Computational Mechanics of Materials and Structures

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Abstract. This paper contains a report on a selection of recent research projects carried out at the Institute for Mechanics of Materials and Structures of Vienna University of Technology. The aim of this report is to demonstrate that Computational Mechanics of Materials and Structures is a scientific field with many characteristics of an electronic golem.

1 Introduction

Resting on rather abstract mechanical principles with a strong "artificial touch", such as principles of virtual work, computational mechanics may be viewed, in a metaphorical sense, as a golem – an artificial creation of enormous strength. It was the advent of the digital computer that has opened the door to computational mechanics which has become a scientific discipline with a tremendous influence on our lives. Hence, it is justified to characterize computational mechanics more precisely, again in a metaphorical sense, as an electronic golem. In any case, it is a field that is full of "interdisciplinary aspects of human-machine co-existence and co-operation", to quote the title of the workshop to which this paper was invited.

Institute for Mechanics of Materials and Structures (IMWS) is the new name of the former Institute for Strength of Materials of Vienna University of Technology. The new designation stands for an old scientific program, which can be described as symbiosis of material and structural mechanics. Material mechanics without challenging applications to real-life structures may degenerate to *l'art pour l'art*. Structural mechanics with material laws that are not based on sound physical principles, on the other hand, may result in inadequate modeling of the mechanical behavior of structures. More recently, multiscale methods have gained momentum in material mechanics. Such methods may require information from the atomistic level. Homogenization strategies then serve the purpose to finally arrive at a constitutive law on the macroscopic level.

Mechanics is not the only scientific discipline that governs the behavior of engineering structures. Frequently, it is necessary to consider the interaction of several scientific fields such as chemistry, heat conduction, and mechanics, to capture this behavior. Consideration of such an interaction is commonly referred to as "multiphysics approach".

This paper contains a report on a selection of recent research projects carried out at the IMWS of Vienna University of Technology. The aim of this report is to demonstrate that Computational Mechanics of Materials and Structures is indeed a scientific field with many characteristics of an e-golem.

2 Computational Mechanics at the Institute for Mechanics of Materials and Structures

This Chapter contains four Subchapters. Each one of them is devoted to a pertinent research topic. Some of these topics haven an industrial background. Their treatment involves both basic and applied research.

2.1 Revealing Universal Principles of Micromechanical Design in Biological Materials – Wood, Bone, Skin

Biological materials are characterized by an astonishing variability and diversity. Their hierarchical organizations are often well suited and seemingly optimized to fulfill specific mechanical functions. This has motivated research in the fields of bionics and biomimetics. The aforementioned optimization is primarily driven by selection during the evolution process. However, it is of great importance to notice that selection is realized at the level of the individual plant or animal (and not at the material level). Therefore, material optimization in the strictest sense of the word does not take place. Rather, once a (hierarchical) composite material has been adopted within a living organism, its fundamental building principles (morphologies or universal patterns of architectural organization [1]) remain largely unchanged during evolution. Hence, entire material classes of biological materials exhibit common (universal) principles of (micro)mechanical design.

These principles can be qualitatively derived from experiments. In this way, the human skin can be characterized as a multiphased material: Intertwined networks of collagen and elastin are embedded in a viscous matrix containing proteoglycans [2]. By varying the direction of the principal components of strain, incrementally increased to different levels, one can separate the elastic and viscous contributions to the stress components. The strain level-dependent visco-elastic behavior of skin can be correlated to the structure of the collagen fiber networks of skin samples from different body sites [3].

Based on the evaluation of mechanical and chemical experiments, the bones of all vertebrates were shown to be hydroxyapatite mineral foams reinforced, at a characteristic length of some microns, by collagen strands and perforated, at an observation scale of several hundred microns, by prolate pores [4,5]. Hellmich et al. [6,7] recently expressed this building principle in quantitative terms, allowing for a prognosis of tissue-specific (inhomogeneous and anisotropic) elasticity properties from tissue-specific mineral, collagen, and micropore content. It is based on universal elastic properties of collagen, hydroxyapatite, and water. Related material models were developed in the framework of continuum micromechanics.

In continuum micromechanics [8], a material is understood as a microheterogeneous body filling a representative volume element (RVE) of characteristic length *l*, $d \ll l$, *d* standing for the characteristic length of inhomogeneities within the RVE. The 'homogenized' mechanical behavior of the material, i.e. the relation between homogeneous deformations acting on the boundary of the RVE and resulting (average) stresses, can then be estimated from the mechanical behavior of different homogeneous phases (representing the inhomogeneities within the RVE), their dosages within the RVE, their characteristic shapes, and their interactions. If a single phase exhibits a heterogeneous microstructure itself, its mechanical behavior can be estimated by introduction of RVE's within this phase, with dimensions $l_2 \ll d$, comprising again smaller phases with characteristic length $d_2 \ll l_2$, and so on, leading to a multistep homogenization scheme (Fig. 1).

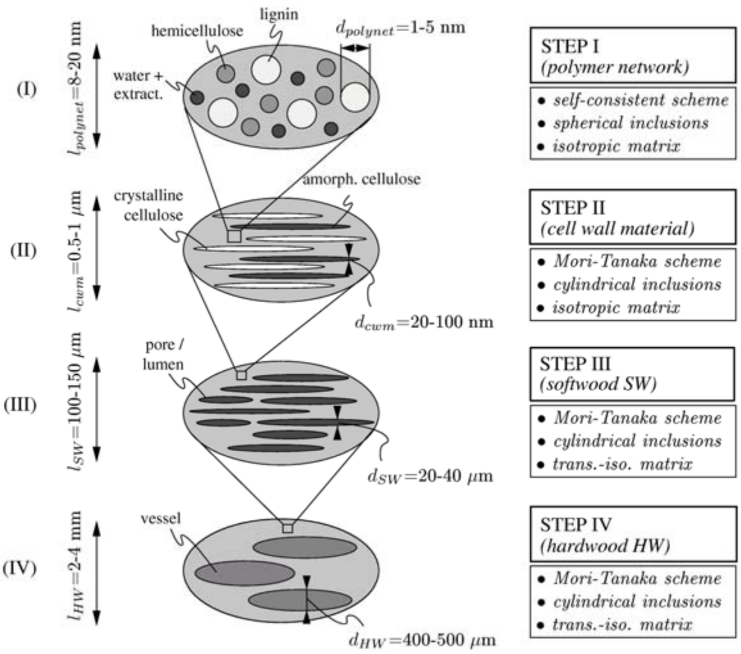


Fig. 1. Four-step homogenization scheme for wood

Such a multistep homogenization scheme, developed by Hofstetter et al. [9], suitably represents the intrinsic structural hierarchy of another class of biological materials, namely wood across all different tree species [10]. The nanoscaled components of the wood cell wall, namely crystalline cellulose, amorphous cellulose, hemicellulose, lignin, and water, exhibit universal elastic properties inherent to all wood species.

They allow for prediction of wood tissue-specific macroscopic elastic properties from tissue-specific chemical composition and microporosity, by means of the four-step homogenization scheme of Fig. 1 [9].
Validation of such a micromechanical model rests on statistically and physically independent experiments: The macroscopic stiffness values predicted by the micromechanical model on the basis of tissue-independent ('universal') phase stiffness properties of hemicellulose, amorphous cellulose, crystalline cellulose, lignin, and water (*experimental set I*) for tissue-specific composition data (*experimental set IIb*) are compared to corresponding experimentally determined tissue-specific stiffness values (*experimental set IIa*) [5,6,7,9]. For the elastic moduli in the longitudinal direction (aligned with the stem axis), E_L, and in the transversal direction (in the cross-sectional plane of the stem), E_T, as well as for the longitudinal shear modulus, G_L, model estimates and experimental results show good agreement over a large variety of softwood and hardwood species (Fig. 2).

This micromechanical model for wood is expected to support optimization processes in wood drying technology as well as structural analyses of wood structures [11] (Fig. 3a,b). Validation of such analyses is preferably done by structural testing [12] (Fig. 3c).

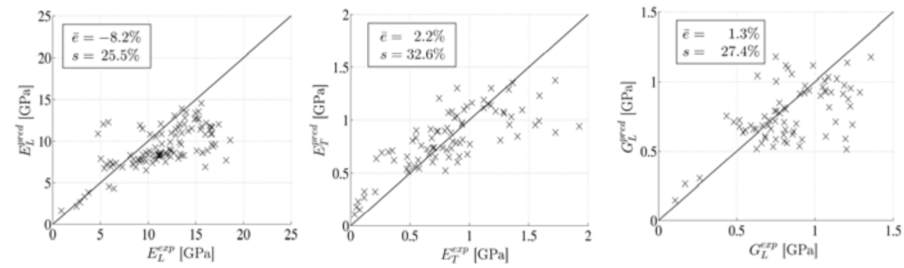


Fig. 2. Comparison of predicted and measured elastic constants

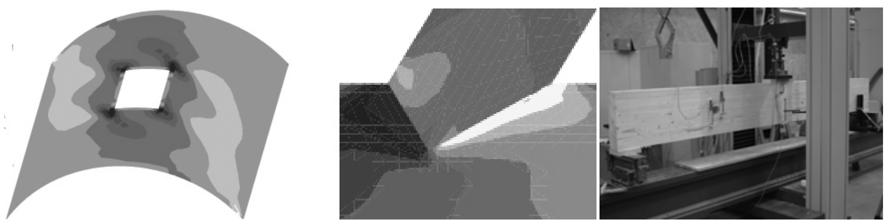


Fig. 3. Experimental investigation and FE analyses of realistic wooden structures

2.2 Computational Model for Assessment of Protection Systems for Buried Steel Pipelines Endangered by Rockfall

The climate change in the last decades has led to an increasing number of rockfalls in the European Alps. This has raised the need for designing rockfall protection systems.

Such systems commonly consist of a load-carrying structure buried by an energy-absorbing and load-distributing layer made of gravel.

FE analyses of such structures require realistic modeling of the material behavior of gravel, i.e., failure laws for gravel under quasi-static mechanical loads and penetration laws for boulders impacting onto gravel. The former were based on (macroscopic) multisurface elasto-plasticity theory [13], the latter were developed in dimensionless form, based on knowledge about projectiles impacting onto soil and concrete targets [14]. The material parameters were identified from related experiments, including dynamic stiffness measurements in gravel [15] and large-scale rock impact experiments on gravel [14].

Considering gravel-buried pipelines endangered by rockfall, a 3D, quasi-static, elasto-plastic FE model was developed. This model was validated by comparing FE-predicted stresses in the pipe with stresses determined in a real-scale structural impact experiment onto a gravel-buried steel pipe (see Fig. 4). This test is *independent* of the experiments used for identification of the material parameters representing input for the FE model [16]. Accordingly, the developed FE model is well suited for prognoses of the loading of a gravel-buried pipeline also for modes of impact, which were not considered in the experiments. Therefore, the FE model was used for studying the structural behavior of gravel-buried steel pipelines subjected to rockfall and for assessing the performance of different rockfall protection systems for such pipelines [17].


(a)


(b)

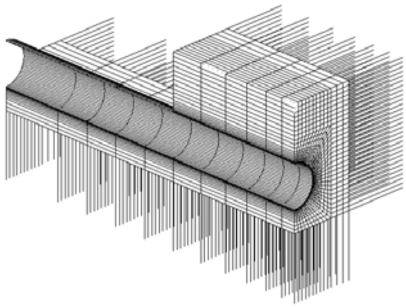

(c)

Fig. 4. Validation of the developed 3D FE model based on a real-scale structural impact test: (a) installation of the pipe for real-scale test, (b) real-scale impact test: 18260kg boulder falling down from a height of 18.85m onto the gravel-buried pipe, (c) 3D FE mesh used for validation of the FE model

2.3 Innovative Methods for Durability Assessment in Civil Engineering

For the solution of a large range of engineering problems, such as transport tunnels subjected to fire load (see Fig. 6), the degradation of road infrastructure, quality assessment during ground improvement (jet grouting), early-age cracking of cement-based materials, etc., techniques formulated exclusively at the macroscale are not able to provide a basis for the development of engineering solutions. Instead, treatment of these problems requires, on the one hand, a multiscale approach, taking into account fundamental material characteristics (building blocks and their arrangement) as well as their changes in the course of time, and, on the other hand, a multiphysics approach, covering the main couplings (e.g., thermo-chemo-hydro-mechanics) within these structures.

The development of models and solution techniques accounting for processes at different scales of observation and their verification by experimental techniques represent a central part of ongoing research at the IMWS. Four examples are given in the following.

Multiscale Modeling of Cement-Based Materials – Fine-Scale Optimization with Structural Impact. A multiscale model for cement-based materials focusing on autogenous shrinkage has recently been developed. Hereby, elastic, shrinkage, and creep parameters are related to finer scales of observation. The model accounts for:
(a) hydration kinetics of clinker phases and the microstructural composition of the cement-based material,
(b) the effect of capillary depression of the liquid material phase, entailing membrane-type internal forces at the solid-liquid-vapor interface, and
(c) crystallization pressure of hydration products, resulting, e.g., from the formation of ettringite in the early stages of hydration.

The identification of creep properties at the nano and microscale of cement paste is part of ongoing work. Hereby, experimental results from nanoindentation are analyzed by means of finite-element and analytical back-calculation of the obtained load-penetration-time data.

The results from multiscale modeling, i.e., intrinsic material functions (related to the degree of hydration) permit for structural analyses on the macroscale [18,19].

Heat Release and Reaction Kinetics of Early-Age Concrete – Innovative Methods for Quality Control in Ground Improvement. The temperature in concrete members influences the hydration kinetics via thermo-chemical couplings and, thus, the early-age properties of cement-based materials. Recently, these couplings were exploited to specify properties of jet-grouted soil obtained from ground improvement [20]. During hydration, both the amount of heat as well as the rate at which this heat is released depends on the chemical reactions taking place in early-age concrete.

The development of an analysis tool for determination of properties of jet-grouted columns (see Fig. 5) comprises:
(a) Differential calorimetry – heat flux differential calorimetry: water and cement (or binders used for jet grouting) are mixed in the test chamber, then the heat flux [J/g] and the heat-flux rate [J/(g h)] required to keep the hydrating sample at a pre-specified temperature are recorded.
(b) Micromechanical hydration model – kinetic laws for clinker phases: the degree of hydration represents the set of chemical reactions taking place during hydration [20]. The hydration process can be divided into three main stages: (a) induction, (b) nucleation/growth, and (c) diffusion considered for the four main clinker phases (C3S, C2S, C3A, and C4AF) [21]. In order to assess the performance of these kinetic laws for the different clinker phases, the rate of heat flow monitored in differential-calorimetry tests was re-analyzed.

(a) (b)

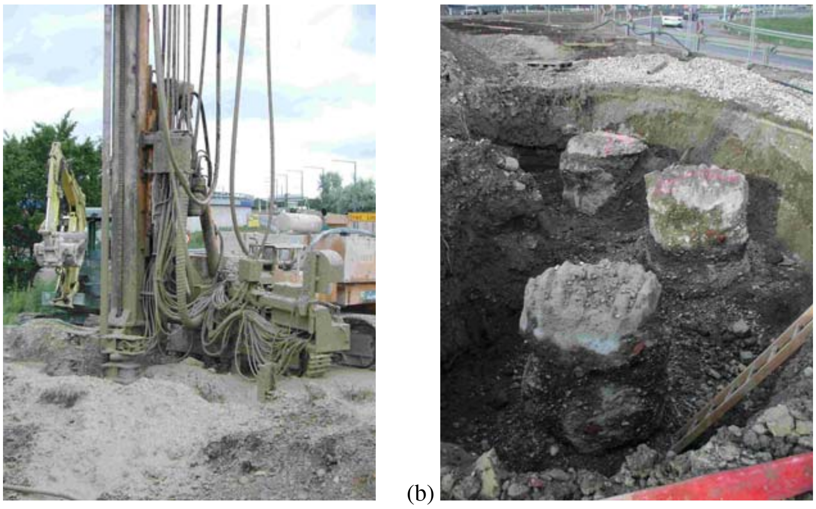


Fig. 5. Process of jet-grouting: (a) drilling rig, (b) jet-grouting columns

(c) Temperature measurements in jet-grouted columns on site: temperature measurements are started immediately after the end of the grouting process. Temperature sensors are located at the center of the jet-grouted column.
(d) Finite element simulation: the temperature history measured at the site is analyzed and compared to FE-simulated data to estimate the aforementioned properties of jet-grouted columns.

Concrete Subjected to High Temperatures – Safety Assessment of Tunnels under Fire Load. When concrete is subjected to high-temperature loading, thermo-hydro-chemo-mechanical processes cause (a) degradation of stiffness and strength of the lining materials, i.e., concrete and steel, and (b) spalling of near-surface concrete layers. As a consequence, the load-bearing capacity of the tunnel structure is reduced.

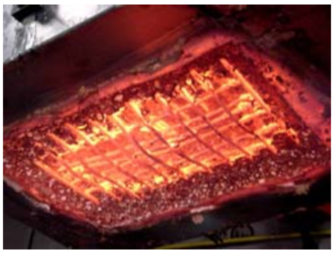


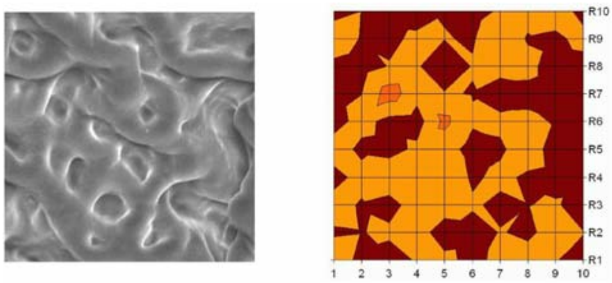
Fig. 6. Large-scale fire experiments: heated surface after fire loading

Large-scale fire experiments on concrete blocks (see Fig. 6) represented the starting point for the research work at the IMWS, consisting of
(a) Large-scale fire experiments: the main objective was to investigate spalling of different concrete mix designs under different temperature and mechanical loading.

The obtained results showed a strong influence of the amount of PP-fibers on the spalling behavior [22].
(b) Material characterization: in order to assess the influence of PP-fibers on the transport properties of concrete, permeability tests are conducted on concrete with and without PP-fibers [23]. Additionally, mercury intrusion porosimetry and thermo-gravimetric measurements were conducted. Nanoindentation experiments provide insight into temperature-dependent changes of the mechanical properties.
(c) Coupled thermo-hydro-chemo-mechanical analysis: the effect of changing material properties with temperature on the loading of the concrete microstructure is investigated by means of a fully-coupled finite element program developed at the University of Padua. This program is based on the governing energy and mass-balance equations outlined in [24].
(d) Structural safety assessment: the influence of the loading of the concrete microstructure and, thus, of the spalling behavior on the structural performance of concrete tunnel shells is determined by finite element simulations [25]. Hereby, layered finite elements are employed. They account for both different material properties in the layers (depending on the temperature profiles) and spalling by de-activation of the layers.

The described research endeavor provides the necessary tools for a performance-based optimization of concrete tunnel linings within a fire-safety assessment.

Multiscale Modeling of Creep of Asphalt – Performance-based Optimization of Flexible Pavements. The rapid degradation of the road infrastructure was a reason for installing the Christian-Doppler Laboratory for "Performance-based optimization of flexible pavements" at TU Vienna. In this laboratory, a multiscale model for asphalt is currently developed, allowing identification of fundamental mechanisms of asphalt at several observation scales. By means of application of advanced upscaling methods, the gain in understanding at the finer scales is translated to the structural scale, and finally used for the design of new pavement structures and the assessment of existing ones.



(a) (b)

Fig. 7. Bitumen microstructure by means of (a) ESEM and (b) NI (50x50 μm)

The binder material of asphalt is bitumen. It is responsible for the time and temperature-dependent behavior of asphalt. Bitumen itself is a multicomposed material emerging from the wide range of hydrocarbon molecules. The microstructure built up by these molecules was observed earlier by means of Atomic Force Microscopy (AFM) [26] and Environmental Scanning Electron Microscopy (ESEM) [27,28].

According to the ESEM results, the microstructure of bitumen consists of string-like structures with a diameter of about 10 μm embedded into a matrix material. In order to detect the viscoelastic behavior of the different bitumen phases, nanoindentation (NI) was employed, providing the spatial distribution of the mechanical properties at different temperatures.

The observed material phases, the identified microstructure (see Fig. 7), and the mechanical properties of the individual phases will serve as input for upscaling within a multiscale model, aimed at assessing the effect of the bitumen microstructure on the macroscopic properties of asphalt.

2.4 Rubber Materials and Products

The treatment of rubber materials and products is characterized by a synthesis of experimental and numerical investigations and the consideration of the raw material as well as industrial products made thereof. Currently, main issues are the frictional behavior of rubber tread blocks and the viscoelastic behavior of rubber blends during extrusion. The respective projects are performed in cooperation with industrial partners.

Rubber tread blocks establish contact between a car tire and the road. Thus, the frictional properties of these blocks are of crucial importance for the performance of tires in breaking events and in rolling turns. Investigation of the frictional sliding behavior by means of numerical simulations using the Finite Element Method allows for a detailed analysis of the sliding process and for comprehensive parameter studies. Application of the numerical simulation tools for industrial product development enables considerable cost savings because of the possible reduction of prototype tests.

Rubber tread blocks undergo very large deformations close to the contact zone, resulting in a curling of the front edges of the blocks in the worst case. Figure 8 shows this deformation behavior for a sliding tread block with parallelogram-shaped base and three sipes (parameters of the simulation as in [29]) together with the distribution of vertical normal stress σ_y in a middle cross-section of the block.

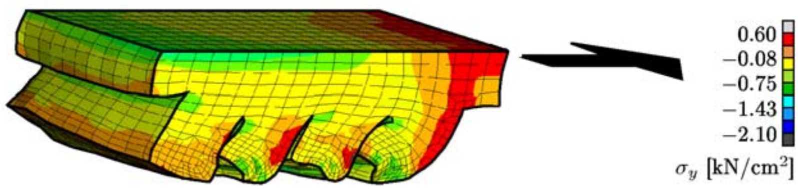


Fig. 8. Distribution of vertical normal stress in rubber tread block with parallelogram-shaped base and three sipes during frictional sliding

Reproduction of the sliding behavior in the numerical simulations is a challenging task, in particular with respect to the numerical stability of the simulation procedure and the appropriate description of the material behavior [30].

Complementary to numerical simulations, the sliding behavior of the tread blocks is also investigated experimentally. Experiments are performed at a test rig at the

Laboratory of the Institute, the so-called *Linear Friction Tester* [31]. At this device, rubber blocks are pulled over various friction surfaces (e.g. asphalt, concrete, ice, snow). Measurement of the reaction forces in tangential and vertical direction allows for evaluation of the average friction coefficient. In addition, the temperature distribution at the bottom surface of the rubber block can be scanned by means of a radiation pyrometer, which is installed at the end of the friction surface. Experimentally determined friction coefficients serve as the basis for identification of frictional parameters of the numerical model. In addition, measured temperature distributions and observed deformations of the rubber blocks allow for validation of the simulation procedure.

In another research project, the material behavior of rubber blends was investigated. Standard material characterization methods do not allow for a realistic determination of the viscoelastic properties. Because the die swell is the determinant criterion for the production of rubber profiles by means of extrusion, its experimental investigation and numerical treatment are necessary. In order to characterize the materials, several experiments were performed by means of a capillary-viscometer and the rubber process analyzer. According to these experiments, two different nonlinear solution algorithms were adopted. With the help of the generalized Newton-Raphson procedure the coupling between the viscosity and the shear strain rate can be considered. For validation, a genetic algorithm was adopted [32]. Furthermore, consideration of the die swell is planned.

2.5 Conversion from Imperfection-Sensitive into Imperfection-Insensitive Elastic Structures

In case of loss of stability by means of symmetric bifurcation, a qualitative improvement of the postbuckling behavior of originally imperfection-sensitive elastic structures is their conversion into imperfection-insensitive structures by means of modifications of the original design. Such a conversion is restricted to symmetric bifurcation. Designation of a structure as either imperfection sensitive or insensitive depends on the initial postbuckling behavior which is often relevant to the entire postbuckling response. The search for specific modes of stiffening that result in the aforementioned conversion is of fundamental as well as of practical importance.

Koiter's initial postbuckling analysis is applied in the framework of the Finite Element Method (FEM) to deduce mathematical relations associated with the transition from imperfection sensitivity to insensitivity [33]. This mode of analysis primarily serves the purpose of deducing important theoretical results which facilitate the verification of specific numerical results. New mathematical conditions for symmetric bifurcation from nonlinear prebuckling paths are presented [34].

Attempts to achieve the aforementioned conversion include the increase of the thickness of the structure and of the stiffness of a spring attached to the structure (see Fig. 9), respectively, and the reduction of the rise of the undeformed structure [34]. The results of this investigation include different modes of conversion from imperfection-sensitive into imperfection-insensitive structures as well as failure to achieve such a conversion.

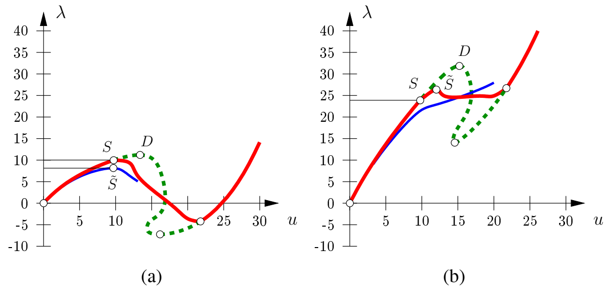


Fig. 9. Load-displacement path for a perfect as well as for an imperfect cylindrical shell (a) without and (b) with a spring attached to the shell [33]

An important ingredient of the numerical investigation are accompanying linear eigenvalue analyses based on the so-called consistently linearized eigenproblem [33, 34]. At the transition from imperfection sensitivity to insensitivity, the resulting eigenvalue curve, in general, has specific geometric properties (saddle points or planar points) at the bifurcation point.

One of the conclusions is that increasing the stiffness of a structure by means of a uniform increase of its thickness does not result in the conversion from imperfection sensitivity into insensitivity. Another one is that reducing the initial rise of an imperfection-sensitive structure eventually results in the transition from bifurcation buckling to no loss of stability. Unfortunately, such a reduction is associated with a decrease of the stability limit. Increasing the stiffness of an elastic spring, suitably attached to the structure, however, usually enables its conversion from an imperfection-sensitive into an imperfection-insensitive structure. Hence, additional supports of a structure may be effective means to achieve the desired conversion [34].

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