AWARDS

Acknowledgement of a member of the Editorial Board

It is a great pleasure to inform the readers that Prof. Herbert A. Mang, an active member of Editorial Board, on April 30, 2007, was given a prestigious award, the Carl-Friedrich-Gauß-Medal, by the Braunschweigische Wissenschaftliche Gesellschaft (BWG). Congratulations!
This medal has been awarded annually once since 1949. Among the awardees are several laureates of the Nobel Prize.The laudation was held by Prof. Peter Wriggers, President of the Gesellschaft fuer Angewandte Mathematik und Mechanik (GAMM). On this occasion Prof. Mang gave a lecture. We expect that printing of a translation of this lecture, reflecting the achievements in Computational mechanics of a research group led by Prof. Herbert A. Mang (*http://www.imws.tuwien.ac.at/en/team/management/herbert-mang.html*), a prominent and world-renowned scientist, would be interesting for the readers.

Editors of *Journal of Civil Engineering and Management*

ON CONTEMPORARY COMPUTATIONAL MECHANICS

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1. Introduction

"When I shall say to the instant: "Stay! You are so beautiful! Then", so Dr. Faustus to Mephistopheles when they sealed their contract (Fig. 1), "you will be free from your services. The clock may stop, its hands may fall. The time for me be over!" Because of the dynamics inherent to Computational Mechanics, its present state certainly does not invite to stay but rather suggests, as Johann Wolfgang von Goethe lets the angels say in the second part of Dr. Faustus' tragedy, continuously striving efforts which promise redemption.

In view of the title of the original (German) version of this paper[1], it is deemed appropriate to briefly comment on the virtual relationship between the *prince of poetry* Johann Wolfgang von Goethe and the *princeps mathematicorum* Carl Friedrich Gauß (Fig. 2). In real life they have never met. There is speculation that Gauß was not interested in such a meeting because of rejecting Goethe's theory of colors which Gauß considered lacking sufficient scientific foundation. He also wanted to avoid a dispute with Goethe. This may have prompted Goethe to replace the name *Gauß* by *Kant* in the following words of his stage arrangement of Kotzebue's comedy *Victims of Theft*: "may you be scholarly like Leibniz or Gauß".

Let us stay with Gauß. In 1842, the German astronomer Christian Schumacher wrote to him regarding the possible offer of an appointment at the University of Vienna: "I have generally heard that the often discussed idea of founding a Society of Sciences is now being seriously deliberated. If you are now really drawn to Vienna, I think it is because of the wish that you found this Society and be its president". In fact, the foundation of this institution had been discussed for almost 150 years. Finally, it took place in 1847 under the name of *Imperial Academy of Sciences in Vienna* (Fig. 3). In the invitation to the solemn inaugural session on February 2nd, 1848, a remark to the "presence of the supreme imperial court", including Archduke Franz, was made (Fig. 4). Exactly 10 months later, after the abdication of his uncle, Emperor Ferdinand I., Franz ascended the throne as Emperor Franz Josef I. In the aforementioned session, the election of Carl Friedrich Gauß to honorary member of the newly founded Academy was proclaimed. In his letter of thanks of March 31st, 1848 (Fig. 5) Gauß also addressed the March revolution in this year. "It is not possible", he writes, "to separate in thought the epoch in which the new Academy was founded from the world historic era that has begun almost immediately thereafter for the Imperial State and also for the whole of Germany in both the interior and exterior affairs".

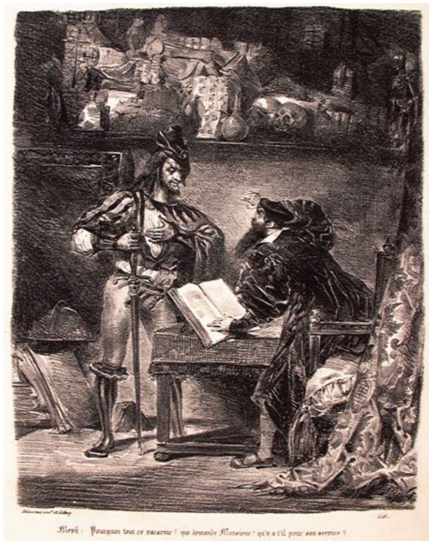

Fig. 1. Faust: First part of the tragedy, study; setting the seal of his contract with Mephistopheles

[1] Translation of "In Computational Mechanics sollt' nie zum Augenblick man sagen: Verweile doch! du bist so schön!", Braunschweigische Wissenschaftliche Gesellschaft, Jahrbuch 2007, 187–216, J. Cramer Verlag, Braunschweig, 2008, into English. The original (German) version of the paper is the manuscript of a lecture delivered on May 4, 2007, in Braunschweig, on the occasion of the award of the Gauß-Medal by the Braunschweigische Wissenschaftliche Gesellschaft.

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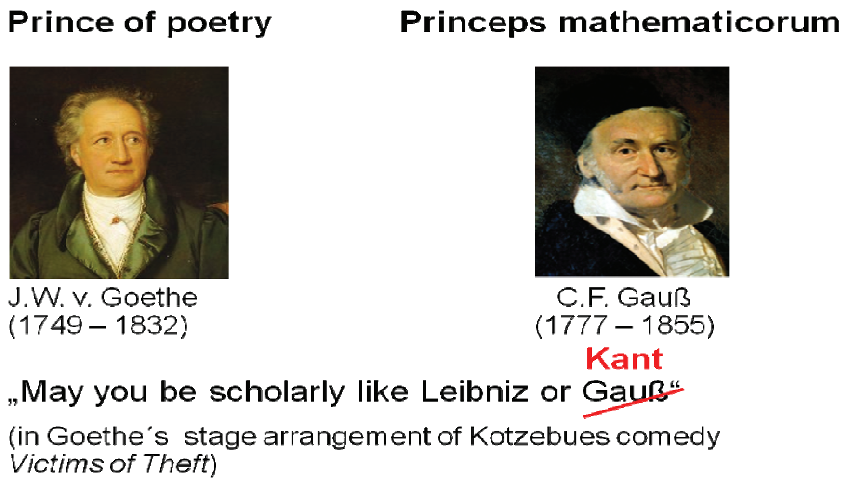


Fig. 2. Goethe and Gauß

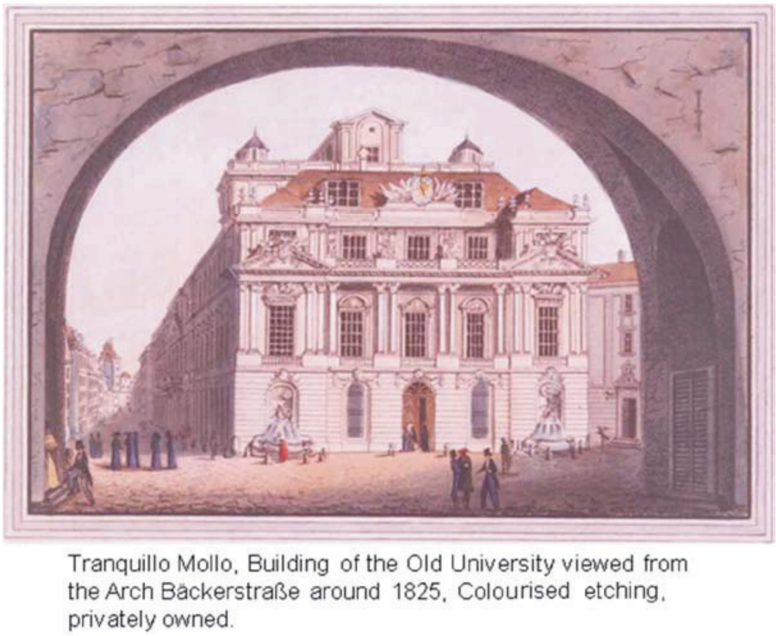


Fig. 3. Imperial Academy of Sciences in Vienna

Einladung
zur
feierlichen Eröffnungs-Sitzung
der
kaiserlichen Akademie der Wissenschaften
am 2. Februar 1848 um 12 Uhr
im grossen Sitzungs-Saale der nied. österr. Herren Stände.
In Gegenwart des allerhöchsten Hofes.
Vom Präsidenten
Hammer-Purgstall.

Fig. 4. Invitation to the Solemn Inaugural Session of the Imperial Academy of Sciences in Vienna, in 1848

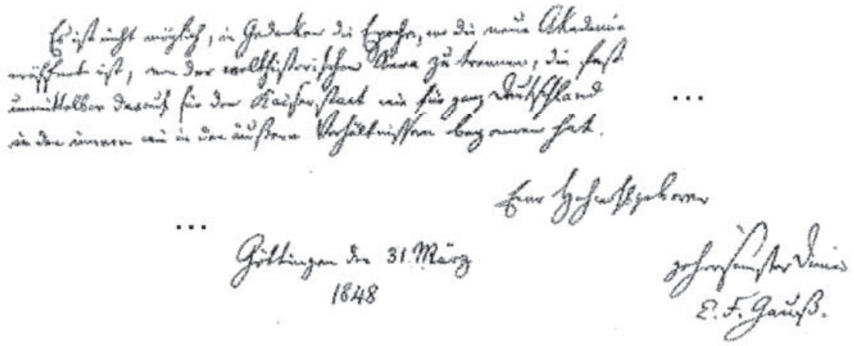


Fig. 5. Letter of thanks by Gauß after his election to Honorary Member of the Imperial Academy of Sciences in Vienna

Fig. 6. Institute for Mechanics of Materials and Structures of Vienna University of Technology

Gauß has laid important foundation stones to the edifice of knowledge of Computational Mechanics. What about is this field of knowledge actually? Let us begin with a definition of the term "mechanics". According to "Meyers Enzyklopädisches Lexikon", mechanics is a basic subarea of physics, concerned with the motion of bodies under the influence of external forces and mutual interaction forces. The special case of rest is included in this definition. It refers to the subfield statics which is important for the engineering sciences. With the help of mathematics, mechanics erects its edifice of knowledge by means of theorems based on experience, i.e. laws of nature exhibiting axiomatic character. The term "computational" refers to numerical operations which follow specific repetitive schemes, i.e. algorithms. The great increase in importance of algorithms in the younger and youngest history of mechanics is a consequence of the strongly increased and continuously further increasing use of computing machines.

If the noun "mechanics" is expressing the fundamental orientation of this field and the adjective "computational" is characterizing its methodology, then computational mechanics, in view of its application to civil engineering, mechanical engineering, bio- and medical engineering, and geotechnical engineering, is a basics-oriented engineering science with a strong methodical reference.

The main emphasis of this presentation is computational quantification of material and structural failure in civil engineering. This agrees with the new name of my workplace at Vienna University of Technology: Institute for Mechanics of Materials and Structures (Fig. 6). The new name of the former Institute for Strength of Materials accounts for the change of paradigm in a traditional field of academic education of civil and mechanical engineers.

2. Pioneers of computational mechanics

Out of the great number of direct and indirect pioneers of computer assisted mechanics only a few can be named here (Fig. 7).

Let me begin with Gottfried Wilhelm Leibniz, a founder of infinitesimal calculus who also introduced the binary number system to mathematics. Beyond its central role in representing numbers in digital computers, it has also gained importance in fields ranging from information theory to digital information transfer.

Carl Friedrich Gauß was already saluted. Indirectly, he has been a pioneer of computational mechanics, among other things, because of his fundamental contributions to numerical integration and to the solution of systems of linear algebraic equations.

Karl Zuse developed basic concepts of program-steered computing machines, beginning in 1934, when he was still a student of civil engineering at Technical University Berlin-Charlottenburg. In 1936, he started building test models. In 1941, he completed the first program-steered computing machine of the world, the relay-controlled Z3.

Let me finally name Ray W. Clough, an American pioneer of the Finite Element Method, who is still alive. As a professor at the University of California at Berkeley, he published a paper, together with 3 colleagues, in 1956 about this method without originally referring to it as the Finite Element Method.

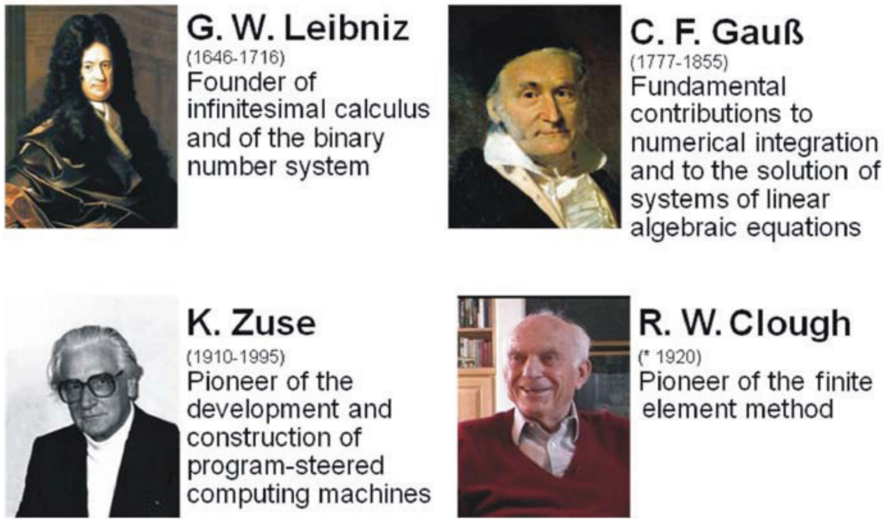
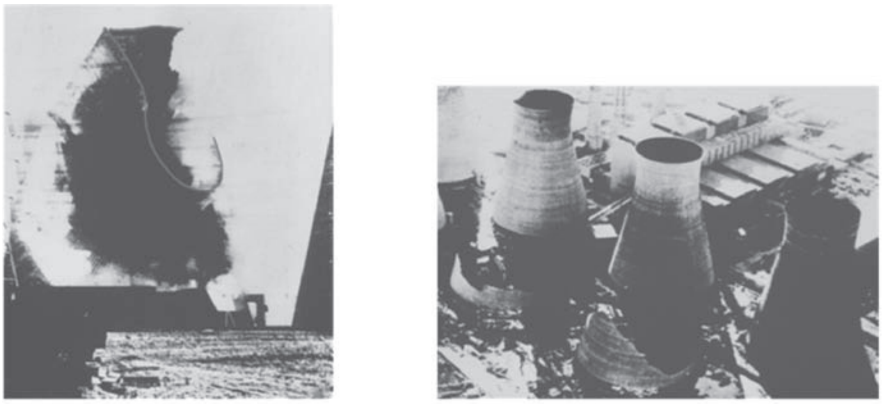


Fig. 7. Pioneers of computer-assisted mechanics



Collapse of the cooling tower in Ferrybridge, England

Cooling towers in Ferrybridge, England, after collapse

Fig. 8. Reinforced concrete – collapse of cooling towers

3. Examples of material and/or structural failure

The following presentation of examples of such failures should not be used as an opportunity for unjustified, discriminating criticism of civil engineering. Especially, the wrong impression of generally insufficient safety against collapse and loss of suitability for utilization should not arise. However, to avoid predictable cases of damage and to minimize unforeseeable catastrophes, scientific research has to deal with real cases.

The first example is concerned with reinforced concrete and refers to the collapse of 3 cooling towers, with a height of 114 m, in England, during a hurricane (Fig. 8).

The second example is concerned with steel and refers to the collapse of a temporary bridge in Bosnia caused by buckling of the upper chord (Fig. 9). The reason for this collapse was overloading by a heavy vehicle, for which the temporary bridge was not designed.

Fig. 9. Steel – collapse of a temporary bridge in Bosnia caused by buckling of the upper chord

The third example is concerned with wood as a building material. It refers to the collapse of an ice-skating hall in Bad Reichenhall/Germany (Fig. 10), in the beginning of January 2006. Although this collapse was triggered by an unusually big snow load, this load was still smaller than the design load. One of the reasons for this collapse was the humidity causing considerable damage of the joints of the roof construction glued with an adhesive consisting of urea-formaldehyde.

Fig. 10. Wood – collapse of an ice-skating hall in Bad Reichenhall, triggered by an unusually big snow load

The fourth example is concerned with asphalt. It refers to damage of roads caused by temperature changes and traffic (Fig. 11), leading to a reduction of traffic safety. The repair including roadblocks resulted in high costs.

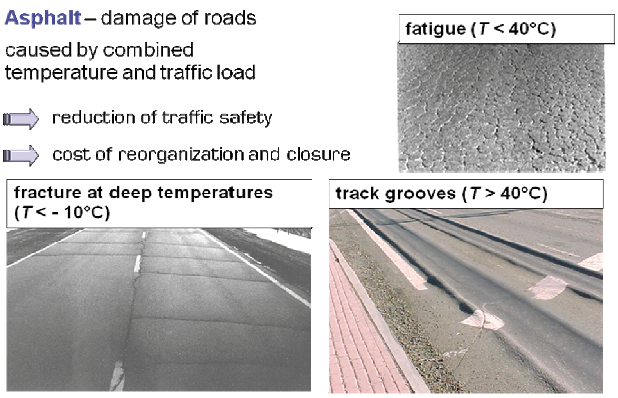


Fig. 11. Asphalt – damage of roads caused by temperature changes and traffic

The last example was taken from the wide area of biological materials. It refers to the fracture of a human bone. Experimental and numerical biomechanical research was conducted both on the level of the entire bone (left illustration in Fig. 12) and on the one of crack propagation (upper right illustration in Fig. 12). The lower right illustration shows molecules of collagen, which seem to impede crack propagation by means of bridging, resulting in increased viscosity of the material.

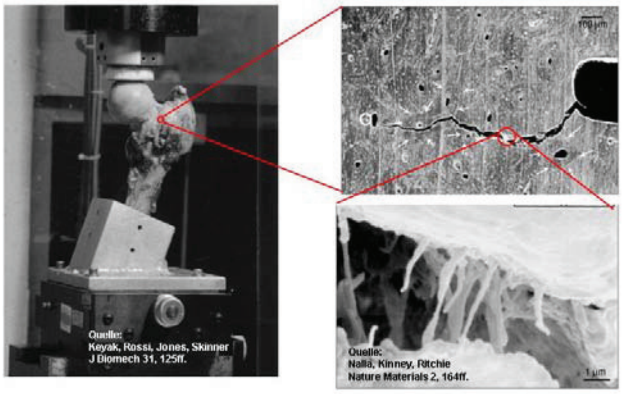


Fig. 12. Biological materials – fracture of a human bone

4. Fundamentals of the finite element method

For damage analysis, the finite element method is usually the most effective numerical analysis technique. What about actually is this numerical method whose triumphal progress occurred parallel to the one of the digital computer? To keep the explanation short, let me consider the application of this method to in-plane loading of a plate (Fig. 13). Such a plate is a plane surface structure whose middle surface remains plane under mechanical and thermal loads. If one wanted to determine analytically the states of displacements, strains, and stresses of the plate, supported and loaded along parts of the external boundary (upper left illustration in Fig. 13), the plate would have to be considered as an assemblage of infinitesimal elements. The resulting initial and boundary value problem would, however, not be amenable to an analytical solution. If, however, one is satisfied with a numerical approximate solution of the problem, it will be sufficient to consider the plate as an assemblage of finite elements, as shown in the upper right illustration in Fig. 13. The lower left illustration in Fig. 13 shows such a finite element. However, it is now necessary to interpolate between the unknown nodal displacements of the finite element, representing the local degrees of freedom. The lower right illustration in Fig. 13 shows a typical interpolation function. In general, the accuracy of the results increases with increasing numbers of elements.

In the intellectual transition from infinitesimal to finite elements, a system with infinitely many degrees of freedom is converted into one with a finite number of degrees of freedom. This intellectual process is referred to as discretization. The equation of motion for a discretized plate with n degrees of freedom has the same form as the one for a system with just one degree of freedom, characterized by the mass m, the damping constant c and the spring stiffness k (Fig. 14). The displacement q of the one-degree of freedom system under the excitation force P at time t corresponds to the vector **q** of the discretized plate. The quantities m, c, k, and P of the one-degree of freedom system correspond to the mass matrix **M**, the damping matrix **C,** the stiffness matrix **K**, and the excitation force **P** of the plate. Consequently, the vector **P** has n rows, whereas the 3 matrices have n rows and columns.

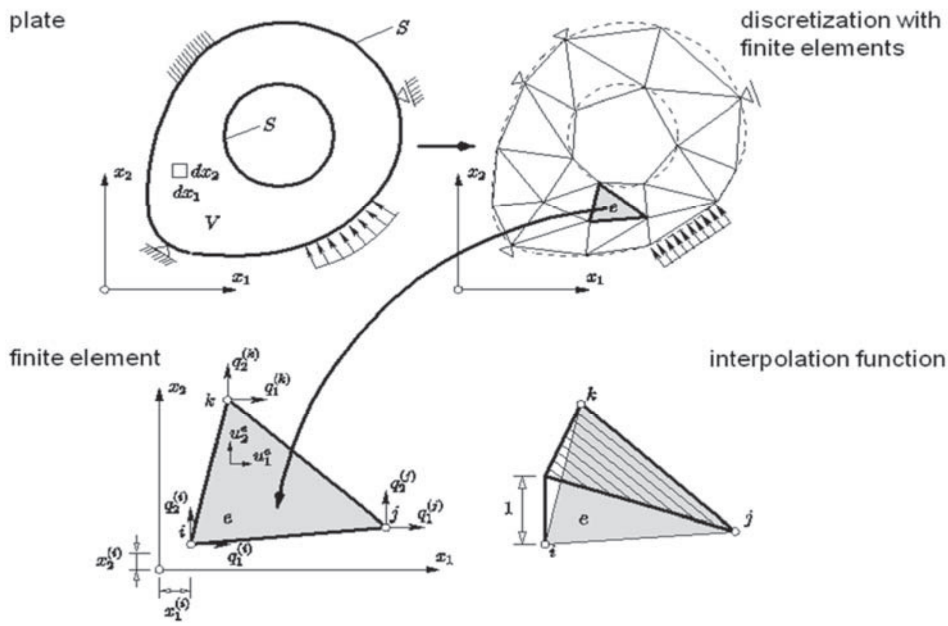


Fig. 13. Fundamentals of the finite element method by way of example of a plate (1)

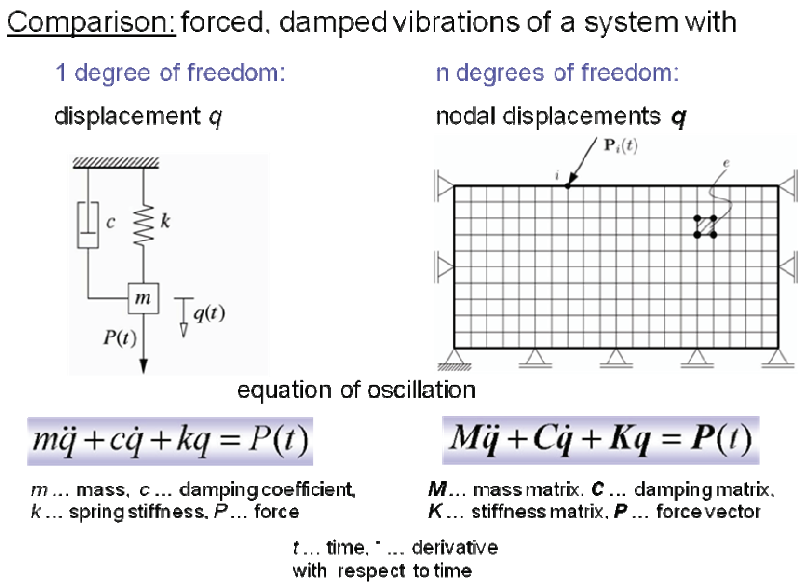


Fig. 14. Fundamentals of the finite element method by way of example of a plate (2)

The same applies to the vectors $\mathbf{q}$, $\dot{\mathbf{q}}$, and $\ddot{\mathbf{q}}$, where dots symbolize derivatives with respect to time. The mentioned matrices are structure-oriented, i.e. global. They are suitably assembled of element-oriented, i.e. local matrices with the exception of the damping matrix which is usually considered as a linear combination of the mass matrix and the stiffness matrix.

So far, I have tacitly restricted myself to linear problems. If, however, the spring stiffness k is not constant but dependent on the displacement q, the problem is non-linear and has to be solved incrementally with an equilibrium iteration at each increment (Fig. 15). The left diagram shows a non-linear load history including the first and the m-th load and time increment. The right diagram refers to iterative determination of the load increment Δq_{m+1} for a system with one degree of freedom. For a system with n degrees of freedom restricted to static loading, a system of linear algebraic equations is obtained for the iteration step r+1 of the increment m+1. In this system, $\mathbf{K}_T$ denotes the tangent stiffness matrix depending on the state of displacements before the iteration step, $\mathbf{R}$ is the residual force vector before this step, representing the imbalance of inner and outer forces, and $\mathbf{\Delta q}$ stands for the increment of nodal displacements, which is to be computed. The iteration is terminated if a specified error tolerance is met.

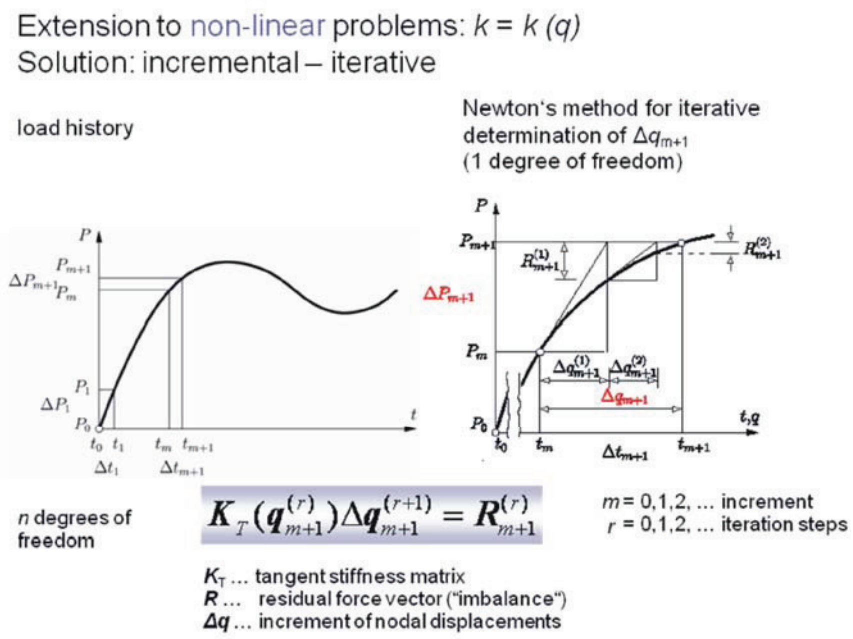


Fig. 15. Fundamentals of the finite element method: extension to non-linear problems

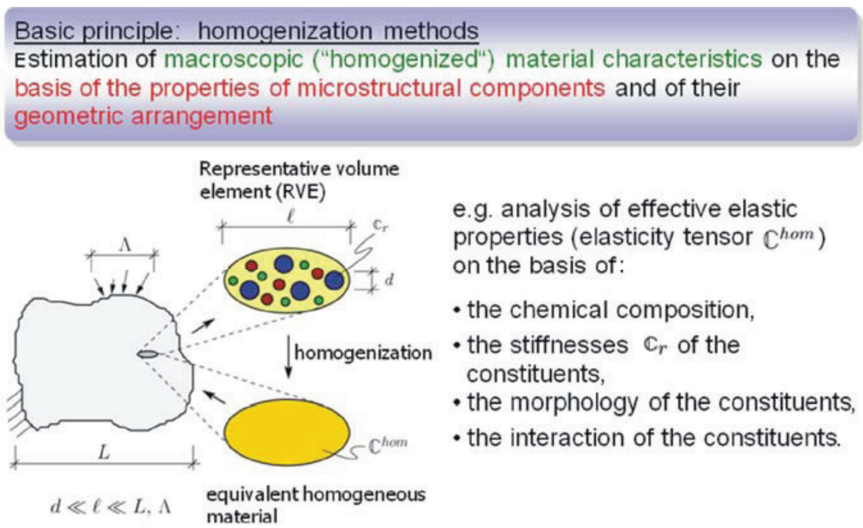


Fig. 16. Multi-scale formulations

The initially addressed dynamics of computational mechanics, which does not render staying at a specific instant of time advisable, manifests itself in two important irreversible tendencies of development, termed multi-scale formulations and multi-physics methods.

5. Multi-scale formulations and multi-physics methods

What are multi-scale formulations about? Notwithstanding their macroscopically homogeneous appearance, many materials have inhomogeneous microstructures. They contain different constituents which are distinguishable on a sufficiently small length scale. To assess the influence of the micro-structure on the macroscopic behavior of such materials, homogenization methods must be applied (Fig. 16).

For such methods, effective material properties such as e.g. strength, stiffness, thermal expansion, thermal conduction and specific further transport properties, electromagnetic characteristics etc. are deduced from corresponding properties of the individual constituents and from their geometric arrangement. A condition for the applicability of such methods is the possibility to define a representative volume element (RVE). Its characteristic length ℓ should at least be an order of magnitude smaller than the characteristic dimensions L and Δ of the investigated structure and of the load acting on it, respectively. The corresponding mathematical relation is $d \ll \ell \ll L, \Delta$, where d denotes the characteristic dimension of the individual components. It is referred to as the *condition of separation of scales*. Homogenization consists of determination of a mechanically equivalent homogeneous material for the RVE. Its stiffness matrix $\mathbb{C}^{hom}$ may e.g. be determined by means of continuum mechanics from the chemical composition of the RVE, the stiffnesses of the individual constituents, their morphology, e.g. spherical or cylindrical, and their interaction, characterized by a transitional matrix phase or else, by mutual contact of all phases.

What are multi-physics mechanical problems about? They are methods to solve problems where mechanics interacts with other branches of the natural sciences and/or the technical sciences need to be considered (Fig. 16).

As an example, let me mention thermo-chemo-mechanical couplings which play an important part in the development of stiffness and strength of young shotcrete, particularly used in tunnel construction. The scientific basis of such couplings is the thermodynamics of chemically reactive porous media. The macroscopic description of microscopic phenomena occurs with state variables and energetically conjugate thermodynamic forces. In the equation of evolution for the hydration of shotcrete, the degree of hydration ξ is the state variable, whereas the chemical affinity A, depending on ξ, is the corresponding thermodynamic force. In the given case, the thermo-chemo-mechanical analysis can be decomposed into 2 successive analyses: the thermo-chemical and the chemo-mechanical analysis. Components and fundamentals, respectively, of thermo-chemical analysis are the hydration heat L, which appears in the first principal theorem of thermodynamics, and Fourier's law of thermal conduction. The output of the analysis, consisting of the degree of hydration and the temperature fields, becomes the input for the chemo-mechanical analysis resulting in the stress and strain fields of the investigated structure that may be e.g. a tunnel shell.

6. Applications

In the following, I want to report on current applications of computer-assisted numerical mechanics at the Institute for Mechanics of Materials and Structures of Vienna University of Technology.

6.1. Rockfall on an oil-bearing pipeline

The first application deals with rockfall on a pipeline conducting oil (Fig. 17). In the Transalpine oil line, 35 million tons of raw oil are transported per year from the oil harbor Triest over the main ridge of the Alps to Southern German refineries. In the National Park *Hohe Tauern* the diameter of the tube is 1 m and the wall thickness 11 mm. The tube is embedded in widely gradated sandy gravel at a depth of 1 m. The route partly proceeds along nearly vertical walls of rock. According to estimates by geologists, rock boulders may drop from a height of up to 100 m. The Institute for Mechanics of Materials and Structures of Vienna University of Technology was entrusted with the investigation of the safety of the pipeline in case of rockboulders hitting the filler.

To quantify the load-carrying behavior of the tube, a model based on continuum mechanics, on the one hand, and the penetration process of a rock boulder hitting the gravel, on the other hand, was considered (Fig. 18). For prediction of the maximum impact and of the corresponding depth of penetration into the gravel, real-size experiments were conducted. Stimulated by dimensional analysis, the experiments were evaluated with the help of dimensionless mathematical penetration laws for metal projectiles into concrete. As results, formulae for the prognosis of the penetration depth of rock boulders into the gravel as well as for the maximum impact were obtained. By means of a statistical evaluation of the conducted rockfall experiments the expectation value of the penetration resistance of the gravel and its 5% and 95% quantiles were determined.

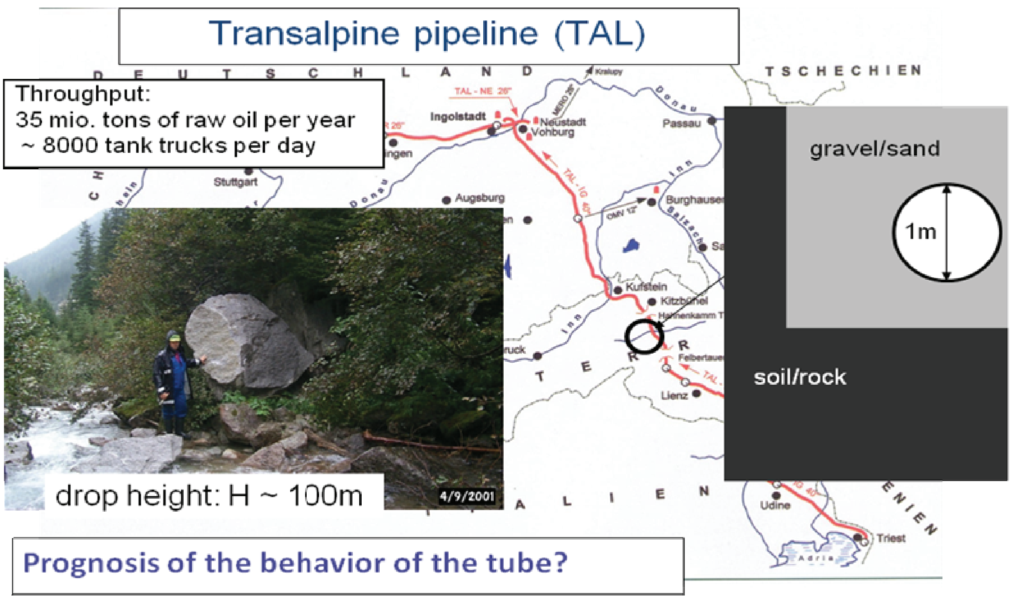


Fig. 17. Rockfall on a pipeline: posing the problem

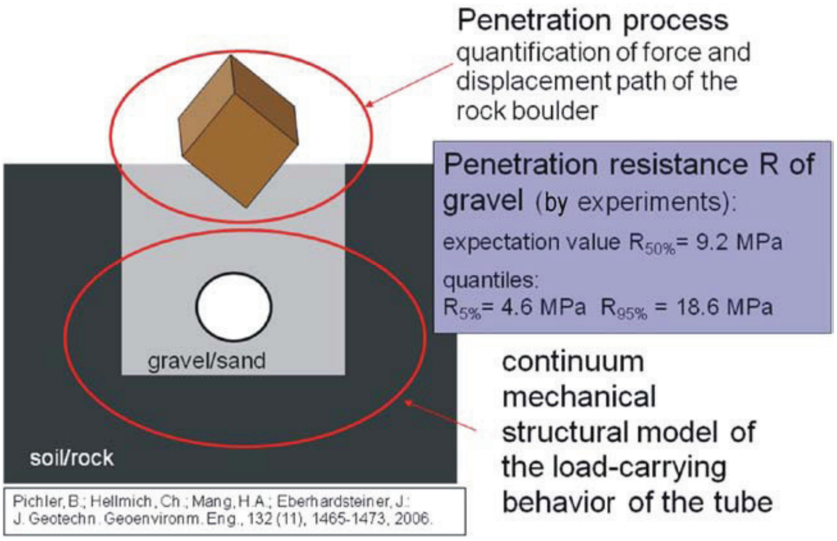


Fig. 18. Rockfall on a pipeline: problem treatment

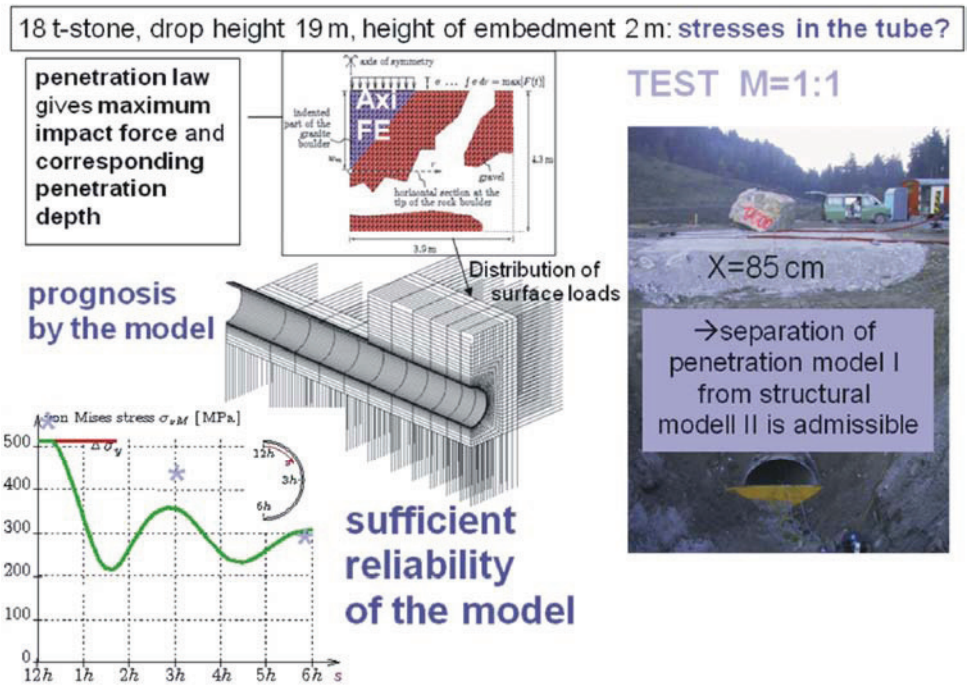


Fig. 19. Rockfall on a pipeline: design and validation of the analysis model

With the help of an axisymmetric finite element analysis the stress distribution that is mechanically equivalent to the maximum impact was obtained (Fig. 19). The stresses are boundary values which are needed for finite element analysis of a dimensional structural model. For consideration of the penetration depth of the rock boulder, the real height of the embedment of the tube was reduced in the analysis by the depth of penetration of the boulder at maximum impact. Since the duration of the penetration process is very much greater than the natural period of the structure at impact of the rock boulder, a quasi-static determination of the stress in the tube is admissible.

To validate the structural model, structural experiments were conducted. A rock boulder of approximately cubic shape, with a mass of 18 tons, was dropped from a height of approximately 19 m such that with its cusp it was hitting the surface above the pipeline buried under 2 m of gravel into which the block penetrated 85 cm.

From the structural model for quantifying the stress in the tube, a diagram was obtained, with the ordinate representing the von Mises stress, and the abscissa showing the circumferential coordinate measured from the highest point on the inner face of the tube and ending at the deepest point. In the structural experiments the strains were measured with strain gauges at selected points of the tube during the process of penetration. Knowing the strains, the stresses can be computed. The maximum value of the stresses in the areas of the maximum load agrees very well with the stresses predicted from the structural model. Hence, the structural model can be used for assessing the pipeline safety in case of rock boulders hitting the embedment.

To show that a depth of the embedment of only 1 m does not offer sufficient protection against rockfall, another structural experiment was carried out. The rock boulder of 18 tons was dropped from a height of 19 m, hitting the embedment surface of a pipeline buried at a depth of 1 m (Fig. 20). Immediately below the embedment of the impact, large plastic deformations of the pipeline occurred. Although the tube remained leak-tight, such deformations are inadmissible under normal working conditions.

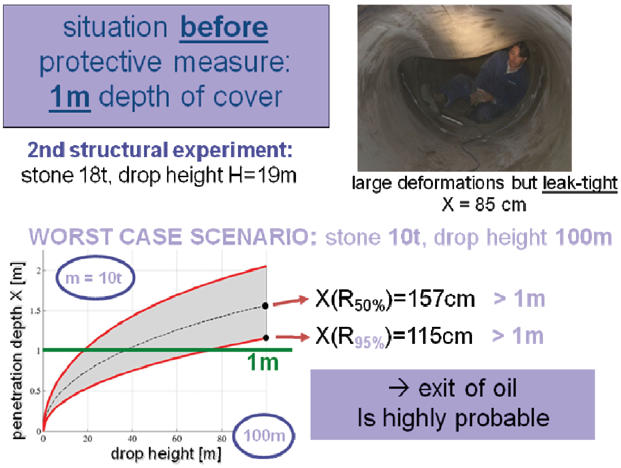


Fig. 20. Rockfall on a pipeline at an embedment depth of 1 m

The structural experiment and the validated structural model permit an assessment of *worst case scenarios,* according to prognoses by geologists. They have assumed that a rock boulder of 10 tons may fall down from a height of 100 meters. The situation for an embedment of 1 m depth can be assessed on the basis of the predicted penetration depth which is plotted in the diagram in Fig. 20 over the drop height. The dashed curve conforms to the expectation value of the penetration resistance of gravel. The two solid curves refer to the 5% and 95% quantiles of the penetration resistance. For a drop height of 100 m of a block of 10 tons a penetration depth of approximately 1.5 m into the gravel must be expected. Hence, the penetration depth is greater than the depth of the tube cover. Consequently, the stone would reach the tube and cause at least similar, inadmissible deformations as in the aforementioned structural experiment. If the penetration depth analysis is based on the 95% quantile of the penetration resistance of the gravel, the expected penetration is smaller but still greater than the existing depth of cover of the tube. Therefore, the exit of oil is highly probable. A depth of cover of 1 m is not sufficient for an adequate protection against rockfall.

For a depth of cover of 3 meters, however, the simulation of the previously presented structural model, based on the Finite Element Method, results in maximum values of the von Mises stress which are significantly below the yield limit (Fig. 21). Hence, large deformations of the tube are improbable and the exit of oil is even more improbable.

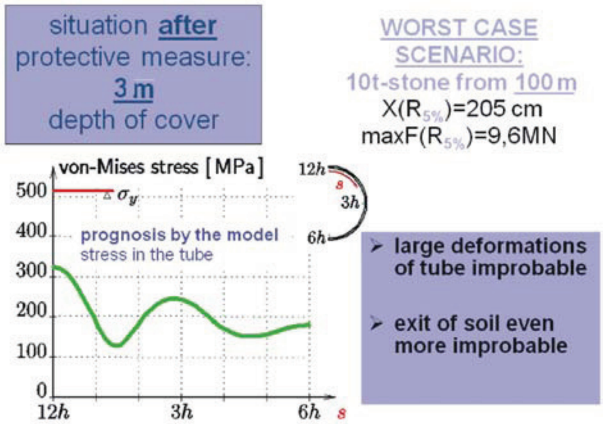


Fig. 21. Rockfall on a pipeline at an embedment depth of 3 m

6.2. Improvement of the postbuckling behavior

When presenting cases of damage, I discussed the collapse of a bridge because of buckling of the upper chord. For slender structures, loss of stability occurs before the yield limit of the material is reached. Hence, structural failure occurs.

The consequences of stability loss of a perfect structure, i.e. of one without deviations from the actual design, which does not occur in engineering practice, depends on the mechanical behavior at and after reaching the stability limit. It correlates with the mechanical behavior of the real structure which is imperfect. In the upper left part of Fig. 22, a cylindrical shell is shown which, in contrast to the one illustrated in the upper right part of Fig. 22, does not contain an elastic spring. Otherwise, the two shells are identical. For the shell without the spring, the consequences of stability loss are worse than for the one with the spring. This manifests itself in the form of the load-displacement diagrams after reaching the stability limit S which is a bifurcation point. In both diagrams, λ is a dimensionless parameter by which the point load $\overline{P}$ is multiplied and w_A is the deflection in the direction of this load (Fig. 22). After reaching S, it is necessary to distinguish between the dashed primary path and the projection of the secondary path, called post-buckling path, into the drawing plane. The spring does not only result in an increase of the stability limit S, but also in an increase of the slope of the mentioned projection of the secondary path at S (Fig. 22).

For engineering practice it is essential to know whether the perfect structure is imperfection-sensitive or imperfection-insensitive. The qualitative difference of these terms becomes obvious if the third curve in the two load-displacement diagrams is compared with each other.

For the same imperfection, for the case of the imperfection-sensitive shell without the spring, a non-monotonous load-displacement diagram, with $\bar{S}$ referring to the maximum value of the load parameter, is observed. However, for the case of the imperfection-insensitive shell, stiffened with a spring, a monotonously increasing load-displacement path is obtained. Point $\bar{S}$ characterizes the beginning of snap-through of the imperfection-sensitive shell. This is a dynamic process which, because of damping, decays quickly.

Through conversion of an imperfection-sensitive into an imperfection-insensitive structure, the stability loss of the imperfect structure can be avoided. Let us conceive the implications of, say, additional columns supporting a shell that spans an auditorium. Their role corresponds to the one of the spring in Fig. 22. This illustrates the possibility of undesirable architectural consequences of the aforementioned conversion.

For basic investigations, the function $\mathbf{G}^+$, which appears in the equilibrium condition of the secondary path, must be developed as a Taylor series for an arbitrary point on this path, denoted as D, at the bifurcation point C (Fig. 23). (Point D is not to be confused with the snap-through point D in Fig. 22). In this series, the asymptotic developments for the difference $\mathbf{v}^+$ between D and the corresponding point on the primary path have to be inserted together with the load difference $\Delta\lambda$, referred to C. Setting the coefficients of η, η^2, η^3, etc. in the obtained result equal to zero – η describes a parameter along the secondary path – yields relations allowing stepwise determination of $\mathbf{v}_1$ and λ_1, $\mathbf{v}_2$ and λ_2, etc.

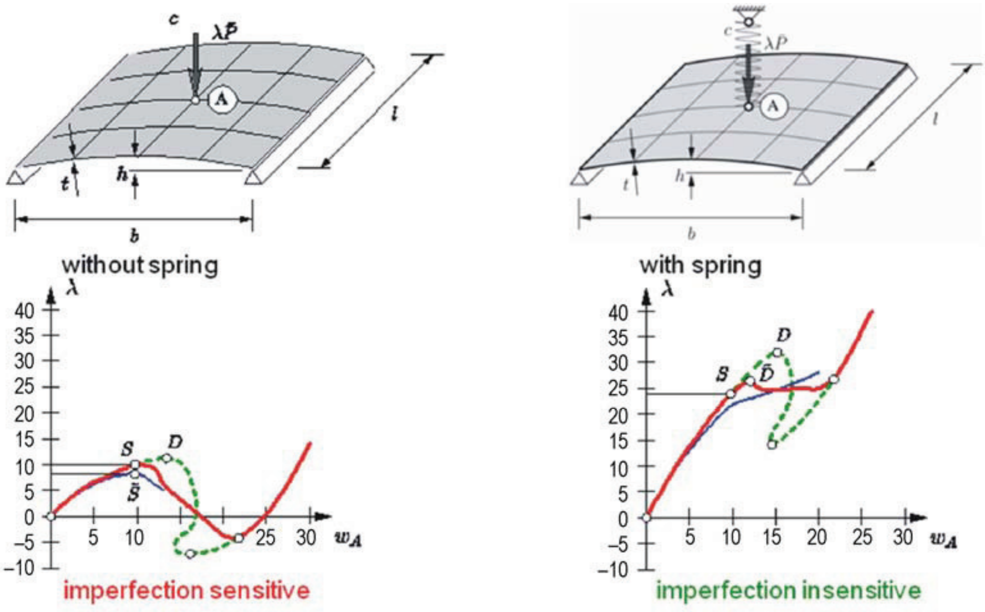


Fig. 22. Improvement of the postbuckling behavior

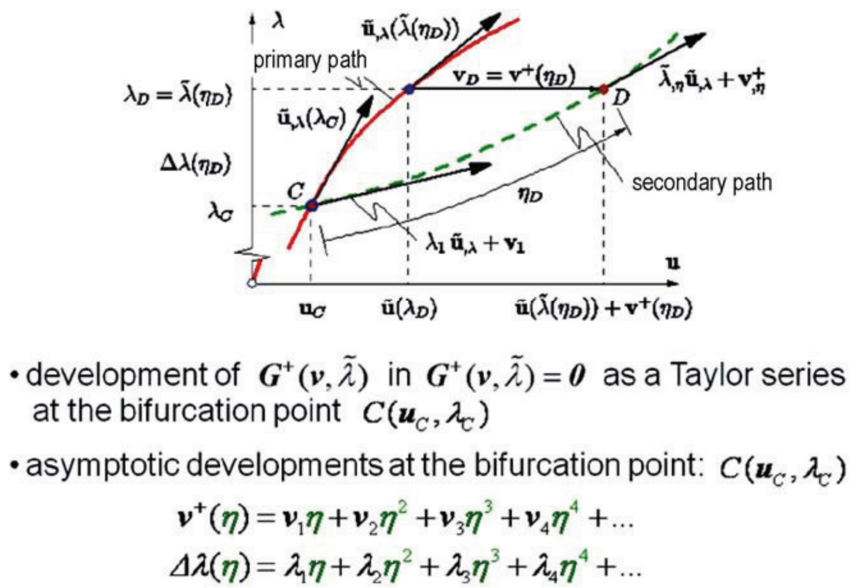


Fig. 23. Mathematical description of the initial postbuckling behavior

A special form of transition from imperfection sensitivity to imperfection insensitivity occurs for a specific system with 2 degrees of freedom. It consists of two elastically supported rigid bars that are connected by a hinge (Fig. 24). At point 1, a vertical force $\lambda\overline{P}$ is applied. The stiffness c_1 of the spring is the design parameter. In this case, the mathematical conditions for the transition from imperfection sensitivity to imperfection insensitivity are characterized by the vanishing of all coefficients λ_i in the expression for $\Delta\lambda(\eta)$. Hence, this expression becomes zero.

The transition from imperfection sensitivity to imperfection insensitivity occurs for $c_1 = 1.5$ (Fig. 25). The $\lambda^* - \lambda$ curves correspond to the load-displacement paths. They are part of the solution of the consistently linearized eigenvalue problem. The full eigenvalue curves refer to the bifurcation mode and the dashed eigenvalue curves to the snap-through mode: for $c_1 = 5.6$, the so-called nonlinearity parameter a_1 vanishes non-trivially. In this case, the eigenvalue curve has a saddle point at C, representing the stability limit.

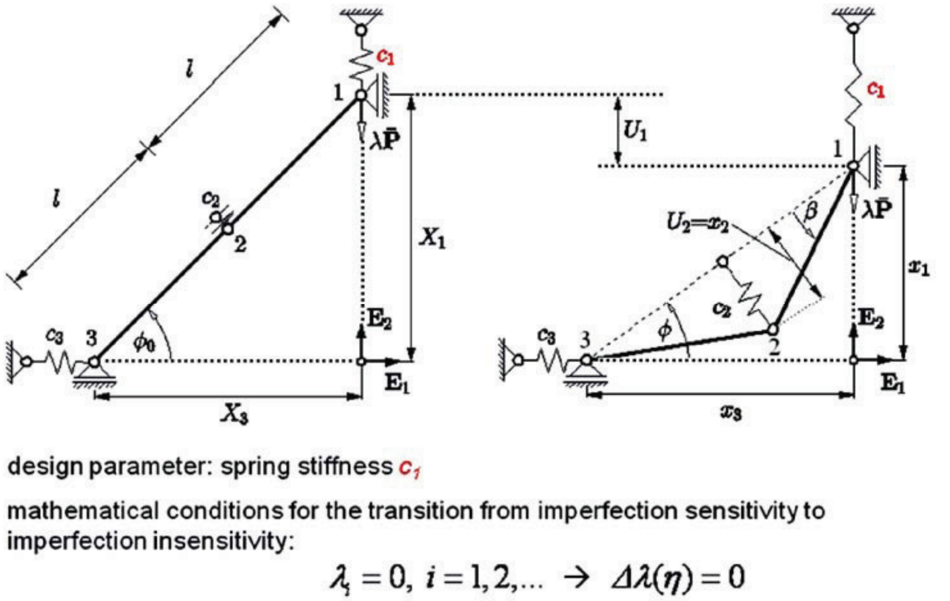


Fig. 24. Elastically supported rigid bars, connected by a hinge (system with 2 degrees of freedom)

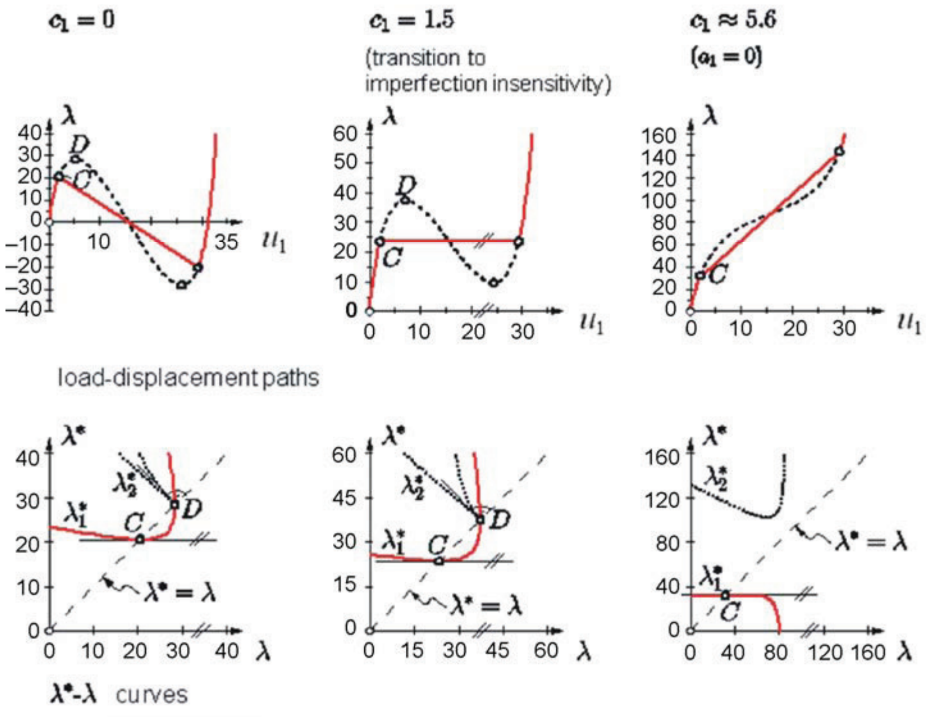


Fig. 25. Conversion of an imperfection-sensitive into an imperfection-insensitive structure

6.3. Thermo-chemo-mechanical couplings during the development of stiffness and strength of young shotcrete

To view computational mechanics just as a tool for numerical solutions of problems of mechanics would fail to appreciate the strong synergetic effect resulting from the increasing interweaving of mechanics and material science. Modern material science without adequate mechanical modelling would remain patchwork just as up-to-date mechanics without appropriate comprehension of processes that determine and change, respectively, observable phenomena of material behavior.

Let me continue where I stopped when explaining the fundamentals of multi-scale formulations and multi-physics methods. These were thermo-chemo-mechanical couplings during the development of stiffness and strength of young shotcrete. The following considerations, however, will not be restricted to this special type of concrete.

Generally, concrete is exposed to environmental influences such as variations of temperature and transport of aggressive fluids. A realistic description of the material behavior requires, in addition to inclusion of lower action planes in the frame of consideration of the deformation of structural elements and structures, the distribution and possible transport processes (Fig. 26). Hence, several fields of variables must be considered. Consequently, for solving a combined multi-scale and multi-field problem, a multi-field ansatz is required in addition to multi-scale modelling.

At hydration of young concrete, a rise in temperature occurs in the structural element which results in improving of the mechanical properties of young concrete. On the other hand, the temperature has an influence on the chemical reaction between cement and water. Temperature strains result in an additional load of the structure. Young concrete is characterized by the interaction of chemistry, temperature, and mechanics. Consideration of this interaction is typical for the problem-specific multi-physics method.

Because of hydration, the composition of young concrete is changing. In the present multi-scale modelling, this change is considered at the two lowest levels – the hydrate and the clinker level, respectively – and on the level of cement stone (Fig. 27). In addition to these two levels, the illustrated multi-scale model for young concrete has two more levels of observation: the mortar level and the macro level. With the help of suitable mathematical models for homogenization of mechanical properties based on the morphology of the components and on their mechanical properties at the three lower action planes, the macroscopic material properties are obtained.

Identification of these properties was facilitated by recent developments in the area of nano-indentation (Fig. 28). In nano-indentation (upper right illustration in Fig. 28) the tip of a diamond of given shape penetrates into the concrete. The forces and the penetration depth are recorded as functions of time. From the obtained force-penetration diagrams, elastic and viscous characteristic features and strength properties can be determined. Because of the heterogeneity of concrete, indentation experiments needed for a statistical evaluation are performed at the points of a quadratic grid. The three contour plots in Fig. 28 show the distribution of the modulus of elasticity on the rasterized surface for three cements of different grinding finesses. The distance between two neighbouring raster points is approximately 5 micrometers. With the so-obtained mechanical properties, the elastic properties of concrete can be determined on the basis of its composition through homogenization. The quality of the prognosis of elastic properties of concrete can be verified by means of validation experiments. As shown in the lower right illustration of Fig. 28, the predicted modulus of elasticity of a typical shotcrete, as a function of the degree of hydration, agrees well with experimentally determined values of the elasticity modulus.

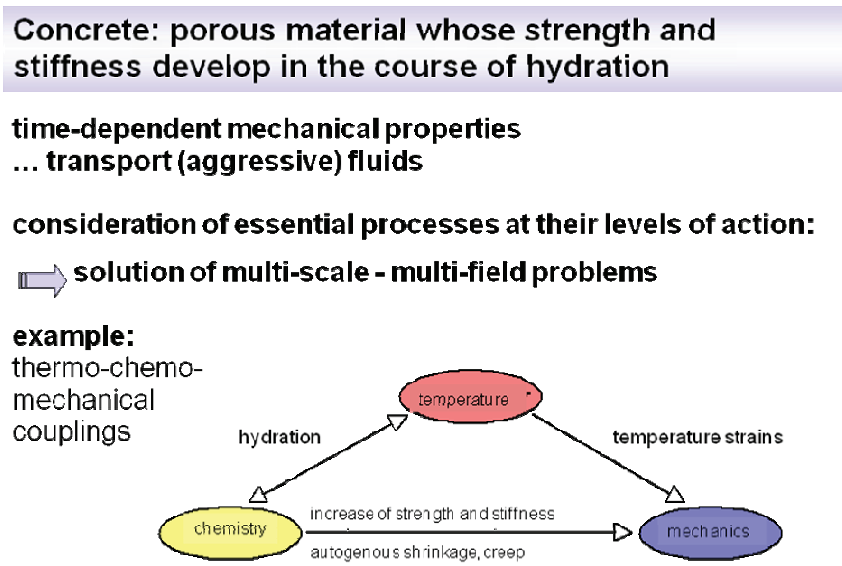


Fig. 26. Thermo-chemo-mechanical couplings of concrete

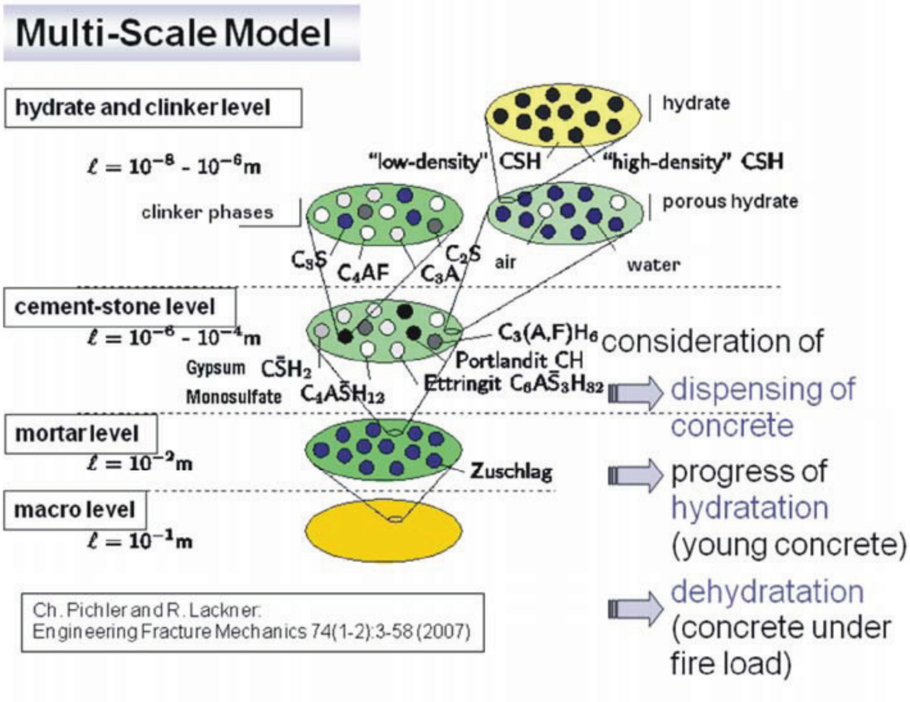


Fig. 27. Multi-scale modelling of concrete

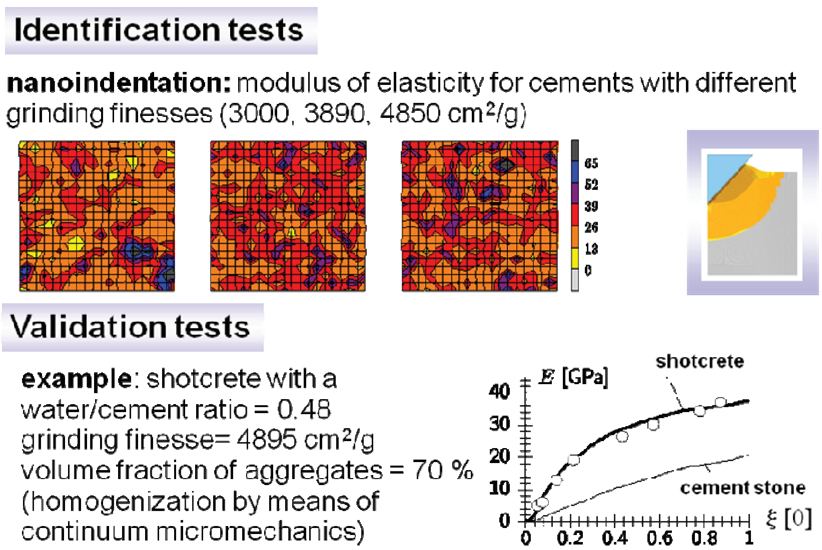


Fig. 28. Identification and validation of the multi-scale model for concrete

The presented multi-scale model of concrete was implemented in a hybrid, i.e. an experimental and computational method for determining the degree of utilization of shotcrete shells during tunneling (Fig. 29). With the help of this model, the elastic properties as well as the creep and shrinkage behavior of shotcrete can be determined in the frame of this method. In this way, the particular composition of this material and the construction situation enter the analysis. The displacements of the tunnel surface are obtained through interpolation between values of displacements measured at individual points of the tunnel surface. Thus, time-dependent boundary values are available for numerical determination of the time-dependent states of strain and stress through solution of a combined boundary and initial value problem. Knowledge of the time-dependent development of the stress state allows determination of the evolution of the utilization degree. The latter is characterized by the distance of point *a* in the lower right illustration in Fig. 29 from point *b* located on the failure surface. Point *a* represents the stress state at the considered point of the shotcrete shell. The failure curve is the geometric locus of all critical stress states. Its shape depends on the chosen material model. A degree of utilization of 100% signals material failure.

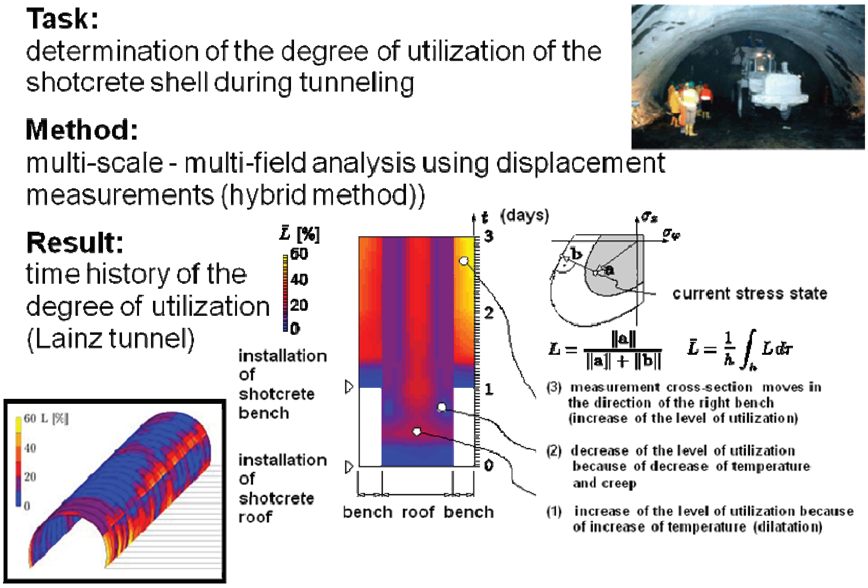


Fig. 29. Degree of utilization of the shotcrete shell during tunneling

The left illustration in Fig. 29 and the middle one show the time course of the distribution of the utilization degree of a particular cross-section of a railway tunnel excavated in the outskirts of Vienna. At first, only the roof area and later the bench areas are excavated and secured with shotcrete. With the elastic and viscous properties of the material, obtained from the multi-scale model, a multi-field analysis is carried out. In this way, the temperature increase in the shotcrete shell, in an early phase of hydration, can be modelled realistically. This allows for a realistic quantification of the resulting degree of utilization. The strongly pronounced creep capability of young shotcrete results in a fast degradation of the compressive stress that was originally built up in the shell. This entails a reduction of the utilization degree. During hydration, the stiffness and the strength of concrete are increasing as the hydration products are forming. For a temperature load, however, these mechanical quantities are decreasing strongly because of dehydration of the reaction products. This property of concrete is significant in case of a fire load, characterized by a fast temperature increase and by maximum values of the temperature exceeding 1000°C. The quick expansion of vaporizing water in the concrete does not only lead to the destruction of its structure, but also to spalling of concrete close to the surface. Modelling the corresponding increase of pressure in the pores of the heated concrete and changes of the mechanical properties of concrete requires again a multi-scale approach and a multi-field ansatz (Fig. 30).

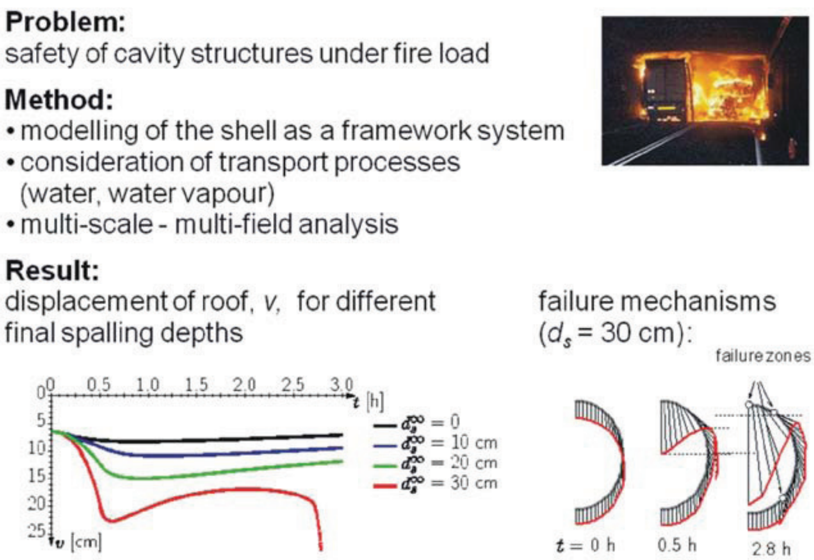


Fig. 30. Safety of cavity structures under fire load

Special characteristics of the analysis are modelling the shotcrete shell as a frame and consideration of transport processes when water evaporates. One of the results obtained from numerical simulations of the tube of a single-track tunnel subjected to fire load is the history of the roof displacement in the investigated cross-section of the tunnel for four different spalling scenarios characterized by different final depths of spalling (see the left illustration in Fig. 30).

According to the analysis, collapse of the tunnel shell occurs when a final spalling depth of 30 cm is reached. It is characterized by a fast increase of the roof displacement. The lower right illustration in Fig. 30 shows the corresponding collapse mechanism which has three failure zones.

7. Perspective and conclusion

Would one in computational mechanics ever say to the instant "Stay! You are so beautiful!", he or she would run the risk of getting captivated by complacency and of failing to clearly recognize the future perspectives of this comprehensive field characterized by continuous further development.

But how will the near future of this fundamental discipline of the engineering sciences, which at the same time represents an important spearhead of technological progress, actually look like?

Networking of mechanics with other fields of the material and engineering sciences will increasingly become an indispensable condition for the solution of challenging technical problems. Multi-physics will mutate from an occasionally overstrained catchword to a term that no longer can be imagined not to be there. It remains to be seen whether this will have an effect on university structures.

More fundamental analysis models will repel concepts that are mainly empirically founded. Multi-scale formulations will contribute decisively to better understanding of, according to Johann Wolfgang Goethe, "what the world (of engineering structures) holds together in the innermost". Mathematical methods that are considerably more powerful than the ones known today and algorithms based on these methods will exhaust the potential of models based on multi-physics methods and/or multi-scale formulations. Irrespective of the possibility to realize the dream of the quantum computer, the performance of computers will further increase. Not least, experimental validation of numerical results will become standard.

What is the conclusion that can be drawn from this perspective into the future of computer-assisted numerical mechanics? To answer this question I am going back, on the one hand, to the original version of the final speech of Dr. Faustus. On the other hand, I am referring to the title of the original (German) version of this paper. Then, the answer briefly reads: "In computational mechanics one must never say to the instant: 'Stay! You are so beautiful!' ".

8. Acknowledgements

I wish to express my sincere thanks for the active support when preparing this article to the Dean of the Faculty of Civil Engineering of Vienna University of Technology, Prof. Josef Eberhardsteiner, and to the collaborators from this Institute, especially to Prof. Friedrich Firneis and Ms. Gabriele Ostrowski, who helped with the translation of the German manuscript into English and with its preparation for publication, respectively, to Prof. Christian Hellmich, Dr. Karin Hofstetter, Prof. Roman Lackner, now at the University of Innsbruck, and to Dr. Herbert Müllner, Dr. Bernhard Pichler and, last not least, to Mag. Martina Pöll.

Information on the scientific work on which the lecture is based is available on the Website of the Institute for Mechanics of Materials and Structures of Vienna University of Technology: *http://www.imws.tuwien.ac.at*