DESIGN OF NONLINEAR MATERIAL BY MATHEMATICAL PROGRAMMING

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SUMMARY

The material planning is an important and developing part of applied mechanics. The problem is usually solved with FEM, which leads to highly non-linear equations and this cause several numerical problems. This paper presents a method where the problem is solved with mathematical programming and uses the theorem of virtual force. The material model is included in the compatibility equations. The material parameters appear as unknowns in the non-linear object function, while the conditions remain linear. The uniqueness and stability of the material model (e.g. Drucker-postulates) is assured by inequality conditions. The boundary conditions are considered. Sample problems were run by a program for non-linear mathematical programming problems written in Fortran 77.

Keywords: Mathematical Programming, Material Design, Non-linear Material Models

1. INTRODUCTION

The material design is now an important and developing part of applied mechanics. There are several ways to achieve our design goals, but the problem is usually solved with FEM. The greatest disadvantages of this method are that they lead to highly non-linear equations and this cause several numerical problems (Popper Gy., Csizmás F., 1993). In contraire, the problem can be formulated using the concept of virtual energy. This formulation leads to a mathematical programming problem (Karush, W. 1939).

The state of equilibrium of a structure is usually determined by solving the system of the equilibrium and compatibility equations. Another possibility is to use the extremum principles of virtual energy with the strain energy and complementary strain energy function (Vásárhelyi A., Lógó J., 1989).

At first assume the principle of small displacement is valid and the material law is linear. The primal problem expresses the virtual force theorem by the help of a quadratic programming problem (Cohn, M. Z., Maier, G., 1979), where the equality conditions are

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the equilibrium equations concerning to the structure and the object function is the complementary strain energy. In this problem, we are looking for the minimum of the object function.

Forming the dual problem, one can find that it contains the compatibility equations as equality condition with the strain energy function as object function. Again, the problem is to find the minimum of the object function. The complementer problem gives the usual formulation.

This formulation allows wide possibilities in

- delimiting the stresses and displacements,
- satisfying the boundary conditions,
- defining yield domain,
- choosing either elastic or elasto-plastic constitutive laws.

These can be built into the mathematical programming problem as equality or inequality conditions, iff the conditions are consistent.

The main advantage of the mathematical programming formulation can be seen, if we introduce different material parameters (e.g. elastic modulus, cross-section parameters, etc.) as unknowns. Using the primal formulation, the object function becomes of higher order even in the case of linear material law, but the equality conditions remain linear.

In the rest of the paper this formulation is shown, and applied to a simple, statically indeterminate beam structure with a Green-type hyperelastic material model (Bojtár I., 1988)

$$\mathbf{å}_{ij} = \frac{\partial \Omega}{\partial \mathbf{ó}_{ij}}.$$

The integration of the stresses (**ó**) concerning the volume were calculated by the Gauss-Legendre scheme, and thus the coefficients can be represented by the diagonal matrix $\langle r \rangle$. These coefficients are independent of the stresses and therefore the order of the derivation and the numerical integration can be changed.

2. THE MATHEMATICAL PROGRAMMING PROBLEM

The elastic state of a structure can be determined through the equilibrium and compatibility equations in the following form (Szabó J., Roller B., 1978)

$$\mathbf{T}^* \cdot \mathbf{B}^* \cdot \langle r \rangle \cdot \mathbf{ó} + \mathbf{P} = 0, \qquad \text{(equilibrium equations)}$$

$$\mathbf{B} \cdot \mathbf{T} \cdot \mathbf{u} + \langle r \rangle \cdot \nabla \Omega(\mathbf{ó}) = 0, \qquad \text{(compatibility equations)}$$

$$\mathbf{P}\big|_{S_P} = 0, \qquad \text{(stress boundary conditions)}$$

$$\mathbf{u}\big|_{S_u} = 0. \qquad \text{(displacement bound. conditions)}$$

Here **ó** is the stress vector, **P** is the vector of external forces, **u** is the displacement vector, **B** is the geometric matrix, **ă** is the strain vector, **T** is the transformation matrix

between the local and global coordinate systems. The unknowns are the **u** and **ó** vectors.

The structure of this system of equations can be visualized as in Fig.1. The **F** matrix is hyperdiagonal, and if the material law is linear, the elements are constants, otherwise they are functions.

The static and kinematic boundary conditions can be considered at the adequate equations The simplest method in the case of prescribed zero displacement or zero stress is to clear the appropriate row and column as shown in Fig. 1. This is impossible only if the material law is not linear and thus the **F** matrix can not be explicitly stated. In this

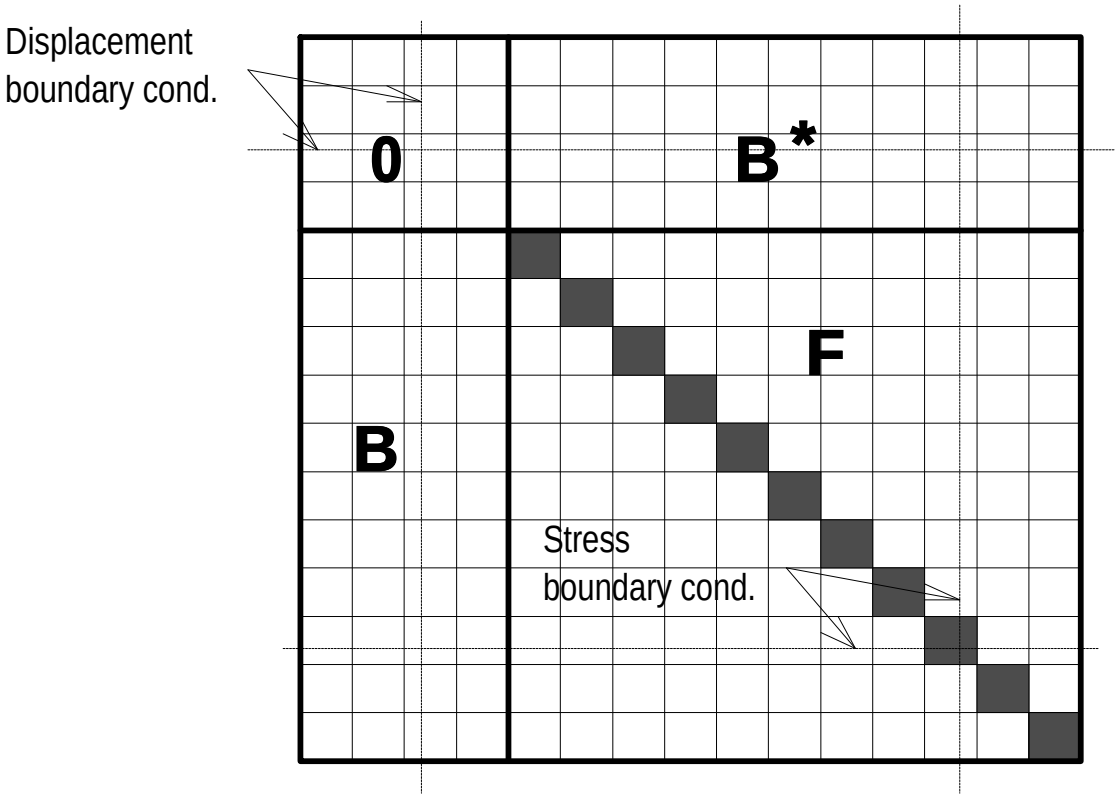

Fig. 1 The structure of the equilibrium and compatibility equations. The boundary conditions can be considered by clearing the appropriate rows and columns.

case, the appropriate stress in the material law must be substituted with zero, but in the geometric matrix (**B**), the appropriate row can be deleted. Otherwise, the boundary conditions can be included as additional equality constrains.

Based on the principle of virtual force theorem, it is possible to give a pair of mathematical programming problem, either of them defines the equilibrium state of a structure, and which are in primal-dual relationship. The primal problem expresses the minimum of virtual complementary energy

$$\min\left\{\int_V \Omega(s)\,dV\right\}$$

$$\mathbf{T}^* \cdot \mathbf{B}^* \cdot \langle r \rangle \cdot \boldsymbol{\acute{o}} + \mathbf{P} = 0\,, \qquad \text{(equilibrium equations)}$$

$$\mathbf{P}\big|_{S_P} = 0\,, \qquad \text{(stress boundary conditions)}$$

$$\mathbf{u}\big|_{S_u} = 0\,. \qquad \text{(displacement bound. conditions)}$$

The Wolf-dual of this problem is

$$\min\left\{\int_V W(\boldsymbol{\mathring{a}})\,dV - \mathbf{P}^*\mathbf{u}\right\}$$

$$\mathbf{B} \cdot \mathbf{T} \cdot \mathbf{u} + \langle r \rangle \cdot \nabla\Omega(\boldsymbol{\acute{o}}) = 0\,, \qquad \text{(compatibility equations)}$$

$$\mathbf{P}\big|_{S_P} = 0\,, \qquad \text{(stress boundary conditions)}$$

$$\mathbf{u}\big|_{S_u} = 0\,, \qquad \text{(displacement bound. conditions)}$$

which expresses the minimum of the virtual energy. The complementer problem, which includes the equality conditions of both the primal and dual formulation, recalls the usual system of equilibrium and compatibility equations.

The theorem of virtual forces and virtual displacements gives a necessary condition for the existence of the optimum for the primal and dual problem, respectively. On the other hand, the convexity of the feasible domain gives the sufficient condition. Moreover, if the energy function is convex in the domain of material stability, the optimum is global optimum and it is the same for the primal and dual problem.

3. THE MATERIAL MODEL

The most simple and convenient material model is based on Hooke's law, and expresses a linear function between the strains and stresses

$$\boldsymbol{\mathring{a}} = \nabla\Omega(\boldsymbol{\acute{o}}) = \mathbf{F} \cdot \boldsymbol{\acute{o}}\,.$$

In this case, the equality constraints are linear either in the primal or in the dual problem, and the object function is quadratic.

$$\min\left\{\sum_{elements} \tfrac{1}{2}\boldsymbol{\acute{o}}^* \cdot \mathbf{F} \cdot \boldsymbol{\acute{o}}\right\} \qquad \text{(primal problem)}$$

$$\mathbf{T}^* \cdot \mathbf{B}^* \cdot \langle r \rangle \boldsymbol{\acute{o}} + \mathbf{P} = 0\,, \qquad \text{(equilibrium equations)}$$

$$\min\left\{\sum_{elements} \tfrac{1}{2}\boldsymbol{\acute{o}}^* \cdot \mathbf{F} \cdot \boldsymbol{\acute{o}} - \mathbf{P}^* \cdot \mathbf{u}\right\} \qquad \text{(dual problem)}$$

$$\mathbf{B} \cdot \mathbf{T} \cdot \mathbf{u} + \langle r \rangle \nabla\Omega(\boldsymbol{\acute{o}}) = 0\,. \qquad \text{(compatibility equations)}$$

The boundary conditions for both problems are

$$\mathbf{P}\Big|_{S_P} = 0, \qquad \text{(stress boundary conditions)}$$

$$\mathbf{u}\Big|_{S_u} = 0. \qquad \text{(displacement bound. conditions)}$$

In the linear case, the stability of the material is automatically satisfied. From the computational point of view, one of the most simple non-linear material behavior is a Green-type hyperelastic model. In a three-parameter quadratic model, the relation between stresses and strains can be stated as

$$e_{ij} = \nabla\Omega(s_{ij}) = \Phi_1 d_{ij} + \Phi_2 s_{ij} + \Phi_3 s_{ik} s_{jk},$$

where Φ_1, Φ_2 and Φ_3 are material parameters. The complementary virtual energy is

$$\Omega(s) = \int_0^s \nabla\Omega(s_{ij}) ds_{ij}.$$

The integral was calculated numerically with a three-point Gauss-Legendre scheme

$$\Omega(s) = \tfrac{s}{2} \sum_{i=1}^{3} c_i \nabla\Omega\left[\tfrac{s}{2}(x_i + 1)\right].$$

Here, c_i are the Gauss-weights at the integration points x_i, and s is the unknown upper limit of the integration.

If the material law is non-linear, the stability of the material is not automatically satisfied. The stability can be ensured by the Drucker-postulate (Drucker, D. C., 1962), which states that the work of any external effect rate ($\dot{T}_i, \dot{F}_i$) on the displacement rate ($\dot{u}_i$) is positive,

$$\int_A \dot{T}_i \dot{u}_i dA + \int_V \dot{F}_i \dot{u}_i dV > 0.$$

Using the principle of virtual work, one can rewrite this in the following form

$$\acute{o}_{ij} \mathring{a}_{ij} > 0.$$

The rate of the stresses and strains can be understood as the change of the effect in each iteration step (r) of the non-linear programming solver and therefore

$$\Delta\acute{o}_{ij} = \acute{o}_{ij}^{r+1} - \acute{o}_{ij}^{r},$$

Using the definition of the Green-model one can write

$$\mathbf{H}'_{ijkl} \Delta\acute{o}_{ij} \Delta\acute{o}_{kl} > 0,$$

where $\mathbf{H}'_{ijkl}$ is the Hessian of the complementary energy function. This non-linear inequality condition ensures the stability and convexity of the material, however, it is more strict than it would follow form the laws of thermodynamics.

4. A SIMPLE BEAM STRUCTURE

The above described method was applied at the calculation of the a simple, 2D, statically indeterminate structure shown in Fig. 2. The structure consists of two elements, each

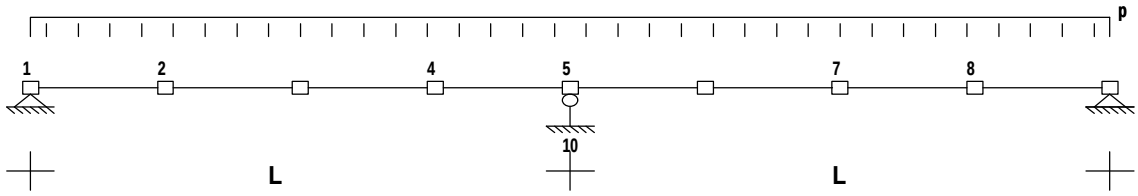

Fig. 2 The beam structure

with three internal Gauss-Legendre integration points for the integration of the energy function. Each node has three degrees of freedom (e_x, e_y, g_{xy}) and the stress state of each node is described by the three element vector

$$s = \begin{bmatrix} s_x \\ s_y \\ t_{xy} \end{bmatrix}.$$

The modified geometric matrix ($\tilde{\mathbf{B}}$), concerning the boundary conditions (shaded rows and columns) in the global coordinate system is

		1			2			3			4			5			6			7			8			9		5		10	
	1			-1																											
12		1	l_{12}		-1																										
			1			-1																									
				1			-1																								
23					1	l_{23}		-1																								
						1			-1																						
							1			-1																					
34								1	l_{34}		-1																				
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510														-1															l_{510}	1		
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The vector of external forces (**P**) can be formed by concentrating the distributed load to the nodes.

The material law described in chapter 3 is now simply

$$e_x = \Phi_1 + \Phi_2 s_x + \Phi_3 (s_x^2 + t_{xy}^2),$$
$$g_{xy} = \Phi_2 t_{xy} + \Phi_3 s_x t_{xy}$$

The complementary virtual energy can be written as the function of the stresses

$$\Omega(s,t) = \int_0^s \int_0^t e_x \, dt_{xy} \, ds_x + \int_0^s \int_0^t g_{xy} \, dt_{xy} \, ds_x ,$$

where the upper limits of the integrals are unknowns. Using three-point Gauss-Legendre integration scheme

$$\Omega(s,t) = \frac{s}{2}\frac{t}{2}\sum_{i=1}^{3}\sum_{j=1}^{3} c_i c_j e_x\left(\tfrac{s}{2}(x_i+1), \tfrac{t}{2}(x_i+1)\right) +$$
$$\frac{s}{2}\frac{t}{2}\sum_{i=1}^{3}\sum_{j=1}^{3} c_i c_j g_{xy}\left(\tfrac{s}{2}(x_i+1), \tfrac{t}{2}(x_i+1)\right).$$

The total complementary strain energy of the structure can be obtained by the volume integration along the two elements

$$\Omega_t = \sum_{n=1}^{2} \frac{l_n}{2} \sum_{i=1}^{3} c_i \Omega(s_i, t_i).$$

Again, a three-point Gauss-Legendre integration scheme was used for the volume integration. s_i and t_i denotes here the stress state in the *i*-th Gauss point.

The non-linear mathematical programming problem now can be stated as

$\min\{\Omega_t\}$	(object function)
$\tilde{\mathbf{B}}^* \cdot \langle r \rangle s + \mathbf{P} = 0$	(equality conditions)
$\Delta s^* \cdot \mathbf{H}' \cdot \Delta s > 0.$	(inequality conditions)

The unknowns are the stress vectors in the Gauss-Legendre integration points and the three material parameters. The structure has one degree of statical indetermination and therefore, eliminating the equality conditions, one variable remains free. Altogether, there are 4 independent variables, and two inequality constrains for each integration point.

The problem was run on a non-linear programming solver (Fiacco, A. V., McCormick, G. P., 1968) written in Fortran 77 in a Silicon Graphics workstation environment. Since there was not defined any yield function, the Drucker-postulate was the active criterion at the stop of the iteration.

The numerical computation has shown clearly that this formulation gives the desired results and thus it can be the base of future extensions.

5. CONCLUSION

A mathematical programming formulation has been shown for the calculation of statically indeterminate structures in the framework of virtual force and virtual displacement theorems. A Green-type hyperelastic material model has been used with three unknown parameters to be optimized. This simple model has shown the applicability of the mathematical programming formulation.
This may serve as a base to further extension which includes the use of more sophisticated material models, the yield condition and plasticity features, and the consideration of time dependency.

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