HYPERELASTIC MATERIAL MODEL DEVELOPMENT USING SIMBOLIC PROGRAMMING

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Abstract – *Very important function in development of the Finite Element Method (FEM) have several material models. This paper presents that simbolic programming represents one powerful tool in the generating material models. The main attention is given on the hyperelastic material model development for 3D eight-node finite element. The secound part of this paper presents example of tension and compression cubes.*

1. INTRODUCTION

Finite element method (FEM) is the most revolutionary and most general numerical method, which has now become necessary in solving scientific and practical tasks in many areas of science, technology and medicine. Important role in the development of FEM has a large number of material models, including hyperelastic material model, which will be presened in this paper. The advantage of symbolic programming in the development of new material models is that the corresponding finite element code generated automatically. The paper uses a system for symbolic and algebraic programming (Mathematica) and within it a developed modules AceGen [1], AceFEM [2] and AceShare [3], which together constitute a system named of Symbolic Mechanics System [4].

Mathematica is a basic and very powerful tool for working with formulas and to perform various mathematical operations and expressions with the help of computers. Modern versions include the possibility of presenting results and numerical analysis.

The Mathematica package ***AceGen*** is used for the automatic derivation of formulae needed in numerical procedures. Symbolic derivation of the characteristic quantities (e.g. gradients, tangent operators, sensitivity vectors,…) leads to exponential behavior of derived expressions, both in time and space.
AceGen offers multi-language code generation (Fortran/Fortran90, C, Mathematica language, Matlab language) and automatic interface to general numerical environments (MathLink connection to Mathematica, Matlab) and specialized finite element environments (AceFEM, FEAP, ELFEN, ABAQUS, …)
The ***AceFEM*** package is a general finite element environment designed to solve multi-physics and multi-field problems. The AceFEM package explores advantages of symbolic capabilities of Mathematica while maintaining numerical efficiency of commercial finite element environment. The main part of the package includes procedures that are not numerically intensive, such as processing of the user input data, mesh generation, control of the solution procedures, graphic post-processing of the results, etc.

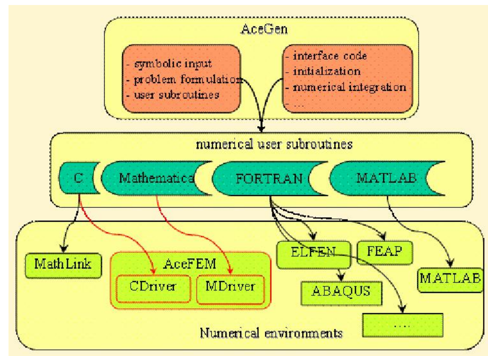


Figure 1. System for generating a finite element code and its further analysis

Those procedures are written in Mathematica language and executed inside Mathematica. The numerical module includes numerically intensive operations, such as evaluation and assembly of the finite element quantities (tangent matrix, residual, sensitivity vectors, etc.), solution of the linear system of equations, contact search procedures, etc.. The numerical module exists as Mathematica package as well as external program written in C language and is connected with Mathematica via the MathLink protocol. This unique capability gives the user the opportunity to solve industrial large-scale problems with several 100000 unknowns and to use advanced capabilities of Mathematica such as high precision arithmetic, interval arithmetic, or even symbolic evaluation of FE quantities to analyze various properties of the numerical procedures on relatively small examples. On Figure 2. is shown the organizational structure of a AceFEM.

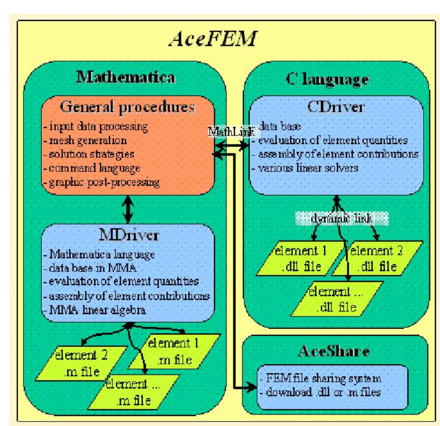


Figure 2. The structure of AceFEM organization

The AceFEM package comes with a library of finite elements (solid, thermal, contact,... 2D, 3D,...) including full symbolic input for most of the elements. Additional elements can be accessed through the AceShare finite element file sharing system. The element oriented approach enables easy creation of costumized finite element based applications in Mathematica. In combination with the automatic code generation package AceGen the AceFEM package represents an ideal tool for a rapid development of new numerical models.
The AceFEM environment comes with a small build-in library including standard solid, structural, thermal and contact elements. Additional elements are accessed and automatically downloadable through the AceShare system. The AceShare system is a file sharing system built in AceFEM that makes AceGen symbolic descriptions and generated finite element user subroutines available for other users to download over the Internet. The AceShare system enables: browsing the on-line FEM libraries; downloading the finite elements from the on-line libraries; formation of the user defined library that can be posted on the internet to be used by other users of the AceFEM system.

2. THEORETICAL BASIS

3D isoparametric eight-node finite element is used to model three-dimensional bodies of general shape (3D Continuum). Interpolation of geometry and displacements are in the form [5]

$$\mathbf{x} = \begin{Bmatrix} x_1 \\ x_2 \\ x_3 \end{Bmatrix} = \begin{Bmatrix} x \\ y \\ z \end{Bmatrix} = \mathbf{NX} \tag{1}$$

$$\mathbf{u} = \begin{Bmatrix} u_1 \\ u_2 \\ u_3 \end{Bmatrix} = \begin{Bmatrix} u \\ v \\ w \end{Bmatrix} = \mathbf{NU} \tag{2}$$

where are: interpolation matrix **N** and vectors coordinates of nodes **X** and displacement of nodes **U**. Note that equation (1) and (2) can be written in component form as

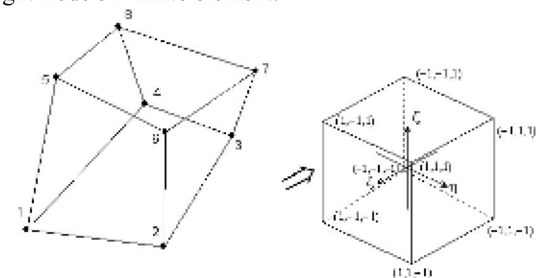
$$x_i = \sum_{k=1}^{N_{node}} N_k X_i^k \qquad i = 1, 2, 3 \tag{3}$$

$$u_i = \sum_{k=1}^{N_{node}} N_k U_i^k \qquad i = 1, 2, 3 \tag{4}$$

where i = 1 corresponds to the x axis, and j= 2 - y axis, and k= 3 – z. In the case of a finite element with 8 nodes, interpolation functions are in the form:

$$N_i(\xi,\eta,\zeta) = \frac{1}{8}(1+\xi\xi_i)(1+\eta\eta_i)(1+\zeta\zeta_i); \quad i = 1,2,.....,8 \tag{5}$$

Functions $N_i(\xi,\eta,\zeta)$ are linear in ξ,η,ζ and because of this fact this element is called a linear. Its surfaces are the planes in physical space, as shown in Figure 3. Element from x-y-z space is mapped into a cube whose coordinates of nodes ξ_i, η_i, ζ_i are equal ±1, as it is given with table on Figure 3. This procedure of marking and input of nodes is characteristic for AceGen defining of eight-node 3D finite element.



NODE	ξ_i	η_i	ζ_i
1	-1	-1	-1
2	1	-1	-1
3	1	1	-1
4	-1	1	-1
5	-1	-1	1
6	1	-1	1
7	1	1	1
8	-1	1	1

Figure 3. 3D eight-node finite element

If we introduce a Jacobian transformation between Cartesian and natural systems, as

$$\mathbf{J} = \left[\frac{\partial \mathbf{x}}{\partial \boldsymbol{\xi}}\right] = \begin{bmatrix} \frac{\partial x}{\partial \xi} & \frac{\partial y}{\partial \xi} & \frac{\partial z}{\partial \xi} \\ \frac{\partial x}{\partial \eta} & \frac{\partial y}{\partial \eta} & \frac{\partial z}{\partial \eta} \\ \frac{\partial x}{\partial \zeta} & \frac{\partial y}{\partial \zeta} & \frac{\partial z}{\partial \zeta} \end{bmatrix} \tag{6}$$

and inverse Jacobian

$$\mathbf{J}^{-1} = \left[\frac{\partial \boldsymbol{\xi}}{\partial \mathbf{x}}\right] = \begin{bmatrix} \frac{\partial \xi}{\partial x} & \frac{\partial \eta}{\partial x} & \frac{\partial \zeta}{\partial x} \\ \frac{\partial \xi}{\partial y} & \frac{\partial \eta}{\partial y} & \frac{\partial \zeta}{\partial y} \\ \frac{\partial \xi}{\partial z} & \frac{\partial \eta}{\partial z} & \frac{\partial \zeta}{\partial z} \end{bmatrix} \tag{7}$$

We introduce the gradient of the displacement,

$$\mathbf{D} = \left[\frac{\partial \mathbf{u}}{\partial \mathbf{x}}\right] = \begin{bmatrix} \frac{\partial u}{\partial x} & \frac{\partial v}{\partial x} & \frac{\partial w}{\partial x} \\ \frac{\partial u}{\partial y} & \frac{\partial v}{\partial y} & \frac{\partial w}{\partial y} \\ \frac{\partial u}{\partial z} & \frac{\partial v}{\partial z} & \frac{\partial w}{\partial z} \end{bmatrix} \tag{8}$$

and tensor of deformation gradient

$$\mathbf{F} = \mathbf{1} + \mathbf{D} \tag{9}$$

Hyperelastic (Neo-Hookean) material model. Hyperelasticity refers to the material, where the final elastic strain is reversible. Rubber and many other polymeric materials belong into this category. Stresses for these materials are calculated using the strain energy.
Second Piola-Kirchhof stress tensor is defined as first derivative strain energy function by right Cauchy-Green deformation tensor [6]

$$\mathbf{S} = 2\frac{\partial \Pi}{\partial \mathbf{C}} \tag{10}$$

where right Cauchy-Green deeformation tensor is equal

$$\mathbf{C} = \mathbf{F}^{\mathrm{T}}\mathbf{F} = \begin{bmatrix} \lambda_1{}^2 & 0 & 0 \\ 0 & \lambda_2{}^2 & 0 \\ 0 & 0 & \lambda_3{}^2 \end{bmatrix} \tag{11}$$

and function is expressed in terms of streches $\lambda_1, \lambda_2, \lambda_3$.

Invariants of tensor $\mathbf{C}$ are:

$$\begin{aligned} I_1 &= Tr[\mathbf{C}] = \lambda_1^2 + \lambda_2^2 + \lambda_3^2 \\ I_2 &= \frac{1}{2}((Tr\mathbf{C})^2 - Tr(\mathbf{C}^2)) = \lambda_2^2\lambda_3^2 + \lambda_3^2\lambda_1^2 + \lambda_1^2\lambda_2^2 \\ I_3 &= Det(\mathbf{C}) = \lambda_1^2\lambda_2^2\lambda_3^2 \end{aligned} \tag{12}$$

Deformation gradient can be divided on volumetric and distortional component.

$$\mathbf{F} = {}^{iso}\mathbf{F}\,{}^{vol}\mathbf{F} \tag{13}$$

As we know that the determinant of deformation gradient gives the ratio of initial and current volume, we can conclude that the determinant of the distortional component is equal to:

$$\det {}^{iso}\mathbf{F} = 1 \tag{14}$$

to satisfy this requirement distortional component must be in the form:

$${}^{iso}F_{ij} = F_{ij}J^{-1/3} \tag{15}$$

Distortional component of right Cauchy-Green deeformation tensor C_{ij} may be defined as:

$${}^{iso}\mathbf{C} = J^{-2/3}\mathbf{C} \tag{16}$$

as follows from the definition of deformation distortional gradient:

$$\begin{aligned} {}^{iso}\mathbf{C} &= {}^{iso}\mathbf{F}^T\,{}^{iso}\mathbf{F} = J^{-1/3}\mathbf{F}^T J^{-1/3}\mathbf{F} = \\ &= J^{-2/3}\mathbf{F}^T\mathbf{F} \end{aligned} \tag{17}$$

Right Cauchy-Green deformation can be expressed in terms of streches:

$${}^{iso}\lambda_A^2 = J^{-2/3}\lambda_A^2 \tag{18}$$

$${}^{iso}\lambda_A = J^{-1/3}\lambda_A \tag{19}$$

from definition of Jacobian we have:

$$J^2 = \det\mathbf{C} = \begin{vmatrix} \lambda_1^2 & 0 & 0 \\ 0 & \lambda_2^2 & 0 \\ 0 & 0 & \lambda_3^2 \end{vmatrix} = \lambda_1^2\lambda_2^2\lambda_3^2 \tag{20}$$

$$J = \lambda_1\lambda_2\lambda_3 = \det(\mathbf{F}) \tag{21}$$

$${}^{iso}\lambda_A = (\lambda_1\lambda_2\lambda_3)^{-1/3}\lambda_A \tag{22}$$

$${}^{iso}I_A = J^{-1/3}I_A \tag{23}$$

Strain energy function in the case of isotropy is shown as function expressed in terms of streches:

$$\Pi = \Pi(\lambda_1, \lambda_2, \lambda_3) \tag{24}$$

This fuction is simetric function expressed in terms of streches $\lambda_1, \lambda_2, \lambda_3$.

Neo-Hookean material model of rubber is model defined with two parametars (constants). Hyperelastic potencial in this case is represented as sum of isohoric and volumetric part.

Isohoric part of strain energy is set as:

$${}^{iso}\Pi = \frac{1}{2}\mu({}^{iso}\lambda_1^2 + {}^{iso}\lambda_2^2 + {}^{iso}\lambda_3^2 - 3) \tag{25}$$

and volumetric part:

$${}^{vol}\Pi = \frac{1}{2}K(J^2 - 1)^2 \tag{26}$$

Total strain energy function of Neo-Hookean material model of rubber [7] i [8] is given as

$$\Pi = \Pi({}^{iso}I_1, {}^{iso}I_2, J) = \Pi({}^{iso}\lambda_1, {}^{iso}\lambda_2, {}^{iso}\lambda_3, J) \tag{27}$$

and equal :

$$\begin{aligned} \Pi &= {}^{iso}\Pi + {}^{vol}\Pi = \frac{\mu}{2}\left({}^{iso}I_1 - 3\right) + \frac{K}{2}\left(J-1\right)^2 \\ \Pi &= \frac{\mu}{2}\left(J^{-\frac{1}{3}}I_1 - 3\right) + \frac{K}{2}\left(J-1\right)^2 \\ \Pi &= \frac{\mu}{2}\left(J^{-\frac{1}{3}}Tr[\mathbf{C}] - 3\right) + \frac{K}{2}\left(\det\mathbf{F} - 1\right)^2 \end{aligned} \tag{28}$$

where μ present shear modulus (other literature G or C_1) which is equal:

$$\mu = \frac{E}{2(1+\nu)} \tag{29}$$

and K (C_3 or K_b) is bulk modulus equal to:

$$K = \frac{E}{3(1-2\nu)} \tag{30}$$

where E is Young elasticity modulus, and ν Poisson coeficient.

Some authors [4] i [9], define strain energy function of Neo-Hookean material modelof rubber in the different shape:

$$\Pi = \frac{\lambda}{2}(\det\mathbf{F} - 1)^2 + \mu\left(\frac{Tr[\mathbf{C}] - 3}{2} - Log(\det\mathbf{F})\right) \tag{31}$$

where μ present shear modulus, and λ Lame's constant equal to:

$$\lambda = \frac{E}{(1+\nu)(1-2\nu)} \tag{32}$$

Green-Lagrange deformation tensor defined by deformation related to the initial configuration.

$$\boldsymbol{\varepsilon} = \frac{1}{2}(\mathbf{C} - \mathbf{1}) \tag{33}$$

Cauchy stress tensor $\boldsymbol{\sigma}$ is equal

$$\boldsymbol{\sigma} = {}^t\rho\frac{\partial \Pi}{\partial \mathbf{F}}\mathbf{F}^T \tag{34}$$

where ${}^t\rho$ is current density. For definition of Cauchy stress tensor was used free energy per unit of current volume ${}^t\rho\Pi$. If for definition of stress tensor use free energy per unit of initial volume ${}^0\rho\Pi$, we have Kirchhoff stress tensor $\bar{\boldsymbol{\sigma}}$. Determinant of tensor of deformation gradient is equal:

$$\det(\mathbf{F}) = \frac{{}^0\rho}{{}^t\rho} \Rightarrow {}^t\rho = \frac{{}^0\rho}{\det(\mathbf{F})} \tag{35}$$

so we have

$$\begin{aligned} \boldsymbol{\sigma} &= \frac{{}^0\rho}{\det(\mathbf{F})}\frac{\partial \Pi}{\partial \mathbf{F}}\mathbf{F}^T \\ \bar{\boldsymbol{\sigma}} &= \frac{1}{J}\frac{\partial \Pi}{\partial \mathbf{F}}\mathbf{F}^T \end{aligned} \tag{36}$$

for Cauchy stress tensor and Kirchhoff-stress tensor.

3. GENERATION OF HYPERELASTIC (NEO-HOOKEAN) MATERIAL MODEL AND ANALYSIS OF OBTAINED RESULTS

AceGen procedure for generating code to work in finite element environment consists of a several steps:

1. **Step 1 – Initialization**

- Read of AceGen code generator

```
<<AceGen`;
```

- Select the working environment

```
SMSInitialize["test","Environment"→"AceFEM"];
```

- Select the type of finite element (**H1**- 3D eight-node finite element)

```
SMSTemplate["SMSTopology"→"H1","SMSSymmetricTangent"→True];
```

2. **Step 2 – Definition of user subroutine**

```
SMSStandardModule["Tangent and residual"];
```

- Definition of input-output variables
- Kinematics of the selected type of finite element
- Definition of test function
- Definition of governing equations
- Definition of Jacobian matrix
- Definition of stiffness matrix

3. **Step 3 – Definition of output variables using subroutine for postprocessing**

```
SMSStandardModule["Postprocessing"];
```

4. **Step 4 – Generation of code**

```
SMSWrite[];
```

Standard AceFEM procedure consists two basic phase.

1. **Phase Data Entry**

- phase starts with `SMTInputData`
- description of the material model of finite element (`SMTAddDomain`) defined by code which must be generated before analisys
- mesh generating (`InputData, SMTAddElement`)
- setting boundary conditions (`SMTAddEssentialBoundary`)
- setting loads (`SMTAddNaturalBoundary`)

2. **Phase analysis**

- phase starts with `SMTAnalysis`
- solution procedures are executed by the user enters inputs (`SMTConvergence`)
- solving problem by standard Newton-Raphson iterative method
- postprocessing of results as part of analisys (`SMTShowMesh`) or later independently of the analysis (`SMTPut`)

Example. Tension and compression of 3D eight-node finite element

Observes the example of tension and 3D eight-node finite element (length 2cm, Young modulus $E = 11.83 \, N/cm^2$ and Poisson coeficient $\nu = 0.499$), boundary conditions are shown on Figure 4. Nodes 5,6,7,8 are free and set to prescribed displacement in the z-direction and increment of displacement is equal 0.1 .

$u = v = w = 0$ for nodes 1,2,3,4

$u \neq v \neq w \neq 0$ for nodes 5,6,7,8

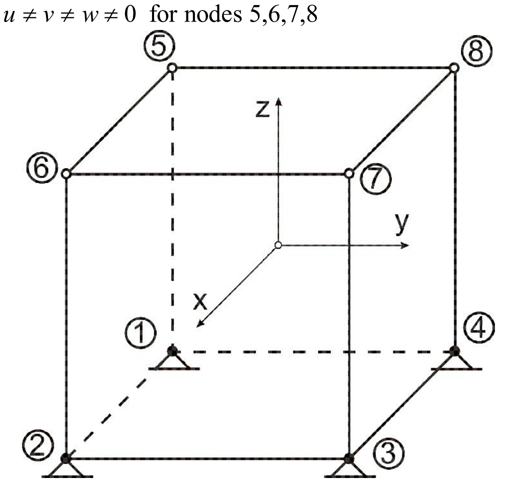


Figure 4. Boundary conditions

Displacement field for case of tension of cube is shown on Figure 5 and displacement field for case of compression of cube is shown on Figure 6. Beside displacement in z direction, it is possible to show the other two displacement, as well as the normal and shear components of stress and strain by simply selecting from Field palette, which is located in the main menu of AceFEM window.

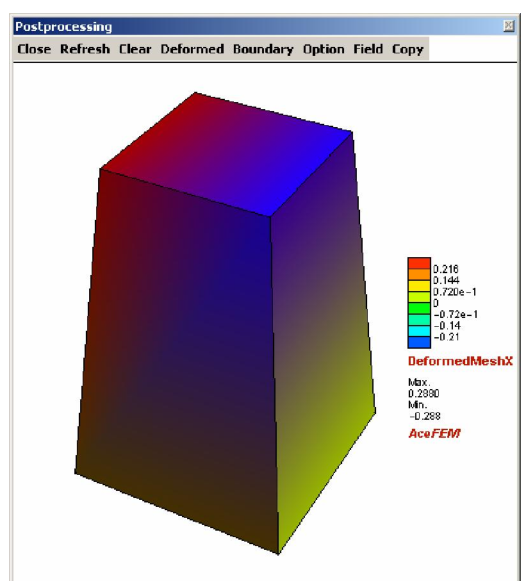


Figure 5. Displacement field for case of tension of cube

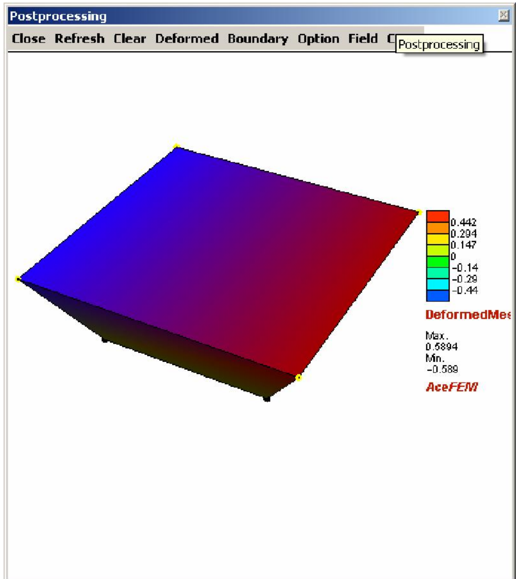


Figure 6. Displacement field for case of compression of cube

The results of numerical solutions are consistent with the results presented in the literature. In the future it is necessary to compare the calculation for this example and for the other benchmark examples with other FEM softwares as ABAQUS, ANSYS, NASTRAN, and PAK software package [10], which is being developed at the Faculty of Mechanical Engineering in Kragujevac.

4. CONCLUSIONS

The primary objective of this paper was to show that the symbolic programming is a powerful tool for generating the material models. The main attention is given on the hyperelastic material model development for 3D eight-node finite element, but it is given basis for creating other material models if it is known total energy of deformation and other constitutive relations that describe the desired material model.

AceGen is presented as multilanguage code generator, which can generate different material models for different types of finite element. It is as an independent FEM environment and AceShare on-line library with material models for different types of finite element. All three modules present complete FEM system.

All this represents an indicator that the application of symbolic programming with knowledge of the total energy of deformation and constitutive relations, we can generate other, new material models. This new symbolic approach can make a huge, all available, a library of material models, which can always be upgraded with new material models.

Acknowledgments

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5. REFERENCES

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