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From Experiments to Predicting the Component Behavior in Solid Mechanics[†]

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Abstract

Modern computer programs for the calculation of the deformation behavior of components under external loads require physical models. These so-called material models are either available for specific materials, or they have to be developed for this purpose. The parameters occurring in the mathematical equations must then be adapted to special measurements. Then, it is possible to implement these material models in computer programs in order to predict complex structures or components. This overall process requires knowledge of executing experiments, of concept formation for developing models, of the numerical implementation of mostly coupled partial differential equations, as well as of identifying the material parameters occurring in the models. In addition, concepts for verification and validation of the calculations must be taken into account and further developed. The entire procedure is relevant in many other scientific fields. Here, we concentrate on problems of the mechanics of solid bodies.

1 Introduction

One thing natural scientists, life scientists, and engineers have in common is that they have to predict the behavior of buildings, ground (soils), machines, or generally of the behavior of technical, biological, pharmaceutical systems, and structures. To this regard, mathematical models are used that reflect the behavior of experimental observations and are used for predictions. This requires a broad range of knowledge and experience in the areas of conducting experiments, mathematical modelling, numerical calculation and further development of numerical calculation methods as well as calibrating the models to measurement data. In addition, statements should also be made about the accuracy, not only regarding the precision of the numerical calculation of the occurring equations (verification), but the prediction quality (validation) as well. The difficulty associated with this is that each subject area in itself requires special challenges, knowledge or experience and individual possibilities in the form of cooperation partners from different disciplines in their environment. In this article, we therefore limit ourselves to questions of solid mechanics, i.e. the description of the motion or deformation of material (solid) bodies due to external influences.[1] This shows that materials technology, materials science and production engineering are coupled with mechanics via the experiment. To some extent, there is also a change into microstructural modelling, due to the possibility of including information from the atomic and molecular scale. On the other hand, applied mathematicians find a playground in mathematical modelling and numerics (simulation of boundary value problems as well as the development of non-linear optimization methods in parameter identification). Therefore, solid mechanics, due to its interdisciplinarity, occupies a special position as a possible cooperation partner, especially in larger research cooperations. Fig. 1 illustrates the four pillars of solid mechanics, which are completed by complex component simulations with predefined computer programs. All questions should then be embedded in the research field of verification and validation, see, for the terminology, (Babuska and Oden, 2004). In the following, the topics experiment, modelling, numerics, and material parameter identification as well as verification and validation in mechanics are addressed in more detail.[2]

[†]This is a translation of the original article "Vom Experiment zur Vorhersage des Bauteilverhaltens in der Festkörpermechanik" published in "Jahrbuch 2018" of the Braunschweigische Wissenschaftliche Gesellschaft, Cramer Verlag, Braunschweig, 73 – 94, 2019.

[1]The transition from solid to liquid state is seamless. The distinction in mathematical modelling is discussed in (Truesdell and Noll, 1965, Sect. 32-33) and (Haupt, 2002, Sect. 7.3.2).

[2]Only an extract of existing literature is given. The contribution therefore represents a small personal point of view.

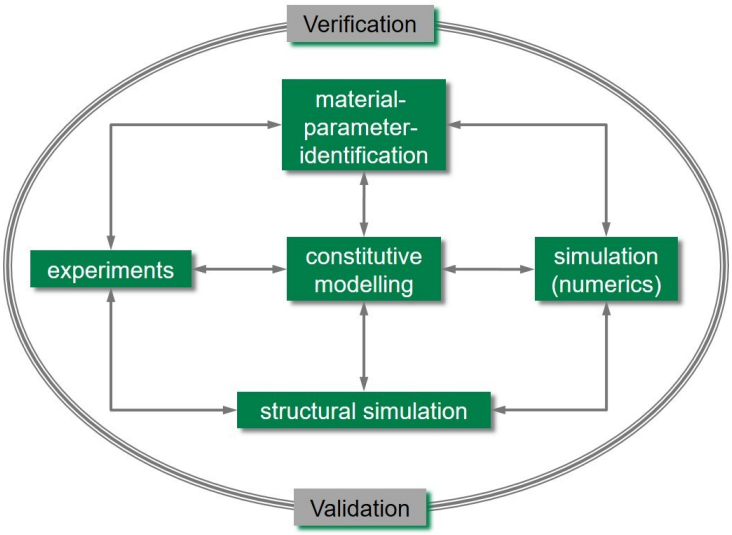


Figure 1: Tasks in solid mechanics

2 Experiments

Experimental solid mechanics, after originally flourishing in the post-war period, was increasingly scaled back by the increase of computational mechanics at German universities since the 1980s. It has mainly dealt with the investigation of material behavior under tensile, compressive, shear, bending, internal pressure, biaxial, and torsion loads. This was initially driven primarily by the incipient power plant construction with the associated safety-related aspects and later by forming technology, which was mainly concerned with the challenges of the automotive industry. This meant that metallic materials were of particular interest. In recent years, however, this has changed in the direction of many other materials (polymers, ceramics, concretes, wood, ...). In addition, due to increasing progress in the field of electronics, the experimental sample contacting measuring systems have been further developed and ever higher accuracies have been achieved. Due to the higher maintenance costs of laboratories in Germany with their experimental equipment and the associated personnel expenditure - in comparison to purely theoretical work or the development of computer programs - this branch of mechanics has been reduced more and more and has been taken over by application-oriented material technology disciplines. Since the 1960s, the German research society in mechanics has developed in the direction of computational mechanics – largely due to the increasing importance of a certain computational method, namely the *finite element method*, which is now to be seen as the tool of choice to simulate the behavior of complex component geometries in the industry. For a few years now, however, laboratories of several universities have been rebuilt. On the one hand, as it has been shown, the experimental implementation with different process controls for the mathematical modelling of the occurring physical problems can only be carried out in own laboratories. On the other hand, it has become clear that the development of many material models – in the following also called *constitutive models* – and the calculation of complex components and structures, without own experimental findings or their experimental underpinning, only allow for a very limited gain of knowledge (and partly also appear questionable). In addition, optical, i.e. non-contact measuring methods are available today, allowing to monitor the temperature and deformation behavior on a part of the sample surfaces during the tests. In addition, due to considerably improved microscopic possibilities (μ-CT images, FIB, SEM, ...), the physical causes of the deformation can also be better interpreted. This opens up completely new possibilities to analyze test results of component behavior, which has made mechanics a very heterogeneous field of research in recent years. On the one hand, this is due to the modelling of multiphysical causes (chemical, electrical, magnetic and thermal effects on the deformation behavior) and, on the other hand, the integration of micromechanical processes for the interpretation of the macroscopic component behavior. This results in multiple scales in space and time, which pose great challenges for both the experimental treatment and the model development. In addition to the pure development of measurement technology, there are three major objectives in experimental mechanics:

1. Initially, the focus will be on conducting experiments to present physical observations.

2. After the development of constitutive models to describe these effects, the material parameters occurring in the models shall be adapted, which is referred to as *material parameter identification* or *calibration*.

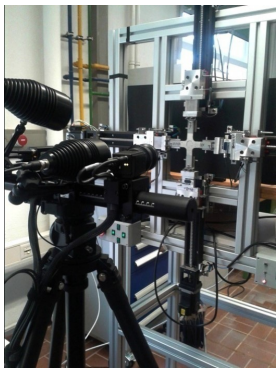
3. To validate the models, independent experiments with other process controls or other (more complex) sample geometries must then be carried out.

In solid mechanics, these purposes are connected to an interest in temporal loading processes, i.e. how the deformations within a material body occur under an external loading process, or vice versa, what the stress response looks like due to a given deformation process. This is usually not the case in materials or production engineering, where key measures are used to characterize material properties.

2.1 Mechanical testing equipment

In mechanics, as explained above, experiments mostly focus on a displacement- or angle-controlled or a force- or moment-controlled temporal processes. If there is optical access to the specimen or if so-called *strain gauges* or *strain transducers* are applied to the specimen, "local quantities" can also be used to measure or control the specimen holder movement of a testing machine. A distinction must therefore be made between test equipment and measurement options. The examination of materials is carried out using uniaxial tensile and compression testing machines, biaxial or triaxial testing devices,[3] shear, torsion, bending and indentation tests or many other more complex examination options. Fig. 2 shows various classical test facilities, while Fig. 3 shows associated

(a) Tension, compression, torsion testing device



(b) Biaxial testing machine

(c) Shear tool

Figure 2: Examples of experimental testing

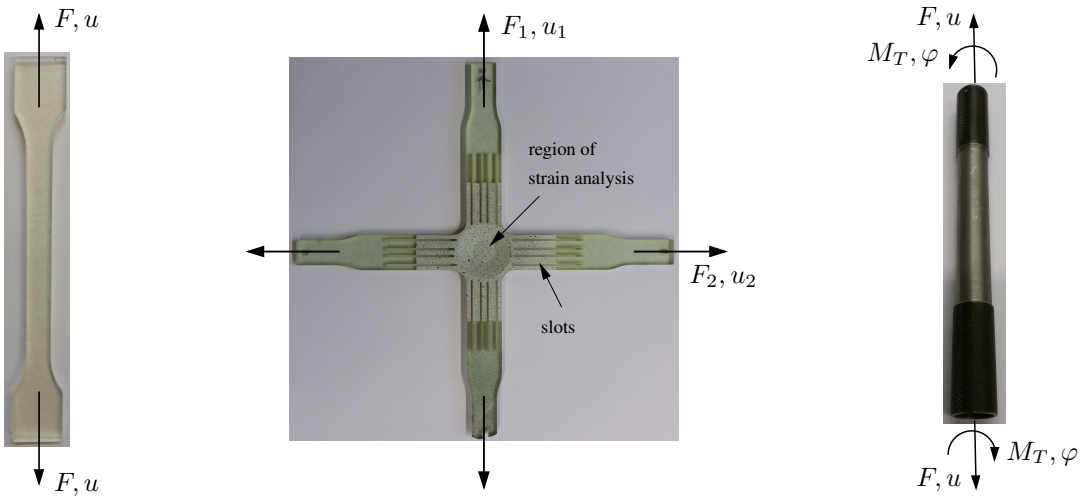
tensile, biaxial and torsional specimens.

2.2 Measurement Technique of Deformation

The aforementioned experiments must be completed with the measurement of physical quantities, in which strains on the surface are of interest. They represent a quantity averaged over a certain range which can be measured by means of strain gauges (adhesive bonding of small electrical components which show a change in electrical resistance in the event of deformation, see Fig. 4(a)), strain transducers (measurement of the change in distance between two contact points on the specimen surface, Fig. 4(b)), or also the total change in length, measured with the movement of the specimen holder in the testing machine. Nowadays, optical methods can also be used if optical access to the sample is available.

Either a few or very many markers (dot patterns) are applied to the sample in order to determine the surface strains from the movement of the dots using image correlation methods, see (Sutton et al., 2009). This is not only a scalar information, but a spatial distribution of the strains and displacements in the sample surface, see Fig. 4(c). For further optical methods see also (Hild and Roux, 2013). If there is no optical access, as for example in forming processes, one can only look at the distance changes of the points (usually by etching the markers on the surface

[3] In addition to the possibility of a pipe under internal pressure and superimposed tensile and torsional loading, there are also complete triaxial loading devices, see (Calloch and Marquis, 1999).

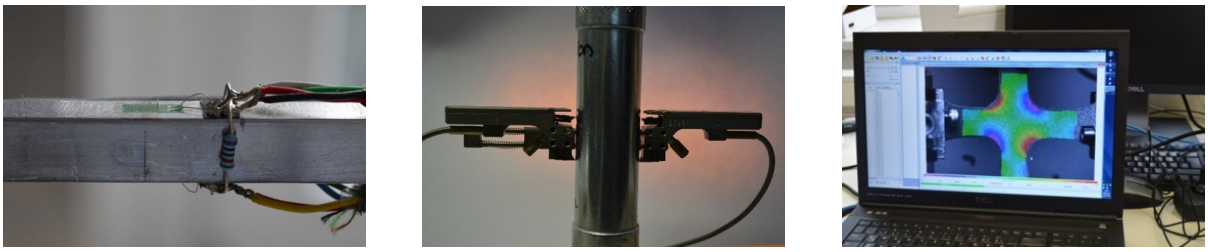


(a) Flat samples for tension

(b) Biaxial sample with slots for lateral strain minimization and point pattern for optical strain analysis

(c) Cylindrical torsion and tension sample

Figure 3: Sample shapes (either prescription of force $F(t)$ and measurement of elongation $u(t)$ or control of $u(t)$ and measurement of $F(t)$; in analogy, for $F_1(t)/F_2(t)$ and $u_1(t)/u_2(t)$ as well as torque $M_T(t)$ and torsional angle $\varphi(t)$)



(a) Strain gauges for local strain measurement

(b) Strain transducers for an integral measurement of the strains

(c) Digital image correlation for strain measurement on the surface, see Fig. 2(b) of the camera system

Figure 4: Examples of testing capabilities

of the sample) before and after the experiment – meaning that no strain information is obtained in situ. Thus, in most cases, only the integral values of the testing machine, such as force and displacement as a function of time t, are known.

2.3 Process Control

In experiments, there is an infinite number of process control options (cyclic processes, creep and relaxation paths, rate dependence, fracture tests, ...). In (Haupt, 1993) and (Haupt, 2002) a classification of experimental observations in isothermal experiments into four categories has therefore been proposed, in order to classify, on the one hand, a clear linguistic separation of observation (rate independence, equilibrium curve or hysteresis), and, on the other hand, the constitutive models based on these observations (elasticity, plasticity, viscoelasticity, viscoplasticity). There are basic experiments to determine in which category the material (and later the constitutive model) belongs. First, the rate dependence of the material is investigated at different strain rates. It must be remarked that it is not sufficient to choose a process control that is twice as fast, since most materials react insensitively to this. Rather, four experiments with different strain rates are considered for each change in the power of ten. In addition, unloading and reloading are carried out as well. Here, it can be seen whether the material exhibits rate-dependent or rate-independent material behavior with or without equilibrium hysteresis. For the latter a theoretically infinitely slow process would have to take place. This is not practicable and it can be replaced by a multi-stage relaxation experiment, see (Haupt and Sedlan, 2001; Hartmann, 2006; Sguazzo and Hartmann, 2018;

Martinez Page and Hartmann, 2018) for details regarding a practical application. The load is gradually increased and the strain is kept constant over a holding time. This holding time depends on the respective material. Usually the stresses decrease and the stress rates tend towards zero. Unfortunately, this can take a very long time, so that frequently estimates (extrapolations) of the behavior are assumed here. In addition to these experiments, cyclic processes (up to fatigue) or processes up to fracture of the material – depending on the interest or objective – can also be characterized more precisely. A major drawback of mostly uniaxial process control systems is that the constitutive models based on such systems can only poorly reflect the multi-axial loading processes. Therefore, there is the tendency to consider triaxiality of material properties, both experimentally and by modelling. For this purpose, combined tensile-pressure-torsion tests are available, see for example (Haupt and Lion, 1995; Haupt and Sedlan, 2001), or tubes under axial, torsional, and internal pressure load. In the case of soils, triaxial cells are used which rather represent a two-dimensional load of axisymmetrical samples under external pressure and axial load (Wood, 1990).

3 Constitutive Modeling

The description of material bodies is subjected to natural laws. These have been developed in the form of balance equations of thermomechanics. In connection with the formal separation of a body from its environment, a balancing must take place – including the *mass*, *momentum*, *rotational momentum*, *energy* and *entropy balances*. If electrical and magnetic influences are taken into account, further balance equations are available, see (Eringen and Maugin, 1990). In addition to these balance equations, constitutive models exist which relate deformation and temperature to forces (stresses) and heat flow. Within the field of thermomechanics of solid bodies, two partial differential equations result, allowing to determine the displacements (local balance of linear momentum, here only for the case of quasistatic processes, so that wave propagation phenomena do not occur) and the temperature (local heat equation),

$$\begin{aligned} \operatorname{div} \mathbf{T} + \rho \vec{k} &= \vec{0} \\ c_\Theta(\vec{u}, \Theta, \mathbf{q}) \dot{\Theta} &= -\kappa_\Theta(\vec{u}, \Theta, \mathbf{q}) \operatorname{grad} \Theta + r(\vec{u}, \dot{\vec{u}}, \Theta, \mathbf{q}). \end{aligned} \tag{1}$$

c_Θ and κ_Θ describe the heat capacity and heat conductivity, r a heat source (sink), and $\vec{k}$ the acceleration due to gravity. Mass and angular momentum balance each provide two trivially satisfiable relationships (the density ρ in the current configuration of the material body is coupled via the deformation gradient with the density in the initial configuration ρ_R, $\rho_\mathrm{R} = \rho \det \mathbf{F}$, and the symmetry of the stress tensor, $\mathbf{T} = \mathbf{T}^\mathrm{T}$). The entropy balance, on the other hand, motivates an inequality, namely that entropy production cannot become negative. This is usually formulated with the help of the Clausius-Duhem inequality, which in turn has a direct influence on the constitutive models still to be formulated. For many decades it has been the task of solid mechanics to develop constitutive models. These were initially developed by engineers and contradicted some basic physical assumptions. Those basic assumptions were finally formulated and ordered in (Truesdell and Noll, 1965), representing various axioms such as *causality*, *determinism*, *equipresence*, *observer invariance*, *objectivity*, and *material objectivity*, see also (Eringen, 1980; Krawietz, 1986) and (Haupt, 2002). Furthermore, symmetry properties for the model development of anisotropic materials have to be considered. Constitutive models describe the stress state $\mathbf{T}$ (Cauchy stress tensor) at the material point $\vec{X}$ in the reference configuration at time t as a function of the past deformation and temperature history

$$\mathbf{T}(\vec{X}, t) = \underset{\tau \le t}{\mathcal{F}} \big[\mathbf{F}(\vec{X}, \tau), \Theta(\vec{X}, \tau), \vec{X} \big], \tag{2}$$

where $\mathcal{F}$ is a functional (which can be formulated by ordinary differential or integral equations), $\mathbf{F} = \operatorname{Grad} \vec{\chi}_\mathrm{R}(\vec{X}, t)$ defines the deformation gradient and Θ reflects the absolute temperature. $\vec{x} = \vec{\chi}_\mathrm{R}(\vec{X}, t)$ is the motion of the material point $\vec{X}$, which is at position $\vec{x}$ at time t. Since it is difficult to analytically or numerically solve integral equations, ordinary differential equations have prevailed in order to describe history dependence of the material behavior. This led to the *theory of internal variables*, variables that can be motivated physically but not identified experimentally, see (Coleman and Gurtin, 1967). The evolution equations of the internal variables serve to describe the non-linear, history-dependent hardening behavior and condition the art of the modeler to develop suitable models, which must satisfy in particular the second law of thermodynamics (entropy equation) as well as the above-mentioned axioms. For this purpose a multitude of constitutive models have been developed, which have

the following mathematical structure,

$$\begin{aligned} \tilde{\mathbf{T}} &= \tilde{\mathbf{h}}(\mathbf{C}, \Theta, \mathbf{q}) \\ \mathbf{A}\dot{\mathbf{q}}(t) &= \mathbf{r}(\mathbf{C}, \Theta, \mathbf{q}) \end{aligned} \tag{3}$$

or with small strains

$$\begin{aligned} \mathbf{T} &= \mathbf{h}(\mathbf{E}, \Theta, \mathbf{q}) \\ \mathbf{A}\dot{\mathbf{q}}(t) &= \mathbf{r}(\mathbf{E}, \Theta, \mathbf{q}), \end{aligned} \tag{4}$$

see also (Lemaitre and Chaboche, 1990). $\mathbf{C} = \mathbf{F}^{\mathrm{T}}\mathbf{F}$ is the right Cauchy-Green Tensor and $\tilde{\mathbf{T}} = (\det \mathbf{F})\mathbf{F}^{-1}\mathbf{T}\mathbf{F}^{-T}$ the 2nd Piola-Kirchhoff stress tensor. $\mathbf{E}(\vec{x}, t) = (\operatorname{grad} \vec{u}(\vec{x}, t) + \operatorname{grad} \vec{u}(\vec{x}, t)//2$ defines the linearized Green strain tensor, and $\mathbf{q}^T = \{q_1, q_2, \dots q_{n_q}\}$ represents the vector of the internal variables (which can be scalar- or tensor-valued; only the components are assembled here). Since algebraic constraints can also occur, for example in models of rate-independent plasticity with yield function, $\mathbf{A}$ can represent a singular matrix. The stress state depends on the strain state $\mathbf{E}$, which in turn is determined by the three displacement components $\vec{u}$. Moreover, the dependence on the temperature is Θ. On the other hand, there are four partial differential equations for the momentum and the temperature. The internal variables, however, are commonly not determined by partial but only by ordinary differential equations.

Before addressing the computation of $\vec{u}$, Θ, and $\mathbf{q}$, further remarks regarding further modeling concepts have to be made. In addition to this approach, which is regarded as classical modelling, there are other modelling approaches. For example, the internal variables can also be formulated as partial differential equations to describe, for instance, the damage behavior in materials, see e.g. (Nedjar, 2016). These so-called *non-local models* are also used to consider size effects of sample materials, the so-called gradient plasticity, see (Bertram, 2017; Grammenoudis and Tsakmakis, 2005). Also micromechanical (and also in the scales below) models are solved numerically to include more physical effects in the modelling (molecular dynamics, homogenization methods, FE^2, FFT, ...), see also (Geers et al., 2010; Müller et al., 2015). The big challenge here is the numerical implementation or the numerical effort to reproduce real component simulations.

4 Numerical Simulation

Originally, the numerical simulation of the initial boundary value problem (1) in connection with constitutive models of type (3) or (4) – caused by the historical code development of the finite element method – was experience driven. Thus, the partial differential equation $(1)_1$ was converted into the weak formulation required for the finite element method, into the principle of virtual displacements, and former finite element programs for linear problems were changed to non-linear problems. This was done first for an incremental formulation of the balance of linear momentum $(1)_1$ and only later on into the currently most common form of the principle of virtual displacement. Intuitively correct the load was incrementally applied – which corresponds to the time integration – and the resulting system of non-linear equations was iterated until it converged against a solution under integration of the constitutive models (4), see (Zienkiewicz, 1984)[4]. The main difficulty was the integration of constitutive models of evolutionary-type. With the fundamental article on the treatment of such material models (initially a model of elastoplasticity), Simo and Taylor (1985) coined the term *consistent* linearization for this issue. Here they intuitively applied the implicit-function theorem correctly when evaluating their equations in order to obtain a method that converges quadratically at any point in time. Due to numerical investigations of the iterates, however, they had unfortunately interpreted the overall procedure as a Newton-Raphson procedure. Many researchers continue to follow this not always correct terminology. A more detailed explanatory memorandum must be added to this effect. A reference to the aforementioned question of numerical solid mechanics to mathematical methods for the solution of partial differential equations was made in the dissertation of (Wittekindt, 1991), where the aspect was addressed by applying the vertical line method. There, the space discretization is carried out first – in this case the finite element method – followed by applying a time discretization method to the equations arising from the space discretization, see Fig. 5. This leads after the space discretization of the Eqns. (1) and (4) to a system of differential-algebraic equations (DAE-system)

$$\begin{aligned} \boldsymbol{g}(t, \boldsymbol{u}, \boldsymbol{q}) &= \boldsymbol{0}, \\ \boldsymbol{A}\dot{\boldsymbol{q}}(t) &= \boldsymbol{r}_{\mathrm{q}}(t, \boldsymbol{u}, \boldsymbol{q}), \end{aligned} \tag{5}$$

[4]German translation of the third edition of the English edition of 1977.

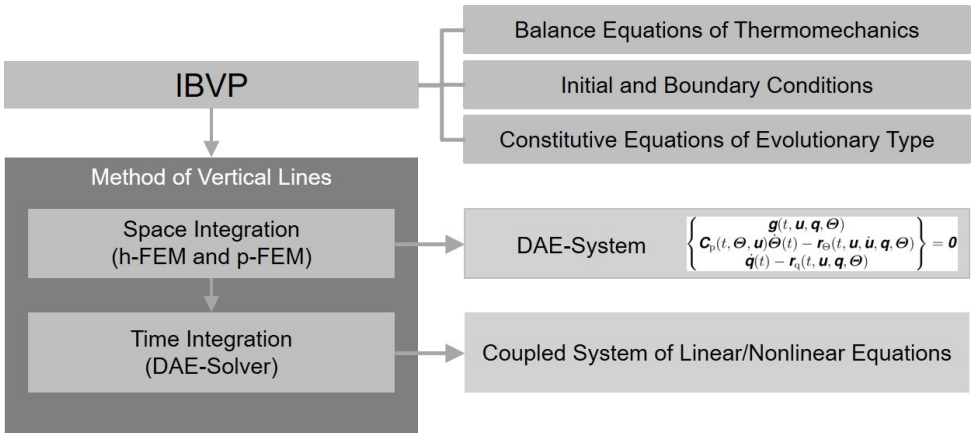


Figure 5: Vertical line method for solving thermomechanical problems using evolutionary equation type constitutive models

for isothermal problems or for thermomechanically coupled problems to

$$\begin{aligned} \boldsymbol{g}(t, \boldsymbol{u}, \boldsymbol{\Theta}, \boldsymbol{q}) &= \boldsymbol{0}, \\ \boldsymbol{C}_{\Theta}\dot{\boldsymbol{\Theta}}(t) &= \boldsymbol{r}_{\Theta}(t, \boldsymbol{u}, \dot{\boldsymbol{u}}, \boldsymbol{\Theta}, \boldsymbol{q}), \\ \boldsymbol{A}\dot{\boldsymbol{q}}(t) &= \boldsymbol{r}_{\mathrm{q}}(t, \boldsymbol{u}, \boldsymbol{\Theta}, \boldsymbol{q}), \end{aligned} \tag{6}$$

$\boldsymbol{g} \in \mathbb{R}^{n_{\mathrm{u}}}$, $\boldsymbol{r}_{\Theta} \in \mathbb{R}^{n_{\Theta}}$, $\boldsymbol{r}_{\mathrm{q}} \in \mathbb{R}^{n_{\mathrm{Q}}}$, plus appropriate initial conditions. Here $\boldsymbol{u} \in \mathbb{R}^{n_{\mathrm{u}}}$ and $\boldsymbol{\Theta} \in \mathbb{R}^{n_{\Theta}}$ represent the unknown nodal displacements and temperatures, and $\boldsymbol{q} \in \mathbb{R}^{n_{\mathrm{Q}}}$ represents the vector of all internal variables to be evaluated at all spatial integration points (usually Gauss points). $\boldsymbol{C}_{\Theta} = \boldsymbol{C}_{\Theta}(t, \boldsymbol{u}, \boldsymbol{\Theta}, \boldsymbol{q}) \in \mathbb{R}^{n_{\Theta} \times n_{\Theta}}$ reflects the heat capacity matrix. Fritzen (1997) then continued this procedure at the same department of the TU Darmstadt, applying numerical methods of higher convergence order in the time domain to the DAE-system (5). Peter Ellsiepen, who was influenced by this approach at the same alma mater of the two predecessors (and who moved to the University of Stuttgart for his doctorate), transferred this to the theory of porous media, (Ellsiepen, 1999). The class of stiffly accurate, diagonal-implicit Runge-Kutta methods (SDIRK) was used for the time integration of the DAE-systems, whereby the simplest of the procedures represents the backward Euler method. This method (shown in the following) leads to a coupled system of non-linear equations

$$\begin{aligned} \boldsymbol{G}(t_{n+1}, \boldsymbol{u}_{n+1}, \boldsymbol{\Theta}_{n+1}, \boldsymbol{q}_{n+1}) &= \boldsymbol{0} \\ \boldsymbol{L}(t_{n+1}, \boldsymbol{u}_{n+1}, \boldsymbol{\Theta}_{n+1}, \boldsymbol{q}_{n+1}) &= \boldsymbol{0}, \end{aligned} \tag{7}$$

at any point in time t_{n+1}. $\boldsymbol{G} \in \mathbb{R}^{n_{\mathrm{u}}+n_{\Theta}}$, $\boldsymbol{L} \in \mathbb{R}^{n_{\mathrm{q}}}$. Parallel to these findings and investigations, the author pursued the question of which solution method should be used to calculate the non-linear system of equations (7), which corresponds to the nested iterative calculation common in the finite element method (global Newton-Raphson method for calculating the nodal displacements $\boldsymbol{u}_{n+1}$ (and nodal temperatures $\boldsymbol{\Theta}_{n+1}$) and the inner loop for calculating the internal variable $\boldsymbol{q}_{n+1}$ at the spatial integration points (Gauss points)) with the method characterized by Simo and Taylor (1985). In (Hartmann, 1998) it has been shown that this corresponds to the so-called Multilevel-Newton Algorithm (MLNA), which was already known in connection with the numerical solution of electrical networks, (Rabbat et al., 1979), as well as non-linear optimization problems, (Hoyer and Schmidt, 1984).[5] This was treated in the fundamental contribution of Ellsiepen and Hartmann (2001), see also (Hartmann, 2005). Thus, it is now clear that the numerical procedure presented in (Simo and Taylor, 1985) does not correspond to the Newton-Raphson procedure. On a closer look it should also be noted that the entire algorithm of applying the backward Euler method and the MLNA to the solution of a DAE-system was already known in (Rabbat et al., 1979), i.e. to another scientific community, see also (Hartmann, 1998). A number of further investigations and applications were carried out based on these findings, such as the reaction force calculation with displacement control, the integration of constraints such as plastic incompressibility by projection methods, the application of different non-linear equation solvers, the transfer to questions of dynamics, the transfer to large deformations, as well as the extension

[5] At this point the author would like to thank Professor Hubert Schwetlick (TU Dresden), who gave the reference to the publications when asked.

to multi-field problems such as thermal fluid-structure interaction and electro-thermomechanics in sintering processes. The numerical time integration of the SDIRK-method has – apart from higher accuracies – the advantage that a step-size control based on the estimation of the time steps is provided, with close to no additional effort, so that nowadays especially processes like creep or relaxation are possible in reasonable calculation times. Furthermore, time adaptivity also solves the question of a suitable step-size $\Delta t_n = t_{n+1} - t_n$ for coupled field problems by error estimators. There was also the question of whether other time integration methods were more attractive in order to reduce the effort of the calculations. Attempts to treat the DAE-system (6) using BDF methods were done for example by Eckert et al. (2004), or applying Rosenbrock or semi-explicit Runge-Kutta methods in (Rothe et al., 2012). Further, the question has been addressed whether not only the time discretization error can be reduced by higher order methods in combination with time adaptivity, but also whether the spatial error can be combined with finite elements of higher order in order to minimize the discretization error for the solution of the partial differential equations (1) in combination with the constitutive models of the evolution equation type. The p-version of the finite element method, see (Szabo and Babuska, 1991; Düster, 2002), has been combined with SDIRK and Rosenbrock methods, (Netz et al., 2013; Netz and Hartmann, 2015). Recent investigations are so-called *contact problems* in which two deformable bodies come into contact, which were coupled with SDIRK methods and step-size control as well as a mortar contact formulation, (Grafenhorst, 2018). However, there are also disadvantages to this approach. For example, the temporal order of convergence in non-linear Dirichlet boundary conditions of parabolic and hyperbolic problems is not achieved and is only considered by a trick, (Alonso-Mallo, 2002; Alonso-Mallo and Cano, 2004; Rothe et al., 2015). Currently, there are also open questions regarding problems with different time scales, as they can occur in multi-scale and multiphysical problems.

5 Material Parameter Identification

The constitutive models occurring in the Eqns. (3) and (4), and also in the heat conduction equation, have so far still undetermined material parameters $\boldsymbol{\kappa} \in \mathbb{R}^{n_\kappa}$, which are based on suitable experimental data $\boldsymbol{d} \in \mathbb{R}^{n_\mathrm{d}}$, and have to be adjusted. A conceptual approach is the *least-square method*, where the square of the distance $\tilde{\boldsymbol{r}}(\boldsymbol{\kappa})$ from the model $\boldsymbol{s}(\boldsymbol{\kappa})$ and the experimental data $\boldsymbol{d}$ should be minimal

$$f(\boldsymbol{\kappa}) = \frac{1}{2}\tilde{\boldsymbol{r}}^T(\boldsymbol{\kappa})\tilde{\boldsymbol{r}}(\boldsymbol{\kappa}) = \frac{1}{2}\{\boldsymbol{s}(\boldsymbol{\kappa}) - \boldsymbol{d}\}^T\{\boldsymbol{s}(\boldsymbol{\kappa}) - \boldsymbol{d}\} \rightarrow \min. \tag{8}$$

This question has been intensively examined especially in the 1970s for general questions, see (Beveridge and Schechter, 1970; Beck and Arnold, 1977) or (Draper and Smith, 1998). Thereby either linear or non-linear systems of equations to be solved arise – iteratively solved with so-called *numerical optimization methods* with and without constraints, see for example (Spellucci, 1993; Dennis and Schnabel, 1996; Nocedal and Wright, 1999). Regarding the application of such methods in the context of solid mechanics we first refer to (Thielecke, 1997). However, it can be said that only relatively few German scientists work in this field, since the range of experiments, modelling and numerics is required, and an experience-based procedure to determine the parameters must be carried out as well. Unfortunately, there is currently no procedure that can be applied to any model. The identification of material parameters represents a so-called *inverse problem*, since a limited amount of measurement information must be used to deduce the corresponding parameters of the model prediction. This only leads to unique solutions in special cases. Therefore, there are a number of questions that are of interest:

1. Which numerical method is suitable to efficiently solve the problem (8) even with inequality constraints?
2. What (numerical) procedures exist to determine the material parameters of problems (3) or (4)?
3. How and with which experiment can the material parameters (possibly individually) be addressed? What are the experimental data that can be delivered by an experiment?
4. What is the quality (sensitivity to measurement errors, uniqueness, ...) of the parameters found?
5. Are there any experiments and loading processes at all that address the material parameters?
6. Do special sequences of identification procedures exist, i.e. using special measurements to determine the entire set of parameters with subsets of parameters from $\boldsymbol{\kappa}$?

Usually, Gauss-Newton-like methods are used to treat the minimum problem (8), which can only detect local minima. Other methods, such as the evolution strategy, see (Rechenberg, 1973), require a very high number of evaluations and are inefficient for expensive calculations of $\boldsymbol{s}(\boldsymbol{\kappa})$. Nowadays, the algorithms are so stably programmed that they usually yield a set of parameters. Unfortunately, some parameters might be outside physically meaningful ranges, they vary with changing starting values of the mostly iterative procedures, or the solutions of the model $\boldsymbol{s}(\boldsymbol{\kappa})$ look insufficient. Therefore, there is the question of the quality or measures for characterizing the quality of the identification process. Due to the usually non-linear least-square problem, one can approach the problem in the solution $\boldsymbol{\kappa}^*$ by a linear least-square problem and use estimative measures like the confidence interval or the correlation between parameters as well as with the help of the Hesse matrix the concept of identifiability, (Beveridge and Schechter, 1970; Beck and Arnold, 1977), see also (Hartmann and Gilbert, 2018; Hartmann et al., 2018). In particular, the concept of identifiability can be used to find out which experiments are suitable for addressing certain material parameters. It is also very easy to see that it is sometimes impossible to identify all material parameters at the same time. Here, certain subsets of parameters have to be adapted to special experiments (example: constitutive models of the overstress-type). In other words, knowledge of the behavior of the model must be available in order to identify parameters, and conversely, knowledge of the identifiability of the parameters must also be included in the modelling. It is precisely these questions that have led to constitutive model development that is dependent on the concept of identifiability. Parameter identification, i.e. the calibration of the model to measurement data, is therefore an experience-based process. Since there is usually no optical measurement data concerning the deformation (or the temperature) on the surface of the specimens, but only resulting traverse displacements – or local strains (strain gauges, strain transducers, see section 2) – or forces are recorded from the experiments, tensile tests (or torsion tests of thin-walled pipe cross-sections) are usually the first choice to evaluate the constitutive equations (3) or (4) component-wise under the assumption of homogeneous deformations and stresses (the strains and stresses are regarded as constant in a certain area of the sample). A common fallacy is that instead, one-dimensional constitutive models are used and not the three-dimensional equations for the special case of the uniaxial tension are evaluated, which usually leads to different relationships and thus to different material parameters. Therefore, (Krämer et al., 2015) present a method which consistently bypasses this problem by means of the DAE-interpretation, with the advantage that the stress algorithm required for the finite element calculation including the generated consistent tangents can be used directly. If there are no homogeneous deformations in a sample (which is usually the case, except for the very few experiments mentioned above), the entire initial boundary value problem (1) and (4) must be solved to determine $\boldsymbol{s}(\boldsymbol{\kappa})$. This was intensively advanced by (Andresen et al., 1996; Mahnken and Stein, 1996, 1997) (for further literature see (Hartmann, 2017)). Unfortunately, however, the consistent interpretation of the solution concept of the vertical line method from Section 4, i.e. the solution of DAE-systems, has not been used here. If looking for mathematical literature that addresses the identification of parameters in ordinary differential equations, DAE-systems, or also partial differential equations, the work of Schittkowski (2002) has to be mentioned. Here, instead of the numerical differentiation of the entire code (external numerical differentiation), the functional matrices required in Gauss-Newton-like procedures are set up analytically (internal numerical differentiation), which promises an enormous gain in computing time. In addition, a consistent representation has been found which can be adapted to many other DAE-solvers and problems. This is examined in (Hartmann, 2017) and transferred to the DAE-system (5) so that a consistent representation and algorithm exists. For each time t_{n+1} from the system (7) in the form (here only shown for the isothermal case and problems without forces as measured data)

$$\begin{aligned} \boldsymbol{G}(t_{n+1}, \boldsymbol{u}_{n+1}(\boldsymbol{\kappa}), \boldsymbol{q}_{n+1}(\boldsymbol{\kappa}), \boldsymbol{\kappa}) &= \boldsymbol{0}, \\ \boldsymbol{L}(t_{n+1}, \boldsymbol{u}_{n+1}(\boldsymbol{\kappa}), \boldsymbol{q}_{n+1}(\boldsymbol{\kappa}), \boldsymbol{q}_n(\boldsymbol{\kappa}), \boldsymbol{\kappa}) &= \boldsymbol{0}, \end{aligned} \tag{9}$$

determines the $\partial \boldsymbol{u}_{n+1}/\partial \boldsymbol{\kappa}$ matrix required for the Gauss-Newton-like procedure. As an alternative to Gauss-Newton similar methods for solving least-square problems, there are alternatives such as the *virtual-field method*, (Pierron and Grédiac, 2012), probabilistic methods, (Tarantola, 2005; Rosić et al., 2013), or also neural network schemes, (Huber and Tsakmakis, 1999a,b). However, they cannot improve the quality of the parameters. These procedures have not been specifically dealt with here.

6 Verification and Validation

Since numerical models are used to predict the real component behavior, there is the question of the quality of such a prediction. There are a number of uncertainties that need to be taken into account. Initially, the findings are based

only on a limited number of experiments that already lead to erroneous data. Then, identification tools are used to determine the material parameters of selected constitutive models, and finally simulations are performed where uncertain initial and boundary conditions (bearings, loads) and approximate algorithms are used for calculation. On the one hand, it therefore has to be asked how the results are produced – and what significance they have on the other? This problem is coupled with the research branch *Verification and Validation (V&V)*. First of all, it is necessary to differentiate the terms *verification* and *validation*, since they are very often used as synonyms. This aspect has been treated in the fundamental contribution of Babuska and Oden (2004). A very rough illustration in the form of questions can be given as follows: *verification* deals with the question "Do we solve the equations correctly?", and *validation* discusses "Do you solve the right equations?". Verification is understood in such a way that the first thing that matters is not whether the physics is described correctly, but whether the numerical calculation method provides "correct" answers. This means that statements about the numerical accuracy of the solution of the partial differential equation have to be given – on the one hand connected to *code verification* and on the other hand with *calculation verification*. In this sense, verification is a process that ensures the accuracy and reliability of the calculation. The code verification therefore represents the verification of the implementation of the mathematical model, which sometimes implies a comparison to analytical solutions or a comparison to high-precision solutions of other methods. Calculation verification, on the other hand, describes the evaluation of the accuracy of the calculation and is associated with time and space adaptivity of the solution method in order to remain below user-defined error tolerances. Unfortunately, there is currently no universal adaptive method for the problem (1) and (4). Validation, on the other hand, involves a comparison of component experiments and numerical predictions, using measures of quality. Validation is also a process that deals with the accuracy of the physical model in relation to its intended use. The concept of V&V has meanwhile been included as a recommendation in the standards of the "American Society of Mechanical Engineers" (The American Society of Mechanical Engineers, 2006), and is strongly connected with the consideration of uncertainties, see also (Oberkampf and Trucano, 2002; Roache, 1998; Schwer, 2001). In particular the model adaptivity is pointed out, i.e. not only the discretization procedures are adapted to numerical inaccuracies, but also the constitutive models, (Oden, 2018). In this sense, the objective of the model, which is in demand at the beginning of any modelling, is of particular interest, since too complex models are sometimes far too demanding and therefore not necessary for the actual, causal objective. Currently, V&V is quite an important and very open field – and it is, unfortunately, only dealt with selectively in the field of solid mechanics in Germany.

7 Conclusions

The modelling of material properties for materials of daily use – while in use or during production – is primarily subject to the question what exactly the model is supposed to be used for. Based on this, a process is developed for the execution of experiments, the development of mathematical models under consideration of physical restrictions, a consistent numerical treatment and the calibration to the previously performed experiments or their experimental data. This process is almost complete in its understanding of the numerics used. However, this does not imply the effort involved in new physical phenomena for materials that have not yet been modelled, both in carrying out the experiments and in modelling and parameter identification. All in all, this is a complex and experience-based process. For multi-field problems, the effort is exposed by the physical couplings and with multi-scale problems, and the treatment of the overall problem of experiment, modelling, numerics and identification is currently a completely open field. This is embedded in the continuous process of verifying the programming and validating the physical modelling – under consideration of uncertainties. Looking at the past 50 years as an evolutionary process, we can be confident that it will be possible to solve many problems that lie ahead.

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