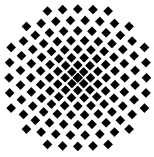
BOOK OF SUMMARIES



1ST SIMTECH PHD WEEKEND

OCTOBER 2–4, 2009

SÖLLERHAUS

Preface

This book documents the course of the first PhD weekend of the SimTech Graduate School held at the Söllerhaus in Hirschegg, Austria, October 2 - 4, 2009. It is intended to serve as a reference book in two respects: On the one hand, it contains a synopsis of the simulation methods used in the SimTech cluster and provides references for introductory reading. On the other hand, it gives an overview over the researchers using these methods and thus allows the quick identification of a suitable contact person.

From our perspective, the success of interdisciplinary research depends on various factors: Firstly and most importantly, it is not possible without the participating researchers' awareness of methods and approaches used in other disciplines that could be useful in the context of his scientific problem. Secondly, it is often made very difficult by the use of diverging terminology in the different disciplines. And thirdly, like all other forms of research involving team work, it depends on a successful social interaction between the involved individuals.

We hope that the talk about interdisciplinarity given by Dr. Rudolf Kötter created some awareness for these factors and that the following interdisciplinary workshops and the social program including a long hike to the nearby Walmendinger Horn helped to lay some foundations for interdisciplinary cooperation between the doctoral students and postdocs in all three respects.

From our point of view and judging from the feedback of the participants, the weekend successfully achieved many of its objectives. This is largely due to the enormous effort that the workshop groups put into the preparation of their presentations. Itself a challenge given their multidisciplinary composition (the group dealing with ordinary differential equations consisted e.g. of a mathematician, a systems biologist, an automatic control engineer and a philosopher).

However, it was also visible during this weekend and its preparation that there are still some bridges to cross between the disciplines and that only continued efforts can guarantee true interdisciplinary cooperation within SimTech in the near future. We dearly hope that a repetition of the PhD weekend will be part of these efforts - a hope that all participants emphasized in their feedback.

We very much enjoyed a weekend full of vivid and fruitful discussions, scientific inspiration and a very pleasant and constructive atmosphere. We warmly thank all participants for their openness, their commitment and their great motivation to meet the various challenges of interdisciplinarity. We are also very grateful for the organizational assistence of the SimTech management team and the financial support of the SimTech directorate without which this great weekend would not have been possible.

Marianne, Felix and Jonas

Friday, October 2, 2009

14:00	Departure from the University of Stuttgart to the Söllerhaus in Hirschegg, Austria
18:30	Dinner
19:30	Design and Engineering Game
20:00	SINN UND UNSINN VON INTERDISZIPLINARITÄT Dr. Rudolf Kötter, Institut für Philosophie, Universität Erlangen

Saturday, October 3, 2009

8:00	Breakfast
9:00	THE FINITE ELEMENT METHOD – BASICS (see p. 4)
10:00	THE FINITE ELEMENT METHOD – APPLICATIONS (see p. 12)
11:00	Coffee break
11:15	PARTICLE METHODS (see p. 18)
12:30	Hiking to the top of the Walmendinger Horn
16:30	Tea and coffee
17:30	REALTIME SIMULATIONS (see p. 26)
18:30	Dinner
19:30	INVERSE PROBLEMS (see p. 32)

Sunday, October 4, 2009

8:00	Breakfast
9:00	ORDINARY DIFFERENTIAL EQUATIONS (see p. 37)
10:00	POROUS MEDIA (see page 44)
11:00	Coffee break
11:15	STOCHASTIC METHODS (see p. 50)
12:30	Price for the best presentation and feedback
13:30	Lunch at the restaurant Sonna-Alp
15:30	Departure from the Söllerhaus to Stuttgart University

THE FINITE ELEMENT METHOD: BASICS

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Finite Element Method – Basics

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Keywords: *weak formulation, bilinear form, Lax-Milgram theorem, test function, variational calculus, Finite Element Method, stiffness matrix, isoparametric concept, heat conduction, discretization, workflow, BPEL, programming in the large*

Introduction

An analytical solution to realistic (initial) boundary value problems is in most cases not available. Thus, approximate solutions are common practice. The Finite Element Method (FEM) is a numerical technique for the solution of elliptic and parabolic partial differential equations (PDE), where it is mainly used for the spatial discretization. Though it is not necessarily better than other methods, e. g., the finite difference method, its users appreciate its geometric flexibility.
The FEM originated from the need for solving complex elasticity and structural analysis problems in civil and aeronautical engineering. Its development can be traced back to the work by Alexander Hrennikoff (1941) and Richard Courant (1942). Courant's contribution was evolutionary, drawing on a large body of earlier results for PDE developed by Rayleigh, Ritz, and Galerkin. Development of the finite element method began in earnest in the middle to late 1950s for airframe and structural analysis and gathered momentum at the University of Stuttgart through the work of John Argyris and at Berkeley through the work of Ray W. Clough in the 1960s for use in civil engineering. Today, the FEM is used for the solution of all kinds of PDE in many fields of mathematics, physics, and engineering.
The method is based upon the discretization of the modeled domain into elements and nodes. In 2-d, triangular and quadrilateral elements are most often used; in 3-d tetrahedron and hexahedron shaped elements are common. When applying the FEM, first the governing equation is transferred to a weak formulation, which is then approximated with piecewise polynomials that are locally defined on the respective elements. Instead of looking for a continuous solution, it is sought for an approximate function for each element. For an engineering based introduction to the finite element method the reader is referred to [1, 2], while a mathematically approach is presented in [3].
Due to the complexity and number of involved steps, it is useful to split the solution algorithm into several different tasks by means of workflow techniques.

In this contribution, we explain the general procedure for the simple problem of heat conduction. In the stationary case, the two equations $\operatorname{div} \mathbf{q} = f$ and $\mathbf{q} = -\boldsymbol{\kappa} \nabla T$ are combined to give

$$- \operatorname{div} (\boldsymbol{\kappa} \nabla T) = f \,, \tag{1}$$

where $\boldsymbol{\kappa}$ is the thermal heat conductivity tensor, T denotes the temperature, and f represents external loads, such as local sources and sinks.

Stationary Problem

Classical and Weak Solutions

Let $\Omega \subset \mathbb{R}^d$ be a bounded polygonal or polyhedral domain in two ($d = 2$) or three ($d = 3$) space dimensions, respectively, and let Γ denote its boundary. We consider the second-order elliptic boundary-value problem

$$-\mathrm{div}(\boldsymbol{\kappa}\nabla T) = f \quad \text{in } \Omega, \tag{2}$$

$$T = 0 \quad \text{on } \Gamma, \tag{3}$$

where the thermal conductivity $\boldsymbol{\kappa}$ is a given second-order tensor, the temperature $T : \bar{\Omega} \to \mathbb{R}$ is the unknown and the source/sink term $f : \Omega \to \mathbb{R}$ is a given function. The constraint $T = 0$ on Γ is called (homogeneous) Dirichlet boundary condition.
Note that the more general case of inhomogeneous Dirichlet boundary conditions can be reduced to the present case.

Assuming $f \in C(\Omega)$, a function $T : \bar{\Omega} \to \mathbb{R}$ is called a classical solution of the boundary value problem (2), (3) provided that $T \in C^2(\Omega) \cap C(\Gamma)$ and equations (2) and (3) hold in the corresponding sets.
Solving a boundary-value problem in the classical sense means writing down a formula for a classical solution or at least showing that a classical solution exists. Naturally, it is desirable to find a classical solution. But, unfortunately, in most cases a classical solution can be found only by means of a challenging computation or does not even exist. It turns out that the regularity assumption of classical solutions is most often too restrictive. Therefore we have to investigate a wider class of candidates for the solution.

In order to introduce a more general notion of solution of the boundary-value problem at hand, we assume that T is a smooth function and $f \in L^2(\Omega)$. We multiply (2) with a smooth test function $v \in C_0^\infty(\Omega)$, then integrate over Ω and use Green's theorem, to find

$$\int_\Omega \boldsymbol{\kappa}\nabla T \nabla v \,\mathrm{d}x = \int_\Omega f v \,\mathrm{d}x. \tag{4}$$

There are no boundary terms because $v = 0$ on Γ. By approximation we conclude that the same equation holds with any function $v \in H_0^1(\Omega)$ instead of requiring $v \in C_0^\infty(\Omega)$. Moreover, the resulting equation makes sense if only $T \in H_0^1(\Omega)$. We define the bilinear form $a : H_0^1(\Omega) \times H_0^1(\Omega) \to \mathbb{R}$ by

$$a(T, v) := \int_\Omega \boldsymbol{\kappa}\nabla T \nabla v \,\mathrm{d}x,$$

and the linear form $L : H_0^1(\Omega) \to \mathbb{R}$ by

$$L(v) := \int_\Omega f v \,\mathrm{d}x.$$

Then, we call a function $T \in H_0^1(\Omega)$ a weak solution of the boundary-value problem (2), (3) provided

$$a(T, v) = L(v) \quad \text{for all } v \in H_0^1(\Omega).$$

We note that a classical solution is always a weak solution and a weak solution is also a classical solution whenever it lies in the space $C^2(\Omega) \cap C(\Gamma)$. But a weak solution may exist in cases when no classical solution exists. Moreover, the proof of existence of an unique weak solution is straightforward using the Lax-Milgram theorem.

Spatial Discretization Using Finite Elements

In general it is difficult or even impossible to find an exact solution $T(\mathbf{x})$ of the weak form (4). Therefore an approximation is necessary. In the Finite Element Method the idea is to divide the whole domain Ω into individual subdomains Ω_e, the so-called *Finite Elements*, and to approximate the unknown function $T(\mathbf{x})$ with piecewise polynomials $T^h(\mathbf{x})$. This means to take the values of $T(\mathbf{x})$ at the nodes of the elements $\mathbf{T}_{node}$ and to interpolate in between with so-called shape functions $\mathbf{N}(\mathbf{x})$. The test functions v are generally chosen to be the variation of the temperature δT and approximated with the same shape functions as the temperature itself (Bubnov-Galerkin). The approximated functions are then:

$$\begin{aligned} T(\mathbf{x}) \approx T^h(\mathbf{x}) &= \mathbf{N}(\mathbf{x}) \cdot \mathbf{T}_{node} \\ \delta T(\mathbf{x}) \approx \delta T^h(\mathbf{x}) &= \mathbf{N}(\mathbf{x}) \cdot \delta\mathbf{T}_{node} \end{aligned}$$

Introducing this into the weak form (4) and assuming isotropic thermal conductivity where $\boldsymbol{\kappa}$ reduces to $\kappa\mathbf{I}$, one gets:

$$\mathbf{T}_{node}^T \int_\Omega \kappa\mathbf{I}\, (\nabla\mathbf{N})^T\, \nabla\mathbf{N}\, \mathrm{d}\mathbf{x} \cdot \delta\mathbf{T}_{node} = \int_\Omega \mathbf{N}^T\, f\, \mathrm{d}\mathbf{x} \cdot \delta\mathbf{T}_{node}$$

By additionally replacing the gradient of the shape functions $\nabla\mathbf{N}$ with the B-operator $\mathbf{B}$ and applying the fundamental lemma of variational calculus, we end up with

$$\mathbf{T}_{node}^T \underbrace{\int_\Omega \kappa\, \mathbf{B}^T\mathbf{B}\, \mathrm{d}\mathbf{x}}_{\mathbf{K}^T\text{: "stiffness matrix" (symmetric)}} = \underbrace{\int_\Omega \mathbf{N}^T\, f\, \mathrm{d}\mathbf{x}}_{\mathbf{f}\text{: "load vector"}}$$

which is a linear system of equations of the form

$$\mathbf{K}\, \mathbf{T}_{node} = \mathbf{f} \tag{5}$$

that we can solve for the only unknowns $\mathbf{T}_{node}$. This yields an approximate solution $T^h(\mathbf{x})$ of the function $T(\mathbf{x})$.

In general one may get now an approximate solution for the temperature field and the problem is solved. However, integrations over an arbitrarily shaped domain Ω have to be performed, which is difficult or sometimes even impossible. Another difficulty is finding shape functions for an arbitrary domain. These two problems can be solved by additionally approximating the geometry, which, according to the *Isoparametric Concept*, can be done with the same shape functions taken earlier for the approximation of $T(\mathbf{x})$:

$$\mathbf{x} \approx \mathbf{x}^h = \mathbf{N}(\mathbf{x})\, \mathbf{x}_{node}$$

The shape functions are chosen such that they are 1 at the node they are defined and 0 at all others. Therefore the problem reduces to a local problem where each element can be considered separately. Another big advantage of this choice of shape functions is that the matrix becomes a sparce matrix and the system of equations is cheap to solve.

On the element level each element is transformed to a reference element which is the same for all elements. The reference element is a quadratic element of size 2 x 2 and is defined in a parameter space with a ξ-/η-coordinate system ($-1 \leq \xi, \eta \leq 1$). The shape functions are defined on the reference element and are hence the same for all elements. Furthermore, all integrations can be performed on a

quadratic element where for a numerical integration the quadrature points are the same in all elements.

However, therefore a transformation between the Cartesian coordiates and the local coordinates is necessary. The derivatives needed for this transformation (e.g. to get the B-operator) are collected in the so-called Jacobian matrix $\mathbf{J}$ and its inverse $\mathbf{J}^{-1}$, which for a 2-dimensional problem are the following matrices:

$$\mathbf{J} = \begin{bmatrix} \frac{\partial x}{\partial \xi} & \frac{\partial y}{\partial \xi} \\ \frac{\partial x}{\partial \eta} & \frac{\partial y}{\partial \eta} \end{bmatrix} \qquad \mathbf{J}^{-1} = \begin{bmatrix} \frac{\partial \xi}{\partial x} & \frac{\partial \eta}{\partial x} \\ \frac{\partial \xi}{\partial y} & \frac{\partial \eta}{\partial y} \end{bmatrix}$$

To transform an infinitessimal area element one needs the determinant of the Jacobian:

$$\mathrm{d}\mathbf{x} = \mathrm{d}x\,\mathrm{d}y = \det \mathbf{J}\,\mathrm{d}\xi\,\mathrm{d}\eta$$

The stiffness matrix for one individual element is then finally:

$$\mathbf{K}^e = \int_{\Omega^e} \kappa\, \mathbf{B}^T\mathbf{B}\,\mathrm{d}\mathbf{x} = \int_{-1}^{1}\int_{-1}^{1} \kappa\, \mathbf{B}^T\mathbf{B} \det \mathbf{J}\,\mathrm{d}\xi\,\mathrm{d}\eta$$

where $\mathbf{B}$ and $\mathbf{J}$ are expressed in terms of ξ and η. The integration can hence be performed easily in the parameter space with Gauss quadrature.

To come from the element stiffness matrix $\mathbf{K}^e$ to the global stiffness matrix $\mathbf{K}$ for the whole domain, an assembly has to be done. The degrees of freedom of each node (here just one temperature value per node) in the reference element have to be numbered in one specific way which has to be kept the same for all elements. Also globally one has to define and number the degrees of freedom of each element node. The local ordering has then only to be linked to the global ordering. To link them one usually defines a so-called ID-matrix, where in one row one has the numbers of the global degrees of freedom belonging to one element, ordered in the sequence defined for the local element. By using this matrix one can define a simple procedure which places the entries of the element stiffness matrices to the right positions in the global stiffness matrix. The same has to be done for the right hand side of the system of equations, the "load vector" $\mathbf{f}$.

After finishing the assembly the boundary conditions have to be included into the system of equations. This means to include the known values of the free variables, which here is only the temperature, and to rearrange the system of equations such that no information gets lost.

Finally, one again has a linear system of equations like the one in equation (5) which can be solved for the unknown nodal values $\mathbf{T}_{node}$.

Transient Problem

Classical and Weak Form

In the previous sections, we showed how the classical, local form of an elliptic problem (in our case the stationary heat conduction) can be transformed into a global, so-called weak form that imposes less restrictions on the solutions. The weak form allows the introduction of a spatial discretization by use of piecewise polynomial approximation functions with a finite amount of degrees of freedom,

which leads to the approximate solution of the elliptic problem via the solution of a linear system of equations.
We now want to illustrate that a similar approach together with a suitable time discretization can be used to approximately solve parabolic problems. To do so, we consider the problem of transient heat conduction: Let $\Omega \subset \mathbb{R}^d, d \in \{2,3\}$ be a bounded domain and let $\Gamma := \partial\Omega$ denote its boundary. We consider the second order parabolic initial-boundary-value problem (in so-called strong form)

$$\rho c\dot{T} = \operatorname{div}(\boldsymbol{\kappa}\boldsymbol{\nabla}T) + f \quad \text{in } \Omega \text{ for } t \in [0,T], \tag{6}$$
$$T = T_D \quad \text{on } \Gamma \text{ for } t \in [0,T], \tag{7}$$
$$T = T_{ini} \quad \text{in } \Omega \text{ for } t = 0, \tag{8}$$

where ρ is the density, c is the heat capacity, $\boldsymbol{\kappa}$ the conductivity and f a heat source. Equation (7) prescribes the temperature on parts of the boundary (Dirichlet boundary condition) and equation (8) prescribes the initial temperature of the body. To derive the weak formulation of (6) to (8), we multiply (6) with a so-called test function $\delta T \in H_0^1(\Omega)$ and integrate over Ω. We obtain

$$\int_\Omega \delta T \rho c \dot{T} \mathrm{d}\mathbf{x} = \int_\Omega \delta T \operatorname{div}(\boldsymbol{\kappa}\boldsymbol{\nabla}T)\mathrm{d}\mathbf{x} + \int_\Omega \delta T f \mathrm{d}\mathbf{x}\,.$$

Applying Green's theorem and making use of the fact that $\delta T = 0$ (Dirichlet boundary conditions) or $\boldsymbol{\nabla}T = \mathbf{0}$ (zero Neumann boundary conditions) on the surface Γ, this simplifies to

$$\int_\Omega \delta T\ \rho c\ \dot{T}\ \mathrm{d}\mathbf{x} + \int_\Omega \boldsymbol{\nabla}\delta T\ \boldsymbol{\kappa}\ \boldsymbol{\nabla}T\ \mathrm{d}\mathbf{x} = \int_\Omega \delta T\ f\ \mathrm{d}\mathbf{x}\,, \tag{9}$$

which is called the weak form of (6), (7).

Spatial Discretization Using Finite Elements

Making use of the approximations

$$\begin{aligned}
T(\mathbf{x},t) \approx\ & T^h(\mathbf{x},t) = \sum_{nodes} N_I(\mathbf{x}) T_{node,I}(t) = \mathbf{N}(\mathbf{x}) \cdot \mathbf{T}_{node}(t),\\
\delta T(\mathbf{x}) \approx\ & \delta T^h(\mathbf{x}) = \sum_{nodes} N_I(\mathbf{x}) \delta T_{node,I} = \mathbf{N}(\mathbf{x}) \cdot \delta\mathbf{T}_{node},\\
\dot{T}(\mathbf{x},t) \approx\ & \dot{T}^h(\mathbf{x},t) = \sum_{nodes} N_I(\mathbf{x}) \dot{T}_{node,I}(t) = \mathbf{N}(\mathbf{x}) \cdot \dot{\mathbf{T}}_{node}(t),\\
\boldsymbol{\nabla}T(\mathbf{x},t) \approx\ & \boldsymbol{\nabla}T^h(\mathbf{x},t) = \sum_{nodes} \boldsymbol{\nabla} N_I(\mathbf{x}) T_{node,I}(t) = \mathbf{B}(\mathbf{x}) \cdot \mathbf{T}_{node}(t),
\end{aligned}$$

where $N_I(\mathbf{x})$ are nodal shape functions that are 1 at node I and 0 at all other nodes and where $\mathbf{B}(\mathbf{x})$ contains the derivatives of the nodal shape functions, equation (9) can be rewritten as

$$\delta\mathbf{T}_{node}^T \cdot \left(\underbrace{\int_\Omega \mathbf{N}^T\ \rho c\ \mathbf{N}\ \mathrm{d}\mathbf{x}}_{\text{"damping matrix" } \mathbf{C}} \cdot \dot{\mathbf{T}}_{node}(t) + \underbrace{\int_\Omega \mathbf{B}^T\ \boldsymbol{\kappa}\ \mathbf{B}\ \mathrm{d}\mathbf{x}}_{\text{"stiffness matrix" } \mathbf{K}} \cdot \mathbf{T}_{node}(t) = \underbrace{\int_\Omega \mathbf{N}^T\ f\ \mathrm{d}\mathbf{x}}_{\text{"load vector" } \mathbf{f}(t)} \right).$$

Making use of the fundamental lemma of calculus of variation, this results in

$$\mathbf{C} \cdot \dot{\mathbf{T}}_{node}(t) + \mathbf{K} \cdot \mathbf{T}_{node}(t) = \mathbf{f}(t). \tag{10}$$

Time Discretization

To discretize equation (10) in time, we introduce $t_n = n \cdot \Delta t$ and use the scheme

$$\mathbf{C} \cdot \underbrace{\left[\mathbf{T}_{node}^{n+1} - \mathbf{T}_{node}^{n}\right] / \Delta t}_{\text{approximation of } \dot{\mathbf{T}}_{node}} + \mathbf{K} \cdot \underbrace{\left[\alpha\, \mathbf{T}_{node}^{n+1} + (1-\alpha)\, \mathbf{T}_{node}^{n}\right]}_{\text{approximation of } \mathbf{T}_{node}} = \underbrace{\left[\alpha\, \mathbf{f}^{n+1} + (1-\alpha)\, \mathbf{f}^{n}\right]}_{\text{approximation of } \mathbf{f}},$$

where α is a numerical parameter that yields a so-called explicit (forward) Euler scheme for $\alpha = 0$ and a so-called implicit (backward) Euler scheme for $\alpha = 1$. These schemes have different properties regarding stability and convergence, see e.g. [5, 6, 7]. Rearrangement yields the final algorithm

$$\left[\mathbf{C} + \Delta t\, \alpha\, \mathbf{K}\right] \mathbf{T}_{node}^{n+1} = \left[\mathbf{C} - \Delta t\, (1-\alpha)\, \mathbf{K}\right] \mathbf{T}_{node}^{n} + \Delta t \left[\alpha\, \mathbf{f}^{n+1} + (1-\alpha)\, \mathbf{f}^{n}\right], \qquad (11)$$

where $T_{node,I}^{0} = T_{ini}(\mathbf{x}_{node,I})$ accounts for the initial conditions. The treatment of the Dirichlet boundary data is similar to the stationary problem.
We can thus approximately reduce the local problem (6)–(8) by introducing its weak formulation, a spatial discretization using finite elements and a time discretization using a forward/backward Euler scheme to a linear system of equations.

FEM Simulations in the Context of Workflow

To execute FEM-based simulations, today's researchers typically create monolithical applications for each specific problem [8]. A popular tool in SimTech to program such simulation applications is the C++ Framework DUNE (see http://www.dune-project.org/doc/grid-howto/grid-howto.html). This approach to the creation of application is generally called programming in the small. However, if the applications become complex, programming in the small has huge limitations. For instance, if a FEM program needs to be enhanced or the running FEM-simulation needs to be adapted, a researcher must read and understand the source code. This can be extremely difficult, especially if a complex simulation is based on millions of lines of code or if the initial programmer left the institute.
The programming in the large approach [9] can solve those kinds of problems. Programming in the large is based on activities and describes only the structure of a program and the flow of the simulation. The activities are linked to smaller independent computable functions [10].
Based on the interface technology Web Services (see http://www.w3.org/TR/2004/NOTE-ws-arch-20040211) those smaller functions can be connected to a complex simulation. With Web Service technology any functions that are located on the local computer, somewhere on a Network, or in the Internet can be accessed via network protocols. Those executable functions can be called independent of programming languages, operating systems, or platforms. The approach behind this is the common interface definition language WSDL (see http://www.w3.org/TR/wsdl). The flow of the programming in the large approach can be described with the Business Process Execution Language (BPEL) and uses Web services as activity implementations [11]. An example of a Dune based FEM simulation can be found in [12].

Conclusion

In this text, we presented the finite element approach for the numerical solution of the heat conduction problem. To achieve this, we presented the governing equation of the stationary and the transient problem, derived the weak formulations, proceeded with the finite element discretization, and discussed the involved steps using workflow techniques.

Note that the presented example is a very simple problem, and many more sophisticated boundary value problems can be solved via the FEM. A second type of boundary condition, called Neumann or natural boundary condition, can be prescribed which does not provide information about the primary unknown itself (Dirichlet or essential boundary condition) but a term containing the spatial derivative of the unknown field. Besides the presented linear Lagrange element, higher order polynomials are commonly used, e. g., quatratic or cubic, to achieve a better approximation of the solution. Further types of finite element methods which will only be mentioned here for completeness are e. g., the generalized finite element method, the hp-FEM, the XFEM, spectral methods, meshfree methods, discontinuous Galerkin methods, and mixed finite element methods.

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THE FINITE ELEMENT METHOD: APPLICATIONS

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FEM for Electronic Structure Calculations

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Keywords: *electronic structure, density functional, OF-DFT, Finite Element Method*

Electronic structure calculations allow to determine many properties of materials directly from fundamental equations. They describe a many body system consisting of the fermionic electrons and the positively charged nucleons interacting with each other. The central element in the calculations is the energy functional, which only depends on the electron density, i.e. the distribution of the electrons in the system, rendering the name density functional theory (DFT) to these kind of calculations.

Two basic theorems by Hohenberg and Kohn account for modern DFT [1], proofing that the energy functional alone is sufficient to determine the exact ground state energy and density of any system of interacting particles in an external potential. Therefore the Kohn-Sham ansatz replaces the interacting problem by an independent-particle problem with all many-body effects included in an exchange-correlation functional.

The computational complexity of DFT however has made some aspects, especially those involving defects, beyond reach. In special cases orbital free density functionals methods can be used [2], which are based on earlier energy functionals by Thomas and Fermi [3], to get some insight into the defect properties. The minimization of the density functional can be performed by an elaborated FEM ansatz.

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Parameterization Models for Scalable, Predictive Simulation of Production Machines

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Keywords: *Finite Element Method, parameter models, component oriented modeling, substructuring*

Due to increasing computer performance FE models can get even more complex. Such models involve higher versioning management, especially where many versions of the same model are available. With the Help of a component oriented modelling the management effort can be drastically reduced, whereas the error rate decreases. The premise for the component oriented FE modelling however is an as much as possible simple but flexible definition of the model interfaces, so that the coupling of the components can be automatically carried out. The coupling algorithm must reliably support particularly non conform meshes of a variety types. In the present text we will describe a novel nodal based Method for automated coupling of non conform meshes by using MPC contact elements. The success of a new production machine design depends on the predictability of the machine properties during the design stage. Reliable simulation-based predictions about the properties of a new machine require a detailed model description and lead to complex models, usually Finite Element Models (FE-Models). But a good agreement between simulation and reality can only be achieved with precise knowledge about the structure and particularly the parameters of nonlinear components. One problem related to the modelling task is that the required parameters are dependent on a very large number of influencing conditions. Even for a given set of influencing conditions essential parameters are often unknown and cannot be acquired (e.g. through measurements) with justifiable time and effort. As a result parameters for abstract component models are often estimated based on knowledge about the parameters of a seemingly similar system. Thus, incorrect predictions can result from intuitive assumptions that are made during the modelling and parameterization process. The aim of this project therefore is to develop practically applicable methods for handling model parameterization and transferability problems for virtual prototypes of production machines. We propose a layered approach based on parameter models (bottom layer) embedded into linear and nonlinear component models including the join patch between components (intermediate layer), which, in turn, make up the machine model (top layer). Parameters, strategies for parameter determination and the associated general conditions will be analysed and generalised. We will characterise the determinant influences on parameters and analyse the model robustness towards parameter variations. In addition to that, we will study the transferability of model knowledge between

- different model formulations used in different stages of the design process,
- different scales of similar structures, e.g. small and large linear guides,
- different levels of abstraction, e.g. material damping vs. modal damping, and
- different system configurations with different general and boundary conditions.

Based on the won awareness new parameter models will be developed to replace the existing constant parameter models. This shall considerably simplify the system identification and transferability of parameter models. As the result of the research proposed here, methods will be available for efficient and reliable predictive determination and characterisation of model parameters. These can be applied to build efficient, accurate and reliable virtual prototypes on the different levels of abstraction and

formulations required throughout the production machine design process. Re-using parameter models and validated scalable component models will reduce the modelling effort and particularly the modelling error rate, thus enhancing the accuracy and reliability of simulative predictions.

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Using 1D-3D Coupled Skeletal Muscle Models to Realistically Simulate the Influence of Skeletal Muscle Forces on Lumbar Spine Mechanics

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Keywords: *Finite Element Method, coupled problems, biomechanics, coupling of 1D-3D, muscles, lumbar spine*

The goal of this work is to investigate the influence of the skeletal muscles anatomically surrounding the lumbar spine.
State of the current work is that mainly the intervertebral disk and the movement of the bones of the lumbar spine are investigated, see for example [2]. Here often the bones are assumed as rigid. If soft tissue is considered in the model it is mainly the ligaments. Muscles are very seldom included and if only as a lumped parameter model where its line of action is approximated using a straight line (1D model) without accounting higher dimensions. Such lumped muscle models certainly provide an important contribution for analysing the musculoskeletal system as a whole but are not able to depict the spatial enlargement of the muscles which are important to simulate a realistic stabilisation of the lumbar spine. As ROHLMANN et. al. studied in [1] by replacing the L1 vertebrae with an implanted telemeterised vertebral body replacement, the position of the limbs do impact the contraction of the muscle around the spine strongly. He observed, by comparing the loading condition for a 90° abduction, elevation of the arms and normal standing position, the displacement in the vertebral body. These results clearly demonstrate the importance of the skeletal muscles on the lumbar spine. As 3D simulations of the whole human being and also a musculoskeletal system around the spine using anatomically realistic 3D skeletal muscle models, as e.g. [3], are still far too computationally expensive and are therefore nearly impossible to handle, the goal of presented work is to develop a multi-scale skeletal muscle model which is able to couple anatomically realistic 3D skeletal muscle models around the lumbar spine to lumped parameter models. The challenge will be to derive a proper and consistent interface conditions between the 1D and 3D structure. Further the 1D-3D model will be merged with multi-body dynamics simulation to create a framework in which local and geometrical effects on spine mechanics can be investigated using detailed biomechanical models and in which complex upper-body movements can be incorporated as kinematic input.

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3D Scalar Field Visualization

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Keywords: *visualization, raycasting, scalar field, Finite Element Method*

When working with simulations, an important task is the analysis of the resulting data generated by the simulation. This is usually done visually, so visualization plays an important role for simulation technology. In many scientific applications the resulting data of simulations are some kind of scalar field. More specific, simulations based on finite element methods (FEM) generate in many cases one or more scalar fields. Hence scalar field visualization is an important problem. In this work some basic knowledge about the visualization of 3D scalar fields will be presented.
The direct visualization of 3D scalar fields is also called *volume rendering*. Basic informations and further references about volume rendering and other visualization techniques can be found in [1]. Detailed informations about the implementation of volume rendering methods, especially with modern graphics hardware, are presented in [2].
Common volume rendering techniques are *ray casting*, *splatting*, *cell projection* and texture mapping based volume rendering. We will take a closer look on ray casting, because this technique can provide high quality results and can be used for all types of grids on which the scalar field is defined.
The basic model behind common volume rendering methods is a semi-transparent light-emitting medium. Based on this, the idea behind ray casting is to trace light rays through the 3D scalar field for every pixel of the resulting the image. To calculate the color of a pixel, the optical properties along the ray is sampled and accumulated. The accumulation could be done in front-to-back or back-to-front order. The values in scalar fields usually do not represent optical properties (color, transparency) so they have to be assigned to them via the transfer function. With the transfer function it is for example possible, to filter out areas with low values by assigning them high transparency.
The computational effort for ray casting depends on the type of grid the scalar field is defined on. In uniform grids, sampling along the ray is simple and could be done fast. Sampling a scalar field on a irregular grid is more complicated, because the computation of intersection points and interpolation between values is more difficult in this case. There are also different acceleration techniques for ray casting and the usage of moder graphics hardware can also increase the speed of this method.

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PARTICLE METHODS

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Classical molecular dynamics simulations

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Keywords: *MD, molecular dynamics simulations, equations of motion, interactions*

Equations of motion

In classical molecular dynamics simulations [1-4] the motion of a vast number of particles is studied. The energy of the system is given by the sum of the kinetic energy K and the potential energy U, which are functions of the positions $\mathbf{R}$ and momenta $\mathbf{P}$ of all particles. The equations of motion in the Hamiltonian form then become:

$$\dot{\mathbf{R}}_i = \frac{\mathbf{P}_i}{M_i}\,, \quad \dot{\mathbf{P}}_i = -\nabla_{\mathbf{R}_i} U = \mathbf{F}_i\,. \tag{1}$$

$\mathbf{F}_i$ is the force on particle i with the mass M_i. Time is discretized to numerically integrate these equations. The Taylor expansions of the coordinates and velocities $\mathbf{V}_i$ help to calculate these values at a later time. One of the various finite difference methods used is the half-step leap-frog scheme [2]. In this way the trajectories of the particles are approximated in a stepwise manner by applying a sufficiently small time step.

Equations (1) are used to simulate (N, V, E)-ensembles, in which the number of particles N, the volume V and the energy E are conserved. A thermostat can be included in the equations of motion to control temperature. Additionally, the pressure can be steered by adding a barostat.

Interactions

The interactions between the particles are determined by the potential energy U, which may be broken up into contributions from individual particles, pairs, triplets, etc. In a simple approach, just the pair terms are taken into account and the potential only depends on the distance r_{ij} between the particles i and j. To simulate specific materials, a variety of more sophisticated approaches exist, e.g. the embedded atom method (EAM) [5] for metals. The corresponding functions are then matched to reproduce values from experiment or from ab-initio calculations.

For large distances r_{ij} one assumes that the corresponding potential functions vanish. Thus, they are set to zero at and beyond a finite cut-off radius r_{cut}. The functions should be continuous and continuously differentiable everywhere. Dividing the simulation box into cells with sufficient size, it can be guaranteed that a particle only interacts with other particles in the same cell or in the neighboring 26 cells [6].

Setup, simulation and results

Initially, the simulation input contains the positions and velocities of all particles. Subsequently, these are derived from the equations of motion at every time-step during the simulation. Modifications of the equations of motion allow to simulate various ensembles and relaxators. The potentials determine how the particles interact.

To influence the simulated material, it is possible to restrict the motion of selected atoms (e.g. to apply stress or shear). Despite the large number of particles (typically millions) a high percentage of them is located at the sample boundaries. A solid without interfaces can be simulated by periodically extending the simulation box.

Finally, the main simulation results are the potential energies, positions and velocities of all particles for every time step of the simulation. Elastic and transport coefficients, correlation functions and diffraction patterns can be derived from these data.

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The Atomistic Monte Carlo Method

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Keywords: *Monte Carlo, statistics, massive transformation*

Monte Carlo

Introduction

The Monte Carlo method has been developed initially in Los Alamos during the Manhattan Project by Metropolis and Ulam [2]. The Monte Carlo methods are based on repeated random sampling. The basic method is to create a catalog of possible events and letting a random number decide the prevailing event happen. This process is repeated so many times, until a statistically valid result is created. The catalog of events can be updated between each determination to create a sequence of events. The method is named after the famous casino in Monaco, because of its stochastic nature.

Atomistic Monte Carlo

Monte Carlo methods use a catelog of possible events from which the algorithm stochastically determines the event which actually occurs. The events of the envisioned atomistic Monte Carlo are the jumps of the atoms from their initially occupied site to an empty site in a discretisized space. Such a Monte Carlo method has been applied by Kees Bos [1] for simulations of the massive transformation in pure iron. Here the movement of an interface between the fcc(111)//bcc(110) was simulated by allowing from occupied lattice sites to empty lattice sites using the following algorithm:

1. Create a list of all interface atoms
2. Calculate the jumprate k for every valid jump
3. Calculate the total jumprate K_{sum}
4. Select a random number between 0 and K_{sum}
5. Find the corresponding jump with the random number
6. Find the realtime with a second random number
7. Redistribute the unused random sites and move the lattices appropriately
8. Continue with step 1

Using an interaction model of choice, the jumprate k is determined by the energy difference between the situation before and after the jump. The main results are evaluated in terms of relation between the activation energy for single jump and the overall activation energy.

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The Theory of Multibody Systems

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Keywords: *rigid multibody system, elastic multibody system, dynamical analysis, robotics, biomechanics*

Multibody systems consist of rigid and/or elastic bodies that are interconnected by massless coupling and connecting elements. Nowadays, the term multibody system is related to a large number of engineering fields of research, ranging from mechanisms, gyroscopes, satellites and robots to biomechanics, see Schiehlen [11]. In order to analyze the dynamics of multibody systems, it has to be described mathematically by equations of motion. The equations need to be integrated in a following step to receive either trajectory data or forces and torques [8]. Generating these equations of motion is one of the central problems or tasks in multibody simulations, see Hospach [3].

The dynamics of multibody systems is - according to Schiehlen [10] - related "to the origins of analytical mechanics starting with the PRINCIPIA OF NEWTON [7], the CORPORUM RIGIDARUM by Euler [2] and the MÉCANIQUE ANALYTIQUE by Lagrange [6]. Even more important for the computational aspects of multibody dynamics are the contributions of d'Alembert in his TRAITÉ DE DYNAMIQUE [1] and Jourdain with his ANALOGUE AT GAUSS' PRINCIPLE [4]".

The first step in mechanical modeling is the replacement of the engineering or natural system with the elements of the multibody system approach: rigid and/or flexible bodies, joints, gravity, springs, dampers and position and/or force actuators. Bearings and joints are constraints on the system, that is disassembled as a free body diagram, see Schiehlen [9]. Referring to the statement above, a free particle, the most simple element of a multibody system, can be treated by Newton's equation. For describing the movement of a rigid body, compared to a free particle, the equations used and obtained in multibody systems are known as Newton-Euler equations. Rigid bodies are the so called principle elements in multibody systems, introduced by Euler in 1775. In order to apply Newton-Euler equations to multibody systems the free body diagram is used. Omitting all contraints, a system of p free bodies holds $6p$ degrees of freedom. Each body is then described by six equations, three Newton equations describe the translation of a system and three Euler equations describe the rotational movement. Connecting the bodies by joints leads to a reduction of the degrees of freedom, e.g. m additionally acting constraint forces or constraint moments lead to a degree of freedom of $6n - m$. Hereby, the rigid bearings and supports are replaced by adequate constraint forces and torques, resulting in the equations below. These are based on the calculated velocities (ω_i) and accelerations ($\mathbf{a}_i, \alpha_i$), as well as on the applied forces ($\mathbf{f}_i^e$) and applied torques ($\mathbf{l}_i^e$), and on the constraint forces ($\mathbf{f}_i^r$) and constraint torques ($\mathbf{l}_i^r$):

$$m_i \mathbf{a}_i = \quad \mathbf{f}_i^e + \mathbf{f}_i^r \qquad i = 1(1)p \tag{1}$$

$$\mathbf{I}_i \alpha_i + \tilde{\omega}_i \mathbf{I}_i \omega_i = \quad \mathbf{l}_i^e + \mathbf{l}_i^r \qquad i = 1(1)p \tag{2}$$

A multibody system is described completely using the Newton-Euler equations and in a following step the equations can be solved with certain integrators. This is one possibility, but the description of a multibody system using generalized coordinates and retyping the equations of motion by using the mechanical principles by, for example, D'Alembert, Lagrange and Jourdain can sometimes be computationally more efficient.
The following Newton-Euler equations describe a multibody system with holonomic constraints and generalized coordinates $\mathbf{y}$ in matrix notation. Inertia properties are expressed by the $6p \times 6p$-matrix

$\bar{\bar{\mathbf{M}}} = diag\{m_1\mathbf{E}\ m_2\mathbf{E}\dots\mathbf{I_1}\dots\mathbf{I_p}\}$. The $6p \times 1$-vectors $\bar{\mathbf{q}}^{\mathbf{c}}$ and $\bar{\mathbf{q}}^{\mathbf{e}}$ represent the Coriolis forces and the applied forces. Whereas, the vector of the constraint forces $\bar{\mathbf{q}}^{\mathbf{r}}$ is composed by a global distribution matrix $\bar{\mathbf{Q}}$ and the vector of generalized constraint forces λ.

$$\bar{\bar{\mathbf{M}}}\bar{\mathbf{J}}\ddot{\mathbf{y}} + \bar{\mathbf{q}}^{\mathbf{c}}(\mathbf{y}, \dot{\mathbf{y}}, t) = \bar{\mathbf{q}}^{\mathbf{e}}(\mathbf{y}, \dot{\mathbf{y}}, t) + \bar{\mathbf{Q}}\lambda \tag{3}$$

The above equation is retyped, applying d'Alembert's principle by premultiplication of (3) with the transpose of the Jacobian matrix $\mathbf{J}^T$, thereby using the orthogonality of generalized motions and constraints, $\bar{\mathbf{J}}^{\mathbf{T}}\bar{\mathbf{Q}} = 0$, to form the following equation

$$\mathbf{M}(\mathbf{y}, t)\ddot{\mathbf{y}} + \mathbf{k}(\mathbf{y}, \dot{\mathbf{y}}, t) = \mathbf{q}(\mathbf{y}, \dot{\mathbf{y}}, t) \tag{4}$$

Hereby, the number of equations completely describing the multibody system is reduced from $6p$ to $f = 6p - q$. Hence, a reduction of the system's degrees of freedom is achieved. Additionally the $f \times f$-inertia matrix $\mathbf{M}(\mathbf{y}, t) = \bar{\mathbf{J}}^T\bar{\bar{\mathbf{M}}}\bar{\mathbf{J}} > 0$ is completely symmetrized and the constraint forces and torques are eliminated. The remaining $f \times 1$-vector $\mathbf{k}$ decribes the generalized Coriolis forces and the $f \times 1$-vector $\mathbf{q}$ includes the generalized applied forces, see Schiehlen [9][11].

In most cases, generating the equations of motions for a multibody system manually is not purposeful. Since the 1960s, the development of modern computer programs, so called multibody formalisms, has advanced successfully and the problem of developing equations generators and matching integrators can be regarded as solved, see Keppler [5], Schiehlen [11], Simeon [13].

Modern lightweight designs aim to reduce both the moving masses and the energy comsumption of machines and allow higher working speeds. However, lower stiffnisses and higher working speeds lead to an increase of body deformations. Thus, the rigid body model is not valid anymore, and other approaches have to be chosen. Examples of such systems are ground vehicles, robots, space vehicles and structures, or precision machines, see Shabana [12]. In contrast to ridig body mechanics the branch of structural mechanics does not aim to describe nonlinear body motions but their deformations due to loads. In many cases a large number of elastic coordinates and therefore a high mathematical effort is necessary to obtain accurate deformation results. Approaches to model multibody systems that exist of rigid and flexible bodies must be able to describe the large nonlinear working motions as well as important body deformations. Depending on the size of the deformations, two different approaches are available. The relative nodal coordinate formulation (RNCF) can be used for small deformations, whereas for large deformations, the absolute nodal coordinate formulation (ANCF) turns out to be very efficient, see Schiehlen [9].

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Visualization of Dynamic Particle-based Data

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Keywords: *visualization, particle data, glyphs, density fields*

Particle data or point data originates from measurements or simulations in the fields of molecular dynamics, biology, astrophysics, and thermodynamics, to name a few. Other sources are 3D scans of objects and particle systems used for modeling fluids, smoke and other effects. The data sets usually contain up to several tens of thousands particles and are time-dependent. Interactive visualization of this data is important to support data exploration to gain new insights. It can also be used for debugging simulation.

Particle data can be visualized in various ways. Scatter plots are commonly used but they contain only the positions of the data points. Other data values are mapped either to size or color. Glyph-based visualizations use geometric primitives instead of points. A glyph consists of at least one primitive, like ellipsoids, cylinders, or more complex shapes. If several primitives are combined, a glyph can represent dipoles or even chemical compounds. For rendering these glyphs, the graphic processing unit (GPU) can be used [2, 4]. Reina and Ertl use glyph dipoles to render over 500.000 molecules at 10 frames per second. Another example for particle-based data can be found in systems biology. To model the process of signal transduction, Monte Carlo are used to simulate the protein propagation through cells [1]. Here, visualization has to deal with crowded environment of the cell. Apart from the nucleus – the target of the signal – the cytoskeleton and other obstacles take part or actively hinder the signal transduction of the proteins and should therefore be an integral part of the visualization. The proteins are again rendered as glyphs. To emphasize certain effects or regions, focus & context techniques are used for highlighting. This includes data segmentation, depth cues or transparency. Even depth of field can be employed to reduce the visual clutter.

In some cases, however, a discrete glyph-based visualization is not sufficient. Instead a continous representation is sought after, i.e. a density field generated from the particle data. Examples are the mass or charge density in molecular dynamics data or protein concentrations inside cells. Current consumer GPUs allow the computation of such fields with interactive frame rates. For the volume visualization of these fields GPU raycasting techniques can be employed [3, 5, 6].

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REAL-TIME SIMULATION

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Different Aspects of Real-Time Simulations

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Keywords: *real-time, simulation, MPC, GSN, control, disaster prevention*

Introduction

Simulation technology has become a crucial part of today's life with significant impact on science, technology and the economy. When talking about simulation, the notion of real-time is used quite frequently. However, real-time can have a variety of meanings depending on the particular aspect of simulation one is interested in. For this reason, this brief note wants to show some possible meanings of real-time in different contexts regarding the simulation technology.
In particular, Andreas Benzing reports about global sensor grids. Then, Tudor Ionescu explains aspects of real-time simulation for disaster prevention. Marcus Reble gives a brief overview on model predictive control. Onboard simulation for higher quality control is the topic of Peter Sekler's part.

Global Sensor Grid

Wireless sensor networks (WSN) have received growing attention over the last decade. With the increasing deployment of such local sensor networks it has become possible to use their data for a wide range of applications on a global scale as part of a *global sensor network* (GSN). Especially the simulation of the environment has gained attention over recent years to better understand global changes and to gather a complete data set. As the popularity of such applications and the number of users increases, it becomes important to provide middleware solutions and expressive continuous query paradigms for efficient data retrieval. This includes optimized bandwidth usage and the need to avoid the overload of sensors and additional data sources. The concept of *Distributed Stream Processing Systems* (DSPS) is the most promising to handle the huge amount of data produced in this domain. Several (DSPS) [1, 4, 5, 7] have been proposed that process data streams inside the network. So-called in-network processing like filtering and aggregation reduces traffic in the system and therefore improves its efficiency.
While those approaches are an important step in contributing to a scalable deployment for GSN applications, major open research challenges are the provision of timely data access as well as the handling of large bursts of data. Such bursts need to be addressed particularly in real-time simulations where it is important to directly investigate the impact of environmental disasters on habitats and ecosystems. To take countermeasures, civil protection services also have to be provided with up-to-date information to support their planning and monitoring. However, traditional approaches proposed to enable real-time processing like network reservation protocols are likely to fail for GSNs since they are typically not available at the global scale. Moreover, the occurrence of unforeseen data bursts may still cause overload on the reserved capacity on the underlying communication links.

The goal of the Global Sensor Grid project is to enhance current distributed stream processing systems with explicit reuse. Intelligent load shedding will be introduced to allow for graceful degradation of precision instead of random dropping of packets. Furthermore, it will provide support for moving queries that can be set to a new location without the need for cancel and reissue. To achieve this, a highly dynamic system design will be developed which provides the necessary adaptation mechanisms. Finally, by combining moving queries with detection and tracking of phenomena, users will be able to specify a phenomenon that is automatically monitored by the Global Sensor Grid.

Real-time Simulation for Disaster Prevention

Disaster prevention procedures rely on time and mission-critical computer simulation. To comply with strict government regulations in areas such as nuclear and environmental sciences, the simulation codes must be updated with the latest research findings, yet still meet time and mission constraints. While computing environments such as supercomputers, clusters, and grids could meet the increasing demand, the simulation codes pose numerous legacy and certification problems that prevent the trivial adoption of these technologies. Since the simulation codes can date back from the late 1970s, they cannot be executed straightforwardly on larger, distributed computing environments. Depending on the mission, the same simulation can run with different requirements such as result accuracy and maximal execution time.
Our motivating example is the ABR system, a real simulation system for disaster prevention based on dispersion calculations[1] for radioactive pollutants. This application is a part of a broader distributed simulation system for remote monitoring of nuclear powerplants. In case of accidents the simulations are time and mission critical within limits and regulations defined by law. In these situations the simulation must be performed in real-time, i.e. it uses current weather and emission data and provides results every 10 minutes. Emission data, that is, information about the quantity and nature of the released radioactive pollutants are collected at the beginning of each new period (time step). Each sensor information is provided as one of seven possible incident categories which range from an event with little or no radioactive emission (cat. 7) to a catastrophic reactor core meltdown (cat. 1). Weather data such as wind and precipitation conditions are fetched from the database of the National Weather Forecast Center for the area surrounding the point of emission under investigation. The system analyzes the evolution and impact of the physical emission process by using a simulation workflow. The results of the simulation are plotted interactively on a digitized geographical map.
The ABR system offers different simulation workflows depending on the required accuracy of the results and computing time. These workflows are based on existing simulation codes written in FORTRAN and C++ which use proprietary data formats. The dispersion calculation itself is based on the Langrange particle model. The simulation workflow is executed once for each time step. The length of a time step is variable and corresponds to the arrival period of the measured values for radioactive emissions (i.e., contamined gases and aerosols) and weather conditions (e.g., wind speed and direction, precipitations, etc.). After receiving a new set of inputs the state vector of each particle is recomputed according to the new values. A dispersion calculation can be composed of an arbitrarily large number of arbitrarily long times steps.
In this context the goal of my research is twofold:

- To develop a highly flexible and maintainable system for dispersion calculations with an extended lifespan ($>$ 10 years) and

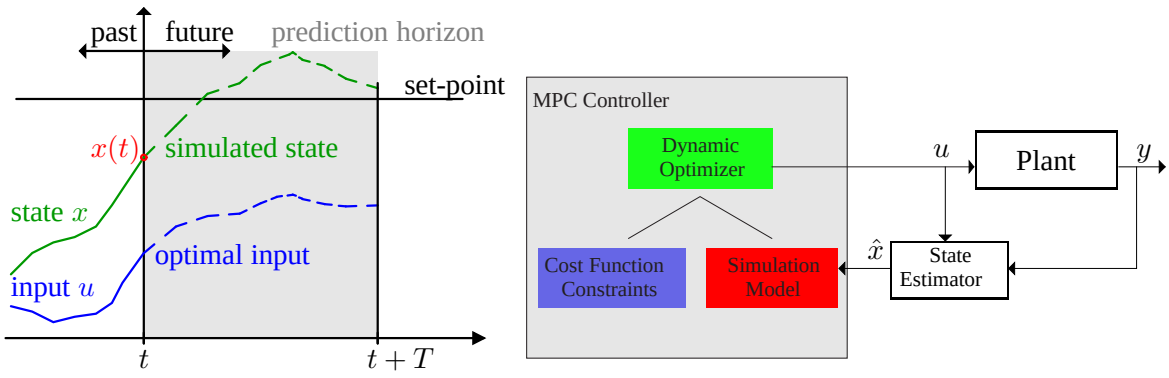
[1] Dispersion modeling is a discipline that provides the mathematical models to calculate the concentration of a substance present in the atmosphere that was released by some source of pollution in any point of an area surrounding it.

- to optimize the ABR workflow in order for it to meet the new real-time computation requirements.

To obtain a highly flexible and maintainable disaster prevention simulation system the possibility of using Aspect Oriented Programming (AOP) is investigated. AOP helps sepparating concerns like distribution (or parallelization), persistence, access control, or tool integration from the functional core of the application. In this way, at first the developer is able to focus on the actual functionality of the simulation application only rather than trying to find tangled solutions to all of the concerns mentioned before.
In order to achieve real-time performance for the ABR workflow the Multicore, Cluster, and Grid computing technologies are considered. The worfklow is modeled as a single instruction, multiple data (SIMD) discrete event based computational pipeline. Thus, a real performance boost can be obtained by parallelizing the different stages of the pipeline rather than rewriting the FORTRAN codes using a parallel programming language.

Model Predictive Control

My main research area is Model Predictive Control (MPC) in general with a particular focus on Nonlinear Model Predictive Control of Networked Control Systems (NCS) and Time-Delay Systems (TDS).
Model predictive control can be explained in a nut-shell as simulation-based optimal control. In contrast to other control methods, e.g. PI-controllers, the calculated input in MPC is not solely based on the current state of the system. Rather the future behaviour of the system is taken into account. For this purpose, a simulation model of the plant is utilised for predicting the evolution of the states up to a certain prediction horizon. Based on this prediction, an optimal input trajectory is calculated which minimises a pre-defined cost functional. Typical cost functionals are based on the squared deviation from a set-point, or reflect the desire for minimum time and energy needed for achieving a certain control task. The calculated optimal input trajectory is applied until new measurement data is available, at which point the procedure of prediction and optimisation is repeated. This recalculation introduces a feedback in the system and allows to react on disturbances which are not known beforehand.
The advantages of model predictive control from an engineering perspective are manifold. Complex nonlinear dynamics, systems with multiple inputs and/or outputs can be treated as well as input and state constraints. Especially the ability to directly incorporate constraints in the controller design distinguishes MPC from almost all other modern control design methods. These advantages are directly connected to the underlying simulation-based prediction of the system's behaviour. However, this also poses the major challenges in MPC. The time required for the simulation causes compuational delays and might result in a degradation of control performance. Typical questions are how a speed-up of the simulation can be achieved and particularly how an efficient simulation model can be found, e.g. based on model reduction.
A good overview on model predictive control can be found in the survey papers [6, 3].
The main focus within MPC I want to concentrate on during my future research are Time-Delay Systems, which appear quite frequently in nature and engineering processes. However, due to the infinite dimension of such systems, control and even mere simulation becomes more challenging. So far, there are only few results even for simple stability of such control schemes, however, with new theoretical results, we have been able to reduce the computational complexity of the optimal control problem to be solved. Thus, a first step towards a 'real-time' application is taken in that respect. For reference, cf. [2].



(a) Basic idea of MPC. (b) Structure of MPC setup.

Figure 1: Model predictive control in a nutshell.

Onboard Simulation for Higher Quality Control

There are several purposes of using modeling and simulation of any system in technical fields. While most of the fundamental researchers like in biology, chemistry, physics etc. use simulation to understand the system, engineers most often use their simulations to parameterize or optimize their systems before the delivery of the product. In contrary some users use simulations to support the running system. But this is very rarely done due to the unpredictability and uncertainty of the simulation. However simulation during the system run helps to reduce sensors, give data about states which are unmeasurable or even allow predicting states of the system. In this manner my research work can be seen and explained:
While traditional production machines obtain high precision despite dynamic motions and process forces through massive design with high mechanical stiffness and high power actuators, today's concepts strive to achieve economical and ecological efficiency through lightweight design, including optimisation of mechanical structures and application of lightweight materials. Even higher mass reduction would be desirable, but this often leads to diminished mechanical stiffness and damping. Advanced control concepts are technically capable of providing good disturbance rejection for this type of machines mechatronically, but they have often been rejected by the manufacturing industry because of the strong theoretical background and expert knowledge which is required for their application to practical problems. A more intuitive approach employs knowledge of a machine's varying instantaneous properties as scheduling input to controllers with variable parameters. To minimise the effort for acquiring information about the instantaneous properties through measurement and storing the resulting large amounts of data on a machine control, I propose to use simulation models. Today, simulation models are typically created during the design of a machine, and methods for their analysis are available, but to implement the proposed approach, new specialised modelling, calculation and simulation techniques have to be developed that allow for computations in real-time ($<$ 1ms cycle time) on the machine control computer. This is the aim of my thesis project proposed here.
The main focus of my thesis work contains the following topics to solve the stated objective: Real-time calculation of eigenvalues, methodologies for real-time system calculation, and vibration reduction on production machines.

Conclusions

As was shown in this brief note, real-time plays an important role in a great variety of issues related to simulation technology. One important thing is that each component in sophisticated technical process, e.g. sensors, simulation, controller etc., has to satisfy its own real-time constraints individually in order to guarantee a good and safe performance.

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INVERSE PROBLEMS

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Inverse Problems

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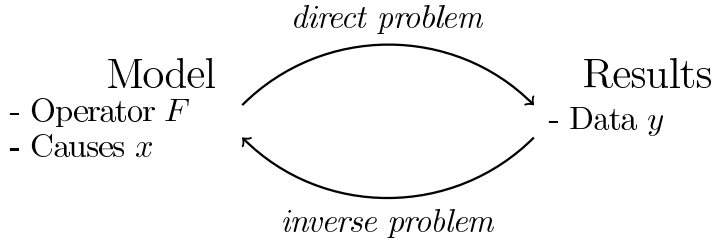
Keywords: *inverse problems, regularization, Bayes theorem, scatterometry, philosophy, isomorphism*

What is an inverse problem?

Inverse Problems have been a field of growing interest in the last two decades. This growth is due to the fact, that inverse problems can be found in almost every field of science and industry. But, what is an inverse problem?
The first question which may arise, is: *inverse with respect to what?* In general we consider two problems: the direct problem (which is in most cases easier to solve) and the corresponding inverse problem. These two types of problems, are called inverse to each other because the formulation of one problem involves the other.
The direct problem can be stated as:
Direct Problem: Given a cause x and a model F, determine the effect y, with $F(x) = y$.
This direct problem directly leads to at least two inverse problems:
Inverse Problem 1: Given the model F and the effect y, estimate the cause x.
Inverse Problem 2: Given the cause x and the effect y, estimate the model F.
In both cases the goal is to use the observed effect to learn something about the system. "Thus, one might say that *inverse problems are concerned with determining causes for a desired or an observed fact.*"[1]



One interesting property of inverse problems is that they are in general ill-posed. Even in case the forward operator F *is well-defined and continuous*, means:

- small changes in x result in small changes in y
- there exits a unique solution

the inverse problem may not be well-posed. This means that the estimate (x or F) strongly depends on y and that the problem may not have a solution. In such situations we call the problem *ill-posed* in the sense of Hadamard (for details see [2]).

Solving ill-posed inverse problem using regularization

In the following we are going to present one frequently used approach to deal with **Inverse Problem 1**, the estimation of x. Therefore, we assume that operator F is known precisely, but (as often the case in practice) the inverse F^{-1} is assumed to be unbounded ($||F^{-1}|| = \infty$). Furthermore, only noisy data y^δ, with $||y - y^\delta|| < \delta$ are available.
According to **Inverse Problem 1** the goal is now to find a solution x such that

$$F(x) = y. \tag{1}$$

As F^{-1} is unbound and only noisy data y^δ are available the formula $x = F^{-1}(y)$ can not be applied. To overcome this problem one may try to consider the mean square error as objective function,

$$J(x) = ||F(x) - y^\delta||^2. \tag{2}$$

Using this objective function an estimate of x is given by

$$x^* = \arg\min_x J(x), \tag{3}$$

in which x^* is the value of x for which $J(x)$ is minimal. Unfortunately, as $||F^{-1}||$ is unbounded the solution of this minimization problem often strongly depends on the measurement noise (this is undesirable!) and the solution x^* may be non-unique.

These problems have already been realized by the famous mathematician Andrey Tikhonov in the 1960s. Therefore, he proposed a regularization of the inverse problem. The idea is that instead of solving the original, ill-posed inverse problem a new problem, closely related to the original one, is solved. This new (regularized) problem is designed such that it has better numerical properties than the original inverse problem. To achieve this the regularized objective function

$$J(x, \alpha) = ||F(x) - y^\delta||^2 + \alpha r(x), \tag{4}$$

is defined, in which $\alpha r(x) > 0 \forall x$ is the regularization term. The first term of $J(x, \alpha)$ forces the estimate to yield a good fit of the available data. The second term on the other hand improves the conditioning of the corresponding minimization problem,

$$x^*(\alpha) = \arg\min_x J(x, \alpha). \tag{5}$$

If the regularization $\alpha r(x)$ is chosen appropriately the solution of (5) is closely related to the solution of the original inverse problem. Additionally, the new problem is far better conditioned and standard optimization algorithms [4] can be employed to determine the optimal solution $x^*(\alpha)$.

Selection of regularization function

As can be seen easily, the function (4) depends not only on x but also on $\alpha r(x)$. Hence, the optimal value x^* also depends on $\alpha r(x)$. This makes the selection of appropriate regularization functions $r(x)$ and regularization parameters α crucial. If α is chosen in the wrong way, the error between exact solution and approximate solution will blow up, as the noise level tends to zero.
In particular for the selection of the regularization function there are several standard approaches. The most common one is probably $r(x) = ||x||^2$. This regularization has already be introduced by Tikhonov himself. An other regularization function which became more and more common during the last years is $r(x) = ||x||_1$ which often yields sparse solutions for x.

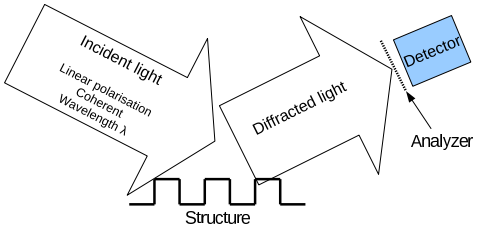
Another possible approach, to solve the inverse problem, is to look at the system as a stochastic model. As y^δ is a realization of a stochastic process, one can use a regularization function based on *a priori* probabilities of x. These are in particular inspired by the Bayes Theorem [5],

$$\Pr(x|y) = \frac{\Pr(y,x)\Pr(x)}{\Pr(y)}, \tag{6}$$

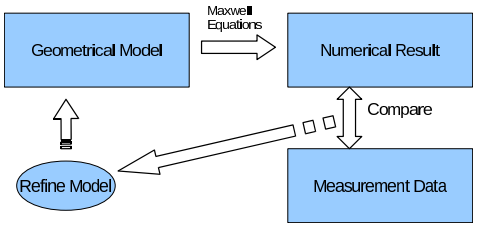
in which $\Pr(x|y)$ is the *a posteriori* probability of x given the data y, $\Pr(y|x)$ is the probability to observe y given x, $\Pr(x)$ is the *a priori* probability of x, and $\Pr(y)$ is the probability to observe the effect y. So if $\Pr(x)$ and $\Pr(y|x)$ is know, one can calculate the a posteriori probability. In case, $\Pr(x)$ is a normal distribution a regularization using $\Pr(x)$ relates directly to the Tikhonov regularization.

A practical Example: Scatterometry

Imaging optical measurement systems (microscopes, etc.) are limited in their resolution by diffraction. The smallest resolvable objects are as big as half the wavelength (λ) of the light. Indirect optical measurements can archieve a much higher resolution, but therefore an inverse problem has to be solved.
Scatterometry is a technique to resolve periodical structures indirectly by measuring intensity and polarisation properties of the light reflected from the structure when illuminated with linearly polarized light under an angle Θ. A rough sketch of the measurement setup is shown in the following figure:



The measurment data consists of the intensity and the polarization changes in the light due to the diffraction at the sample, but the parameters we want to acquire are the dimensions of the periodic structures on the sample (width, height, spacing of the lines ...). So the inverse problem is calculating the surface (cause) from the measured values (effect). The equations that connect both are the well known Maxwell-equations from electrodynamics.
The surface can be retrieved with an iterative method that first simulates the measurement for a initial guess of the structure. The simulation is compared with the measured data and the gradient towards a lower distance (in a least square sense) between the datasets is calculated. A new structure in the direction of the gradient is simulated and tested and the process starts again until a minimum is found.



To speed up the search for the best fit, it is practical to pre-calculate a whole library of possible structures. The computer that drives the measurement then only has to fetch the right structure out of the existing database, without having to use a lot of computation time. The drawback of this method is that one has to calculate a great dataset beforehand to reach sufficient resolution.

Some philosophical questions about inverse problems

Some paradigms of the solution of inverse problems suggest that obtaining "the best" model consist, basically, in 'extracting' a model from the data. This is based on the idea of deducing the model from the data and, therefore, any further data should "fit" into the model. Scientist not only want to know certain system but also infer back to the world *new* information. I use this simplified version to discuss three traditional issues in philosophy of science:

1. *Isomorphism:* A deduction of a model from data presupposes a isomorphism between the data and the model, but it does not oblige us to accept the isomorphism of the model (or data) and the world. As a consequence, we might naïvely be dealing with a *created* phenomena instead of the "*true*" one.

2. *Emergence:* One major objection to computer simulations is that they cannot produce new information. All the information produced is already coded in the model. If we create a model using certain data, it is expectable that similar information will be contained in the model. Quoting Nietszche: "Wenn jemand ein Ding hinter einem Busche versteckt, es ebendort wieder sucht und auch findet, so ist an diesem Suchen und Finden nicht viel zu rühmen: so aber steht es mit dem Suchen und Finden der 'Wahrheit' innerhalb des Vernunft-Bezirkes. Wenn ich die Definition des Säugetieres mache und dann erkläre nach Besichtigung eines Kamels: 'Siehe, ein Säugetier', so wird damit eine Wahrheit zwar ans Licht gebracht, aber sie ist von begrenztem Werte, ich meine, sie ist durch und durch anthropomorphisch und enthält keinen einzigen Punkt, der 'wahr an sich', wirklich und allgemeingültig, abgesehen von dem Menschen, wäre."[6]

3. *Apparatus:* Scientist work with the data obtained from measuring and observation (often by technological means) creating models and, afterwards, inferring back to the world. However, there is no epistemic warranties that the model created is the "true model". Moreover, there is no warranties that the inference back to the world is not based on new, hidden, information created by the apparatus used for manipulating the data.

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ORDINARY DIFFERENTIAL EQUATIONS

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Differential equations: Definition, Application and Philosophical Framework

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Keywords: *ordinary differential equations, phase portrait, Picard-Lindelöf method, philosophy, modeling, representation, model-target relation, qualitative theory, stability, oscillator, synchronization*

Definition

The most general form of an ordinary differential equation (*ode*) is

$$F(y^{(n)}, y^{(n-1)}, \dots, y', y, x) = 0, \quad x \in J \subset \mathbb{R}, \tag{1}$$

where n denotes the order of the *ode*. A special form of (1) is

$$y'(x) = f(x, y(x)), \ y(x_0) = \eta, \tag{2}$$

where $x \in J \subset \mathbb{R}$ and J is a compact interval. A function $\phi(x)$ is a solution of the equation (2) if $\phi(x)$ is differentiable and satisfies (2) for each $x \in J$ and if $\phi(x_0) = \eta$. If the function $f(x, y)$ is continuous, then (2) can be written as an integral equation $y(x) = \eta + \int_{x_0}^{x} f(s, y(s))ds$. This equation can be solved by the method of Picard-Lindelöf

$$y_{k+1}(x) := \eta + \int_{x_0}^{x} f(s, y_k(s))ds, \quad k = 0, 1 =, 2, \dots,$$

where $y_0(x)$ is chosen arbitrarily. The series $y_k(x)$ converges uniformly to the solution $y(x)$ of (2), if $f(x, y)$ is continuously differentiable with respect to y and x, cf. [8]. The method of Picard-Lindelöf is not used to compute a solution of the *ode* but it is suitable for the proof of an existence and uniqueness theorem. So, if the function $f(x, y)$ is continuously differentiable with respect to y and x, then the initial value problem (2) possesses a unique solution. This result holds for systems of *ode*s as well.
To visualize solutions of the *ode*, the vector field $\mathbf{z} = (1, f(x, y))^\top$ is drawn in the (x, y)-plane. Since $f(x, y)$ is the slope of the solution $y(x)$ in a point x, the vector field $\mathbf{z}$ is tangential to the graph of the solution $y(x)$. The standardized vector field and a trajectory to the *ode* $y'(x) = x^2 - y$ is displayed in Figure 1. Solutions of a system of *ode*s $\mathbf{y}' = \mathbf{f}(\mathbf{y})$, $\mathbf{y} = (y_1(x), y_2(x))^\top$, often are visualized in the (y_1, y_2)-plane. The chain rule yields

$$\frac{dy_2}{dy_1} = \frac{dy_2/dx}{dy_1/dx} = \frac{f_2(\mathbf{y})}{f_1(\mathbf{y})}, \text{ if } \frac{dy_1}{dx} \neq 0,$$

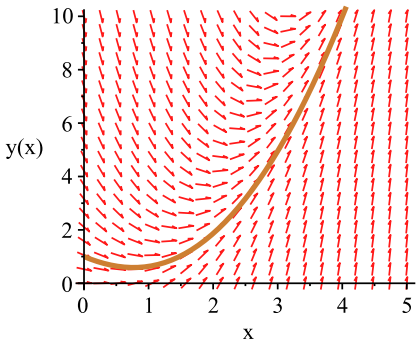

Figure 1: Vector field $\mathbf{z}/\|\mathbf{z}\|$.

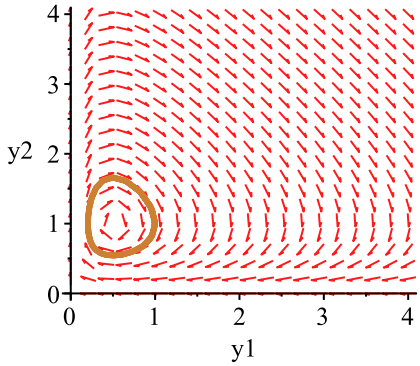

Figure 2: Vector field $\mathbf{f}/\|\mathbf{f}\|$.

and the vector field $\mathbf{f}$ can be written as $\mathbf{f} = f_1(\mathbf{y})(1, \frac{f_2(\mathbf{y})}{f_1(\mathbf{y})})^\top$ if $f_1(\mathbf{y}) \neq 0$. Hence, the vector field is tangential to the trajectory in the (y_1, y_2)-plane. The direction field $\mathbf{f}/\|\mathbf{f}\|$ for the example

$$y_1'(x) = y_1(x) \cdot y_2(x) - y_1(x),$$
$$y_2'(x) = -y_1(x) \cdot y_2(x) - 0.5 \cdot y_2(x)$$

is depicted in Figure 2.

Modeling Biological Systems with ordinary differential equations

Ordinary differential equations *ode*s are commonly used for modeling cell processes such as signal transduction, which rely on a molecular reaction network. The cell defines the system to be considered, and its state can be represented by a vector containing the amount of each molecule species that can be found (or is of interest) in the system. During the time course, reactions cause the molecule amounts to change and thus correspond to an *ode* system

$$\frac{\mathrm{d}x}{\mathrm{d}t} = f(x, p, t), \tag{3}$$

where x is the state vector (amount of each molecule species), p is the vector of parameters, and t is the time.

The application of *ode*s is feasible under certain circumstances which are fulfilled in most common reaction networks: spatial homogeneity within compartments and a high number of molecules. The spatial dimension in cellular systems is given by the partition into compartments; within each compartments a homogeneous medium can be assumed, and spatial transport between the compartments can be considered in the exchange rates. Furthermore, the usually high number of molecules in biochemical reactions makes an ”overall deterministic” approach reasonable. Besides that, stochasticity can be included in *ode* models if desired [9].

Several books address the task of converting a set of biochemical reactions into an *ode* system, e.g. [4]. Suitable software, e.g. SBML (Systems Biology Markup Language) and its corresponding toolboxes for multiple programming languages, allow the user to simply enter the list of reactions, and the resulting *ode* system is generated automatically. For large *ode* systems, as are usually resulting from biochemical reaction networks, it gets intractable to solve the system analytically. Rather, numerical or graphical ”solutions” yielded by simulations serve for further understanding and analyzing the system. Typical approaches include the dynamics (time course), phase portraits, bifurcation diagrams, vector fields and nullclines.

Qualitative Theory

Introduction

The two previous sections introduced the mathematical definition for ordinary differential equations and presented a typical differential equation arising in systems biology. In the following, we give a short overview about some questions that come up during the analysis of odes.

Quantitative and qualitative behavior

If we talk about an ordinary differential equation (*ode*) in the following, we mean an equation of the type

$$\dot{x}(t) = f\big(x(t)\big), \tag{4}$$

where $f : D \to \mathbb{R}$ is a sufficiently smooth function on a region $D \subset \mathbb{R}^n$ and $\dot{x}(t)$ denotes the derivative of x with respect to the independent variable t. As discussed before, solutions $\phi : \mathbb{R} \to D$ of (4) are functions of the independent variable t, if we talk about *behavior* of solutions we mean how the solutions change in dependence of t, i.e. how they *evolve*.
One way to analyze the evolution of solutions of (4) distinguishes between *quantitative* and *qualitative* approaches. By quantitative we mean approaches that aim to determine the solution or a solution family exactly, i.e. as explicit functions of series of functions of t. Such an approach is restricted, since it is only possible to obtain explicit solutions for few equations [6]. Because of the existence and uniqueness of solutions under mild conditions, an approach to obtain a single solution would be the approximation by a time series obtained through numerical integration. This approach still does not solve the problem that a solution is parametrized by the initial condition, hence the information one gets from a single solution is restricted. Furthermore, there are cases where numerical integration fails to produce an approximate solutions of a system, see e.g. [1]. The qualitative approach aims to solve these problems. In the qualitative setting one looks at properties that mostly do not involve the calculation of an explicit solution. Furthermore the goal is to give statements about whole sets of solutions, i.e. solutions with initial conditions inside a subregion of the domain D of the *ode*.

Stability theory

There are many different questions of interest for the evolution of solutions of an *ode* on the qualitative level. It is possible to pose all the questions on a higher abstraction level, which is the topic of the theory of dynamical systems, see e.g. [3]. Here we want to concentrate on properties that are connected to the long term behavior of solutions. The reason for the interest in the long term behavior lies in the requirement that we want to investigate properties which do not depend on a single initial condition but rather on whole sets of initial conditions. One technical term that deals with questions related to long term behavior is *stability*.
There are various stability definitions that came up throughout history. We present two definitions that treat various types of stability of solutions of (4). For a comprehensive treatment of stability theory see [2].

Lagrange stability In case of Lagrange stability we are interested whether solutions that go through a point $x_0 \in D$ stay bounded. In $D \subset \mathbb{R}^n$ we would say that a solution ϕ through a point x_0 is Lagrange stable if there is a solution $\phi : \mathbb{R} \to D$ such that $\phi(s) = x_0$ for one s and there exists a $\alpha \in \mathbb{R}$ such that for all t we have $\|\phi(t)\| \leq \alpha$.

Lyapunov stability Lyapunov stability is the formalization of stability of solutions ϕ under perturbation. Formally, a solution ϕ is Lyapunov stable if for every $\varepsilon > 0$ there is a $\delta > 0$ such that all solutions starting within a δ-neighborhood of ϕ stay in an ε-neighborhood of ϕ. More descriptively, if we find a tube around our solution ϕ such that no solution leaves the tube, then it is Lyapunov stable. The importance of stability analysis for practical problems is immediately evident. For all dynamical processes described by an *ode* it is desirable to know whether a process stays within certain bounds or close to a certain point. We now want to give a small example which shows the importance of stability problems in a more complex situation.

Example for a stability problem

For our example of stability we want to consider an effect observable in connection to oscillating phenomena. Periodic processes are quite common in nature, simple everyday examples stem from physiology, e.g. the heartbeat. We want to consider an effect that occurs if oscillators interact — the phenomenon of *synchronization*. The term synchronization refers to the emergence of patterns

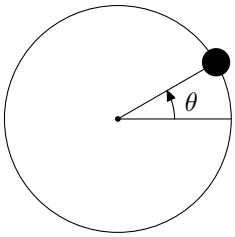

Figure 3: A scheme for a single oscillator. We model the oscillator as point moving around the circle with constant speed ω, i.e. if we measure the position of the point on the circle with the angle θ, then it grows according to $\dot{\theta} = \omega$. We call θ the phase of the oscillator.

in interacting oscillators, e.g. a group of oscillators agrees on a common frequency or a common phase. To describe the effect in more detail consider a network of oscillators, where a single oscillator is described by a point that moves on a unit circle with a constant speed, i.e. we can describe the evolution of the phase θ of the oscillator by the differential equation

$$\dot{\theta} = \omega, \tag{5}$$

see also Figure 3. For the network of oscillators we consider a set of N oscillators coupled by a function that respects the configuration space of the single oscillator, i.e. we choose a 2π-periodic coupling. As result we obtain a model of the from

$$\dot{\theta}_i = \omega + \frac{K}{N} \sum_{k=1}^{N} \sin(\theta_k - \theta_i), \tag{6}$$

where $\sin$ is the coupling function and K is the coupling strength. The model (6) describes now the evolution of the phases of N oscillators who interact. The effect we are interested in now would be an agreement of all oscillators on a common phase, i.e. for all i, j we have $\lim_{t\to\infty} \theta_i - \theta_j = 0$, in other words they behave like one system. Such an effect is a typical synchronization phenomenon, for a more detailed description of the possible effects, see [5]. From the mathematical point of view the problem behind the phenomenon is a stability problem: we want to know whether the difference of all solutions approaches zero and stays there irrespective of disturbances. Thereby we reduced a complicated phenomenon to a problem which is tractable with tools from the qualitative theory from differential equations.

Conclusion

We gave a sketch about aspects of qualitative theory in the context of ordinary differential equations with a particular focus on stability. Therefore we explained several types of stability and showed the importance of the definitions on an example for complex behavior.

Ontological and Semantic Viewpoints on Models in Science

The word ”model” is frequently used, even though in (i) different and often (ii) non-terminological (i.e. ambiguous) ways [7]. According to the Stanford Encyclopedia of Philosophy diverse things are commonly referred to as models, namely ”physical objects, fictional objects, set-theoretic-structures, descriptions, equations or combinations of some of these” [10]. Apparently, this (exemplary) listing demands further conceptual clarifications: First, the ontological categories need to be specified more carefully in order to provide clearer distinctions (e.g. between fictional objects and set-theoretic structures). Second, the underlying model-concepts need to be exposed in order to re-examine the extension(s) of the term.

The revelation of conceptual differences furthermore helps to distinguish between types of models and sheds light on their respective roles in various processes of acquiring knowledge. The classification of different usages of technical terms thus is crucial with respect to multi- and interdisciplinary contexts, insofar as it provides a common point of reference.

The attempt to expose different types of models leads to their representational function. Models play an important role in the process of acquiring knowledge and understanding by means of representing data, phenomena or theories in a modifiable way. While models of data and phenomena refer to certain target systems (models for sth.), models of theories are derived from theories in the way that they interpret the axioms of the theory (models of sth.). Especially in terms of computer-based simulations, one can further investigate on the compatibility and simultaneity of different representational functions.

Yet, not only the type of target-relation is crucial with respect to the epistemic function of models, but also the mode of target-representation. The Stanford Encyclopedia of Philosophy suggests corresponding differences between scale models, idealized models, analogical models and phenomenological models [10]. Again, one could demand for further specifications, since at first glance all of these model types seem to require (quantitatively more or less divergent) idealizations in the sense of abstractions of relevant target-properties.

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THEORY OF POROUS MEDIA

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Theory of Porous Media - Basics: Flow through Porous Media

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Keywords: *porous media, multiphase flow, Darcy*

In nature as well as in technical applications, a multitude of materials can be considered as porous media which consist of a matrix of solid material like soil material in the subsurface (e.g. sand, clay, rock) and void spaces in between, which are also called pores. Flow through the pores of a porous medium can be directly calculated by solving different conservation equations like mass balance equations and momentum balance equations, which could be Navier-Stokes or Stokes equations. However, it would be necessary to know the detailed structure and geometry of all pores of a porous medium as well as the location of all fluid-fluid interfaces in case of multi-phase flow. This is extremely expensive with regard to computational costs and in most cases, it is just impossible to describe the detailed geometry of the pore structure. Therefore, a continuum approach in which the microscale properties are averaged over a representative elementary volume (REV) is used in most porous media flow models. Through this averaging process a set of new macroscale parameters like the saturation and the porosity is generated. Additionally, closure relations have to be defined relating multiphase fluid behavior on the microscale to the macroscale parameters. (For a detailed overview of this topic, see e.g. [1] or [2])

Porosity A porous medium consists of a solid matrix and the pores. The ratio of the pore space within the REV and the total volume of the REV is defined as porosity ϕ:

$$\phi = \frac{\text{volume of pore space within the REV}}{\text{total volume of the REV}}. \tag{1}$$

The porosity appears in the macro scale (Darcy scale) equations to reduce the volume of the porous medium to the volume usable for flow. If the solid matrix is assumed to be rigid the porosity is constant and independent of temperature, pressure or other variables.

Permeability When considering flow through porous media, the interaction between a fluid and the solid matrix is essential. In a macroscopic approach these interactions are covered by one parameter, the hydraulic conductivity $\mathbf{K}_f$, which accounts for the influence of fluid viscosity and adhesion at the surface of the solid matrix. The hydraulic conductivity can be defined as

$$\mathbf{K}_f = \mathbf{K}\frac{\varrho_f g}{\mu} \qquad \left[\frac{m}{s}\right], \tag{2}$$

where ϱ_f is the fluid density, μ the fluid viscosity, g the gravity and $\mathbf{K}$ the intrinsic permeability. $\mathbf{K}$ is a tensor characterizing the porous medium and is only dependent on the solid matrix.

Saturation In multiphase flow of immiscible or only partly miscible fluids in porous media the pore space is divided and filled by the different phases. In the macroscopic approach this is expressed by the saturation of each phase α. It is defined as the ratio of the volume of phase α within the REV and the volume of the pore space within the REV:

$$S_\alpha = \frac{\text{volume of phase } \alpha \text{ within the REV}}{\text{volume of the pore space within the REV}}. \tag{3}$$

Capillarity Due to interfacial tension, forces occur at the interface of two phases. This effect is caused by interactions of the fluids on molecular scale. Therefore, the interface between a wetting and a non-wetting phase is curved and the equilibrium at the interface leads to a pressure difference between the phases called capillary pressure p_c:

$$p_c = p_n - p_w, \tag{4}$$

where p_n is the non-wetting phase and p_w the wetting phase pressure. On the microscale, the capillary pressure can be formulated as Laplace equation, depending on the radius of the pore space and the interfacial tension of the different fluid combinations.
In a macroscopic consideration of multiphase systems a macroscopic capillary pressure can be related to the saturation. The most common capillary pressure-saturation-relations for a two-phase system are those of *Brooks and Corey* and *van Genuchten*.

Darcy's law Usually, momentum equations have to be solved to get phase velocities at the pore scale. However, in a macroscopic treatment of porous media *Darcy*'s law which was originally obtained experimentally for single phase flow can be used to calculated the velocity directly:

$$\mathbf{v}_\mathrm{f} = -\frac{1}{\mu}\mathbf{K}(\nabla p + \varrho g \nabla z). \tag{5}$$

For multiphase systems a generalized *Darcy* law can be formulated for each phase

$$\mathbf{v}_\alpha = -\frac{k_{r_\alpha}}{\mu_\alpha}\mathbf{K}(\nabla p_\alpha + \varrho_\alpha g \nabla z), \tag{6}$$

where $\mathbf{K}$ is the intrinsic permeability, μ the dynamic fluid viscosity, p the pressure and ϱ the density of phase α, and g is the gravity constant acting in z-direction. Flow in porous media is strongly influenced by the interaction between the fluid phase and the solid phase. This is taken into account by the concept of a hydraulic conductivity and intrinsic permeability respectively. If more than one fluid phase fill the pore space, the presence of one phase also disturbs the flow behavior of another phase. Therefore, a relative permeability k_{r_α} is introduced which can be considered as an additional scaling factor.

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Theory of Porous Media

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Keywords: *Finite Element Method, porous media, theory of mixtures*

Mixture kinematics

Each constituent within a Porous Media has its own motion function $\boldsymbol{\chi}_\alpha(\mathbf{X}_\alpha, t)$. The motion function gives the actual position $\mathbf{x}$ at time $t \geq t_0$ of every material point $\mathcal{P}^\alpha$, identified by its position $\mathbf{X}_\alpha$ in the reference configuration $t = t_0$. Every spatial point $\mathbf{x}$ is occupied by as many material points as constituents exist within the porous media model.
The motion of the solid constituents is ussally given in a material (*Lagrange*ian) description by the displacment vector $\mathbf{u}_S$. Therein the observer is moving with the the observed material. In an FEM calculation the net is deforming according to the deformation of the solid contituent.
Fluid flow within the pores of the solid matrix is described by a modified *Euler*ian describtion using the seepage velocity $\mathbf{w}_{FR}$. In an *Euler*ian description the observer has a fixed spatial position which does not change during the observation. In the TPM the observers position is not spatially fixed but fixed to the deformation of solid constituent. This allows to use the same FEM net for the solid and the fluid constituents.

Balance equations and interactions

In the TPM the balance equations, as in continuums thermodynamics are introduced via axioms. The local balance equations of the constituents are obtained in analogy to those of a single-phase materials. But additionally the interaction between the constituents must be taken into account by additional production terms.
The local change of the partial density of each constituent is discriped by the mass balance. Therein $-\rho^\alpha \operatorname{div} \mathbf{x}'_\alpha$ denotes the change of mass due to deformation processes. The interaction or mass exchange between the constituents is described by $\hat{\rho}^\alpha$. In a closed system no mass is produced, this leads to the restriction that the sum over $\hat{\rho}^\alpha$ must be equal to zero.
The balance of momentum introduces *Newton*'s second law of motion (force equals mass times acceleration) into the TPM. Therein $\operatorname{div} \mathbf{T}^\alpha$ and $\rho^\alpha \mathbf{b}^\alpha$ are forces due to contact or volume forces. The momentum interaction between the constituents is described by the direct momentum production $\hat{\mathbf{p}}^\alpha$. Within a mixture no forces are produced, therefore the sum over the global momentum production must be equal to zero. This results in a condition for the direct production terms, which also includes terms from the mass balances.
The local changes of the internal energy are described in the energy balance equation. The interaction between the constituents is included into the equation by the direct energy production $\hat{\varepsilon}^\alpha$, which, since no energy is produced within a mixture, must fulfil a summation condition, where the direct production of energy and production terms from the lower balance equations are included.

Constitutive modelling

The mechanical problem, given by the complete motion and temperture situation cannot be solved by the balance equations alone. The remaining quantities must be calculated using constitutive assumption, which must fulfil the entropy inequality. More details on this topic can be found in [1].

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Theory of Porous Media - Applications

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Keywords: *transvascular processes, micro-/macromodels, Stokes equation, porous media*

Flow and transport processes in porous media occur in many different fields of application. Basically, natural, technical and biological applications can be identified. A classical natural porous medium is the subsurface. Here, the spreading of contaminants and their remediation, the migration of methane emanating from exhausted coal seams and evaporation processes at the interface between atmosphere and subsurface are of interest. Recently, the modeling of the behavior and fate of CO_2 during underground storage came to the fore. Technical applications are, for example, gas and/or liquid flow processes through filters, the behavior of ink in paper, the gas-liquid-solid interactions in baby diapers or the processes that occur in the gas diffusion layers of fuel cells ([1]). The biological field of application mainly deals with the distribution of therapeutic agents in the human body. As possible applications the modeling of enhanced drug delivery to brain tumors, the distribution of agents within the human lung or the investigation of transvascular processes are to be mentioned.

One example for an application to biological systems is the detailed investigation of the flow and transport processes between blood vessels and surrounding tissue, with the main focus on a detailed description of the structure and influence of the microvascular wall ([2]). This is done in the research project *"Coupling of micro- and macromodels for complex flow and transport processes in biological tissue"* in the framework of the"Research Center for Simulation Technology".
The objective of the project is the development of a coupled micro-macro-model. Micromodels are used in regions which are highly active with respect to transfer processes, like the blood-vessel-interstitium interface, while much faster macromodels are applied in less active parts such as the interstitial space. Hence, the vascular and the interstitial compartment are described using a continuum approach. Blood flow within the capillaries is described with the STOKES equation for free, laminar flow of a NEWTONIAN fluid, while the tissue space is modeled as a rigid, porous medium ([3]). These macromodels are coupled with a discrete model resolving the structure of the microvascular wall. A coupled model allows us to benefit from the advantages of both micro- and macro models: physically correct description of the transfer of mass and energy processes and resolution of the biological structure versus computational efficiency.
Furthermore, the project aims at applying an analytical upscaling to the three-dimensional PDEs that describe the capillary wall on the microscale, in order to obtain a two-dimensional interface with the respective equations and properties. If possible, further simplifications will be carried out to derive coupling conditions that can be implemented in other models describing flow and transport processes in whole organs.

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Theory of Porous Media: Turbulent flow at porous medium interface

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Keywords: *porous media, turbulent flow, coupled problems, direct numerical simulation*

Transport phenomena at the interface between porous medium and a free flow play a crucial role in many areas. Filters, catalytic reactors, ground water pollution, benthic boundary layer are common applications. Numerous investigations have been made in the past, concerning the physics of the flow at this fluid-porous interfacial region. Most of the studies are concentrate on laminar flows. The earliest investigation can be contributed to Beavers and Joseph [1] in this work it is assumed that, the velocity within the porous media, away from the interface, should follow the Darcy's law and they propose that the flow outside the porous media satisfies the following slip boundary condition:

$$\frac{\partial u}{\partial y}|_{y=0} = \frac{\alpha}{\sqrt{k}} (u_s - u_d) \tag{1}$$

where k is the intrinsic permeability of the porous medium and α is the slip coefficient. Many investigators have been trying to determine this slip coefficient for different porous media. It has been found that α is strongly dependent on the geometry of the interface, internal structure of the porous medium and a choice of the interface position i.e. the discontinuity inside the transition region.
There are significant studies on turbulent flows adjacent to a porous interface. Many studies in turbulence of plant canopies indicate the existence of large-scaled coherent vortices having a size comparable to the height of the canopies [2, 3]. These structures enhance heat and mass transfer between the air and the canopies. Finnigan [2] proposes that these coherent vortices is initiated from a Kelvin-Helmholtz instability. In open channel flow, Shvidchenko found a very large vortex can have a vertical size of the flow depth (h). It is thus unlikely that the simple interface condition above will be able to represent these complex structures.
In this talk, we present the interface conditions applied to turbulent flows available in the literature. We then present an investigation of the interface condition using a pore-scaled simulation of turbulent flows using direct numerical simulation of the Navier-Stokes equations. The preliminary findings suggest that the existing interface conditions are not physically correct and better interface conditions are needed.

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STOCHASTIC METHODS

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Joint Data Compression and Model Reduction for Conditional Stochastic Modeling of Subsurface Flow and Transport Processes

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Keywords: *inverse modeling, geostatistics, Bayes theorem, data assimilation*

Variability of geological materials in combination with the scarcity of data lead to a geostatistical description of subsurface systems coupled with stochastical simulation. Experimental site data e.g., from well tests or tracer tests, are assimilated into stochastic simulation via Bayesian updating, and help to reduce the prediction uncertainty. This type of approach is indispensable, e.g., in the stochastic definition of well capture zones in the prediction of human health risk from groundwater contamination.

The computational costs of Baysian updating can quickly become intractable when large quantities of data have to be processed. Regardless of the specific tool for stochastic simulation or Baysian updating, numerical simulations have to be run repeatedly. The computational load rises with the number of data points, with the discretization of the spatially random material properties, and with the complexity of the simulation model. In many cases, the vast computational costs prohibit the use of rigorous stochastic approaches.

Well and tracer tests are important experimental tools that help to reduce the uncertainty of predictions in heterogeneous and uncertain subsurface systems. Yet, they yield time series data with very limited information per individual data point. In this project, temporal moments will be used to compresse down time series data to a low number of characteristic features, while minimizing the information lost by the compression [1]. The compression will be designed to fit with a simultaneous model reduction from transient to steady-state equations. By matching data compression and model reduction, the original model equations can be entirely avoided. This will drastically reduce the computational costs of the stochastic modeling and data assimilation task, and hence make stochastic approaches applicable to larger and more complex problems.

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Joint Design and Probabalistic Risk Assessment for CO_2 Storage

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Keywords: *polynomial chaos, carbon dioxide, multiphase flow, porous media, risk assessment, uncertainties, stochastic response surfaces*

The present work deals with the environmental problem of carbon dioxide (CO_2) emissions influencing the global climate. Large-scale industrial CO_2 injection into deep geologic formations bears an inherent risk of leakage back into atmosphere. The potential of CO_2 injection as a large-scale interim solution will vastly depend on our ability to quantify its uncertainties and risks. Current numerical simulation models are inadequate for stochastic simulation techniques, because they are too expensive for stochastic approaches based on repeated simulation. Even single deterministic simulations require parallel high performance computing. Because the involved multiphase flow processes of CO_2 in porous media have a significantly nonlinear character, the problem is too non-linear for quasi-linear and other simplified stochastic tools. As an alternative approach, we propose a massive stochastic model reduction which is based on the probabilistic collocation method [1]. The model response surface is projected onto a higher-order orthogonal basis of polynomials [2], allowing for non-linear propagation of model uncertainties onto the predicted leakage risk. The variable parameters include uncertain model parameters, such as porosity, permeability, etc. and a list of design parameters (injection rate, depth, etc.). The chosen degree of the polynomial balances between computational effort and accuracy. The proposed stochastic approach was validated through Monte Carlo simulation using a common 3D Benchmark [3]. The reasonable compromise between computational efforts and precision was reached with 2nd order polynomials. In this case study, our proposed approach yields a computational speed-up of 100: 1000 Benchmark runs for Monte Carlo evaluation are comparable to 10 Benchmark runs using the probabilistic collocation method. At the same time, our collocation methodology is an integrative powerful tool for optimizing design variables and uncertain variables into one approach (via integrative response surfaces). Thus the design tasks explicitly includes uncertainty, leading to robust designs with minimum failure probability over the entire range of uncertainty.

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