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Scientific Program - Timetable

Sunday 22	Time	Monday 23	Tuesday 24	Wednesday 25	Thursday 26	Friday 27
	9:15		Contributed sessions (15 in parallel)	Plenary Lecture Moritz Diehl	Contributed sessions (15 in parallel)	Contributed sessions (14 in parallel)
	9:30					
	9:45					
	10:15	Registration		von Mises prize lecture		
	10:30					
	10:45					
	11:15		Coffee Break	Coffee Break	Coffee Break	Coffee Break
	11:30					
	11:45					
	12:15		Plenary Lecture Thomas Böhlke	General Assembly	Plenary Lecture Ferdinando Auricchio	Contributed sessions (11 in parallel)
	12:30					
	12:45					
	13:15	Opening	Lunch	Lunch	Lunch	
	13:30					
	13:45	Univ. Chorus Performance				Closing
	14:15	Prandtl Lecture Keith Moffatt	Plenary Lecture Enrique Zuazua	Contributed sessions (15 in parallel)	Plenary Lecture Daniel Kressner	
	14:30					
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	15:15	Plenary Lecture Giovanni Galdi	Plenary Lecture Nikolaus Adams		Plenary Lecture Stanislaw Stupkiewicz	
	15:30					
	15:45					
Registration pre-opening	16:15	Coffee Break	Coffee Break Poster session	Coffee Break	Coffee Break Poster session	
	16:30					
	16:45	Minisymposia & Young Reseachers' Minisymposia (10 in parallel)	Contributed sessions (14 in parallel)	Contributed sessions (15 in parallel)	Contributed sessions (15 in parallel)	
	17:15					
	17:30					
	17:45					
	18:15		Public lecture Francesco D'Andria			
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	19:15	Opening reception at Castle of Charles V				
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	20:15			Conference dinner at Hotel Tiziano		
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S07: Coupled problems

Coupled problems arise in several applications. From a general point of view each problem containing more than one primary field is called a coupled one. Usually the class of coupled problems is subdivided into volumetrically coupled problems and problems with surface coupling. The class of volumetrically coupled problems contains e.g. the fluid flow in porous solids described by mixture theory, thermo-mechanically coupled problems, chemo-mechanically coupled problems and electro- or magneto-mechanically coupled problems while in the second class problems like the fluid-solid interaction via an interface are included.

All problems is in common that the presence of different fields in the numerical treatment requires special attention with respect to the multi-field formulation and the solution strategy. The session on coupled problems deals with all aspects mentioned above, i.e. ranging from modelling aspects to numerical solution strategies.

Thermo-mechanical modelling of cellular ceramic composites by a multiphase approach of porous media

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Refractory materials have a wide range of applications in steel-making industry as lining of furnaces, oxygen converters or for ladles. Often, magnesia carbon bricks (MgO-C) are used. These consist of a periclase phase (MgO) with inclusions of carbon and gas filled pores. In their applications, refractories are subjected to thermal and mechanical loads causing damage. In recent studies, the thermo-mechanical properties of MgO-C composites could significantly be improved using cellular MgO-C composites based on carbon foams [1, 2]. Modelling of MgO-C composite foams is not only a multi-phase, but also a multi-physics problem, in which the displacement field and the temperature field have to be taken into account. Cellular materials, as foams, are micro heterogeneous materials consisting of three different hierarchical levels reaching from the macro scale, dealing with whole components, over the meso scale, dealing with several pores, up to the micro level, comprising single struts. Hence, in experiments and modelling as well, cellular materials can be described on these different scales. In previous work, a mesoscopic elastic thermo-mechanically coupled model was used to investigate the structure-property relationship of MgO-C hybrid foams, in order to reduce thermally induced stresses and accompanying damage [3, 4, 5].
In the present contribution, based on the optimized micro structures of the meso scale model, a fully coupled phenomenological thermo-mechanical continuum model was developed. The theory of porous media (TPM) with a kinematic coupling of the displacement and temperature fields of all constituents was used. It was assumed, that there is no interdiffusion of the three constituents (MgO, C and pore gas) with the result that the motion functions and hence the deformation gradients of all phases are equal. Linear thermoelasticity with a multiplicative decomposition of the deformation gradient into an elastic and a thermal part for isotropic materials according to the Duhamel-Neumann relation was extended to the mixture of MgO and C phase. The difference in the coefficient of thermal expansion (CTE) leads to different thermal induced stresses in both phases. For the pore gas, the ideal gas law was used as equation of state for the evolution of pressure as function of the density and the temperature. The total macroscopic stress was calculated using the theory of mixture, inclusing the contributions from the pore pressure and the two solid phases.

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Thermo-mechanical computation of inelastic pavement structures under rolling tire loads

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Pavements, as one main part of the world wide infrastructure, are exposed to increasing traffic loads. Especially, in case of asphalt pavement structures, the formation of ruts depends beside the tire loads also on the temperature dependent behavior of asphalt. In order to predict the long term behavior of pavements after a multitude of tire overruns, first the structural behavior of pavement structures at single tire overruns has to be investigated.

Therefore, this contribution presents, a coupled tire-pavement-model based on Finite Element Method (FEM) and an Arbitrary Langrangian Eulerian (ALE) formulation. Within this ALE formulation, the reference configuration is no more fixed in space (like in Lagrangian formulation) but moves with the rigid body motion of the tire through the space. In case of a steady state rolling tire, the deformation, stress and strain state of the tire and the pavement are then time independent with respect to this moved reference frame, what allows for a numerical efficient computation compared to a transient Lagrangian one [1]. Nevertheless, this model implies a material flow through the FE mesh of tire and pavement, so that the material history has to be followed through the mesh in case of inelastic materials. The presented ALE formulation of the pavement includes an unsplit solution technique for the time derivative of internal variables at inelastic material models, e.g. for asphalt, that utilizes the material history of the previous integration point in case of a regular FE mesh [2].

The staggered tire-pavement-iteration is organized by a program interface that is required, since, the pavement model is included in an inhouse FE code while the tire and contact formulation is computed by a commercial FE code. The program interface manages the transfer of the contact forces and the deformed shape of the contact surface between the two FE codes. In order to avoid an oscillating and slow convergence in case of large pavement deformations (e.g. at soft soil materials), a stabilization scheme is included.

For the investigation of the temperature dependent structural pavement behavior, first, the temperature field induced by climatic influences of a pavement cross-section is computed by a transient thermal FE model. Then, the FE ALE simulation of the coupled tire-pavement-model can be conducted at different points in time, by transferring the associated temperature field of the pavement cross-section to the ALE pavement model. Further, an inelastic material model for asphalt [3] is utilized with temperature dependent material parameter functions, that are fitted based on experimental test results. The numerical results show a significant influence of the temperature field on the structural behavior of pavements under rolling tire loads.

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Shock structure for macroscopic multi-temperature model of binary mixtures: comparison with kinetic models

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The present study deals with the shock wave profiles in the macroscopic multi-temperature (MT) model of binary gaseous mixtures. For that purpose we have adopted the hyperbolic model developed within the framework of extended thermodynamics [4]. Recently, we used this model restricted to the simplest case of non-viscous and non-heat-conducting inert gases to compare our results with experimental data in the case of helium and argon mixture [2]. With diffusion as only dissipative mechanism the structure of the source terms is determined using the general principles of extended thermodynamics - invariance of equations with respect to the Galilean transformation and the entropy principle. Diffusivity and relaxation times are taken from kinetic theory for mixture of monatomic gases. Excellent agreement was obtained but with restriction on the shock strength, i.e. Mach number.

In the present study we include viscosity and thermal conductivity to eliminate restriction on parameters. This allows as to compare our results with more sophisticated kinetic solutions which were computed for hypothetic mixtures of gases [1]. Numerical implementation of the MT model is considerably simpler than the one for Boltzmann equations for mixtures or the direct simulation Monte Carlo method (DSMC). Analysis of results is carried out with special regard to the temperature overshoot (TO) of the heavier constituent using a large set of values for parameters. The presence of the extra dissipation (viscosity and thermal conductivity) implicitly introduced atomic diameters of the components in the model, which are not present in inviscid approximation. By varying the parameters it has been found that the temperature overshoot changes non-monotonically with the mass ratio of the constituents, like in the inviscid case in [3]. Also, the dependence of the shock thickness parameter, Mach number and equilibrium concentration on mass ratio is analyzed.

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Efficient Simulation of the Heat Flux Input in Moving Contacts

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One approach for increasing the quality of thermal analyses of machine tools is the additional consideration of their structural movement abilities including the related impacts on the temperature field by frictional heating. Therefore, discretely adjusting the position of the moving parts in transient analyses is a very intuitive but computationally expensive way, especially when aiming for the time convergent respectively continuous solution (see [1]). One strategy to reduce the necessary effort of this approach is the usage of a coarse time step size while countering the consequential defects in result quality with computational low cost methods. Based on formerly published work which dealt with the kinematic depended portion of this loss in quality (see [2]), this time we consider the effect of rarely updating a time depended frictional heat flux (NEUMANN-BC) in the contacts of the analyzed, structural variable systems.

We present a method for applying contact loads which are corrected under the consideration of the actual time discretization. This method uses a maximal error heat flux which is pre-determined under the condition of conserving the supplied energy between the continuous and the discrete solution. To ensure this, it is also necessary to appropriately considerate the simulated motion as well as the operating principle of the later used time integration scheme (in our case: backward EULER). For conclusion, we present the performance of the correction for an exemplary motion, executed with ANSYS. It is stated explicitly, that result defects stemming from a coarse discretization in the spatial domain are not considered.

The presented work is embedded within the research activities conducted by the CRC/Transregio 96.

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Simulation of ice under mechanical and thermal load

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The contact physics of the wheel-rail contact of a railway vehicle under presence of water and ice at low temperatures is still not completely understood. Especially for locomotives in cargo operations with a high traction load per wheel and under extreme winter conditions, a significantly higher wheel wear is observed in praxis. For the development of measures to reduce the re-profiling costs exact knowledge about the local contact conditions and the processes in the wheel-rail contact zone are necessary. To investigate these processes a simulation is needed, which is able to calculate the normal and tangential contact, the temperature field and the fluid-structural interaction between wheel and rail at very low temperatures under presence of snow and ice. The effects on the process zone by the behavior of the ice under the contact conditions are a major issue. The typical pressure conditions within the wheel-rail contact are in the range of 0 MPa up to 1500 MPa. At this loads and in the range between -40 °C and 20 °C, ice can exist in several phases (water (w), ice Ih (1), ice III (3), ice V (5), ice VI(6)). At a vehicle speed of 100km/h the contact time for a material point traveling through the contact zone is approximately 500 μs. Publications [1], [2] show that the ice can make rapid phase transitions under similar shock loads. The density anomaly between ice Ih and the other phases leads to volume changes that may be responsible for an additional load on the wheel materials. A numerical simulation of phase changes in the ice under typical conditions at the wheel-rail contact, is presented in this paper. Based on the theory of Tshijov [1], a dimensionless ice probe is loaded by typical wheel-rail contact pressure curves. In a first approximation the ice sample is assumed as an adiabatic system.

$$E(p,T) = \sum_{i\in\Psi} x_i E_i(p,T), \qquad V(p,T) = \sum_{i\in\Psi} x_i V_i(p,T), \qquad p = p(t)$$

$$\frac{\mathrm{d}E}{\mathrm{d}t} + p\frac{\mathrm{d}V}{\mathrm{d}t} = 0, \qquad \frac{\mathrm{d}x_i}{\mathrm{d}t} = F_i(p,T) \qquad (i = w, 1, 3, 5, 6)$$

The data of thermodynamic properties which are necessary for the calculation, such as the specific volume V_i or the specific internal energy E_i, are determined from the individual equations of phase states. The description of the water phase is based on the specific Helmholtz free energy formulated in IAPWS95 [4]. The ice-phase is described with the aid of the specific Gibbs energy according to [3]. The remaining ice phases are formulated via state equations $V_i(p,T)$ by [1].

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Reduction Approaches for Thermogasdynamic Lubrication Problems

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In many technical applications with rotating devices (gas turbines, turbochargers, etc.), oil thrust bearings are used to support a shaft in axial direction. To describe the pressure and temperature distribution in the fluid film of oil thrust bearings, the geometry of thrust bearing pads is frequently simplified and the finite slider bearing is used to analyze and optimize thrust bearing pads.

Instead of oil thrust bearings, gas thrust bearings are often used in order to reduce costs, weight and maintenance effort. Gas thrust bearings may advantageously be applied in low-load applications, e.g. in air cycle machines, in gas turbines or in rotor systems for fuel cell applications [1].

The pressure and temperature distribution in gas thrust and oil slider bearings is described by the generalized Reynolds equation according to Dowson [2] and the 3D energy equation. The numerical solution of the generalized Reynolds equation in combination with the 3D energy equation yields a system of nonlinear integro-differential equations. Solving this system with a finite element approach is related with a high computational effort. Due to the nonlinearity of the problem, also convergence problems are frequently observed.

In this paper, two different approaches are presented in order to reduce the dimension of the governing integro-differential equations system and in order to stabilize the solution process. The approaches are discussed for the thermohydrodynamic and the thermogasdynamic case.

In the first reduction approach, see [3], the temperature in the fluid is averaged across the fluid film yielding an averaged 2D temperature field. Viscosity and density are calculated with the 2D temperature field using appropriate constitutive equations. Due to the averaging approach, the generalized Reynolds equation can be replaced by the classical Reynolds equation. Both, the classical Reynolds equation and the 3D energy equation are discretized by a finite element approach.

In the second approach, Legendre polynomials of different order are used to approximate temperature, density and fluidity across the fluid film, see [4, 5, 6]. The integrals in the generalized Reynolds equation can be calculated approximately using Lobatto point quadrature, see [4]. For calculating the temperature at the Lobatto points, two different weighted residual methods are applied, namely a point collocation approach, see [5, 6], and a general Galerkin approach. The reduction of the 3D energy equation and the consistent formulation of the boundary conditions is discussed in detail for the point collocation and the Galerkin method.

The different reduction approaches are compared with respect to numerical efficiency, accuracy and convergence behaviour for gas thrust and oil slider bearings.

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A phase-field theory for fracture in porous media

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The investigation of crack phenomena has been an elaborate topic for several decades. From a numerical point of view, discontinuities in structures and the generation of internal boundaries coming along with crack propagation complicate the problem. Since the 1920s, pioneering work has been done by Griffith, Irwin and Barenblatt to depict crack phenomena theoretically. In the last twenty years, a new attempt based on the phase-field theory has been exploited by Bourdin, Ralph Müller and Miehe, whose work proves the feasibility and potential of this method. In 2001, Ingo Müller conceptually extended the phase-field theory to multi-phasic material, such as porous media. However, his work is devoted to a general description of phase-field models and their interpretation in a theoretical mixture approach.

The present contribution proposes a new way to describe crack propagation in porous media. It addresses a biphasic material composed of solid and pore fluid by integrating the phase-field theory into the Theory of Porous Media (TPM). The resulting model is advantageous in terms of providing a detailed description of the evolution of cracks in porous solids and the interaction of cracks with the pore-fluid flow.

The realisation of the transfer starts from assigning the motion function to each material and the formulations of the corresponding balance equations. In order to maintain the thermodynamical consistency, proper constitutive equations and evolution equations are postulated to fulfil the Clausius-Planck inequality for both constituents. Here, a new variable ϕ together with its gradient, originated from the phase-field theory, is introduced into the TPM. ϕ depicts the accumulation of cracks in the micro-structure of the solid constituent and therefore measures the current state of material whether the solid constituent is intact or not. Accordingly, a new form of the momentum production due to interaction as well as the Helmholtz free energy is suggested in this paper. Manifestly, the new form must be dependent not only on the motion of solid and fluid but also ϕ and grad ϕ. Finally, a simulation based on a tensile test is performed, where a dramatic change of the flow velocity in the crack zone is observed.

Isogeometric Analysis of Mechanically Coupled Phase Segregation in Li-Ion Battery Electrode Particles

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In pursuit of Lithium-ion batteries with larger capacity, electrode materials such as Silicon, Tin-Oxide have be introduced. However, those electrodes experience irreversible mechanical degradation even after limited charging/discharging cycles due to phase segregation induced high stresses.

In this contribution a mechanically coupled Cahn-Hilliard phase field model in the framework of finite deformation theory is proposed and implemented with isogeometric nonlinear finite element method. In particular, the mechanical properties are assumed to be hyper-elastic and phase-dependent. In the literature [1, 2, 3] the drifting effect due to hydrostatic stress gradient has been considered. The present model includes also the coupling effect due to phase-dependent mechanical properties. In addition, the influence of the volumeric change due to concentration will be fully considered. The influence of these additional coupling effects on phase segregation behavior such as spinodal points and equilibrium concentrations will be demonstrated. The Isogeometric Analysis is employed for the treatment of high-order problem and the smooth boundary geometry. Firstly, the fourth-order spatial derivative of the concentration is required to account for the diffusive phase interface, and the third-order differential appears in the chemo-mechanical coupling term [4]. The smooth shape functions in IGA allow us to straightforwardly treat the high-order differential equations. Secondly, in spinodal region the whole system is sensitive to infinitesimal composition fluctuation, either due to compositional inhomogeneity or computational error. Approximation failing to give a solution with high precision will lead to incorrect results on phase segregation. Compared to traditional FEM, IGA has its advantages in modeling the curved boundary geometry precisely, e.g. spheres and ellipsoids, even with coarse meshes. Thus the numerical effects of the boundary on phase segregation can be avoided.

This work is supported by the "Excellence Initiative" of the German Federal and State Governments and the Graduate School of Computational Engineering at Technische Universität Darmstadt.

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Eulerian large deformation formulation coupled with phase-field

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The presented work deals with large deformation modelling using the Eulerian frame of reference. The authors present a scheme that combines a fast Fourier small strain solver [1] with an explicit consideration of geometrical effects as translation, rotation and stretch. While the translation is applied by advection of the system variables, the stretch and rotation are considered by recalculating anisotropic and density like variables by operators derived from the displacement gradient.

The benefits of the presented approach are the straight forward implementation due to the use of space fixed coordinates, that eliminates the need of the remeshing procedure typically employed in the Lagrangian FEM frameworks like *Simulia Abaqus* [2] and the possibility of combination with other Eulerian modelling frameworks. The developed model is combined with the phase-field framework *OpenPhase* [3]. In the diffuse interface the problem of the appropriate interpolation procedure of the orientation arises. Therefore, the rotation tensors are transformed to quaternions, that can be linearly interpolated. With that procedure at hands, determination of the effective orientation within the diffuse interface becomes possible. Moreover, the linear interpolation simplifies the advection procedure for the orientation information.

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A continuummechanical, bi-phasic, two-scale model for thermal driven phase transition during solidification

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Numerical simulations of hot working processes has gained significant importance for steel making industries in order to improve manufacturing. Hence, a continuum-mechanical, bi-phasic, two-scale model is developed to predict thermally driven phase transition during solidification processes. The solid and liquid physical states are formulated in the framework of enhanced theory of porous media (TPM) [1], by transition rate terms and thermal coupling [2], respectively. Furthermore, finite plasticity superimposed by secondary creep law has been considered to describe realistic material behavior. A linear viscoelastic material law and Darcy's permeability were chosen for the liquid phase material description. The phase transition is formulated by a two-scale approach considering the phase-field model on the micro-scale [3]. Here, a double-well potential consisting of two local minima at completely solid and liquid physical states is utilized. The finite element method and the finite difference method are employed to solve the macroscopic and the microscopic boundary value problem.

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Formability enhancement in deformed AZ31 magnesium sheets via texture evolution: experiments and phase-field study

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Experimental and phase-field studies are conducted to investigate preferential texture modification in AZ31 Mg sheets. The texture and stress states of materials after initial deformation are studied via electron back scattered diffraction (EBSD) technique before and after annealing. Using the EBSD analysis, a phase-field model is constructed to simulate the texture evolution after initial deformation. Current results suggest that the residual-stresses induced by in-plane compression is the main driving force for recrystallization and grain growth. The inhomogeneous stress distribution conducts preferential growth of $\{2\ \bar{1}\ \bar{1}\ 0\}$ texture, which are at lowest stress state, at the expense of initial basal texture. Limited mobility of twin boundaries changes the mixture of textures but the non-basal textures are still preferred. The formability tests confirm a significant enhancement of the final product compared to as-received sheets.

Isogeometric Analysis of size-dependent behavior of Li-ion battery electrode particles

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Lithium-ion batteries find wide application as power source for mobile devices such as cellphones and tablet PCs. Unfortunately, they suffer from gradual capacity fade over their lifetime. Besides electrochemical effects, mechanical degradation has been identified as one of the sources of this deterioration. The repeated intercalation and extraction of Li ions results in high stress levels in the electrodes, leading to delamination of the electrodes' structure and to fracture of individual particles. However, these particles show a distinct size effect and it has been shown that nanostructured electrodes exhibit a higher resilience against diffusion-induced stresses and mechanical degradation.

We have recently developed a coupled three-dimensional constitutive model for bulk diffusion [1], aiming to gain a better understanding of the mechanical processes taking place in the electrodes. In this model, the diffusion is enhanced by a drift term based on the gradient of the stress field. By virtue of the drift term, the model produces enhanced diffusion rates due to mechanical effects which, in turn, induce a stress relaxation effect and lower stress levels in the electrode material. This term requires basis functions of C^1-continuity and is often neglected in Finite Element-implementations which provide only a C^0-continuous basis. Instead of using a mixed-variational formulation, our Finite Element-implementation is based on the concept of Isogeometric Analysis (IGA) [2] which allows for a straightforward and stable discretization of the weak form.

This talk is concerned with the representation of size effects in our model. We achieve this through two approaches, namely gradient elasticity [3] and surface stresses. In particular the latter have been shown to allow for a faithful representation of nanoscale materials [4]. We describe the mathematical models and their implementation by means of IGA. Using a single electrode particle, we discuss the influence of particle size, charge rates, material parameters, and shape parameters on the stress levels in a single electrode particle.

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Variational Principles and Stability of Diffusion in Hydrogels

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Due to their wide range of applications, a precise knowledge of the mechanical behavior of hydrogels is essential. The most important mechanical property attributed to hydrogels is swelling due to diffusion of fluid molecules into the polymer network. Large deformations caused by swelling can lead to instabilities. This stability issue underlines the importance of a robust numerical treatment of the coupled diffusion-deformation problem.

This work shows that the diffusion-deformation problem can be based upon a *variational principle*, which determines the coupled chemo-mechanical response of hydrogels. The proposed formulation requires only two constitutive functions, the free energy function and a dissipation potential function and thus provides a new, canonically compact modeling framework. For this purpose we start by constructing *rate-type potentials* for the coupled chemo-mechanical evolution problem. These potentials can be exploited in the numerical implementation by construction of time-discrete *incremental potentials*, which fully determine the update equations given by typical time stepping procedures. For the space discretization of the problem finite element method is used. This provides the most fundamental approach to the chemo-mechanical problem under consideration, leading to *symmetric algebraic systems of equations* for iterative update procedures.

A well known issue in the treatment of coupled problems is the numerical stability due to the saddle-point structure of the variational principle, which is connected to the Babuška-Brezzi or LBB condition. We propose a new *minimization principle* for the coupled diffusion-deformation problem by applying a Legendre transformation on the introduced potential. With this pure minimization problem, no requirements have to be fulfilled for the numerical ansatz spaces, leading to a unconditionally stable formulation. Furthermore, when dealing with instabilities, using pure minimization principles is more favorable. We demonstrate the capabilities of our model and its performance by means of representative numerical examples with complex instability issues in two and three dimensions.

Modeling of electrodynamic-mechanical coupling phenomena in smart magnetoelectroelastic materials

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The coupling of electric, magnetic and mechanical phenomena may have various reasons. The famous Maxwell equations of electrodynamics describe the interaction of transient magnetic and electric fields. On the constitutive level of dielectric materials, coupling mechanisms are manyfold comprising piezoelectric, magnetostrictive or magnetoelectric effects. Electromagnetically induced specific forces acting at the boundary and within the domain of a dielectric body are, within a continuum mechanics framework, commonly denoted as Maxwell stresses. In transient electromagnetic fields, the Poynting vector gives another contribution to mechanical stresses.

First, a system of transient partial differential equations is presented, comprehensively describing all coupling phenomena. Introducing scalar and vector potentials for the electromagnetic fields and representing the mechanical strain by displacement fields, seven coupled differential equations govern the boundary value problem, accounting for linear constitutive equations of magnetoelectroelasticity. To reduce the effort of numerical solution, the system of equations is partly decoupled applying generalized forms of Coulomb and Lorenz gauge transformations [1, 2], introducing appropriate scalar gauge functions [3]. A weak formulation is given to establish a basis for a finite element solution. The influence of constitutive magnetoelectric coupling on electromagnetic wave propagation is finally demonstrated with a simple one-dimensional example.

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Modeling of the Crosstalk Phenomenon by the Non-Stationary Maxwell Equations Coupled with the Circuit Equations

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In this work, we propose a new modeling approach in a general framework in order to describe the crosstalk phenomenon in an extended way. We investigate the phenomenon within electro-magnetic systems, and in particular, where electrical elements such as inductors, capacitors, and resistors are tightly located within electrical circuits. Crosstalk in electro-magnetic systems, loosely speaking, refers to the undesirable signal coupling where the electrical elements are communicating with each other. We model the crosstalk phenomenon by bilateral coupling of two sets of differential equations where the main set is the set of non-stationary Maxwell equations, and the second set contain the circuit equations formulated in the framework of modified nodal analysis.

For the purpose of modeling the electro-magnetic phenomena where the dynamical behavior of the electrical circuit is also involved, virtually the non-stationary Maxwell equations cannot fully explain the phenomena. Therefore, as a remedy to model the crosstalk we consider the circuit equations in addition to the Maxwell equations. Considering these two sets of equations as input-output systems, the bilateral coupling approach connects the output of one system to the input of the other system and conversely, via coupling and re-coupling relations. These relations, which are in principle physical constitutive relations, are introduced in our model by suitable operator structures. The coupling of these two sets lead to a set of partial differential-algebraic equations modeling the crosstalk phenomenon. In addition to the modeling, a numerical example is also simulated where the crosstalk is considered only between two inductors within a simple electrical circuit .

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Velocity vector field optimization in bioventing

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Bioventing is a technology used to remove some kinds of pollutants from subsoil and it is based on the capability of some bacteria species to biodegrade contaminants. The biochemical reaction requires, among other things, oxygen and, therefore, oxygen is inflated in the subsoil by wells.

The mathematical model describes the movement of the different fluids which are present in the subsoil – air, water, pollutants, oxygen and so on – and the bacteria population dynamics. The presence of source reactive terms in the continuity equations allows the contaminant biodegradation to be described.

The design of a subsoil decontamination intervention concerns bioavailability problems and, in particular, the oxygen concentration. The optimization of the subsoil oxygen velocity field is, therefore, required in the polluted area in order to enhance the biodegradation phenomenon. The goal is obtained by an appropriate choice of the well positions and of the well air or oxygen inflating rates.

In mathematical terms, the design problem consists of obtaining the decontamination of the subsoil in correspondence of a minimal value of an objective function, such as decontamination time or costs, by acting on some control variables which, in our case, are the well positions and inflating rates. The control variables are subject to some physical limitations: the number of the wells and the total air or oxygen flow rate are limited resources.

The state variables of the system are subject to be a solution of the mathematical model, that is they are solutions of the partial differential equations describing the decontamination phenomenon.

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A consitutive and damage model for high cycle fatigue of tetragonal ferroelectrics

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Ferroelectric materials, such as barium titanate, are widely used in smart structures and devices as actuators, sensors etc. To investigate the material behavior, a condensed model for ferroelectric solids with tetragonal unit cells is presented. The approach is microelectromechanically and physically motivated, considering discrete switching processes on the level of unit cells and quasi-continuous evolution of inelastic fields on the domain wall level. To calculate multiple grain interactions, an averaging technique is applied [1, 2]. Hysteresis loops are simulated for a pure electric and an electromechanical loading to demonstrate the influence of a compression preload on the poling and stress-strain behavior. Further, residual stresses are calculated as a result of switching processes and interaction between crystallits. To study the high cycle fatigue damage and to predict lifetime of ferroelectric devices, an accumulation model is proposed based on the growth of microcracks [2]. Here, the Paris law [3] is applied to calculate fatigue crack growth rates. The lifetime is calculated considering different parameters, e.g. initial micro crack lengths, material parameters, loading cases etc. The simulations agree with experimental findings, where actuation efficiency and structural integrity come out to be opposing properties.

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Phase field simulation on mechanically coupled switching dynamics in nanomagnets

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Miniaturization of the magnetic devices is highly recommended for achieving large areal density up to 1 Tbit/in^2 in magnetic data storage. Recently, based on the bit patterned media (BPM) concept, nanomagnets have show huge prospect in this aspect. For the BPM concept, the nanomagnets-based logic and memory applications require a deterministic 180° switching of the magnetization, i.e. the nanomagnet changes its bit state from 0 to 1, or vice versa. Thus, the strategy for switching the magnetization state in nanomagnets is indispensable. Presently, the magnetic field and spin-polarized current are two available ways. In this contribution, we will propose a mechanical strategy, i.e. controlling the switching dynamics in nanomagnets by the magneto-mechanical coupling. This strategy is demonstrated by a constraint-free and mechanically coupled phase field model which was initially developed for simulating domain evolution in ferromagnetics [1].

Taking single-crystal Cobalt nanomagnet as the model material, we find that due to the magneto-mechanical coupling, the mechanically induced switching dynamics in nanomagnets has two regimes, i.e. coherent switching with homogeneous magnetization distribution and incoherent switching with inhomogeneous magnetization distribution. The transition boundary of these two regimes can be identified in terms of the geometry of the nanomagnets. Coherent switching happens in the small nanomagnets while incoherent switching in the large nanomagnets. In the coherent switching which is very interesting for the BPM concept, only a deterministic 90° can be achieved by a constant mechanical loading. But we show that by using the dynamic nature and overrun behavior of the magnetization, a deterministic 180° switching can happen if the mechanical loading is removed once the magnetization rotates to the achievable largest angle. The dependence of the 180° switching time on the mechanical loading magnitude is furthermore investigated. We also studied the switching dynamics under the combination of magnetic filed and mechanical loading. These results have shed light on the design of an optimum mechanically driven nanomagnets-based logic and memory devices.

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The electrocaloric effect in ferroelectrics: nonlinear modeling and simulation

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Due to their special electromechanical properties, nowadays ferroelectric materials are widely used in many technical applications, mostly as actuators or sensors. Advantages compared to other smart devices are the extremely fast reaction times in a range of μm - ms and large actuation forces. Influences of temperature and heat flux due to electrocaloric and thermomechanical effects are mostly neglected in models, although they may have a non-negligible impact on issues like phase transitions, domain wall motion or reliability and lifetime. In particular, the cooling due to domain reorientation in ferroelectrics is under current investigation mostly by physicists, who observed partly high temperature changes due to electric fields [1].

In this paper, the theoretical background of a micromechanically and physically based constitutive model is presented. In addition to the nonlinear ferroelectric behavior, the model considers the mutual nonlinear coupling of thermal and electromechanical fields. Results are presented in terms of analytical solutions for one-dimensional problems and single domain configurations. First steps of a finite element implementation are also demonstrated by implementing a linear mutual coupling between temperature and electromechanical fields into an ABAQUS user element.

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Nonlinear numerical simulation of ferroelectric-ferromagnetic multifunctional composites

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The coupling of magnetic and electric fields due to the constitutive behavior of a material is commonly denoted as magnetoelectric (ME) effect. The latter is only observed in a few crystal classes exhibiting a very weak coupling, mostly at low temperatures, which can hardly be exploited for technical applications. Much larger coupling coefficients are obtained at room temperature in composite materials with ferroelectric and ferromagnetic constituents. The ME-effect is then induced by the strain of matrix and inclusions converting electrical and magnetic energies based on the piezoelectric and magnetostrictive effects.

In this paper, the theoretical background of nonlinear constitutive multifield behavior as well as the Finite Element (FE) implementation are presented. Nonlinear material models describing the magneto-ferroelectric or electro-ferromagnetic behaviors are presented. Both physically and phenomenologically motivated constitutive models have been developed for the numerical calculation of the nonlinear magnetostrictive and ferroelectric behaviors. On this basis, the polarization in the ferroelectric and magnetization in the ferromagnetic respectively magnetostrictive phases are simulated and the resulting effects analyzed. Numerical simulations focus on the prediction of local domain orientations and residual stress going along with the poling process, thus supplying information on favorable electric-magnetic loading sequences. Goals are to improve the efficiency of ME coupling and to reduce damage associated with the poling process. Further, the developed tools enable the prediction of the electromagnetomechanical properties of smart multiferroic composites and supply useful means for their optimization. The resulting final state of a poling simulation can be implemented as a starting condition for approximate linear simulations and multifield homogenization procedures.

Intrinsic symmetries in constitutive modeling of magneto-elastic materials

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We consider a class of non-dissipative materials whose constitutive equations are derived from a suitably constructed thermodynamic potential function. First, we establish an appropriate Helmholtz energy relation in terms of temperature and magnetization. Then by invoking the Legendre transformation we introduce the Gibbs energy relation as a function of stress, strain, magnetic field, magnetization, and temperature, and by minimization with respect to the chosen subset of independent variables seek the condition for local minimum in strains and magnetization. Derivation is essentially three dimensional based on truncated polynomial energy relations. The chosen form of the free energy function leads to the linear elastic and nonlinear ferromagnetic coupling where non-linearity emerges in terms associated with the strength of magnetization. In principle, the adopted order of non-linearity can accommodate nonlinear behavior of ferromagnet in the region of hysteresis with sufficient level of accuracy in qualitative and quantitative sense.

Correction of Characteristics of Subsystems of Torsionally Vibrating Complex Mechatronic Systems as Introduction to Solution of Their Inverse Task

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The mechatronic system composed from many mechanical subsystems having the same length and variable cross section, loaded by the focused moment was analysed e.g. [1, 2, 3, 4, 5]. The main subject of deliberation was to determine the flexibility of the mechanic system with constant cross section using the exact and approximate methods. Next the method comparison and the correction of approximate methods where made. As far as the mechatronic system flexibility determinations concerned the approximate methods has been chosen. Two cases of attachment the systems were considered. The research of subsystems establishes the foundation to complex systems analysis with cascade structure. Analysing the diagrams of characteristics of confirmed system it has been determined that in case of approximate method the resonance frequencies cover with those which have been determined with exact method. However the values of the characteristic in other areas are different. Therefore there is the mistake of approximate method, which in case of studying the single systems does not have any influence because in resonance areas the characteristic values of the system approach to the infinity. However the difference in values of flexibility within two methods has the great influence on the result of complex systems. That is why it was necessary to correct the results of approximate method.

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Modeling a Halfspace with Tunnel using a Coupled Integral Transform Method - Finite Element Method Approach

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Moving loads in an underground tunnel lead to oscillations inside the soil which can cause annoyances or health problems for humans. Moreover, sensitive machines can be disturbed by these oscillations. Due to urbanization and permanent advancements in machine construction, the effects are still increasing. Therefore, an accurate modeling of the system halfspace with tunnel is required.

In this contribution, a coupled Integral Transform Method (ITM) - Finite Element Method (FEM) approach is presented. The soil as first substructure is described analytically using ITM which is appropriate for the description of the infinite extension of the medium. A solution for a halfspace with cylindrical cavity is derived as a superposition of two fundamental systems. The degrees of freedom on the surface of the cavity inside the halfspace are coupled to the degrees of freedom of a finite element mesh. Thus, the complex geometry of the emission system of the tunnel as second substructure can be modeled using FEM.

The solution of a halfspace with cylindrical cavity is obtained superposing the fundamental systems of a halfspace and a fullspace with cylindrical cavity. Both fundamental systems are solved in a threefold Fourier transformed domain. The Lamé equation as basic equation in elastodynamics consists of three coupled, partial differential equations. First, a decoupling is performed using a Helmholtz approach. Afterward, a transformation from partial into ordinary differential equations is done applying a threefold Fourier transformation [2]. Depending on the coordinate system, different Fourier transformations are carried out. The halfspace which is modeled in Cartesian coordinates, is transformed from time into frequency domain and from the spatial coordinates in the plane of the halfspace x and y into the respective wavenumbers k_x and k_y. The fullspace with cylindrical cavity with its cylindrical coordinates is also transformed into the frequency domain and into the wavenumber domain regarding the longitudinal coordinate of the cavity x. As a third transformation, a Fourier series expansion regarding the circumferential angle is applied. The two fundamental systems are superposed with the boundary conditions on the external surfaces [1]. As both calculations are carried out in dependency on the frequency ω and wavenumber k_x, a quasi-static, two-dimensional calculation is done for each combination of ω and k_x.

The finite element mesh for the modeling of the tunnel geometry is also defined in the wavenumber-frequency domain. Therefore, also quasi-static, two-dimensional computations are carried out. A two-dimensional mesh with four-node elements is modeled with three degrees of freedom at each node. The FEM formulation is adapted to the wavenumber-frequency domain and the stiffness matrix is transformed on the same basis as the cylindrical coupling surface of the ITM.

The two substructures are coupled using the substructure technique and the coupling conditions on the cylindrical surface. Thus, the complete system of halfspace with tunnel can be modeled and the response due to loads on the halfspace surface or inside the finite element mesh can be calculated. The effects of mitigation measures e. g. of a mass-spring system inside the tunnel can be assessed and different installation situations can be compared.

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Fluid-Porous-Media Interaction: A Decoupled Solution Algorithm via Localised Lagrange Multipliers

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The fluid-porous-media interaction (FPMI) refers to a surface interaction among several non-overlapping subsystems, composed of either a bulk fluid or a porous medium. This could be the interaction of blood with a blood vessel wall, a body of water with an earth-dam structure, or acoustic waves with acoustic panels used in soundproofing, etc. These are highly coupled phenomena inheriting different coupling mechanisms which take place within the interacting subdomains as well as across common boundaries. Consequently, the mathematical models of such phenomena also consist of sets of coupled differential equations, which are commonly solved numerically, following a monolithic or a decoupled approach. Here, the focus is on the latter.

The design of an algorithm for the decoupled solution of the fluid-porous-media-interaction problem can be advantageous in several ways. First and foremost, the process of decoupling breaks down the problem into several subproblems, which can be solved efficiently employing specialised fluid and porous-media solvers. Furthermore, solution of several decoupled subproblems instead of one highly coupled problem may be more economical in terms of computational costs. This is especially the case if the scheme permits parallel treatment of the produced subproblems.

Here, motivated by the idea of the method of localised Lagrange multipliers, a partitioned solution algorithm for the problem of surface interaction between an incompressible and inviscid fluid with a saturated biphasic porous medium with intrinsically incompressible and inert constituents is proposed. This method facilitates spatial partitioning of the problem and a parallel solution of the interacting components, and allows for using tailored solvers optimised for each subproblem. Moreover, using the method of perturbed Lagrange multipliers within the subsystems, the pressure fields are eliminated. It reduces in the size of the problem, simplifies the formulation of the interface constraints and also removes the burden of using mixed finite elements. It is known that the decoupled solution of a coupled problem may lead to conditional stability of the produced numerical results. In this regard, considering the 1-dimensional (1-d) version of the equations, a stability analysis of the proposed solution method is performed, and the unconditional stability of the partitioned solution scheme is shown. Solving 1- and 2-d numerical benchmark examples, the applicability of the proposed scheme is demonstrated.

Simulation of vortex-induced oscillations within a shear-thinning liquid

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The present study discusses the influence of a viscous shear-thinning fluid flow on the vibration behavior of an elastic bar which is attached behind a rigid obstacle. The problem geometry is defined on the basis of the well-known FSI benchmark described in [1]. Owing to the asymmetric position of the obstacle within a laminar channel flow, a periodical Kármán vortex street occurs and the continuous eddy shedding stimulates the bar to the observed oscillations. In contrast to [1], in this work the fluid corresponds to a model of the Carreau-Yasuda type (cf. [2]). The model represents an explicit equation to determine the local shear viscosity in dependance of the deformation rate. It is well-suited to reproduce the drawdown of viscosity, for instance, taking place in polymer melts. All parameters of the model are chosen according to a test liquid that has been specified in simulations of vortex streets in [3] with non-Newtonian matter.

In the current investigation above illustrated setting is discretized and calculated in the framework of OpenFOAM®: foam-extend-3.1. In order to accomplish the coupling between the liquid and solid region, a partitioned FSI approach is used with the IQN-ILS algorithm (e.g. [4]) serving as coupling scheme. From the numerical solutions different characteristical quantities, which are suitable to describe the interaction, such as the periodic time and the oscillation amplitude, are determined. In a parameter study the level of shear-thinning and the shape of the obstacle are changed. The solutions show remarkable deviations compared to results obtained with a Newtonian fluid. These differences embody the additional nonlinearity introduced by the material model.

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A numerical approach to the dynamics analysis of mooring lines

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Mooring lines in deep water are exposed to the hydrodynamic forces due to the relative motion between the water and the cables. The response may involve complex phenomena such as vortex induced vibration, unsteady lock-in, dual resonance and travelling waves response [1]. This contribution present a novel numerical approach to capture the non-linear behaviour of mooring lines in deep water. A possible way to capture the complex behaviour of a marine cable is using a fluid structure interaction (FSI) solver coupling together a computational fluid dynamic solver (CFD) with a computational structural dynamic (CSD) solver. This approach, with nowadays computational resources, is feasible only for a limited size of the domain. The present work aims to study the local behaviour of the cable using a small scale FSI model in order to gather computational data that may be used to create a reduced order model suitable to solver the full scale problem. The FSI problem is solved with a partitioned approach coupling together a finite volume method (FVM) solver with a finite element method (FEM) solver through the approach of software components [2]. The importance of several parameters, such as the size of the small scale problem, degrees of freedom taken into account, and the characteristics of the imposed motion in terms of amplitude and frequency, is assessed.

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Critical velocities for flow induced vibrations of a U-shaped belt

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A prism with U-shaped cross-section in cross flow offers interesting features to study, in particular for intermediate aspect ratios: frontal height of the U over its length, $B/H \approx 4 \ldots 5$. In engineering applications, slender structures with U-shaped cross section are sometimes encountered in bridge decks of long-span suspension bridges or conveyor belts for bulk materials. Considered from a scholarly point of view, the U-profile has aspects of the rectangular prism and the H-prism as well. It has an unbroken side (rectangular prism) as well as a cavity (H-prism) but is asymmetric and therefore presents an extension to these extensively researched configurations.

In the present study we investigate the flow around a stationary U-profile and excitation mechanisms for flow induced two-degree of freedom (2DOF) vibrations – vertical motion (heave) and rotation about the long axis of the belt (pitch). We consider the case where the respective eigenfrequencies f_y and f_φ are equal, $f_\mathrm{y}/f_\varphi = 1$. The flow field is studied with the help of unsteady RANS simulations using the commercial CFD solver *ANSYS Fluent*, where the belt is modelled as a two-dimensional U-profile. Wind tunnel results for validation comprise Particle Image Velocimetry (PIV) experiments investigating the flow around a stationary model, free 2DOF vibration tests with a rigid section model, and free vibration tests with a tensioned belt.

The presentation will focus on two excitation mechanisms for flow induced vibrations, occurring at two different dimensionless reduced velocities $U^* = u_\infty/Hf_0$, i.e. the far-field flow velocity u_∞ made dimensionless by the product of frontal height H and eigenfrequency f_0.

The most interesting vibrations occur at low reduced velocities, $U^* \approx 14$ due to vortex formation patterns inherent to the U-profile. Normally, vortex induced vibrations would be expected at even lower reduced velocities, $U^* = 7 \ldots 10$ [1]. Naturally, vortices form in the wake of the U-profile, similar to the von Kármán vortices. Additional vortices can form right behind the windward flange of the U. They were observed in the simulations and were confirmed with good agreement by PIV wind tunnel experiments. These vortices can excite torsional vibrations with a very large amplitude. This was mainly observed by means of simulation, and suggested by free vibration experiments with a tensioned belt.

Flutter vibrations at large reduced velocities ($U^* > 30$) were observed in simulations and confirmed experimentally. They occur at the so-called flutter frequency which – generally – does not coincide with the eigenfrequency of the structure. The excitation is not due to von Kármán or other vortices but rather due to the response of the flow-field to a profile motion at a frequency much lower than the vortex shedding frequency. It can be reasoned that the torsional vibration mode first becomes unstable and gives rise to flutter vibrations. An attempt to determine aeroelastic stability by the so-called aerodynamic derivatives was made. They describe the dependency of the aerodynamic forces on a small profile motion [2] and were obtained by forced profile motion simulations. Good agreement with respect to the predicted critical reduced velocity was achieved.

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Hydroelastic stability of multi-plate structures interacting with flowing fluid

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Plate structures consisting of a single or multiple parallel plates partially or totally immersed into a fluid flow are used extensively in modern engineering applications. High flow velocities and server size and weight restrictions necessitate exclusive safety standards and preliminary estimation of the effect of the hydrodynamic pressure in the case of two-way interaction of the elastic stricture-fluid system. In this case it is equally important to investigate the dynamic response of a thin-walled plates subjected to hydrodynamic loading and to estimate the critical flow velocity, exceeding of which leads to the loss of plane stability. The study of this phenomenon is represented mainly by numerical-analytical works. Most of them are usually restricted by either stability analysis of plates having an infinite extent in one of the directions or by two-dimensional model of the flowing fluid [1–2]. Only in [3] proposed a hybrid finite-element method for the analysis of hydroelastic stability of finite length plates placed in three-dimensional channel with rigid walls, containing incompressible flowing fluid. In practice, the structures are often subjected to 3D loads and have complicated clamping, which lead to the onset of different types of spatial vibrations and instability. In this paper we propose a finite element algorithm for calculating the spatial frequencies and vibration modes and also the boundaries of hydrodynamic stability of a multi-plate structure interacting with compressible fluid.

Equations of fluid motion written in the framework of potential theory, as well as the impermeability condition and corresponding boundary conditions are transformed using the Bubnov–Galerkin method. The deformation of elastic plates is determined either in the framework of the elasticity theory, which is based on the Kirchhoff-Love hypotheses, or with the use of Timoshenko's hypothesis. A mathematical formulation of the dynamic problem for thin-walled structures is developed using the variational principle of virtual displacements, which takes into account the work done by the inertial forces and hydrodynamic pressure exerted on the wetted surfaces of the plates. Numerical solution of the three-dimensional problem is carried out by means of the finite element method. The criterion of stability of the system is based on the analysis of the sign of imaginary part of eigenvalues of a coupled system of equations obtained for different values of flow velocity. The eigenvalue problem of asymmetric matrix is solved with the use of algorithm, which is based on the implicitly restarted Arnoldi method for sparse matrices.

The implementation of numerical experiments allowed us to estimate the influence of linear dimensions, the thickness of the gap between the plates and the type of the flow past the plates on the spectrum of eigenfrequencies and the boundaries of hydrodynamic stability of the structure. The analysis of the structure behavior at various combinations of kinematic boundary conditions imposed on the plate ends has revealed the existence of different instability modes. The effect of the walls rigidity of the three-dimensional channel on critical velocities of instability has been estimated.

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Validation with numerical simulations of a simplified model of a hybrid rocket motor

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The hybrid propulsion offers some remarkable advantages like high safety and high specific impulse and thus it is considered a promising technology for the next generation launchers and space systems. The mechanism characterizing hybrid rockets is the boundary layer combustion. The complex interaction between (turbulent) flow and combustion in hybrid rockets arise some scientific challenges like regression rate modeling, the increase of combustion efficiency and instabilities mitigation by active control. Furthermore, the pressure sensitivity of the combustion process, the coupling between the motor and the oxidizer feed system, the vortex shedding in the aft mixing chamber makes indispensable a study of the mutual coupling between the main flow stream, the fuel gasification and combustion and the thermal conduction into the solid fuel. The purpose of this work is to validate through complex numerical simulations a design tool for hybrid rocket motors (HRM). A simpler model is required for performing overall analysis and parametric studies which are necessary for optimisation and for the development of control techniques for instabilities mitigation. In the present work, we use first a simplified HRM model which is based on the coupling of the hybrid combustion process with the complete unsteady flow. The flow model is based on the one-dimensional Euler equations. The flow equations and the fuel regression rate law are solved in a coupled manner. Each propellant combination has its unique regression rate formula and thus such a model includes some key operational parameters that are known and used by engineers in the design process. The platform of the numerical simulations is an implicit fourth-order Runge-Kutta high order cell-centred finite volume method. The FLUENT commercial code is after then used for the numerical simulation of the mutually interacting three-dimensional flow, combustion and heat conduction processes in a very rigorous manner. In order to take into account the modification of the geometry of the combustion port due to the consumption of the solid fuel, one uses an UDF to implement the effects of the regression rate on the moving boundary. The numerical results allow the comparison of the pressure and temperature in the combustion chamber and of the overall thrust with those obtained with the simpler model. The numerical results obtained with both models show a good agreement between them and with published experimental and numerical results.

Thermodynamically consistent description of mass transfer in a porous medium by a singular surface

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Phase transition processes are important and ubiquitous physical phenomena. These processes are not limited to systems like batch reactors or evaporation from open fluid surfaces, e. g. lakes, but can also appear inside porous solids, such as in CO_2 sequestration, drying of paper during production, or in the food industry. In these processes, mainly first-order transitions between the liquid and the gaseous phases of a certain fluid occur and are characterized by a jump in density and the coexistence of both phases during phase change. Second-order transitions, which do not show this behaviour, are not part of this work. The jump at the interface between the two fluid phases is numerically handled by introducing a singular surface. This allows for a thermodynamically consistent description of the mass transfer during phase transition. The mass transfer is driven by the change in internal energy and couples the two mass balance relations of the two fluid phases.

Obviously, the formulation of a model for a multiphasic porous aggregate in a non-isothermal environment, while accounting for the thermodynamics of the fluids and the phase transition, calls for a potent theory for its description. Here, the Theory of Porous Media (TPM) comes into play, since it provides a well-founded, continuum-mechanical basis to model deformable, fluid-saturated porous media. In this particular case, a three-phasic model is proposed, consisting of the thermoelastic solid phase, which is percolated by the compressible gaseous and liquid fluid phases. The thermodynamical behaviour, i. e. the dependency of the fluid densities on temperature and pressure, is governed by the Redlich-Kwong-Soave equation of state and the Antoine equation for the vaporisation/condensation line. Moreover, the representation of the interface between the fluid phases by a singular surface results in additional terms in the balance relations. The evaluation of these terms leads to a consistent formulation of the mass transfer, which basically compares the energy added to the system with the latent heat of the phase transition (energy needed for the phase change of a certain amount of substance). This mass-transfer term is furthermore dependent on the interfacial area, a factor defined by porosity and saturation. Thus, geometrical and fluid-flow-dependent parameters are included into the phase change process.

Finally, the proposed model for phase transition inside a porous medium is based on the mixture momentum balance, the volume balances of the fluid phases and the energy balance. Consequently, the four primary variables are the solid deformation, the effective pore pressures of the two fluid phases and the temperature. This strongly coupled system of partial differential equations is solved monolithically using the finite element program PANDAS with an implicit time-integration scheme. The numerical simulation of condensation or evaporation of CO_2 in a porous solid rock, which can be either caused by changes in temperature or in pressure, allows for the demonstration of possible application areas for the presented model.

A coupled multiphasic description of biological methane oxidation in landfill cover layers

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Under aerobic conditions methanotrophic bacteria are able to convert methane (CH_4) into carbon dioxide (CO_2) and water. This exothermic reaction leads to a significant reduction of the climate impact. Over a period of 100 years, the global warming potential of methane is 25 times higher than that of carbon dioxide.

Since methanotrophic bacteria are situated within the landfill cover layer and therefore can convert the harmful methane emissions arising from the degradation of organic waste to the less harmful carbon dioxide, the biological oxidation of methane can be considered as a method of passive aftercare for landfills to reduce climate-impact.

The application of methanotrophic treatment is limited by the low forecast ability of the biological processes in the landfill cover. These dynamic processes are influenced by a variety of environmental factors. For a full scale implementation a model with high reliability is needed to simulate the behavior of methanotrophic layers on a landfill site.

To model the coupled processes during methane oxidation, the well-known Theory of Porous Media has been used in order to develop a multiphasic FE-calculation concept, see [1]. The thermodynamic consistent model analyzes the relevant gas productions of methane, carbon dioxide and oxygen. The model also accounts for the driving phenomena of production, diffusion and advection. A multiphasic continuum approach is presented, focusing on the constitutive modelling of the gas phase as well as the energy production. For validation, selected numerical results are compared to experimental results.

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Modeling, Simulation and Parameter Identification for Rate-Dependent Magnetoactive Polymer Response

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Magneto-active polymers (MAP), which are composite materials consisting of a polymeric matrix and embedded magnetizable particles, have recently attracted much attention due to their unique magneto-mechanical coupling properties that enable a contactless, kinematically reversible, and continuous tunability of stiffness and viscoelastic (damping) properties through magnetic field application. Another attractive feature is the possibility to equip this active composite material with tailored anisotropies by positioning particles through proper field application during the curing phase of the matrix material. This unique combination of magneto-(thermo)-mechanical coupling, non-linearity, rate-dependence, hysteresis and anisotropy poses new challenges for constitutive modeling. While there has been significant activity in the area of electro- and magnetoactive polymer modeling throughout the past decade, such efforts, particularly for MAP, have been impeded by the lack of sufficiently detailed and reliable experimental data.

In the present work, the magneto-viscoelastic behavior of MAPs is studied by means of a thermodynamically-consistent constitutive model. A finite deformation based framework of nonlinear magneto-viscoelastic coupling is introduced with a multiplicative decomposition of the deformation gradient. Viscous effects, which are entirely attributed to the properties of the polymeric matrix material, are captured by appropriate evolution equations for the internal state variables. A Gent-type model is adopted to describe the hyperelastic energy storage. Another important contribution is the proposition of an energy function that consistently captures the saturation effects in both the magnetization as well as the magnetostrictive behavior. The modeling efforts were strongly supported by the availability of detailed experimental characterization data provided by a collaborating partner as basis for rigorous, nonlinear optimization-based parameter identification. In addition to the model development at the material point level, a numerical finite element-based code for the analysis of magneto-mechanically coupled finite deformation boundary value problems was developed, into which the newly formulated, calibrated and validated MAP constitutive model has been implemented. This tool can for instance be used to predict the behavior of smart MAP structures under complex loading conditions, and some technologically relevant numerical examples are discussed. It is further demonstrated, that FE-analysis is in fact indispensable to ensure material model calibrations that are independent of the sample geometry, so that the model parameters reflect the true constitutive behavior and not the system response which is typically recorded in experiments due to the so-called demagnetization effect.

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On electrostatic-viscoelastic simulation of dielectric actuators

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Modern robotic systems suffer some severe dynamic limitations. The rigid coupling between electrical drives and joints does not allow for dynamic motions like they occur in nature, where muscles act as an energy buffer and store energy. However, this elastic behaviour plays an important role when considering humanoid systems in terms of safety, energy efficiency and robustness. Stacked dielectric elastomer actuators are composed of a series of elastic capacitors. Each capacitor consists of two conductive layers separated by an insulating material with small Young's modulus and large permittivity [1]. As with capacitors, when an external voltage is applied to the conductive layers, an electric field is established. The electric field leads to polarisation. Attracting bound charges then induce a contraction of the silicone. Due to its similarity with real muscles, dielectric actuators are also knows as artificial muscles.

The functional principle can be described by the Maxwell equations, the balance of momentum and constitutive material laws. It is assumed that the electric field $\mathbf{E}$ can be regarded as quasi-static, no external magnetic fields are applied and no free currents and electric charges are present. The mechanical behaviour is covered by the balance of momentum with the deformation gradient $\mathbf{F}$ and its determinant J. In analogy to the Kelvin-Voigt model where the total force is split into the sum of an elastic and a viscous part, the mechanical stress tensor can be split into the sum of a conservative elastic stress tensor and a time dependent viscous part to allow for viscoelastic material behaviour. Coupled by the electrostatic body force [3], these equations set up the strong form of the electrostatic-viscoelastic simulation model.

The coupled strain energy density of the dielectric actuator is given by

$$\Omega(\mathbf{F},\mathbf{E}) = \underbrace{\frac{\mu}{2}[\mathbf{C}:\mathbf{1}-3]-\mu\ln(J)+\frac{\lambda}{2}[\ln(J)]^2}_{\text{Neo-Hooke}} + \underbrace{c_1\mathbf{E}\cdot\mathbf{E}}_{\text{electric}} + \underbrace{c_2\mathbf{C}:[\mathbf{E}\otimes\mathbf{E}]}_{\text{coupling}} - \underbrace{\frac{1}{2}\varepsilon_0 J\mathbf{C}^{-1}:[\mathbf{E}\otimes\mathbf{E}]}_{\text{free space}}, \tag{1}$$

with the Lamé parameters μ and λ, the Cauchy-Green tensor $\mathbf{C}=\mathbf{F}^T\cdot\mathbf{F}$, the identity matrix $\mathbf{1}$, two electrical parameters c_1 and c_2 and the vacuum permittivity ε_0 [4]. Together with the kinetic energy, the Lagrange function L can be evaluated. The Lagrange d'Alembert principle $\delta S + \int_0^T \delta W^{\text{ext}} dt = 0$, with the action $S=\int_0^T L dt$ for a time interval $[0,T]$ and non-conservative contributions W^{ext} (that include viscous terms) then leads to a variational setting of the coupled problem.

The action integral is approximated using quadrature rules. Hexahedral finite elements with linear shape functions are used for the spatial discretisation and finite differences are used for the temporal discretisation. Then, the Lagrange d'Alembert principle is applied to the discrete set of equations, resulting in a variational integration scheme. Variational integration guarantees that important characteristics of the system are preserved exactly [2].

The implicit integration scheme is implemented as C++ code using the library deal.II. Simulation examples illustrate the use of the coupled model for the simulation of dielectric elastomers. In future work, the artificial muscles will be used to actuate humanoid kinematics. The model is then used for the optimal control of motions that are driven by dielectric actuators.

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Microscopic modeling and finite element simulation of magnetorheological elastomers

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Magnetorheological elastomers (MRE) feature mechanical moduli that become enhanced by an applied external magnetic field as well as the ability to generate magnetically induced deformations and mechanical actuation stresses. Typically, these materials represent a two-component system, in which micron-sized magnetizable particles are embedded in a cross-linked polymer network. The spatial distribution of these particles can be either isotropic or anisotropic depending on whether the particles have been aligned by an applied magnetic field before the cross-linking of the polymer. Since the effective material behavior of MRE is essentially determined by the constitutive properties of the individual components and their geometrical arrangement in the composite, this contribution will apply a homogenization approach [1] for coupled magneto-mechanical problems. Based on a microscopically motivated model for the electrodynamics of continua [2, 3] the balance of momentum is expressed in terms of the total stress tensor which is split into a mechanical and a magnetic part.

The governing equations are solved using the extended finite element method [4] that allows for the use of nonconforming, structured meshes which do not have to be adapted to the particle-matrix interfaces. This is advantageous if complex systems representing stochastic and structured particle distributions are considered. Based on the simulation of the magneto-mechanical interactions in a microscopic representative volume element, the effective coupled material behavior has been predicted using periodic boundary conditions for both the magnetic potential and the displacements. Results obtained from computations are comparable to experiments as well as the analytic findings of Ponte Castañeda et al. [5] and are outlined in more detail in [1, 6].

Moreover, a large deformation framework for the magneto-mechanical boundary value problem is derived and compared to the small deformation model. For the nonmagnetic polymeric matrix of the MRE a compressible neo-Hookean material model is used. Since the enclosed particles exhibit a nonlinear magnetization behavior with saturation at higher values of the magnetic field but negligible hysteresis effects, a phenomenological model is used to describe the magnetic nonlinearity. One crucial task is the formulation of thermodynamically consistent constitutive equations for large deformations [6] which, in the limit case, should coincide with the small deformation model used in [1, 4].

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Harvesting energy with a cone-type dielectric elastomer generator

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The realization of large and medium scale dielectric elastomer generators (DEGs) for harvesting energy from sea waves is one of the current challenges in energy-conversion engineering: a feasible and adaptable suitable device is represented by a generator deforming out-of-plane. This note concerns the numerical analysis of the performance, in terms of gained energy and efficiency, of a cone-type DEG deforming non-homogeneously out-of-plane.

A thin circular membrane of dielectric elastomer is constrained at the boundary by a rigid ring and at the centre by a movable rigid plate, where an external load is applied. The generator undergoes an electromechanical cycle where the external load and the charge are alternately held constant. The membrane is first stretched, then charged and afterwards released, so that the charge is finally harvested at high voltage. In order to avoid loss of the tensile stress state, electric breakdown and electromechanical instability, we control the applied voltage limiting in this way the maximum voltage and keeping the maximum stretch in an admissible range.

The prestretch of the membrane is crucial for an improved behaviour of the device. We evaluate its positive effects on the performance employing an hyperelastic formulation. Moreover, fixing the external radius, we compare the behaviour of two generators characterized by different values of the radius ratio R_e/R_i, namely 2 and 4. Numerical results show that the generator characterized by the smaller ratio has a better performance. Even if the membrane volume is smaller, this configuration allows to leverage the material to obtain a better performance in a wider range of prestretch values.

In the final part, a comparison of the capabilities of the cone-type generator with respect to those associated with other explored configurations and some considerations on viscoelastic effects will be provided.

Modeling of thermo-electro-mechanical coupling effects in ionic electroactive polymers within the Theory of Porous Media

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In this contribution we focus on the numerical simulation of ionic electroactive polymers (EAPs) by using the Theory of Porous Media (TPM). For the description of these EAPs, we investigate the material behavior by considering the thermo-electro-mechanical coupling. The presented model consists of a charged polymer (Solid) saturated by an electrolyte solvent (Fluid). The matrix is plated between two deformable electrodes. In the present talk a thermodynamically consistent model based on the TPM will be discussed in consideration of the electrostatic forces and the osmotic and fluid pressure. Representative simulation of a cantilever beam will be demonstrated. The ability of the model in view of the distribution of the concentration of the mobile cations and the volume fractions of the solvent will be analyzed.

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Deformation and interaction of surface energy driven systems

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This contribution presents a general formulation for mechanical bodies governed by surface energy. Both solid and liquid bodies are considered. The surface energy can characterize both membrane and shell-like surface behavior. It leads to a coupling between the surface and bulk fields. Further coupling is introduced by the interaction between different bodies. As an example, a liquid droplet in contact with a deformable solid substrate is considered [1]. This setup can be easily modified to two liquids or two solids in contact. The surface kinematics, essential to the modeling of surface energy driven systems, are described here in curvilinear coordinates [2]. In particular modeling focus are the contact conditions at the interface between the bodies. It is shown that in the case of quasi-statics and hyperelasticity, the governing equations can be derived from a global potential that accounts for contact as well as the energy storage within the bulk and surface domains. Altogether, 21 coupled Euler-Lagrange equation are derived in this manner. Apart from these strong form equations, the governing weak form as well as its complete linearization, which are required for computational methods, are also discussed. It is further shown that in some cases the governing equations can be further simplified into a reduced set of equations that are then suitable for efficient computational implementations of such systems [3, 4]. The presented formulation is illustrated by several numerical examples.

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Parallel solution of volumetrically coupled multi-field problems using an Abaqus-PANDAS software interface

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The appearance of coupled multi-field problems in nature is manifold and can, thus, be assigned to different engineering disciplines, such as mechanical, civil, environmental and biomechanical engineering. In general, coupled problems can be split into so-called surface- and volume-coupled problems. In surface-coupled problems, adjoining subdomains with different physical properties are linked together via common interfaces, for instance, in fluid-structure-interaction problems. In contrast, in case of volume-coupled problems, distinct domain-coupling interfaces cannot be identified. Instead, the coexisting physical fields exhibit intrinsic interacting properties, for instance, in thermomechanical problems. However, the type of physical coupling may depend on the considered length scale. For instance, the micro-structural surface-coupled problem in porous materials (pore-fluid-solid-skeleton interaction) can be recast into a macroscopically volume-coupled problem by employing a suitable homogenisation technique. The present contribution addresses the simulation of macroscopic volume-coupled problems. The reliability of these simulated processes, apart from computational issues, such as numerical stability, strongly depends on the governing material model, especially, when strongly coupled multi-field problems come into play. Basically, material models are developed or improved either during academic or during industrial research projects and are then implemented into existing software packages. However, it often appears that these packages are either not well suited, or it requires considerable efforts to use them for the solution of complex initial-boundary-value problems (IBVP) in order to prove their capability in practically relevant scenarios.

The present work introduces a general interface between the research code PANDAS, which is a multi-field finite-element solver based on a monolithic solution strategy, and the commercial finite-element package Abaqus. The coupling is based on the user-defined element subroutine (UEL) of Abaqus. This procedure allows, on the one hand, a straight-forward embedding of all material models of PANDAS into Abaqus. On the other hand, it provides, in comparison to the native UEL subroutine of Abaqus, a user-friendly programming environment for user-defined material models with an arbitrary number of degrees of freedom. Furthermore, the coupling exhibits minimal-invasive properties with respect to the IBVP definition process in Abaqus and allows for the parallel analysis of large-scale problems on high-performance computing clusters.

The Abaqus-PANDAS linkage can be applied to various coupled multi-field problems, such as partially or fully saturated soils, vacuum-assisted resin injections (VARI) of dry fibre fabrics, or chemically or electrochemically driven swelling phenomena as they appear, for example, within hydrogels. Additionally, discontinuities, such as cracks, can be described for instance via phase-field models or by the extended finite-element method (XFEM).

Application and modification of the POD Method and the POD-DEIM for model reduction in porous-media simulations

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Researchers with a continuum-mechanical background typically use a multi-phasic and multi-component modelling approach for materials with a saturated porous microstructure. Therefore, the mechanical behaviour of porous media is considered in a continuum-mechanical manner and solved using the Finite-Element (FE) Method. The constitutive models for the subsequent FE simulations are based on the well-founded Theory of Porous Media (TPM), leading to macroscopic models of superimposed and interacting constituents.

The developed models need to be, on the one hand, as simple as possible and, on the other hand, complex enough to capture the relevant properties of the investigated materials. In most cases, this requirement results in simulations with a very large number of degrees of freedom (DOF) which are associated with long computing times. The aim of the present contribution is to reduce the computing time and the numerical effort of these simulations through model-reduction methods, while the accuracy of the solution needs to be maintained. Therefore, the method of Proper-Orthogonal Decomposition (POD) for linear problems and the Discrete-Empirical-Interpolation Method (DEIM) in combination with the POD Method (POD-DEIM) for non-linear problems are investigated as model-reduction techniques for FE simulations of porous media.

Using the POD Method, a given data set is approximated with a low-dimensional subspace which ensures a high flexibility in application. To generate this data set, the vector of unknowns of the FE simulation, which contains the values of the primary variables at each node of the FE grid, is stored in a pre-computation in the full (unreduced) system in each time-step. The generated vectors are the so-called "snapshots" of the system.

Dealing with porous-media problems, the primary variables are the solid displacement, the pore pressure and, depending on the particular problem, other primary variables such as the solid velocity and the seepage velocity for dynamic problems or the molar concentration of a therapeutic agent in biomechanical applications. Following this, the primary variables have entries with very huge differences in their absolute values. As a result, rounding errors may occur when applying the POD Method, which are not negligible. To overcome this problems, modifications of the classical POD Method and the POD-DEIM need to be performed for such problems. The present contribution discusses this issue and presents results for the reduced simulations of porous media with different material behaviour.

NURBS-based Approaches in Fluid Flow Simulations

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Fluid flow applications can involve a number of coupled problems. One is the simulation of free-surface flows, which require the solution of a free-boundary problem. Within this problem, the governing equations of fluid flow are coupled with a domain deformation approach. These domain deformation approaches can either fall into the category of interface capturing, such as level-set or volume-of-fluid methods, or interface tracking, where, at least in portions of the mesh, a Lagrangian view point is adopted and the mesh nodes are displaced with the fluid flow. Our solution approach is based on the Deforming-Spatial Domain/Stabilized Space-Time (DSD/SST) finite element method in combination with a boundary conforming interface tracking scheme. In DSD/SST, the variational form is written over the complete space-time domain, thus easily incorporating deforming domains into the formulation. The stabilization is performed using a Galerkin/Least-Squares technique. In order to enhance the aspect of boundary conformation, the scheme employs Non-Uniform Rational B-Splines (NURBS) as a support of the standard finite element representation of geometry and flow solution. As the basis of CAD systems, NURBS are closely connected to any engineering application, particularly since the concept of Isogeometric Analysis (IGA) [1] has introduced NURBS to the numerical analysis. However, the generation of complex three-dimensional grids suited for IGA is still a challenge, restricting its use in the area of fluid mechanics. Nevertheless, methods for fluid simulation can profit immensely from the use of NURBS as a boundary description. Several approaches (here, all connected to FEM) are possible:

1. Certain information needed for the computation (e.g., curvature or normals) is computed from a NURBS representing the boundary [2].
2. The computational domain is represented exactly using NURBS, but the solution is still interpolated using polynomials. This idea is, for example, realized in the NURBS-enhanced finite element method [3].
3. The NURBS represent the geometry and in addition represent the solution at the boundaries.

Such approaches can have a variety of advantages, stemming from both the exact boundary description and the superior approximation properties of NURBS. They involve the computational accuracy reached with a specific computational cost as well as the efficiency and accuracy of coupling schemes. The advantages of the discussed approaches are demonstrated on two numerical examples of fluid flow, namely two-phase flow with drops and sloshing tanks. The case of drops requires an accurate geometry description particularly to evaluate surface tension effects, which rely on the curvature of the boundary. The curvature, and therefore second derivatives of the geometry representation, are often hard to obtain from standard finite element meshes. This information is however provided by NURBS. In the sloshing tank case, we concentrate on representing tank walls of arbitrary shape in an interface tracking context.

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Numerical Approaches towards Plasticity

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Integrated thermomechanical forming processes are developed to optimize mass products' properties application oriented. As an example for this kind of procedures the fabrication of a metal flange shaft can be considered. At first the workpiece is heated inductively creating a heterogeneous temperature field, forged thermomechanically due to the contact with the forming die and in the last step a local cooling using a high pressured air stream is carried out, cf. [1]. One of the main topics characterizing this integrated manufacturing process is the second part where finite thermoviscoplastic deformations take place. Thus, adequate material models as well as proper numerical schemes have to be established.
The first step towards creating and analyzing numerical schemes for finite thermoviscoplasticy, is to generate a series of model problems considering different aspects. As a starting point for numerical investigation a classical small strain plasticity model of the VON MISES typeand its numerical implementation is examined, cf. [2]. Therein distinct time discretization schemes, like RUNGE-KUTTA and GALERKIN, are applied to solve the evolution equations on the GAUSS point level as well as the balance of linear momentum on the element level, cf. [3, 4, 5].
In contrast a consistent variational approach is presented. Therein a dissipation potential is assumed and the principle of JOURDAIN is exploited to generate a multifield formulation of plasticity enabling the usage of one single time discretization scheme on the element level, cf. [6, 7, 8]. An active set strategy is developed to judge whether elastic or plastic phenomena prevail at distinct element nodes.
Hence, a comparison between the conventional and the variational procedure taking into account the different time discretization schemes will be presented.

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