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Validation of Computations: A Synopsis of Criteria

Critères de vérification de calculs par ordinateur

Kriterien zur Überprüfung von Computerberechnungen

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SUMMARY
The most important checks and considerations to validate computations from an engineer's point of view are discussed. A set of general criteria is given which apply to every structural analysis. In addition special checks for dynamic problems are presented. The outlined criteria are illustrated by examples.

RESUME
Les tests et les considérations les plus importants permettant la vérification, du point de vue de l'ingénieur, de calculs effectués par ordinateur sont présentés. Des critères applicables pour tous les types de calcul de structures sont énumérés. Pour les problèmes dynamiques, des tests spécifiques sont proposés. Ces critères sont illustrés par des exemples.

ZUSAMMENFASSUNG
Die wichtigsten Tests und Überlegungen zur Überprüfung einer Computer-Rechnung vom Standpunkt des Ingenieurs aus werden diskutiert. Ein Satz allgemeiner Kriterien wird angegeben, welche für jede Tragwerksberechnung Gültigkeit haben. Für dynamische Probleme werden spezielle Tests zusammengestellt. Die Ausführungen werden durch Beispiele illustriert.

1. INTRODUCTION

Computerized structural analysis has developed rapidly over the past two decades. Powerful computers and a large variety of software packages permit the efficient solution of many static, dynamic and field problems. The scope and complexity of the problems which can be solved as well as the accuracy which can be achieved have steadily increased over the years. New facilities such as computer graphics, CAD/CAE and still more automated, stable and efficient numerical techniques have made the use of computers in structural analysis very attractive.

Today, computerized analysis is no longer a domain of highly specialized engineers. More and more structural analysts with little knowledge of the underlying numerical methods are taking advantage of the existing facilities. All computations, however, have to be verified before the results are further used. It ist therefore indispensable that the analyst is familiar with the validation criteria, a synopsis of which is given in this paper. Furthermore, it is required that the software in use supports this validation by furnishing the appropriate information and also automatically performs certain checks as far as possible and feasible.

2. EQUATIONS OF MOTION

The analysis of a structure is done on an analysis model which contains simplifications and idealisations, but has to reflect the essential physical behaviour of the structure. Today, analysis models usually are built up from finite elements. As sketched in Fig. 1, on each node acts a resulting internal force $\vec{F}$, an inertia force $\vec{T}$, a damping force $\vec{D}$ and an external force $\vec{P}$, which have to be in equilibrium. Representing the forces of all nodes by the vectors $\{F\}$, $\{T\}$, $\{D\}$ and $\{P\}$, respectively, the equilibrium equation

$$\{T\} + \{D\} + \{F\} + \{P\} = \{0\} \tag{1}$$

must hold. In an actual numerical analysis equ. (1) will only be satisfied within a certain accuracy. Introducing

$$\{P\} = \{Q\} + \{R\} \tag{2}$$

where $\{Q\}$ denotes the external loads and $\{R\}$ the reactions, equ. (1) appears in the form

$$\{T\} + \{D\} + \{F\} + \{Q\} + \{R\} = \{\varepsilon\} \tag{3}$$

with the residual nodal forces $\{\varepsilon\}$. If the problem is formulated in constrained nodal displacements $\{q\}$, $\{R\}$ will disappear in equ. (3).

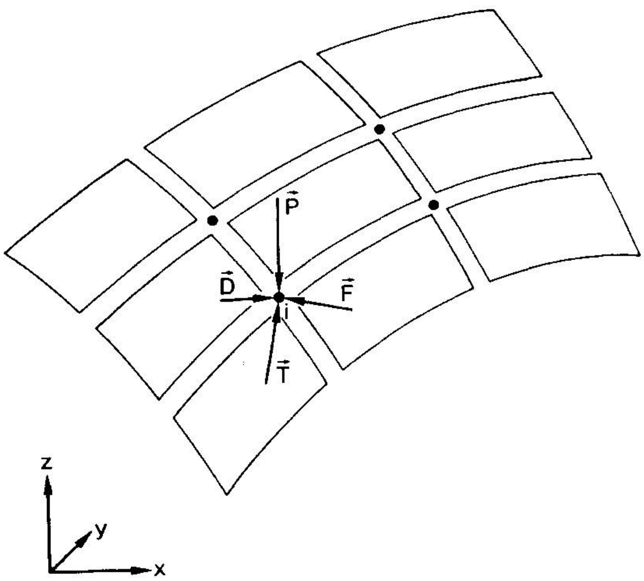


Fig. 1 FE-Model

In a linear analysis, the displacements of the structure depend on the total loads only and not on the loading history. Thus the problem can be formulated in total displacements. In constrained displacements $\{q\}$ the equilibrium equation becomes

$$[M]\ \{\ddot{q}\} + [C]\ \{\dot{q}\} + [K]\ \{q\} = \{Q\} \tag{4}$$

with the mass matrix $[M]$, the viscous damping matrix $[C]$ and the stiffness matrix $[K]$. In addition, two initial conditions exist. Deleting the inertia and the damping term, the basic equation for static analysis is obtained. Dropping only the inertia term, the governing equation of a number of field problems including heat transfer analysis results.

In the nonlinear case, it is advisable to formulate the equations of motion in an incremental form. Usually the internal forces are thereby obtained from a linearised stiffness matrix. Equ. (3), however, must hold for the nonlinearized expressions. Thus a solution obtained from linearized equations eventually has to be improved iteratively until $\{\varepsilon\}$ in equ. (3) is sufficiently small.

The complete time-dependent solution of the equations of motion is obtained by discretisation in the time domain. As shown in Fig. 2, $\{q(t)\}$ is replaced by displacements $\{q_i\}$ at discrete times t_i and a polynomial interpolation in-between. The basic form of the equation for the integration is

$$[A]\ \{\Delta q\} = \{\bar{Q}\} \tag{5}$$

The integration matrix $[A]$ depends on the mass, damping and stiffness matrix and on the integration time step Δt. $[\bar{Q}]$ is a known effective load vector which also contains $\{\dot{q}\}$ and $\{\ddot{q}\}$ at the beginning of the time step. Equ. (5) permits the step by step integration of the equations of motion in the linear and nonlinear case.

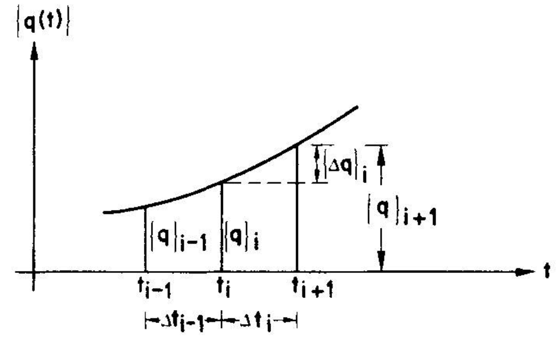


Fig. 2 Discretisation in the time domain

3. VALIDATION OF THE ANALYSIS MODEL

In a first step the analysis model has to be designed conceptually before it is defined numerically. This work is of central importance for the reliability of the analysis. All essential physical properties of the real structure must be reflected in the model. Considerations have to be made on the type of the analysis, the discretisation including the properties of the elements used, the required accuracy, the available computing facilities, the numerical methods to be used and last but not least on the time schedule and costs. In this phase primarily engineering knowledge and experience is required, supported in special cases by preliminary numerical investigations.

Once the model is defined conceptually, it will be described numerically as input data for a particular computer program. In Table 1 the most important checks to validate the model are listed. The geometry and topology of the discretisation are verfied graphically. Modern interactive graphic mesh generators permit the definition and validation in one step. The numerical values of the cross sectional properties and of the material properties have to be checked. For a displacement model only geometric constraints have to be considered. In the general case they appear as linear constraint equations

$$\sum_k a_{ik} - d_i = o \tag{6}$$

where the a_{ik} denote constraint coefficients, d_i is a fixed displacement and the

☐ Geometry and topology
☐ Cross sectional properties
☐ Material properties
☐ Constraints
☐ Applied loads
☐ Number of modes
☐ Time or load steps
☐ Convergence criteria
☐ Simple static load case

Table 1 Validation of the analysis model

q_k are degress of freedom. Linear constraint equations serve for instance to model rigid parts of the structure or to represent generalized tying conditions. The simple constraint $q_i = o$ is a special case of equ. (6). Each linear constraint equation leads to a reaction which is distributed to the degrees of freedom according to the constraint coefficients. These coefficients as well as the position of the constrained degrees of freedom have to be checked. Finally the applied loads have to be validated with respect to magnitude and position.

In a modal dynamic analysis the number of modes has to be chosen according to the frequency content and the participation factors of the loads. In dynamic or nonlinear analyses time steps or load steps have to be selected. The integration time step Δt is critical for the accuracy of the solution. As a rule of thumb, in an unconditionally stable algorithm Δt should satisfy the condition

$$\Delta t \leq \frac{1}{20\ f_{max}} \qquad (7)$$

where f_{max} [Hz] denotes the highest frequency of interest. This leads to approximately 2 % numerical damping in f_{max}. It also should be noted that stability limits of unconditionally stable algorithms usually have been derived for the linear case and may have to be modified for nonlinear analyses. Finally the convergence criteria for iterative solution techniques (eigenvalue extraction, nonlinear analysis) have to be validated or adapted to the problem.

It is always a good idea first to subject a complex model to a simple load case such as gravitational loading and to run a linear static analysis. The inspection of the results frequently leads to the uncovering of hidden errors in the model and thus can save the analyst from useless major computations.

4. VALIDATION OF RESULTS: GENERAL CRITERIA

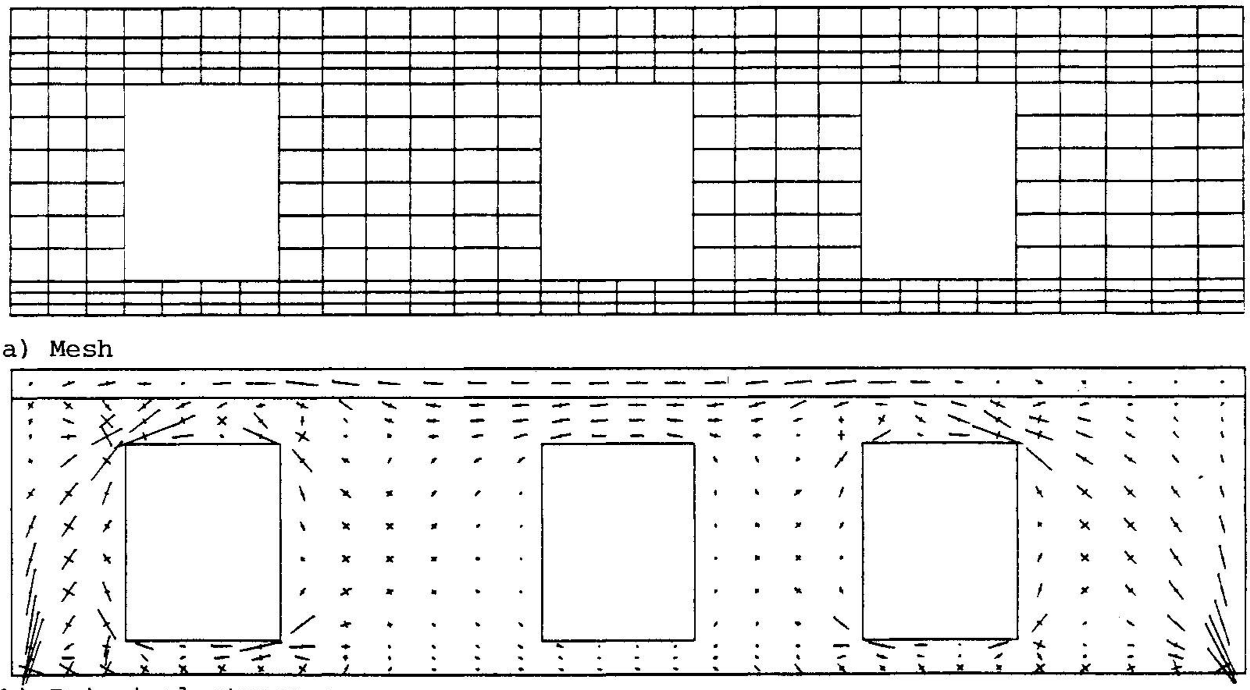
Table 2 shows the most important general criteria to validate results. These criteria are basically applicable to linear and nonlinear static and dynamic analyses as well as to field problems. First of all, global and local equilibrium has to be satisfied. Thus the residual forces according to equ. (3) have to be small for the solution without linearisation. In the case of direct integration, the equilibrium equations may look different depending on the integration

- ☐ Equilibrium
- ☐ Geometric constraints
- ☐ Static constraints
- ☐ Stability
- ☐ Energy
- ☐ Convergence criteria
- ☐ Plausibility checks
- ☐ Experimental results

Table 2 General criteria

algorithm used. Equilibrium also means, that the momentum and moment of momentum theorems etc. are satisfied. It would thus be useful to obtain the resultant vectors of momentum, moment of momentum, damping forces and external forces at selected times from the program. Violation of equilibrium can indicate a program error, a not converged solution, to few modes or an ill-conditioned system matrix.

Geometric constraints are verified by inspecting the reactions and the deformed shape of the structure. It is necessary that the program also calculates the constraint forces of linear constraint equations. Violation of geometric constraints usually stems from input errors. Static constraints, on the other hand, are automatically satisfied in displacement models in the sense of the under-



a) Mesh

b) Principal stresses

Fig. 3 Wall with openings

lying energy expressions. Thus the quality of satisfaction of prescribed stress conditions is an indication of the quality of the mesh near the respective boundaries. Fig. 3 shows as an illustration the mesh and the principal stresses at the centroids of the elements of a supporting wall with three rectangular openings. It is seen that the trajectories reflect well the static boundary conditions along the stress free edges.

Global instabilities will occur when the determinant of the stiffness matrix (static analysis) or of the integration matrix in equ. (5) (direct integration) becomes very small or changes sign. The determinant is easily obtained as product of the diagonal terms of the triangular factor. An unstable solution can indicate a real, physical instability of the structure or may be caused by numerical reasons. Examples of numerical instabilities are static analyses with high differences in the stiffness coefficients or dynamic analyses with an only conditionally stable integration algorithm. Thus care must be taken to identify the causes of an instability.

In a static analysis, the strain energy of the elements is always greater than or equal to zero. A negative strain energy usually stems from erroneous material coefficients. The strain energy per element should be a slowly varying function. This requirement leads to criteria for the mesh quality. In a dynamic analysis, the kinetic energy, the dissipation energy and the work of the external forces are useful quantities to validate the results.

Iterative solution procedures such as eigenvalue extraction or a number of nonlinear techniques are controlled by convergence parameters. The satisfaction of the convergence criteria has to be checked in the solution.

Every analysis should be validated by plausibility checks. In simple cases, global checks suffice. It is important that the analyst is familiar with the appropriate methods such as for instance the Rayleigh quotient for eigenvalues or the limit theorems of plasticity for the determination of collaps loads. In more complex situations, a detailed counter analysis using different methods and/or a different model can clarify questions about a solution.

Finally, the comparison of numerical results with experiments may give further evidence of the validity of a solution. In the machine building industry, tests are frequently possible on prototypes before production starts, whereas in civil engineering the tests usually can be performed only after the completion of the building. Such a posteriori tests, however, are still very useful to calibrate the analysis methods. In all comparisons between numerical and experimental results, the accuracy of the experiment has to be included in the considerations.

5. VALIDATION OF MODAL ANALYSES

There exist a number of additional criteria for the modal analysis of linear dynamic problems which are listed in Table 3. First, the eigensystem of the undamped structure has to be determined. Assuming a harmonic motion, equ. (4) reduces to

$$([K] - \omega^2 [M]) \{\bar{q}\} = \{o\} \tag{8}$$

with the eigenfrequency ω and the eigenvector $\{\bar{q}\}$.

- ☐ Error bounds of eigenvalues
- ☐ Sturm sequence check
- ☐ Shape of eigenvectors
- ☐ Orthogonality
- ☐ Completeness of modal loads

Table 3 Criteria for modal dynamic analyses

In the numerical calculations, equ. (8) will only be satisfied within a certain accuracy. By calculating the corresponding residual vector it is possible to establish error bounds on the eigenvalues $\lambda_i = \omega_i{}^2$. Thus the accuracy of the eigenvalues of the analysis model can be verified.

It is important, that no frequencies have been missed in the interval of interest. This is particularly important if the number of degrees of freedom of the model has been reduced by condensation. Shifting the origin of the eigenvalue axis to a shift-point Λ (Fig. 4), equ. (8) becomes

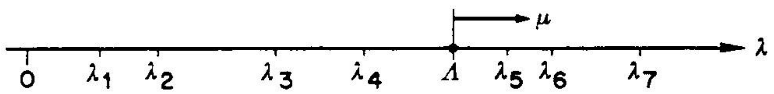


Fig. 4 Shift of eigenvalues

$$([\bar{K}] - \mu[M])\ \{\bar{q}\} = \{o\} \tag{9}$$

with

$$[\bar{K}] = [K] - \Lambda[M] \tag{10}$$

The Sturm sequence check states, that the number of negative terms on the diagonal of the triangular factor of $[\bar{K}]$ is equal to the number of eigenvalues below the shift-point. Applying the check to the uncondensed system at different values of Λ determines the number of eigenvalues in the corresponding intervals.

The discretisation of the structure has to be such that the analysis model can assume the mode shapes corresponding to the eigenvalues of interest. Thus the shapes of the eigenvectors permit a judgement of the quality of the model. In particular, if the spacial wave lengths are of the order of the dimensions of the finite elements, the eigenvector usually reflects properties of the analysis model rather than of the real structure.

The eigenvectors are orthogonal with respect to the stiffness and mass matrix. Thus the quality of satisfaction of the orthogonality conditions is a measure for the quality of the set of eigenvectors.

In a modal analysis, the load vector $\{Q\}$ in equ. (4) is represented by its modal contributions

$$P_i(t) = \{\bar{q}_i\}^T\ \{Q\} \qquad i = 1,...n \tag{11}$$

where n denotes the number of modes included in the analysis. It is important to chose n such that $\{Q\}$ is properly represented with respect to time and space. Usually n is much smaller than the number of degrees of freedom of the analysis model which leads to the omission of high-frequency contents of the solution. If the load is properly represented by the n modes, the neglected structural response will be a quasi-static response. By such considerations the solution can be further improved.

6. CONCLUDING REMARKS

Many structural analysis programs perform certain validation checks automatically or provide options to initiate such tests. The software developers should always keep the validation aspect of an analysis in mind and must make dedicated efforts to enhance the corresponding program capabilities.

It can be expected that the reliability of computerized analysis will still further increase during the next years, especially in the field of nonlinear problems. In particular, self-adaptive discretization and solution techniques in combination with interactive graphics will greatly facilitate the validation of computations in the future. From the experimental side, more and better test data will permit a still better calibration of the numerical procedures as well as for instance of complex material models such as reinforced concrete. All these developments will make computerized structural analysis a still more powerful tool in the hands of the knowledgable and experienced engineer.

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