R. Rannacher. An optimal control approach to a posteriori error estimation in finite element methods. *Acta Numerica*, 10:1–102, edited by A. Iserles, Ed., Cambridge Univ. Press, 2002.
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- [5] J.T. Oden, S. Prudhomme. Estimation of Modeling error in computational mechanics. *J. Comp. Phys.*, 182:496–515, 2002.
- [6] J.C. SIMO: *Numerical Analysis and Simulation of Plasticity*. In P.G. Ciarlet and J.L. Lions, editors, *Handbook of Numerical Analysis (Volume VI)*. North Holland, 1998.

11. An efficient adaptive time-stepping scheme for the wave equation

Michael E. Geiger, Institut für Angewandte Mathematik, Universität Heidelberg

Tuesday, August 24, 14:00–14:30

Main issue of this talk is the construction of an efficient time-stepping scheme for the solution of the acoustic wave equation. The subject of adaptive refinement of the spatial mesh will be neglected here but may be found in papers of W. Bangerth and R. Rannacher [1, 2]. The error estimator for the time variable will be developed for a member of the family of Newmark methods.

The talk can roughly be divided into two parts: First, a well-known relationship between the Crank–Nicolson difference scheme and the so-called average-acceleration method (which belongs to the family of Newmark methods) is briefly recapitulated. The central aspect herein is an interpretation of both time-stepping schemes as a Galerkin method. In the second part, the dual-weighted residual (DWR) method is applied to derive an a posteriori error estimator which can be used for adaptive refinement of the time grid in the context of the undamped acoustic wave equation. The presented method can also be adapted to equations including special types of damping or to the Lamé–Navier equations from elasticity theory. In short, an error estimator for the Newmark scheme will be presented which is reliable, highly efficient and more flexible than some former approaches that can be found in the literature [3, 4]. In the end, all results will be illustrated and verified by numerical examples.

References:

- [1] W. Bangerth and R. Rannacher. Finite element approximation of the acoustic wave equation: Error control and mesh adaptivity. *East-West J. Numer. Math.* 7:263–282, 1999.
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- [4] I. Romero and L.M. Lacoma. A methodology for the formulation of error estimators for time integration in linear solid and structural dynamics. *Int. J. Numer. Methods Engrg.*, 66:635–660, 2006.

12. The MeshWorker Interface: Reusable Structures for Integral Forms

Guido Kanschat, Department of Mathematics, Texas A&M University

Wednesday, August 25, 9:15–10:15

When integrating forms related to the weak formulation of PDE, the same loop over all cells of a mesh is programmed over and over again. In particular, when it comes to discontinuous Galerkin methods on locally refined meshes, this loop becomes too

complicated to copy it by hand between instantiations. Therefore, the MeshWorker Interface has been introduced, which implements the loop in a generic way. From the point of view of applications, only the local integrals on a single cell or face have to be implemented. Complemented by a set of control parameters, they are being fed into the generic loop, such that programming of complex applications becomes much more reliable. In this presentation, we introduce the basic concepts of the MeshWorker, the most important classes and their relation to each other.

13. Coupled problems in non-linear solid mechanics

Andrew McBride and Paul Steinmann, Lehrstuhl für Technische Mechanik, Universität Erlangen–Nürnberg

Swantje Bargmann, Institute of Mechanics, Technische Universität Dortmund

Wednesday, August 25, 10:45–11:15

The problem of interest involves the penetration of a low molecular weight solvent within a polymeric solid. The presence of the solvent causes the polymer to undergo a transition from a glassy to a rubber-like state. This transition occurs at a finite rate and thereby inhibits the solvent ingress. The resulting diffusion process is non-Fickian and wave-like in nature. The molecular rearrangements in the polymeric solid result in significant deformations at the macro-scale. These deformations are best described using a Lagrangian finite deformation viscoelastic model.

The resulting coupled diffusion–deformation problem, known as case II diffusion, presents numerous challenges from a modelling perspective. The system is highly non-linear, stiff and tightly coupled. A robust solution algorithm is essential to capture the key features of case II diffusion.

This work explores the use of spatial and temporal adaptivity to model case II diffusion. Spatial adaptivity is essential to track the solvent wave as it moves through the polymer. Temporal adaptivity is necessary due to the extreme non-linearities. The description of the polymer as a viscoelastic solid requires the use of an internal variable approach. These internal variables are stored at the level of the quadrature point in the discrete model, thereby complicating the spatial adaptivity process.

The objective of the talk is to encourage feedback on the optimal way in which to tackle this complex problem using the deal.II library. A general discussion on the solution of problems in non-linear solid mechanics is also envisaged.

14. Simulation of quasi-static crack propagation with deal.II

Martin Steigemann, Department of Mathematics and Natural Sciences, University of Kassel

Wednesday, August 25, 11:15–11:45

In this talk, we present some ideas, how quasi-static crack propagation for plane problems can be simulated. Based on the Griffith' energy principle, a crack grows in such a way, that the total energy of the solid is always minimal. Recent mathematical results of asymptotic analysis show, that the change of energy can be calculated by means of certain integral characteristics, if the crack grows along a small kink. With these integral characteristics at hand, which depend on the geometry, the material properties and the individual load scenario of the solid, quasi-static crack propagation can be simulated step-by-step.

Considering linear elastic materials, not necessarily homogeneous, the (elliptic) elasticity system defines the underlying partial differential equations which have to be solved numerically with the finite element method. In order to calculate the change of energy, we are not interested in solutions of the elasticity system itself, but in certain functionals of solutions, for example the stress intensity factors. The precise-as-possible and efficient calculation of these functionals is till this days a numerical challenge and adaptive mesh refinement is one of the main keys for accurate results. Clearly, the mesh has to be adapted in such a way, that the error of the functional decreases with mesh refinement and we use an error estimator based on the dual-weighted-residual approach developed by Rannacher/Becker and co-workers.

Besides finite element solvers for the elastic equations itself, there are many aspects which have to be taken into account when simulating quasi-static crack growth. We have to deal with complicated geometries, inhomogeneous material properties and very complex load scenarios, just to name a few. In order to provide a general framework for handling these aspects, the software package MCrack2D was developed at our research group "Applied Mathematics" at the University of Kassel. MCrack2D is a pure research code with the intention to realize an exact-as-possible transfer of analytical models to numerics in order to test and improve theoretical ideas and make them finally applicable to real-world problems. Within MCrack2D the deal.II package is the heart and soul of all finite element calculations, coupled with the mesh generator Cubit 12.0 from Sandia National Laboratories and other in-house developed modules for handling crack problems.

In this contribution, we show ideas for calculating functionals of fracture mechanics using the dual-weighted-residual approach, details of the implementation and the advantages of these ideas by some numerical examples.

Acknowledgements:

This contribution is based on investigations of the collaborative research center SFB/TR TRR 30, which is kindly supported by the DFG.

15. dealing with atomic imagery: A case study of the Hartree-Fock equations and the selfconsistent solver context

Toby D. Young, Institute of Fundamental Technological Research of the Polish Academy of Sciences

Wednesday, August 25, 11:45–12:15

As a case study the many-body problem for finite electron systems is presented [1] in which the self-consistent Hartree-Fock equations are explored for the isolated atom [2] in the finite element basis using `dealii` [3] coupled to SLEPc [4]. Based on work following **step-36** of the `dealii` tutorial, Schrödinger's equation is solved as a vector-valued generalized eigenspectrum problem with computations on parallel machine architecture. Unresolved problems facing the development of a sufficiently abstract self-consistent solver context are discussed. In particular: (i) A possible advanced programming interface; (ii) Memory management of static orbital matrices; and (iii) Speed-up methods with holistic grid adaptivity. To this end, recent developments and pending extensions to the `dealii::SlepWrappers` namespace are given. In particular, (i) The implementation of a new solver for the generalized eigenspectrum problem; and (ii) Exploitation of matrix symmetries.

Acknowledgements:

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References:

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16. 3D FEM-model for the Reconstruction of a Porous SOFC Cathode

Thomas Carraro, Institut für Angewandte Mathematik, Universität Heidelberg

Jochen Joos, André Weber, and Ellen Ivers-Tiffée, Institut für Werkstoffe der Elektrotechnik (IWE) and Center for Functional Nanostructures (CFN), Karlsruhe Institut für Technologie (KIT)

Wednesday, August 25, 13:30–14:00

The performance of a solid oxide fuel cell (SOFC) is strongly affected by electrode polarization losses, which are related to the composition and the microstructure of the porous materials. A model that can decouple the effects associated to the geometrical microstructure and to the material properties can give a relevant improvement in the understanding of the underlying processes.

Based on the method described in [1, 2] a porous cathode can be reconstructed. Focused Ion Beam (FIB) and Scanning Electron Microscopy (SEM) techniques, combined with image processing, lead to an accurate reconstruction of the porous microstructure.

We developed a detailed 3D finite element method (FEM) model for the calculation of the area specific resistance (ASR) as a performance index. In this model the electrochemical and diffusion processes are described by surface exchange parameters and diffusion coefficients. A parametric study of the main processes can reveal important influences on the performance index. In this context we perform a sensitivity study of the model with respect to the material parameters. The reconstruction of the microstructure allows to focus on the material parameters, considering the geometrical ones as accurate given data.

Numerically, the solution of the forward problem is challenging due to the electrochemical couplings between the phases and the large dimension (bigger than 10^7 elements) of the model. Thus an efficient solver is a key component of this work.

We present a 3D FEM-model for the reconstruction of a porous LSCF cathode.

References:

- [1] J.R. Wilson, W. Kobsiriphat, R. Mendoza, H.Y. Chen, J.M. Hiller, D.J. Miller, K. Thornton, P.W. Voorhees, S.B. Adler and S.A. Barnett. Three-dimensional reconstruction of a solid-oxide fuel-cell anode. *Nature Materials*, 5:541-544, 2006.
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17. Statistical Sampling in Bayesian Inverse Problems using deal.II

Jean Marie Linhart, Department of Mathematics, Texas A&M University

Wednesday, August 25, 14:00–14:30

Inverse problems attempt to infer physical parameters from observable data. A PDE model (with deal.II) might be the forward model, or starting point, for solving an inverse problem. The fun has barely started at this point. Solving an inverse problem will demand many evaluations of the forward model, and Bayesian inverse problems, which look at inverse problems from a statistical point of view, demand many many more. I will give an introduction to Bayesian inverse problems, show some preliminary results with a model problem, and describe some of the stresses I put on the computing resources by attempting to do statistical sampling.

Conference Dinner

We invite all people to join the informal conference dinner on Tuesday evening at 19:00h in the old town of Heidelberg. After the discussion round “Ideas for the future” you are invited to walk with us in the old town of Heidelberg and feel the great atmosphere of one of the most beautiful cities in Germany. Along the river Neckar you will find time for relaxing as well as continuing fruitful discussions with colleagues.

The location is

Das Bootshaus
Schurmannstr. 2
69115 Heidelberg

and you will find it in the first map provided on page 2 of this booklet.

In order to keep the organization of this event as easy as possible, each participant pays for one’s own dinner at the venue.

We wish you a stimulating and memorable evening!

Access to Wireless Internet

For connecting to network services at the University of Heidelberg

- **IMPORTANT:** Please make sure that your operating system is updated to the most current version possible. Make sure that you have installed a virus scanner on your computer with regular updates and a full array of scan options.
- Install/activate your network card and set it to “obtain IP-address automatically” (DHCP).
- For WLAN users: Our network ID (SSID) is “UNI-WEBACCESS” (or “UNI-HEIDELBERG”, in case WEBACCESS is not available). At this time we are not employing options for “secure wireless LAN” (WEP/WPA/802.1x/802.11i): Please take your own precautions with regard to sufficient encryption.
- You will be able to use the following Internet services:
 - WWW: http und https
 - Email services: pop, spop, imap, imaps
 - In order to send emails – if not via web interfaces – the following SMTP server (“outgoing mail”) must be entered: `extmail.urz.uni-heidelberg.de`
 - SSH, MS-RDP and VPN (IPsec)
 - H.323 and SIP with the above listed UDP port ranges

Upload of Presentations

In order to avoid tedious switching between different laptops for your talks, we will provide a laptop from which all presentations are started. Therefore, we kindly ask you to upload your presentation during a break before your session. The laptop will be located in the seminar room (item 1 on the map on page 3).

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