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Adaptive solution of problems modeled by unified state variable constitutive equations

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The objective of the work was an efficient, numerical implementation of one of the unified, internal-state-variable constitutive models. Such models are general and convenient in numerical applications since they describe elastic, plastic, viscous, damage phenomena and they do not require neither yielding condition nor loading/unloading criterion. However, they result in so called stiff initial–boundary value problems. Therefore, an efficient numerical implementation demand adaptive techniques, both in space and in time. The paper presents application of such an adaptation approach. It uses an improved version of the semi-implicit Euler method with automatic time step control and the h refinement of the FEM meshes based on the interpolation error estimate and on the reliable, selfequilibrated, implicit, *a posteriori* estimate. Selected problems were solved and both the efficiency and reliability of the unified model were confirmed.

1. Introduction

The paper presents a numerical implementation of a unified, internal-state-variable constitutive model in an "hp" adaptive FEM code. Such theories have evolved over the last 40 years (e.g. Biot [4], Bodner [5], Krempl [10]) and are now the most general, consistent with micro-mechanics and thermodynamics of materials, methods for modeling of the nonelastic behavior of metals. They make use of some functions (internal state variables) which evolve in time, keep track of proportional or nonproportional loading history and are the main factor contributing to the nonelastic strain rates. The most important advantage of such models is the unified treatment of the elastic and various kinds of the nonelastic phenomena including plasticity, creep, relaxation, continuum damage and thermomechanical fatigue. Moreover, the unified models do not require a yielding condition or loading and unloading criterion, therefore, they avoid many of the classical complexities in numerical applications. The internal-state-variable constitutive models can be successfully used in computer codes, however, some research work on their efficient application is still necessary.

From the mathematical point of view, the unified elastic-visco-plastic models together with the momentum and geometric equations result in initial boundary-value problems. We deal here with, so called, stiff differential equations with respect to time, therefore, a special integration with automatic time step control is necessary. Efficient integration in space also requires advanced adaptive methods. Both kinds of adaptation should be based on apropriate error estimates, which are the key to rich high efficiency and reliability of the computation.

The Bodner–Partom constitutive model was chosen as an example of the internal-state variable theories and it was efficiently implemented in a two-dimensional [8] computer code based on the adaptive FEM. The semi-implicit Euler method with automatic time step control is used for integration in time.

The similiar problems were already undertaken in [20, 21]. In this work other error estimates were used and some improvement of integration in time is proposed.

2. Description of the problem

We consider the problem of infinitesimal, quasistatic deformations. It can be formulated as follows

- Conservation of momentum and linear formula for strains result in the relation

$$\mu \dot{u}_{i,jj} + (\mu + \lambda)\dot{u}_{j,ji} = 2\mu \dot{\varepsilon}^*_{ij,j} \qquad \text{in } \Omega \tag{1}$$

  where $i, j = 1, \ldots, N$; $N = 1, 2$ or 3; $\Omega \subset \mathbb{R}^N$ is an open material domain; $\dot{\varepsilon}^*$ is the nonelastic strain rate tensor, λ, μ are the Lame elastic constants and the dot stands for derivative with respect to time (denoted by t).

- The constitutive equations include the Hooke law – Eq. (2), a formula for evolution of nonelastic strains – Eq. (3), and at least one evolution law of parameters which model influence of loading history on the nonelastic deformation – Eq. (4):

$$\dot{\sigma}_{ij} = E_{ijkl}(\dot{\varepsilon}_{kl} - \dot{\varepsilon}^*_{kl}) \qquad \text{in } \Omega, \tag{2}$$

$$\dot{\varepsilon}^*_{ij} = g_{ij}(\boldsymbol{\sigma}, \boldsymbol{\beta}) \qquad \text{in } \Omega, \tag{3}$$

$$\dot{\beta}_{pq} = h_{pq}(\boldsymbol{\sigma}, \boldsymbol{\beta}) \qquad \text{in } \Omega, \tag{4}$$

  where σ_{ij} is the Cauchy stress tensor, $\mathbf{E}$ is the elastic modulus tensor; $\boldsymbol{\beta}$ is a vector of internal state variables, i.e. functions of $\mathbf{x} \in \Omega$ which evolve during the loading process and are the main factor modeling nonelastic behavior of the material; $\mathbf{g}$, $\mathbf{h}$ are functions which depend on some material constants.

- Boundary conditions:

$$\dot{u}_i = w_i \qquad \forall\, t \text{ on } \partial\Omega_u, \tag{5}$$

$$\dot{\sigma}_{ij}\, n_j = \dot{q}_i \qquad \forall\, t \text{ on } \partial\Omega_t, \tag{6}$$

  where n_j are components of the unit vector normal to the boundary. More general cases, e.g. contact condition, elastic foundation, can also be considered.

- Initial conditions:

$$\mathbf{u} = \mathbf{u}_0 \qquad \text{for } t = 0 \quad \forall \mathbf{x} \in \bar{\Omega}, \tag{7}$$

$$\boldsymbol{\varepsilon}^* = \boldsymbol{\varepsilon}^*_0 \qquad \text{for } t = 0 \quad \forall \mathbf{x} \in \bar{\Omega}, \tag{8}$$

$$\boldsymbol{\beta} = \boldsymbol{\beta}_0 \qquad \text{for } t = 0 \quad \forall \mathbf{x} \in \bar{\Omega}. \tag{9}$$

  All functions $\dot{w}_i$, $\dot{q}_i$, $\mathbf{u}_0$, $\boldsymbol{\varepsilon}^*_0$, $\boldsymbol{\beta}_0$ are known.

The above problem can be formulated in the following semi-weak form

Find $\dot{\mathbf{u}} \in \mathbf{V} + \dot{\mathbf{w}}$ *such that:*

$$\int_\Omega v_{i,j}[\mu \dot{u}_{i,j} + (\mu + \lambda)\dot{u}_{j,i}]\, d\Omega = 2\int_\Omega v_{i,j}\mu\dot{\varepsilon}^*_{ij}\, d\Omega + \int_{\partial\Omega} v_i \dot{\sigma}_{ij} n_j\, ds \qquad \forall\, \mathbf{v} \in \mathbf{V}, \quad \forall\, t > 0, \tag{10}$$

where $\mathbf{V}$ is subspace of the Sobolev space $(H^1(\Omega))^N$ of functions satisfying the homogenous Dirichlet boundary conditions.

3. A UNIFIED CONSTITUTIVE MODEL

The first formulation of unified constitutive equations was proposed by Biot [4] and Meixner [14] in the fifties. Some theoretical background for this type of models was also developed by Perzyna [16]. The first practical implementations are due to Bodner [5]. A fast development of internal state variable models, observed in the recent years [3, 12, 20, 21] was mainly due to their significant advantages like:

- a unified treatment of the elastic and different kinds of the nonelastic phenomena (plasticity, creep, relaxation, continuum damage, thermomechanical fatigue),
- theoretical and experimental background,
- lack of yielding condition or loading and unloading criterion, which simplifies the numerical implementation.

Let us now briefly review the Bodner–Partom constitutive equations. It was proposed in the seventies for modeling of metals in wide range of temperatures. The formulas have the following form

$$\dot{\varepsilon}^*_{kl} = D_o \frac{s_{kl}}{\sqrt{\frac{1}{2} s_{ij} s_{ij}}} \exp\left\{ \left[\frac{\left(Z + \beta_{mn} \frac{\sigma_{mn}}{\sqrt{\sigma_{ij}\sigma_{ij}}} \right)^2}{\frac{3}{2} s_{ij} s_{ij}} \right]^n \right\}, \tag{11}$$

$$\dot{Z} = m_1 (Z_1 - Z) \sigma_{ij} \dot{\varepsilon}^*_{ij} - A_1 Z_1 \left(\frac{Z - Z_2}{Z_1} \right)^{r_1}, \tag{12}$$

$$\dot{\beta}_{kl} = m_2 \left(Z_3 \frac{\sigma_{kl}}{\sqrt{\sigma_{ij}\sigma_{ij}}} - \beta_{kl} \right) \sigma_{ij} \dot{\varepsilon}^*_{ij} - A_2 \left(\frac{\sqrt{\sigma_{ij}\sigma_{ij}}}{Z_1} \right)^{r_2} \beta_{kl}, \tag{13}$$

where: D_o, n, m_1, m_2, Z_1, Z_2, Z_3, A_1, A_2, r_1, r_2 are additional to λ, μ, material constants:

D_o [s^{-1}] – limiting strain rate in shear,

n [-] – a kinematic parameter related to the yield limit,

m_1, m_2 [MPa^{-1}] hardening rates (usually $m_1 = m_2$),

Z_1, Z_2, Z_3 [MPa] – limiting values of the hardening parameter Z,

A_1, A_2 [s^{-1}], r_1, r_2 [-] – temperature recovery constants (usually $r_1 = r_2$ and $A_1 = A_2$),

s_{ij} stands for deviatoric components of the stress tensor, $s_{ij} = \sigma_{ij} - \frac{1}{3}\sigma_{kk}\delta_{ij}$, and Z, $\boldsymbol{\beta}$ – internal parameters responsible for isotropic and unisotropic hardening.

A characteristic feature of the unified models is comperatively large number of material constants. They can be determined from a few uniaxial tension and creep tests [13, 18]. One can simplify the above formulas by neglecting some terms (e.g. unisotropic hardening), reducing simultaniously the number of constants. On the other hand it is possible to introduce certain additional parameters which would model other phenomena (e.g. damage).

4. SOLUTION OF THE PROBLEMS WITH INTERNAL-STATE-VARIABLES

Equations (1)–(4) can be treated as an initial-value problem and can be written in the following form

$$\frac{\mathrm{d}\mathbf{Y}}{\mathrm{d}t} = \mathbf{F}(\mathbf{Y}, t) \tag{14}$$

where $\mathbf{Y} = (u_1, u_2, u_3\ Z, \omega, \beta_{11}, \beta_{12}, \ldots)^T$. In fact, Eq. (1) is an implicit formula for rates of displacements, so computation of $\dot{\mathbf{u}}$ requires solution of a linear boundary-value problem. It can be done efficiently using adaptive numerical methods. Their basis is an error estimation. A simple error estimate based on interpolation theory together with h-adaptivity was already used for unified problems [3, 20]. We use here the more reliable implicit residual estimate [1, 2].

The system of Eqs. (14) is so called stiff (ill conditioned), and it demands application of implicit integration methods in time in order to provide stability of the algorithm. On the other hand the more d.o.f. in space are used for better accuracy the worse stability may be observed. Therefore, to obtain high accuarcy and stability of the algorithm, as well as possibly low computational cost we use adaptive approches, both in space and time. Semi-implicit Euler scheme with automatic time-step control is usually applied [12, 20, 21]. However, we have also tested several other strategies. These were the Runge–Kutta (a higher order method) and the Bulirsh–Stoer approach (recommended in textbooks [17]). In order to compare efficiency of these methods we applied them to solution of a simple benchmark problem. The semi-implicit Euler method was used in the original form and in a modified one. In the original version the implicit iteration is performed only once. If the error is too big the time step is decreased. In the modified version an additional implicit iteration was performed without decreasing the time step if the error was slightly (a few per cent) higher than the admissible tolerance. It reduced the time of computation by about 10%.

As the test problem we considered analysis of the uniaxial stress state arising from cyclic load. One cycle was analyzed (tension–compression–tension) with the extremum total strain equal to ±5%. The Bodner–Partom constitutive model in its simplest version was assumed. The results are summarized below.

method	*number of evaluation of right-hand side*
Bulirsh–Stoer	2515
Runge–Kutta	3502
semi-implicit Euler	371
semi-implicit Euler (modified)	343

The number of evaluations of the right-hand side ($\mathbf{F}$ in Eq. (14)) decides about the time of computation, since it involves solution of a boundary-value problem. The above results indicate that the simplest method is the fastest one. Additionally, as a first order approach it requires the least amount of memory. The above observation is very likely to be generalized for more complex problems.

5. Error estimates

Adaptive modification of the FEM mesh and of the time steps is based on error estimates. For adaptation in space an *a posteriori* [1] and an interpolation [15] error estimates were used, while for the time step adaptation an error obtained from the Taylor formula [12] was used. They are briefly described below.

5.1. An idea of *a posteriori* implicit residual error estimate

The finite element approximation of problem (10) is to find $\mathbf{u}_X \in \mathbf{X} \subset \mathbf{V}$ such that

$$B(\mathbf{v}_X, \mathbf{u}_X) = L(\mathbf{v}_X) \qquad \forall\, \mathbf{v}_X \in \mathbf{X}. \tag{15}$$

The error of the solution is defined as the following function from to the space $\mathbf{V}$

$$\mathbf{e} = \mathbf{u} - \mathbf{u}_X \tag{16}$$

which satisfies

$$B(\mathbf{e},\mathbf{v}) = L(\mathbf{v}) - B(\mathbf{u}_X,\mathbf{v}) \qquad \forall\, \mathbf{v} \in \mathbf{V}. \tag{17}$$

Moreover, the standard orthogonality condition for the error in the Galerkin projection holds

$$B(\mathbf{e},\mathbf{v}_X) = 0 \qquad \forall\, \mathbf{v} \in \mathbf{X}. \tag{18}$$

In practice, it is not possible to compute exactly the error $\mathbf{e}$. Error estimation allow one to evaluate the error indicator (η) which should satisfy the property

$$\exists\, C_1, C_2 : C_1\|e\| \le \eta \le C_2\|e\|. \tag{19}$$

In such a case η tends to zero at the same rate as the true error. The ratio

$$\frac{\eta}{\|e\|} \tag{20}$$

is called the effectivity index. Usually

$$\eta = \left(\sum_K \eta_K^2\right)^{\frac{1}{2}} \tag{21}$$

where η_K is a local error indicator on element K evaluated by the approach described in [1].

5.2. Interpolation error estimate

In the non-elastic problems an additional estimate of the error is necessary for nonelastic strain tensor. This field is approximated by shape function derivatives on triangular elements, and it is the input data for the FEM analysis. The interpolation error estimate [15] is useful here. If ε_{ij}^{*h} is an interpolant of nonelastic strain, which has bounded second derivatives, and $e_{ij} = \varepsilon_{ij}^* - \varepsilon_{ij}^{*h}$ is the interpolation error function then the error estimate assumes the form

$$\|e_{ij}\|_1 \le Ch|\varepsilon_{ij}^*|_2 = Ch\sqrt{\int_K \left[\left(\frac{\partial^2\varepsilon_{ij}^*}{\partial x_1^2}\right)^2 + \left(\frac{\partial^2\varepsilon_{ij}^*}{\partial x_2^2}\right)^2 + \left(\frac{\partial^2\varepsilon_{ij}^*}{\partial x_1 \partial x_2}\right)^2\right] dK} \tag{22}$$

with C being a positive constant. The general conclusion from the above formula is that, wherever the second derivatives of the nonelastic strain are high, the mesh should be refined or enriched. We estimate this derivative, using the moving least square approximation.

5.3. Estimation of time integration error

The system of ordinary differential equation (14) is integrated in time. The *k-th* time step lenght is controlled by the following error estimate [12]

$$e_k = \frac{1}{2}\Delta t_k \frac{\|\dot{\mathbf{Y}}_{k+1}^p - \dot{\mathbf{Y}}_k\|}{\|\mathbf{Y}_{k+1}^c\|} \tag{23}$$

where

$\dot{\mathbf{Y}}_{k+1}^p$, $\mathbf{Y}_{k+1}^c$ stand for predictor of solution rate and corrector of the solution at the end of the k-th time step,

$\dot{\mathbf{Y}}_k$ is the rate of the solution at the begining of the k-th time step,

Δt_k stands for the k-th time step lenght,

$$\dot{\mathbf{Y}}^p_{k+1} = F(\mathbf{Y}^p_{k+1}, t_{k+1}),$$

$$\mathbf{Y}^p_{k+1} = \mathbf{Y}_k + \Delta t_k \dot{\mathbf{Y}}_k,$$

$$\mathbf{Y}^c_{k+1} = \mathbf{Y}_k + \Delta t_k \frac{\dot{\mathbf{Y}}^p_k + \dot{\mathbf{Y}}_k}{2},$$

$\mathbf{Y}_k$ is the solution at the begining of the k-th time step.

Finally the following strategy of adaptive solution was developed.

1. Obtain the solution for an adaptively adjusted time step. IF *adaptation in space is not assumed for this time instant* THEN *go to 6.*
2. Evaluate the *a posteriori* error estimate of the BVP solution.
3. Estimate the interpolation error.
4. Modify the mesh, wherever it is necessary (i.e. residual or interpolation error indicator exceed the assumed level), if the errors are small skip the next step.
5. Project the solution onto the new mesh and go back to 1.
6. If it was not the last time step go to 1.

6. Numerical examples

A computer, adaptive FEM code [8] was customized to solution of nonelastic problems modeled by the Bodner–Partom equations. Triangular, second order elements were used in all the examples.

Some selected problems were solved to verify and present possiblities of the model and of the code. They are summarized below.

- Uniaxial tension for different materials (aluminum, steel, B1900Hf alloy) for various strain rates as well as creep and relaxation tests for the alloy at different temperatures (Fig. 1). The tests show possibilities of the model.
- A thick wall cylinder (with radiuses 1 m and 2 m) loaded by the internal pressure 180 MPa. Adaptively refined meshes and results are shown in Figs. 2, 3. This is an example of an adaptation process. The results were compared with solution obatined by another code [11], which makes use of the Perzyna model. The difference for all stress components was less than 1%.
- Tension test of a specimen with a hole of radius 1 m, solved to evaluate a solution with concentration of stresses (Figs. 4–6).
- A railroad rail (American 132RE type, about 0.18 m heigh) in a plane strain (Figs. 7, 8), loaded in the middle of the top surface by continuouosly distributed load 900 MPa. The exapmle shows possible practical applications. In fact this problem will require a 3D model.

In all the examples the following material constants for steel [5] were used in the Bodner–Partom, internal state variable constitutive model with only isotropic hardening taken into account:

$$\begin{aligned}
E &= 203\ \text{GPa}, & m_1 &= 0.030\ \text{MPa}^{-1},\\
\nu &= 0.3, & Z_0 &= 640\ \text{MPa},\\
D_o &= 1.0^8\ \text{s}^{-1}, & Z_1 &= 930\ \text{MPa},\\
n &= 4.0, & m_2 &= 0,\\
& & A_1 &= A_2 = 0.0\,.
\end{aligned}$$

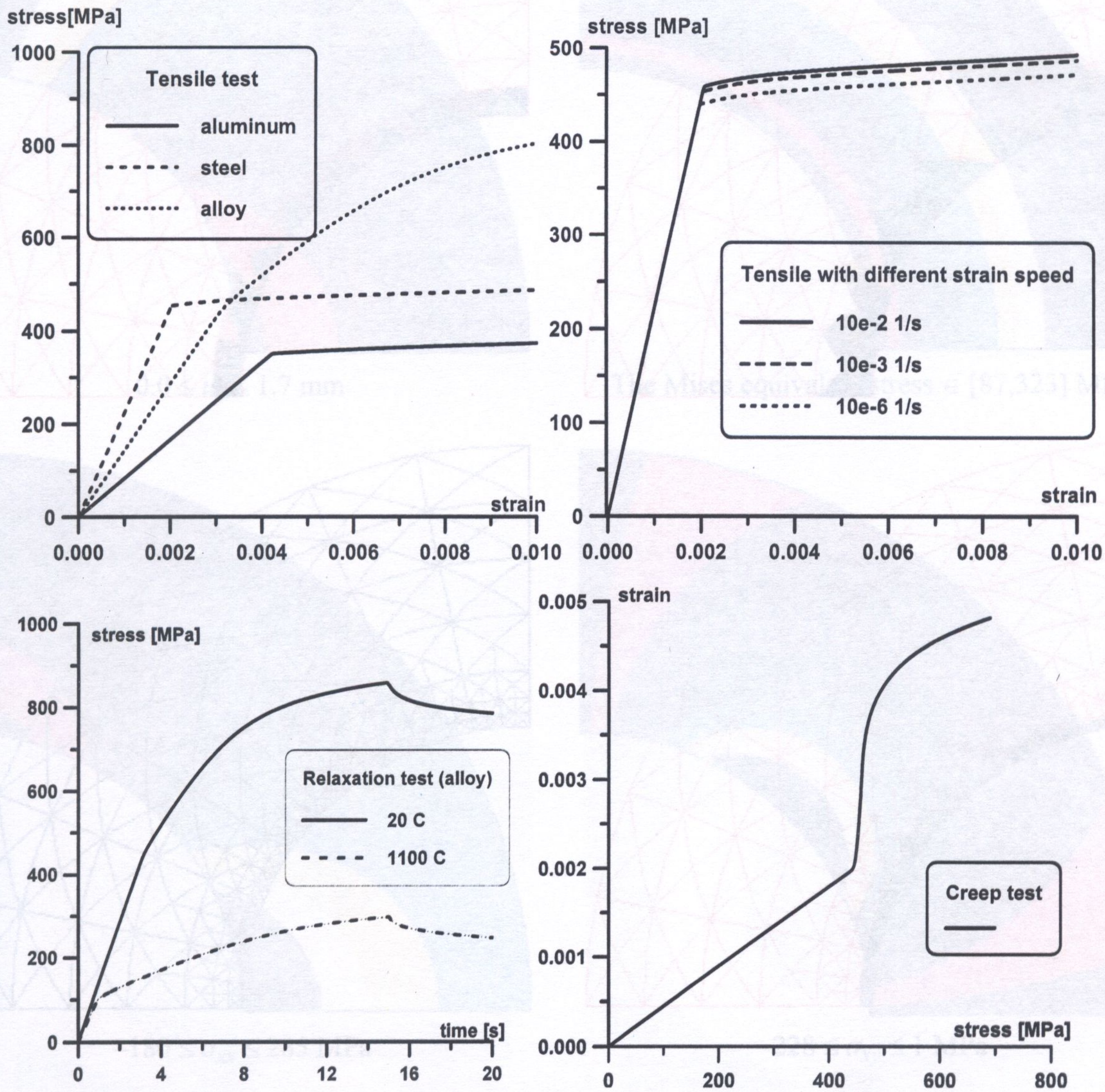

Fig. 1. Uniaxial tests

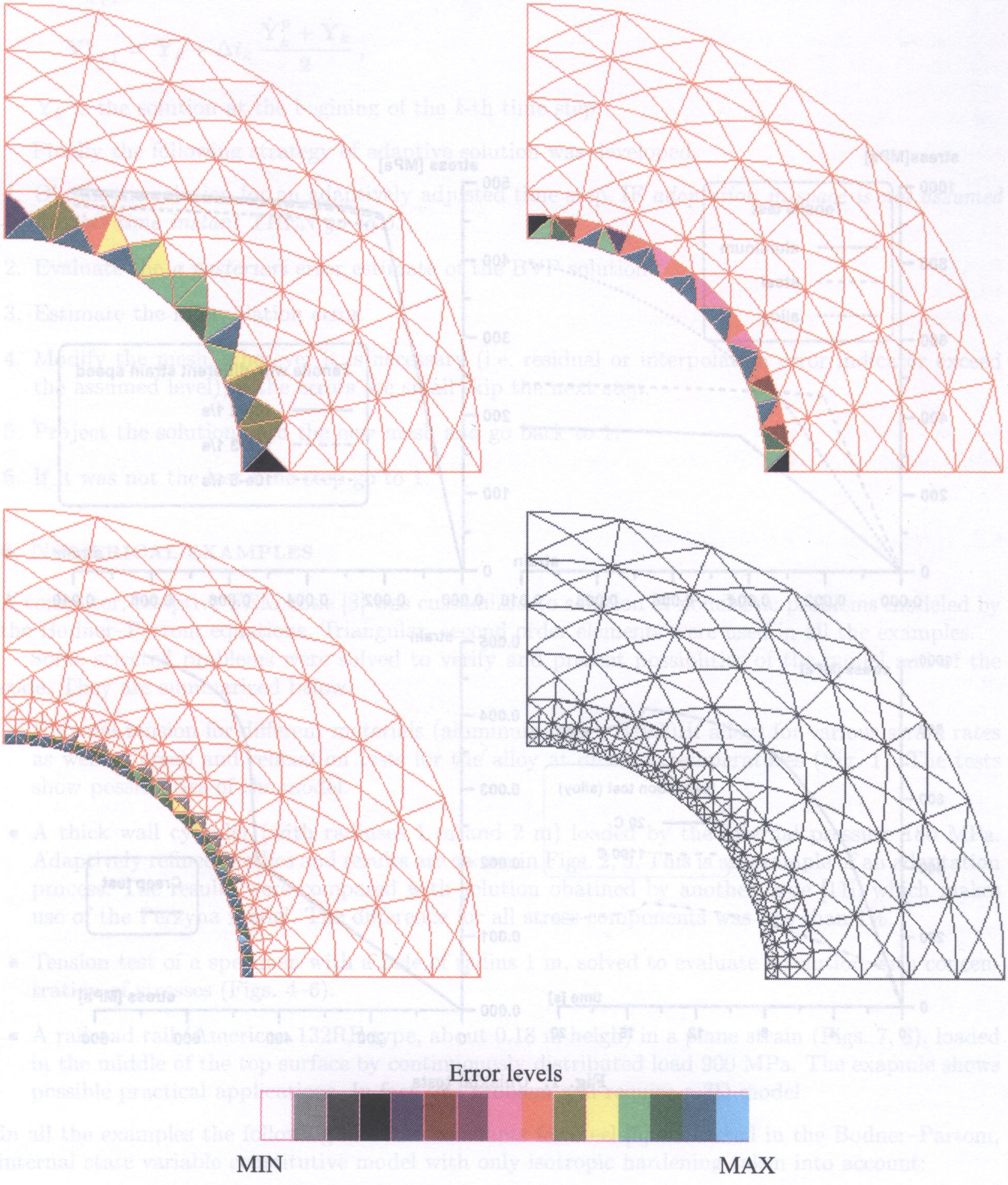

Fig. 2. Cylinder problem. Initial and adaptively refined meshes with error estimates

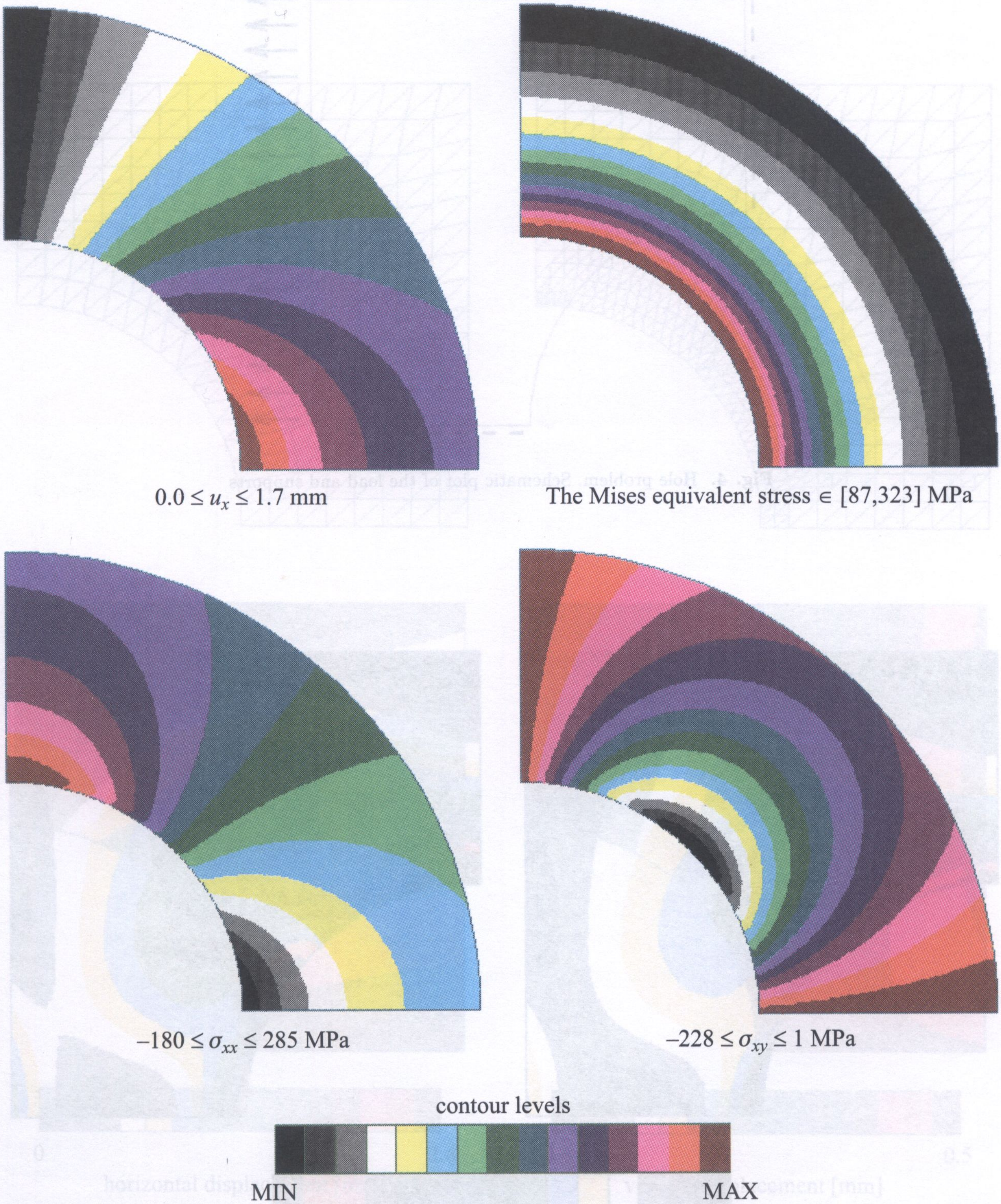

Fig. 3. Cylinder problem. Contour plots of horizontal displacement and stress components for internal pressure 180 MPa

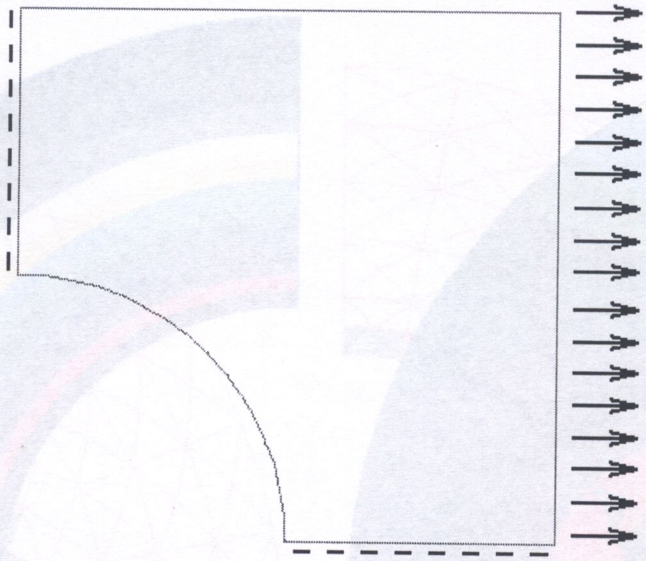

Fig. 4. Hole problem. Schematic plot of the load and supports

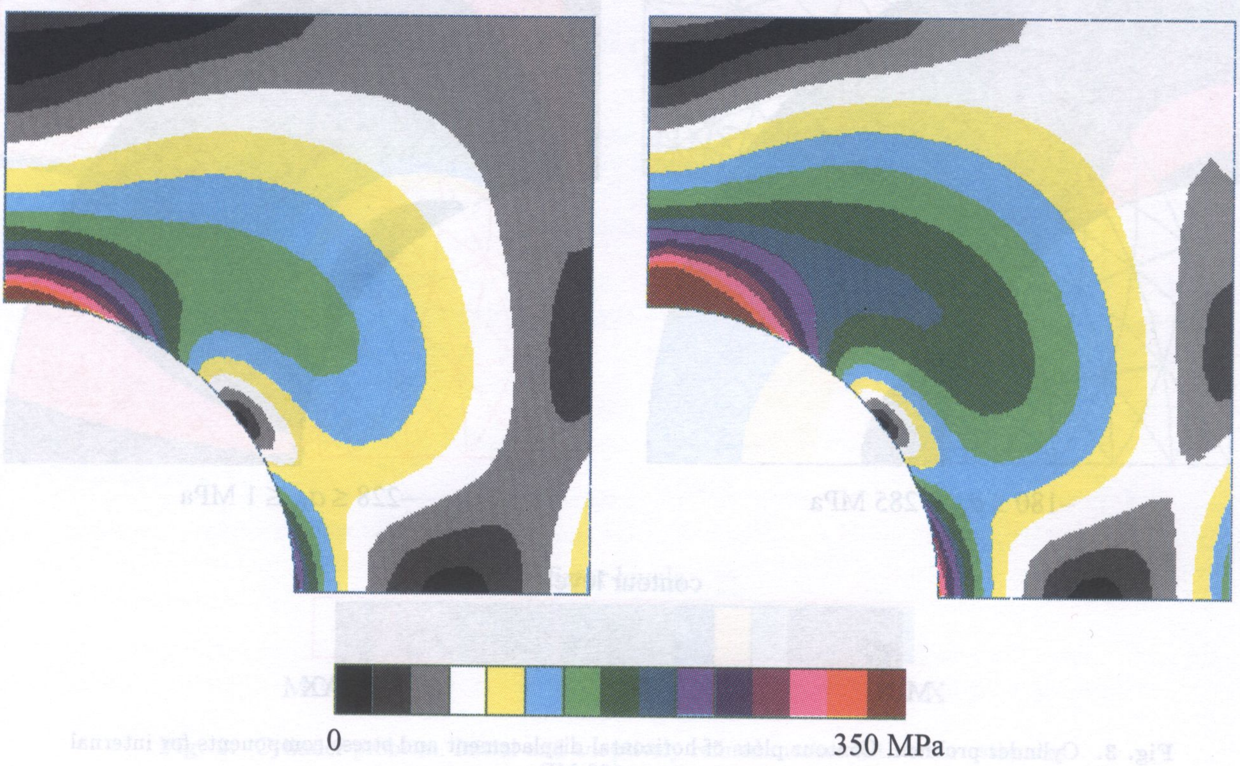

Fig. 5. Hole problem. The Mises equivalent stress for 80 MN/m and 100 MN/m

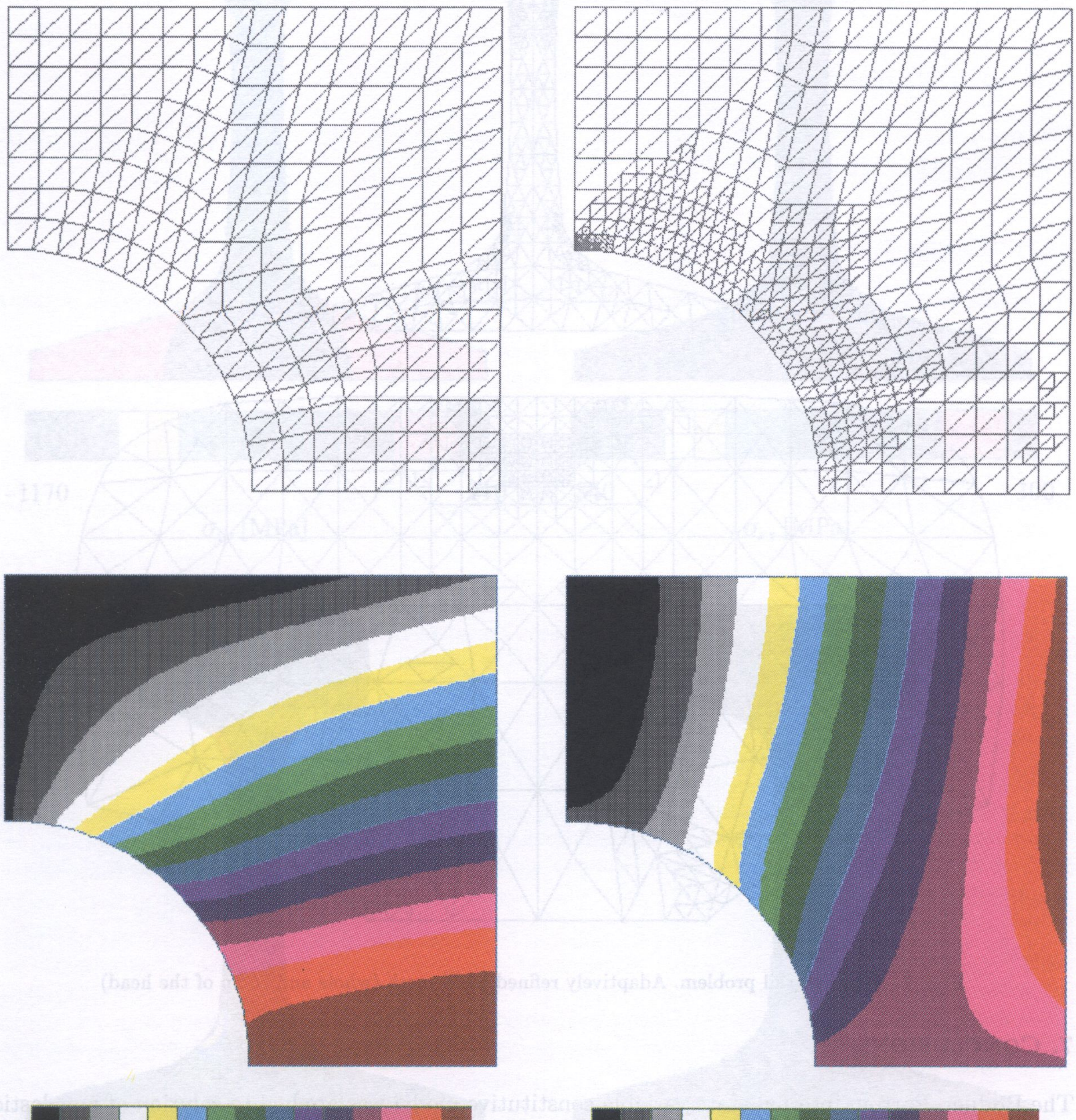

Fig. 6. Hole problem. Initial mesh, refined mesh and displacement fields

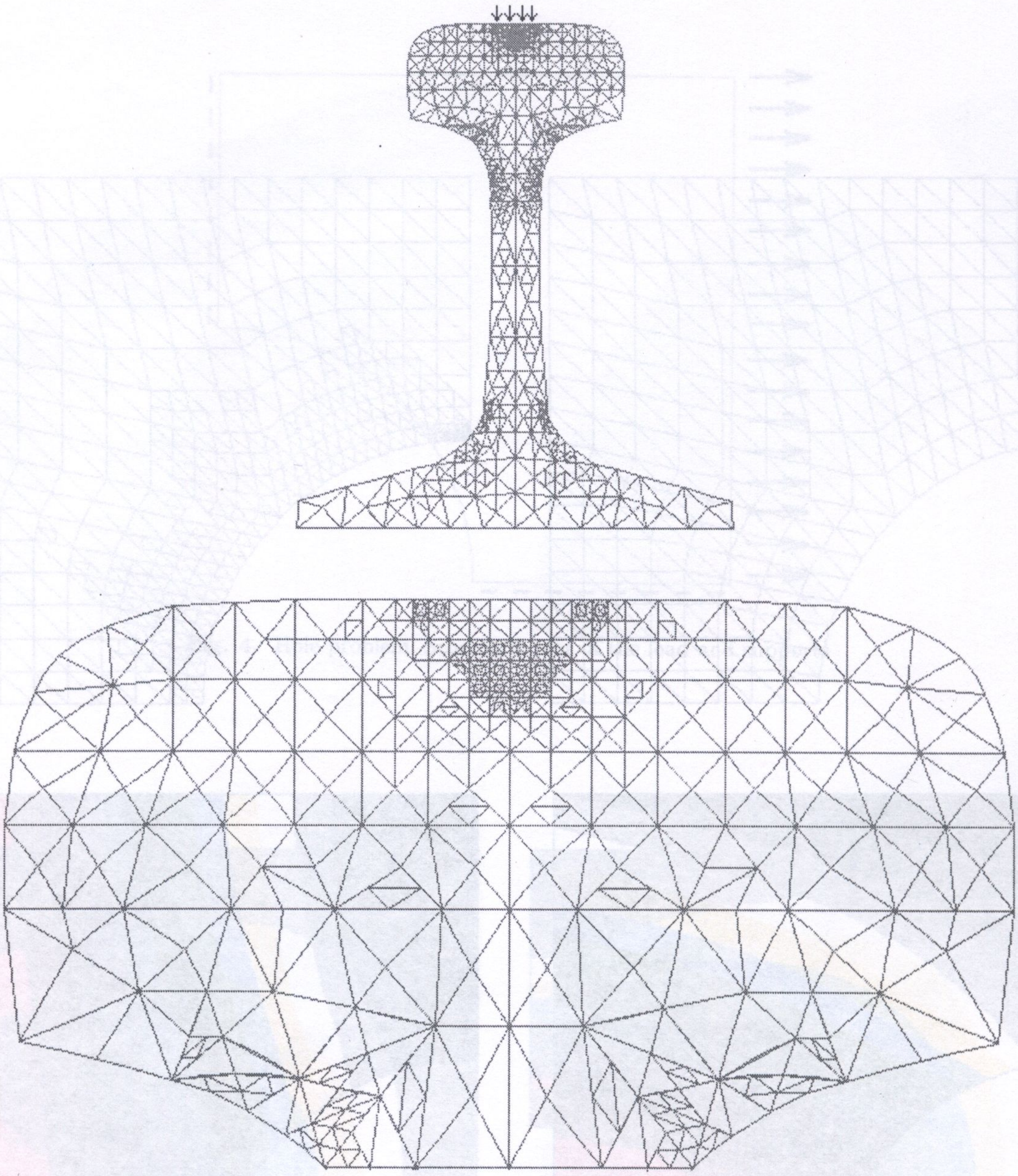

Fig. 7. Railroad rail problem. Adaptively refined FEM mesh (whole and zoom of the head)

7. Conclusions

The Bodner–Partom internal state variable constitutive model was applied to solution of nonelastic problems. These kind of models are very general since they describe elastic, plastic and viscous phenomena. Moreover, they are convenient in numerical applications due to the fact that they do not require neither yield condition nor loading/unloding criterion and they describe material properties more precisely as they were developed on the basis of more accurate experimental measurements than the classical models.

However, their efficient implementation requires to apply an addaptive approach both in space and time. A few methods of adaptive integration in time were compared in order to choose the optimal one. It is the semi implicit Euler scheme with automatic time step control which additionally was speeded up by a modification of the algorithm. On the other hand reliable *a posteriori* and an interpolation *a priori* error estimates were used for adaptation in space.

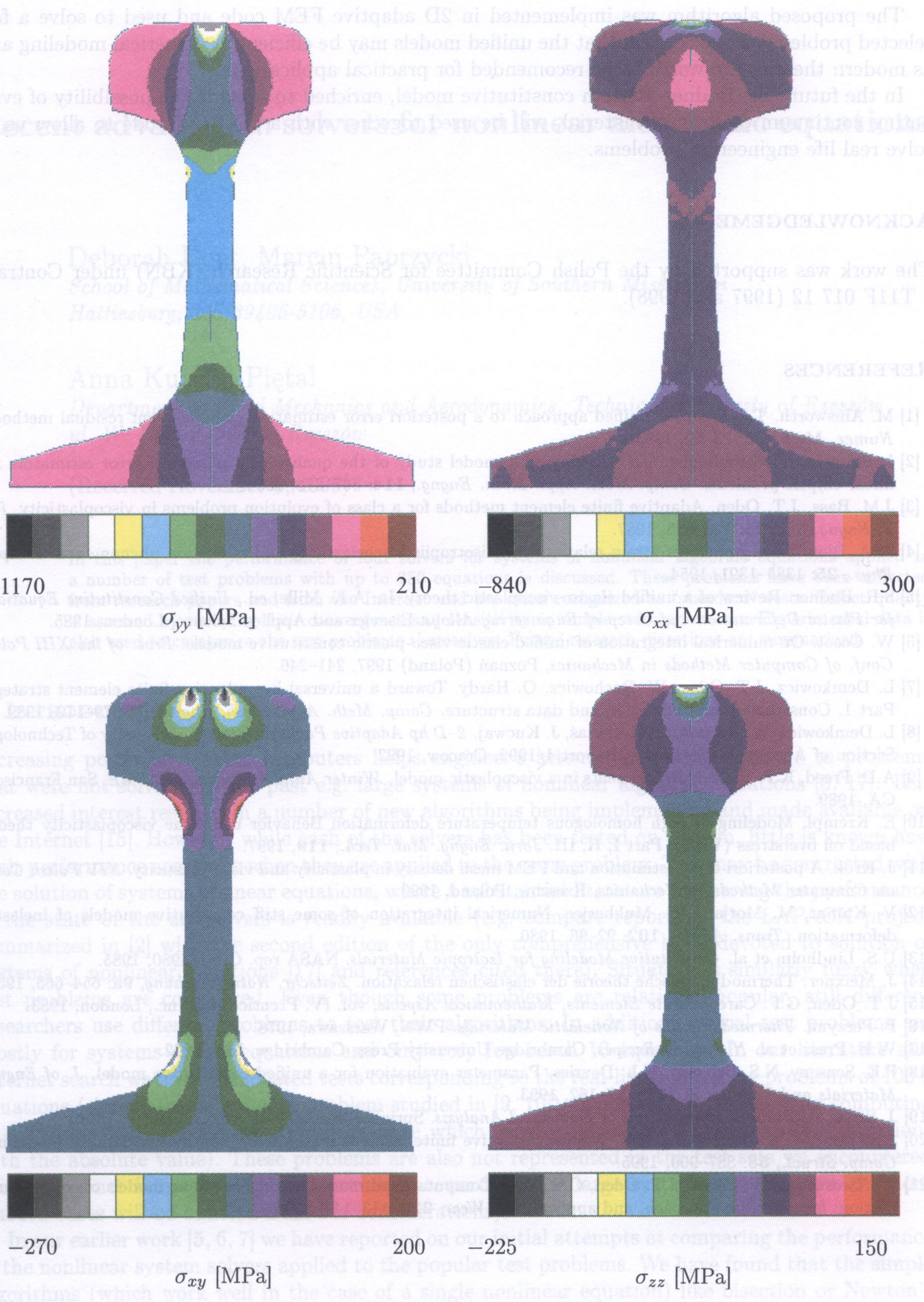

Fig. 8. Railroad rail problem. Stress components for the plane strain state

The proposed algorithm was implemented in 2D adaptive FEM code and used to solve a few selected problems. They confirm that the unified models may be efficient in numerical modeling and as modern theories are worth to be recomended for practical applications.

In the future the Bodner–Partom constitutive model, enriched to provide the possibility of evaluating continuum damage of material, will be used together with a 3D FEM code to allow us to solve real life engineering problems.

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