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Identification of viscoplastic constitutive and creep-fatigue damage coefficients to use in ABAQUS automotive structural calculations with the Zmat library

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***Abstract**--Complex constitutive equations are needed to accurately predict the failure of high temperature components such as car diesel engine cylinder heads or exhaust manifolds. They may have to take into account the evolution of the material behavior relating to aging or phase changes, which strongly affect the stress-strain history and lifetime predictions.*

Such advanced viscoplastic material models are available for ABAQUS users by means of Zmat library, which implements a series of constitutive equations and can be seen by ABAQUS as a huge UMAT subroutine, and also offers numerical tools for making the development of new models easier. Creep-fatigue damage models are also available in a companion code, which can be used as a post-processor with ABAQUS.

*However, one key point for the industrial use of such methods is the identification of material coefficients, which can still be cumbersome considering the large number of parameters involved. The purpose of this paper is to present identification tools called **Zsim** and **Zopt** that can be a great help in this task. The capabilities of this software are demonstrated by the full identification of the cyclic viscoplastic properties of a typical engine material and its creep-fatigue behavior.*

An application to the ABAQUS calculation of a RENAULT SA car engine component will be presented with the aim to derive number of cycles to failure in the low cycle thermomechanical fatigue regime.

1 General description

One of the principal difficulties associated with the use of complex constitutive equations to predict the behavior of high temperature components is the number of parameters to be handled and the quality of experiments performed.

Both modeling and experiments call for good identification tools. To answer this need, **Zmat**, the general material constitutive model library developed by the Ecole des Mines de Paris, contains a general identification and optimization module called **Zopt**. It can handle any kind of constrained optimization problems and is particularly well suited to parameter identification. The optimal model parameters are typically chosen so as to minimize the least-square distance between a set of reference (i.e. experimental data) and simulated curves generated by any finite element code (e.g. ABAQUS). A general description of the optimization procedure is shown in Figure 1.

2 Optimization methods

The **Zopt** optimization module can deal with a broad range of optimization conditions e.g.,: constrained or unconstrained, local or global, with or without gradients of the objective function to be optimized. Amongst the optimization methods used by **Zopt** are:

- two gradient-driven methods, Levenberg-Marquardt (unconstrained, gradient driven method) which is particularly efficient for least-square type cost functions, and an augmented-Lagrangian method for constrained optimization.
- the Nelder-Mead (Simplex) method, a heuristic local method that does not need sensitivity calculations and is very effective on moderate size and strongly non-linear problems. It can also handle constraints.
- a genetic algorithm that can bypass local minima in the case of complex non convex optimization problems and is insensitive to the starting point (although at the expense of requiring a large number of function evaluations). Typically, it can be used to provide gradient -driven methods, with a set of good starting points.

3 Identification tools

3.1 The Zsim simulation module

As described above, the optimal design parameters are chosen so as to minimize the least-square distance between experimental data and simulated curves generated by an external software. In fact, the **Zmat** package includes a simulator module called **Zsim**, which is connected to the optimizer and allows the user to load any representative volume element (RVE) under arbitrary stress or strain controlled conditions instead of forces and displacements, leading to fast and efficient simulations. It has an access to the integration methods, and leads to a very efficient integration of the constitutive equations: the integration time corresponds to one Gauss point only, and run more than 20 times faster than a single finite element. An example of a typical **Zsim** input file is given below.

```
****simulate
***test fatigue                                % Output file name :  fatigue.test
**load cycle 2                                % Beginning of the loading table (2 cycles)
*segment 10                                   % 10 points are stored in the output file for
  time   sig11  eto22  sig33  sig12          % each line of the table
  0.0    0.0   0.0   0.0   0.0
  100.0  0.0   0.01  0.0   0.0           % Loading table for one cycle
  200.0  0.0   0.0   0.0   0.0
  300.0  0.0  -0.01  0.0   0.0
**model
*file id_evp.mat                              % Material behavior defined in file id_evp.mat
**output time eto22 sig22                    % Contents of the output file
***test relax
**load
*segment 10
  time   sig11  eto22  sig33  sig12
  0.0    0.0   0.0   0.0   0.0
  10.0   0.0   0.01  0.0   0.0
  70.0   0.0   0.01  0.0   0.0           % Loading table for relaxation test
**model
*file id_evp.mat
**output time eto22 sig22
****return
```

The input data for the material given in the `id_evp.mat` file corresponds to the standard viscoplastic Chaboche model available in the **Zmat** library:

```
***behavior gen_evp
**elasticity isotropic  elastic behavior
  young 150000.
  poisson 0.3
**potential gen_evp ev
*critterion mises viscoplastic flow
*flow norton
  n      8.
  K      500.
```

```

*kinematic nonlinear kinematic hardening
  C      40000.
  D      250.
*isotropic constant isotropic hardening
  R0     111.
*** return

```

3.2 The Zopt optimization module

The parameters **n**, **K**, **C**, **D** **R** of the previous phenomenological elastoviscoplastic Chaboche type model can be identified by using the **Zopt** package. A typical optimization input file for this set of parameters is as follows:

```

****optimize levenberg_marquardt
***files id_evp.mat
***shell Zrun -S id_evp
***values
  n  9.1      min  1.5      max  30.
  K  200.     min  70.      max  2000.
  c1 90000.   min  10000.  max  150000.
  d1 1990.    min  100.     max  5000.
  r0 250.     min  0.1     max  500.
***convergence iterations 200
***compare
  t_file_file fatigue.test 1 3 fatigue.exp 1 3 weight 1.
  t_file_file relax.test 1 3 relax.exp 1 3 weight 1.
****return

```

The optimization method is given through ******optimize** command, i.e. Levenberg_Marquardt. The ******shell** command allows to run the simulator program that is necessary to the calculation of the distance minimized. Various input files containing design parameters are specified after the ******files** command. Interfacing between the simulation program and the optimizer is then simply done by creating a template for each input file needed by the specified ******shell** commands. In those template input files numerical values of design parameters are replaced by a character string composed by the name of the parameter preceded by a "?" symbol. For instance, the template file **id_evp.mat.tmpl** used in this example is:

```

***behavior gen_evp
**elasticity isotropic
  young 150000.
  poisson 0.3
**potential gen_evp ev
* criterion mises
*flow norton
  n ?n
  K ?K
*kinematic nonlinear
  C ?C
  D ?D
*isotropic constant
  R0 ?r0
***return

```

Figure 3 gives identification results of the optimization procedure in terms of the predicted experimental fatigue and relaxation test data and the optimized simulations.

4 A typical example

In this section, identification of the nodular graphite ferritic cast iron parameters from room temperature to 850°C, will be illustrated using the **Zopt** package.

For this temperature range, the material can be considered to be made up of ferritic (α) matrix and graphite nodules.

4.1 Industrial context

One of the major challenge for car manufacturers in forthcoming years is a drastic reduction of green house effect gas emissions, especially carbon dioxide. These emissions are directly connected to fuel consumption. European car manufacturers have taken an ambitious program, known as CAFE (Corporate Average Fuel Economy), to achieve by 2008 a mean average emission for their whole production of 140 g of CO₂ per km.

One way to meet this requirement by increasing the share of diesel engines in the European market. Diesel engines, associated with turbo charging and common rail direct injection, can achieve high specific output and low fuel consumption. High specific output allows to use down sizing (i.e. smaller engine than before for the same power) which can increase fuel economy. The difficulty associated with high specific output is the important increase of thermal and mechanical loads for constant dimensions of parts.

On the other hand, to develop the share of Diesel engines, it is crucial to propose them to customer at constant price, or better, at lower price, similar to gasoline engines. In this context, the use of low price material, such as cast iron, even for parts undergoing high thermal loads like exhaust manifolds, keeps an interest. But, due to the increase of thermal loads, it will be used very close to its temperature and thermal fatigue limits.

To be able to develop new diesel engine exhaust manifolds for popular cars, it is necessary to have efficient numerical tools to predict thermal fatigue and associated life time. These tools must not only take into account all relevant physical phenomena (e.g. cyclic plasticity, creep, ageing, low cycle fatigue...) but must also be easy to use in an industrial context from material model to the exploitation final results. In coherence with the general use of ABAQUS for non linear and thermomechanical analyses in RENAULT, it has been a natural choice to use in complement the library for material behavior and life prediction tools proposed by Ecole des Mines de Paris.

5 Identification of a Chaboche type model for a graphite ferritic cast iron material

At high temperatures cast iron exhibits a classic viscoplastic behavior whose main features are illustrated on the Figures 4 to 6 extracted from the RENAULT test database. Figure 4 shows the rate dependent effect on a tensile test at several strain rates and at $T=500^{\circ}C$, while Figures 5 and 6 illustrate the cyclic hardening behavior on strain controlled tests.

Chaboche-type models are particularly suited to integrate accurately such a viscoplastic response under cyclic loading. The basic equations are briefly summarized below, in terms of \mathbf{s} the deviator of the stress tensor σ and $J(\sigma)$ the von-mises invariant $J(\sigma) = \sqrt{\frac{3}{2} \mathbf{s} : \mathbf{s}}$:

$$\text{Strain partition:} \quad \varepsilon = \varepsilon^{el} + \varepsilon^v + \varepsilon^{th} \quad (1)$$

where ε^{el} is the elastic strain and ε^{th} the thermal strain

$$\text{Plasticity criterion:} \quad f(\sigma) = J(\sigma) - R \quad (2)$$

$$\text{Normality rule :} \quad \dot{\varepsilon} = \dot{v} \mathbf{n} \quad \text{with} \quad \mathbf{n} = \frac{3}{2} \frac{\mathbf{s}}{J(\sigma)} \quad (3)$$

$$\text{Norton flow :} \quad \dot{v} = \left\langle \frac{f(\sigma)}{K} \right\rangle^n \quad (4)$$

$$\text{Nonlinear kinematic hardening :} \quad \mathbf{X} = \frac{2}{3} C \mathbf{a} \quad \text{with} \quad \dot{\mathbf{a}} = \dot{v} \left(\mathbf{n} - \frac{D}{C} \mathbf{X} \right) \quad (5)$$

$$\text{Nonlinear isotropic hardening :} \quad R = R0 + Q (1 - e^{-bv}) \quad (6)$$

In the above equations, the strain rate dependence is governed by a power law relation (equation 4). Cyclic hardening (evolution of the stress-strain loops from one cycle to the other) is characterized by equation (6), where R is an exponential function of the cumulated plastic strain v : in this expression Q represents the amount of hardening between the first cycle and the stabilized cycle, and b the rate of saturation. This particular cast iron

exhibits in fact cyclic *softening* (figure 5), which can be taken into account by choosing a negative value for Q .

Kinematic hardening (equation 5) is then introduced to characterize the reversible hardening behaviour within each cycle. Integration of equation (5) also yields an exponential form, with C/D the asymptotic value and D the rate of saturation (note that sharper transition from elasticity to plasticity are obtained with higher values of D).

For strain-rate controlled uniaxial tests, the maximum stress level obtained on the stabilized cycle can then be simply evaluated as:

$$\sigma = K(\dot{\epsilon})^{\frac{1}{n}} + R_0 + Q + \frac{C}{D} \quad (7)$$

The **Zmat** library allows to integrate this kind of viscoplasticity models within **ABAQUS** analyses by means of the UMAT interface. The corresponding **Zmat** material file is given hereafter:

```
***behavior gen_evp
**elasticity isotropic
  E temperature ...
  nu ...
**thermal strain isotropic
  alpha temperature ...
**potential gen_evp
**criterion mises
**flow norton
  K temperature ...
  n temperature ...
**kinematic nonlinear
  C temperature ...
  D temperature ...
**isotropic nonlinear
  Q temperature ...
  b temperature ...
***return
```

Within this basic framework, the object-oriented modular design of **Zmat** allows almost infinite variations for instance by :

- changing the type of the material sub-objects: anisotropic elasticity or thermal strain, various types of plasticity criteria (eg. Hill ...), flow (eg. time-independent plasticity, exponential creep ...), isotropic or kinematic hardenings (eg. adding recovery ...)
- complexify the model by adding, for example, an unlimited number of kinematic hardening terms to better control the shape of the elastic-plastic transition, or by adding damage internal variables acting on the elastic or plastic regimes, etc
- building multi-potential models with different hardening mechanisms and flow rules within each potential and add coupling between them,
- defining the individual behavior at each phase in multiphase materials and associate them with an homogeneization rule to build a macroscopic *multi_mat* model.

The identification of the material coefficients for such sophisticated models is indeed a complex process that necessitates efficient dedicated optimization tools. Even for the basic simple Chaboche model described above, there is still seven coefficients to identify at each temperature (in addition of the thermo-elastic parameters): the viscosity coefficients K and n , the isotropic hardening coefficients R_0 , Q and b , and the kinematic hardening coefficients C and D .

The **Zsim** and **Zopt** identification tools are a great help to ease this process as will be demonstrated in the following sections.

5.1 Identification of the Chaboche model coefficients at T=500°C

The first step requires the calibration of coefficients from isothermal tests performed at different temperatures. The RENAULT test database includes such tests from room temperature to 800°C. The following section details the optimization procedure at an intermediate temperature 500°C, for which 3 different tests will be used:

- the **VISC** tensile test at different strain rates already presented on Figure 4,
- two cyclic strain-controlled tests **CYC_02** (Figure 5) and **CYC_03** (Figure 6) performed at a strain rate $5 \cdot 10^{-3}$ 1/s

For the last two, reference will be made to particular stress-strain loops at given cycles denoted as **CYC1_02**, **CYC5_02** and **CYC1000_02** corresponding respectively to cycle 1, 5 and 1000 (stabilized cycle) in the case of test **CYC_02** and **CYC1_03**, **CYC5_03** and **CYC400_03** (cycle 1, 5 and 400) for test **CYC_03**.

To get fast-convergence and good quality solutions when using gradient-driven optimization algorithms (such as the Levenberg-Marquardt method available in **Zopt**), it is strongly advised to use a step-by-step procedure, adding tests and the corresponding sensitive parameters progressively into the optimization loop. In such a procedure, previously calibrated coefficients provide good starting points for the next step, thus allowing the algorithm to escape local minima. Finally, all tests are added and all coefficients identified at the same time, thus yielding a good quality optimal set of coefficients.

a) First evaluation of the viscosity parameters on test VISC

A first estimate of the viscosity parameters K , n and initial yield $R0$ can be obtained using the **VISC** strain-rate sensitive test. The corresponding material template file and the optimization input file are given below. One can see that during this first step all hardening mechanisms are removed from the model. Numerical simulation of this test is performed using the **Zsim** module. The optimizer input file and the material template file (GS500.tpl) are given below.

```
***optimize levenberg_marquardt          ***behavior gen_evp
***shell Zrun -S VISC                    **elasticity ...
***files GS500                           **potential gen_evp
***values                                  **criterion mises
  K    100.  min 1. max 10000.            **flow norton
  n     5.   min 1. max 10.                K ?K
  R0   10.  min 0. max 500.                n ?n
***convergence iter 200                   **isotropic constant
***compare                                  R0 ?R0
  t_file_file VISC.test 1 3 VISC.exp 1 3  ***return
****return
```

Optimizer input file

Material template file : GS500.tpl

The optimizer fast converges to an optimized set of coefficients that provides a fairly good fit of test **VISC** (see Figure 7): in about 20 iterations (this includes the iterations needed to calculate the sensitivity of the cost function to design parameters), the cost function is strongly decreased and a good quality solution is obtained.

b) Calibration of the kinematic hardening parameters C and D from stabilized material response

Stabilization is obtained at about 1000 cycles for test **CYC_02** and 400 cycles for test **CYC_03**. To avoid simulation of a large number of cycles, the response is calculated directly on the stabilized cycle by considering that the nonlinear isotropic hardening is saturated and that the final yield radius is 0 ($R0+Q=0$ in equation 3). This only leaves the kinematic hardening coefficients C and D to completely define the hardening behavior during this cycle.

As the maximum stress obtained during the cycle is defined by equation (7), the coefficient K must also be evaluated during this step. Values of K obtained during step a) (denoted by K_a) is used as a starting point, while the power law exponent n is kept fixed to n_a for the rest of the identification procedure.

The corresponding optimization and material template files are detailed below.


```

****optimize levenberg_marquardt
***shell Zrun -S STAB
***files GS500s
***values
  K K_a min 10. max 10000.
  C 2000. min 10. max 500000.
  D 200. min 1. max 10000.
***convergence iter 200
***compare
  t_file file CYC1000_02.test 1 3
  CYC1000_02.exp 1 3
  t_file file CYC400_03.test 1 3
  CYC400_03.exp 1 3
****return

```

Optimizer input file

```

***behavior gen_evp
**elasticity ...
**potential gen_evp
**criterion mises
**flow norton
  K ?K
  n n_a
**kinematic nonlinear
  C ?C
  D ?D
**isotropic constant
  R0 0.
***return

```

Material template file : GS500s.tmpl

As shown on figure 8 after 30 optimization iterations an optimized set of parameters is obtained that fits closely the stress-strain loops of the stabilized cycle.

c) Calibration of the initial yield stress R0 on the first cycle

Once the K_b , C_b , D_b set of parameters obtained during step b are fixed, the only parameter left to calibrate the model through the overall cyclic history is the initial yield stress $R0$. The corresponding optimization and material template files are:

```

****optimize levenberg_marquardt
***shell Zrun -S CYC1
***files GS500
***values
  R0 R0_a min 0. max 300.
***convergence iter 200
***compare
  t_file file CYC1_02.test 1 3
  CYC1_02.exp 1 3
  t_file file CYC1_03.test 1 3
  CYC1_03.exp 1 3
****return

```

Optimizer input file

```

***behavior gen_evp
**elasticity ...
**potential gen_evp
**criterion mises
**flow norton
  K K_b
  n n_a
**kinematic nonlinear
  C C_b
  D D_b
**isotropic constant
  R0 ?R0
***return

```

Material template file : GS500.tmpl

Optimization results are summarized on Figure 9. As there is only one parameter to fit in this step, fast convergence (10 iterations) is obtained.

d) Final optimization of all parameters on all cycles

At this point the only unknown parameter is the isotropic hardening saturation rate b , that must be fitted on intermediate cycles. Since the current set of parameters already gives a pretty good fit for both the first and the stabilized cycle, all parameters will be released in this step and all tests introduced in the optimization loop at the same time.

Note that during this last step, two material files are used at the same time. As in step b) a "stabilized" material file with constant initial yield parameter $R1$ is used for the last cycle (file GS500s). However this $R1$ value must correspond to the non-linear isotropic hardening saturated value $R0+Q$ defined in material file GS500. A constraint on the design variables is thus introduced in the optimizer input file, and the augmented_lagrangian method that can handle those constraints effectively is activated.

In about 150 iterations (including sensibility analysis function evaluations) the overall least square distance cost function is decreased from a value of about 1000 down to 828. Numerical results obtained with this optimized set of coefficients are compared to experimental results on Figure 10.

The optimizer input file, the material template file (GS500.tmpl) and the stabilized material template file (GS500s.tmpl) are given below.

```

***optimize augmented_lagrangian
***shell Zrun -S CYC1
          Zrun -S CYC5
          Zrun -S STAB
***files GS500 GS500s
***values
K  K_b  min 10.  max 10000.
C  C_b  min 10.  max 500000.
D  D_b  min 1.   max 10000.
R0 R0_c  min 0.   max 300.
Q  -R0_c min -500. max 0.
R1 0.    min 0.   max 300.
***constraint R1 - R0 - Q = 0.;
***convergence iter 200
***compare
t_file_file CYC1_02.test 1 3
CYC1_02.exp 1 3
t_file_file CYC1_03.test 1 3
CYC1_03.exp 1 3
t_file_file CYC5_02.test 1 3
CYC5_02.exp 1 3
t_file_file CYC5_03.test 1 3
CYC5_03.exp 1 3
t_file_file CYC1000_02.test 1 3
CYC1000_02.exp 1 3
t_file_file CYC400_03.test 1 3
CYC400_03.exp 1 3
****return

```

Optimizer input file

```

***behavior gen_evp
**elasticity ...
**potential gen_evp
**criterion mises
**flow norton
      K ?K  n  n_a
**kinematic nonlinear
      C ?C  D  ?D
**isotropic nonlinear
      R0 ?R0 Q ?Q  b ?b
***return

```

Material template file : GS500.tmpl

```

***behavior gen_evp
**elasticity ...
**potential gen_evp
**criterion mises
**flow norton
      K ?K  n  n_a
**kinematic nonlinear
      C ?C  D  ?D
**isotropic constant
      R0 ?R1
***return

```

Stabilized material template file : GS500.tmpl

5.2 Industrial application

With specific power increasing, the exhaust manifold has become one of the most critical component of an engine. This component is submitted to thermomechanical loads which occur at high temperatures. Sometimes, failure occurs by thermomechanical fatigue and creep damage due to the repeated restrained expansion and contraction of the manifold. The following example describes the first results obtained from a diesel engine exhaust manifold finite element simulation using Abaqus and Zmat.

The first step of our procedure is the calculation of the transient thermal field. This thermal cycle is classically chosen to reduce the period of component validation. Using FE , a thermal cycle is computed until a good agreement with experimental measurements is obtained (thermocouples placed in different locations on a real exhaust manifold). The transient temperature is then known at each node of the structure.

The objective of the mechanical calculation is to analyse the thermomechanical low cycle fatigue and creep damage of the hot parts. In a first step, we have to determine the stress/strain field. To predict the durability of the manifold at high temperatures, a formulation of the material behavior which gives accurate mechanical values which control fatigue and creep damage is needed. The behavior of the material (cast iron) has been modelled using the elastoviscoplastic constitutive law previously identified with Zsim and Zpost (i.e. Chaboche type model). Using this elastoviscoplastic law, FE computations were performed to estimate the transient stress/strain fields. For the first cycle, Figure 12 shows the stress range from the end of the maximum power retention time until the end of the idle speed retention time, and Figure 13 shows a cumulative strain field at the end of the idle speed retention time. To take into account the temperature effect and identify the critical areas in the component, a normalised stress range must be considered instead of the stress range shown in Figure 12. After calculating " asymptotic " conditions, we obtain the necessary input to evaluate the durability of the manifold : stress and temperature history during stabilised cycle. The location of the critical zones identified by the cumulated uniaxial equivalent inelastic strain are in good agreement with the experimental data. At present time, calculation of the corresponding fatigue life is in progress.

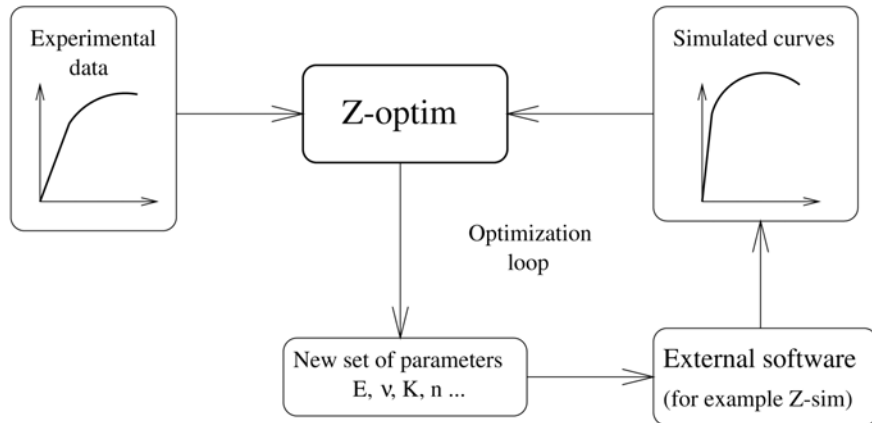


Figure 1: Structure of the optimization module Z-optim

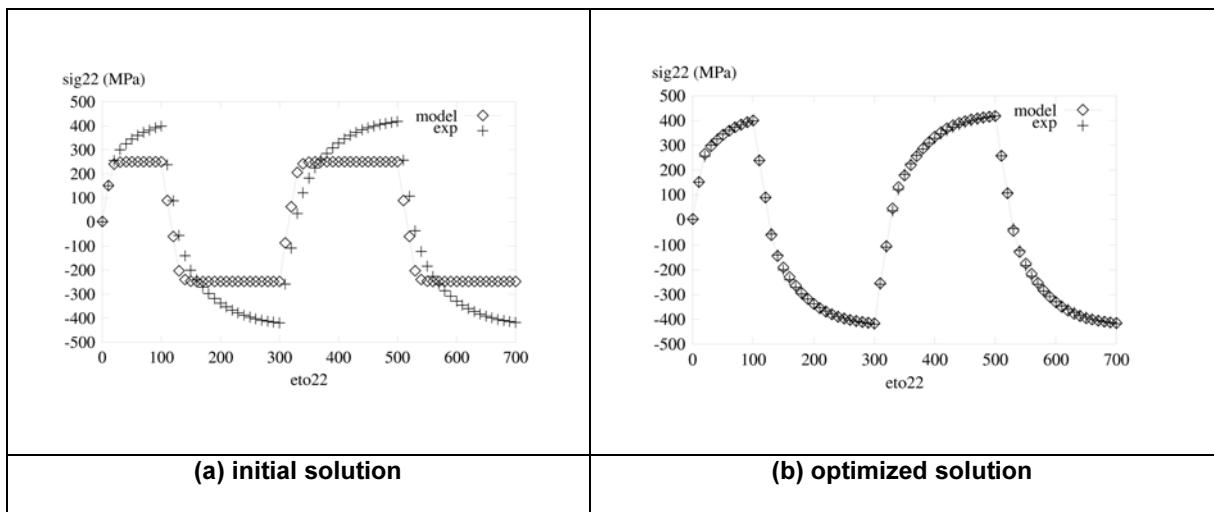


Figure 2: Comparison between experimental data and model simulations of a fatigue test

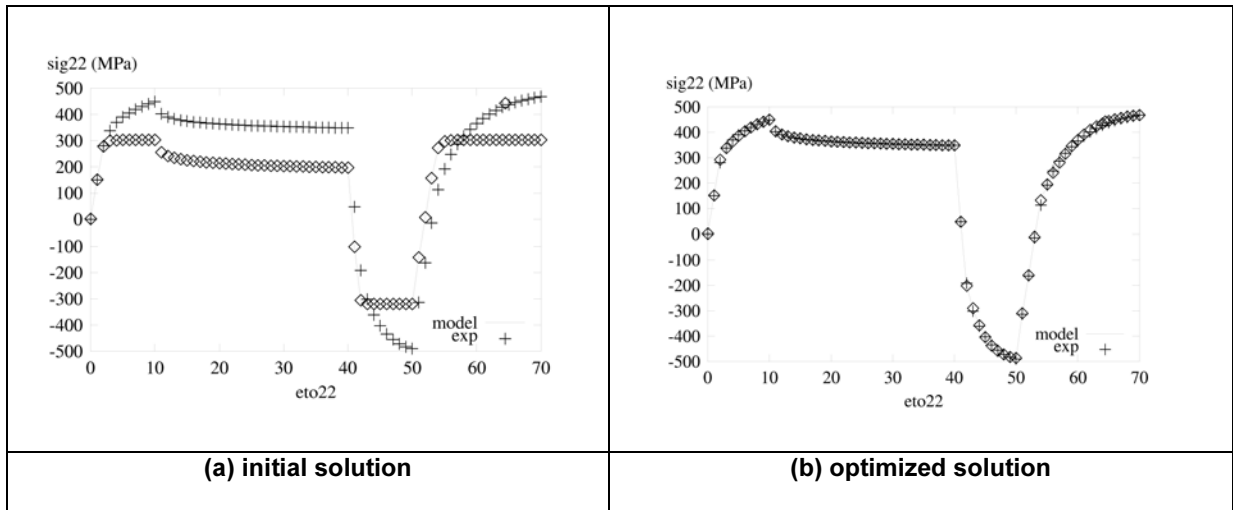


Figure 3: Comparison between experimental data and model simulations of a relaxation test

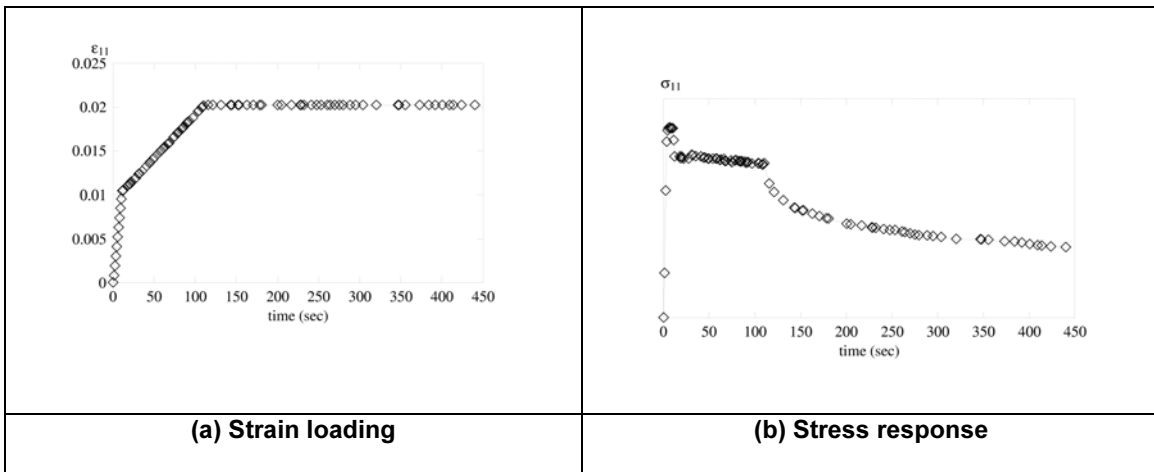
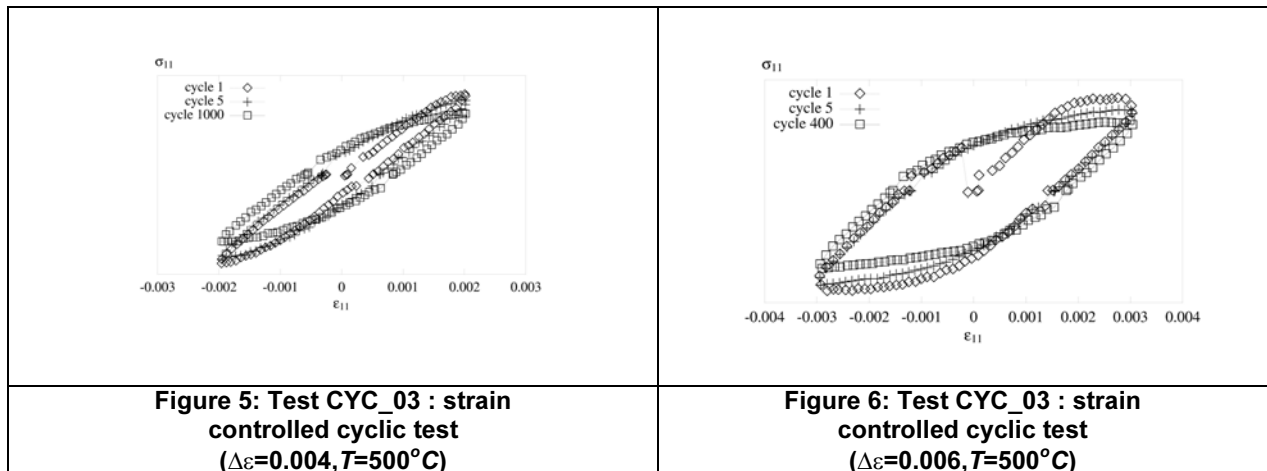
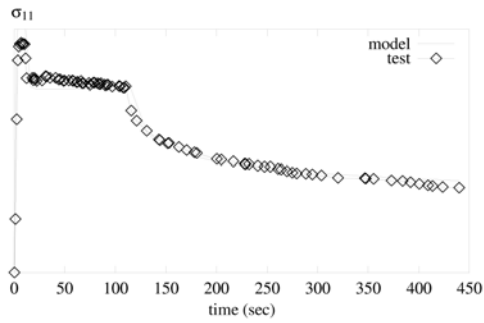
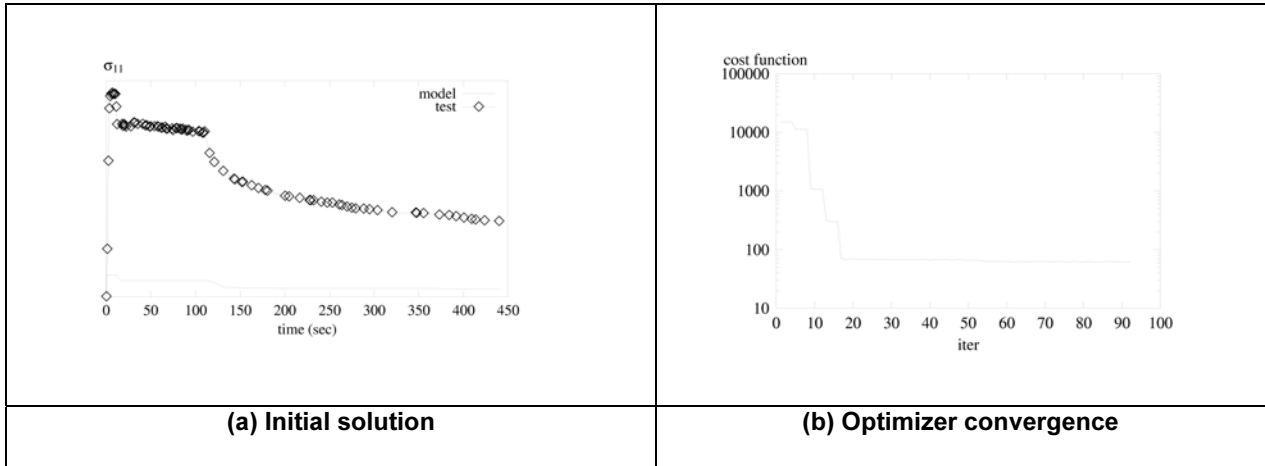


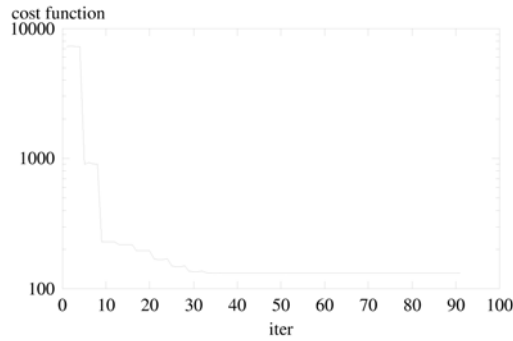
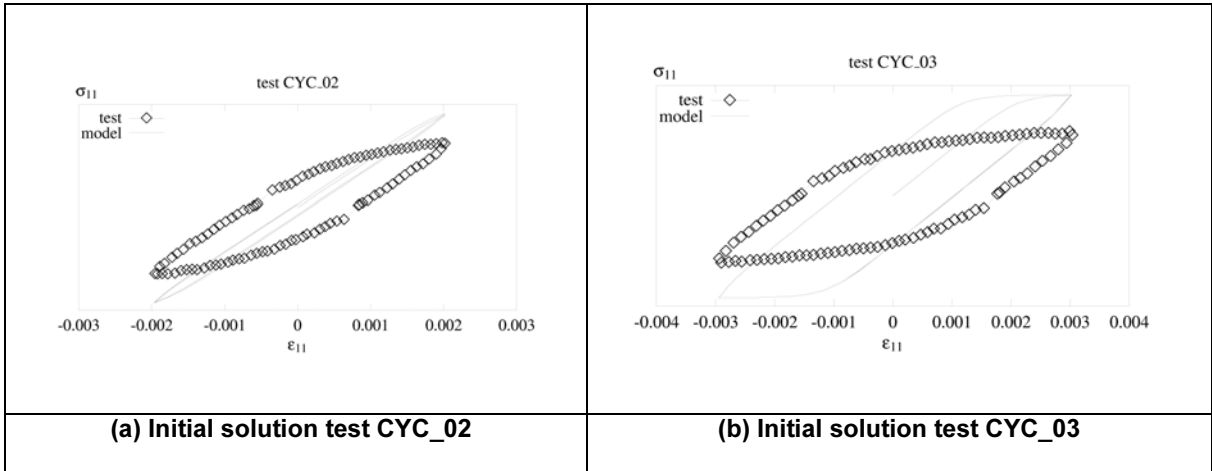
Figure 4: Test VISC: tensile test at various strain rates (500°C)





(c) Optimized solution

Figure 7: First identification of K , n and $R0$ on test VISC



(c) Optimizer convergence

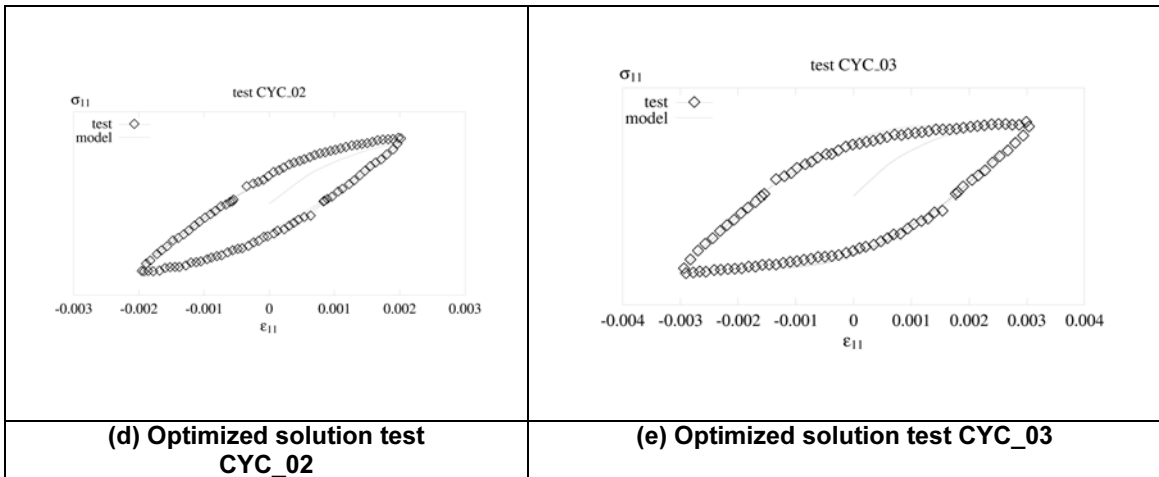
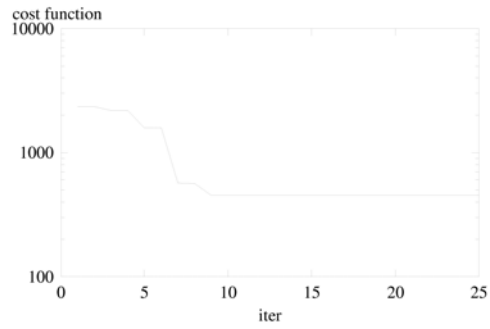
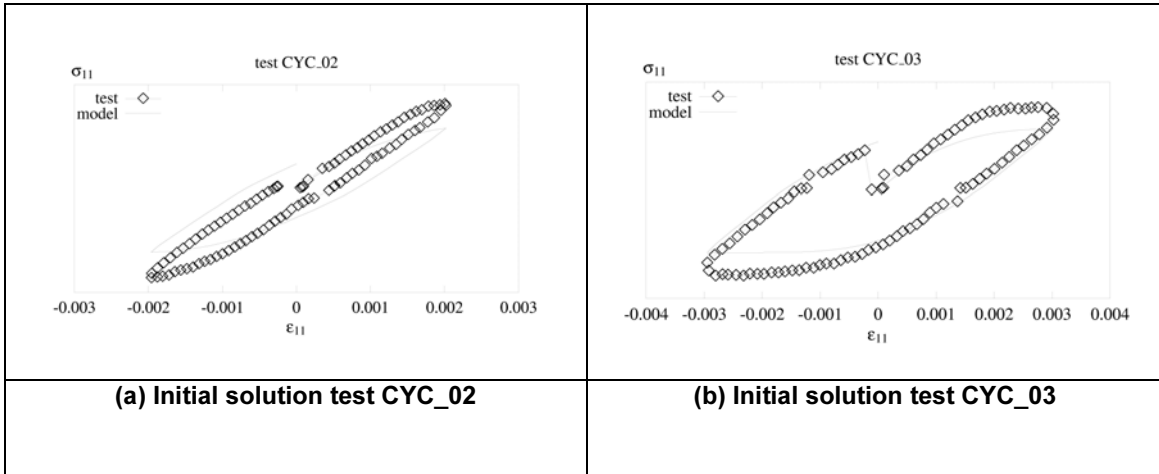


Figure 8: Identification of C and D parameters on the stabilized cycles



(c) Optimizer convergence

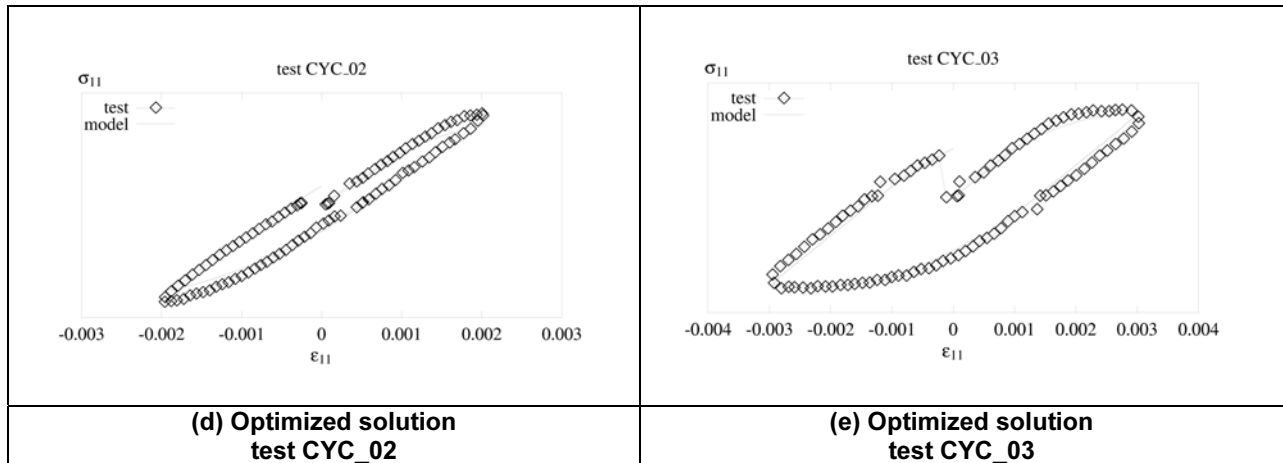


Figure 9: Identification of the $R0$ parameter on the first cycle

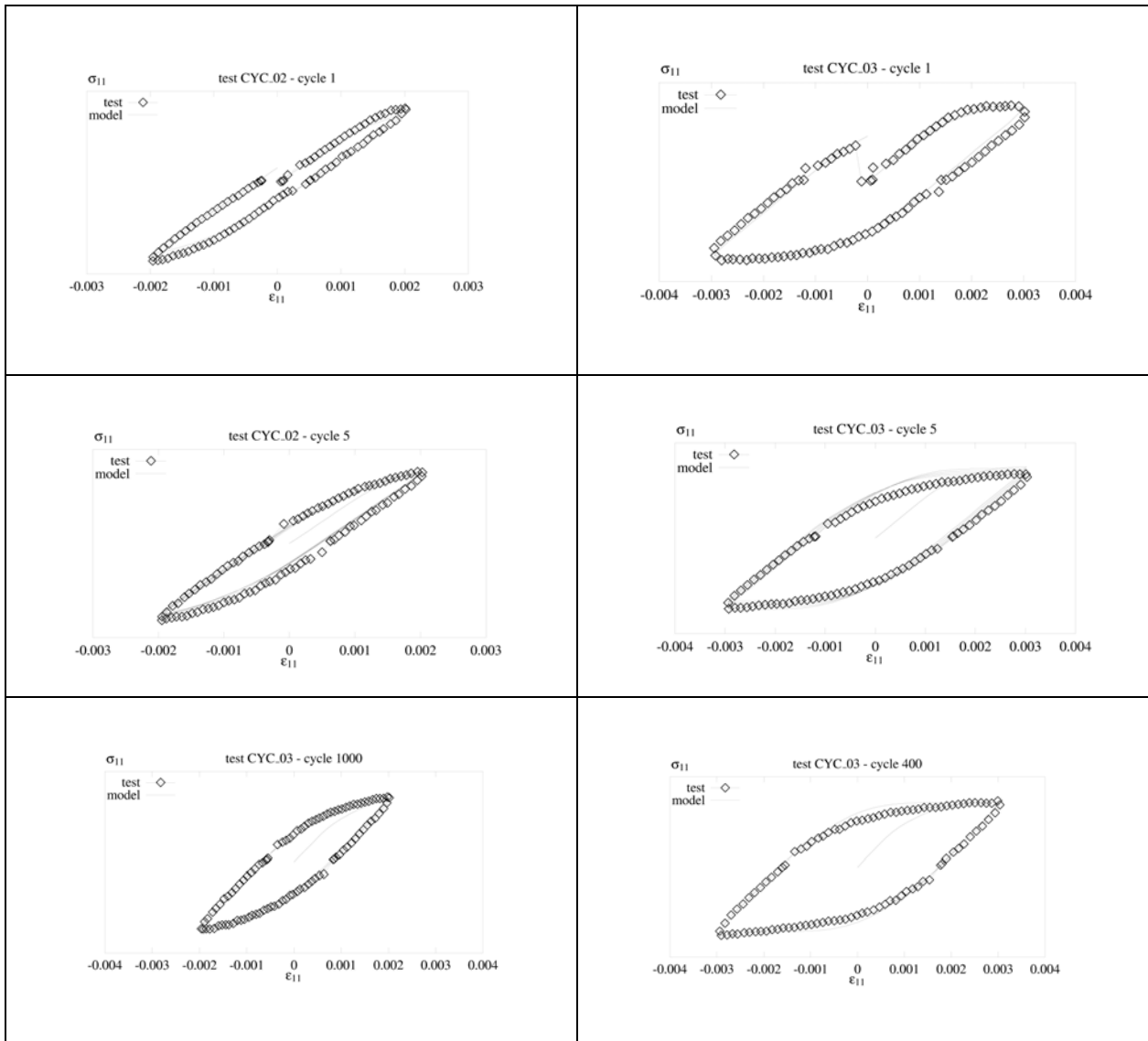


Figure 10: Identification of all parameters on all cycles

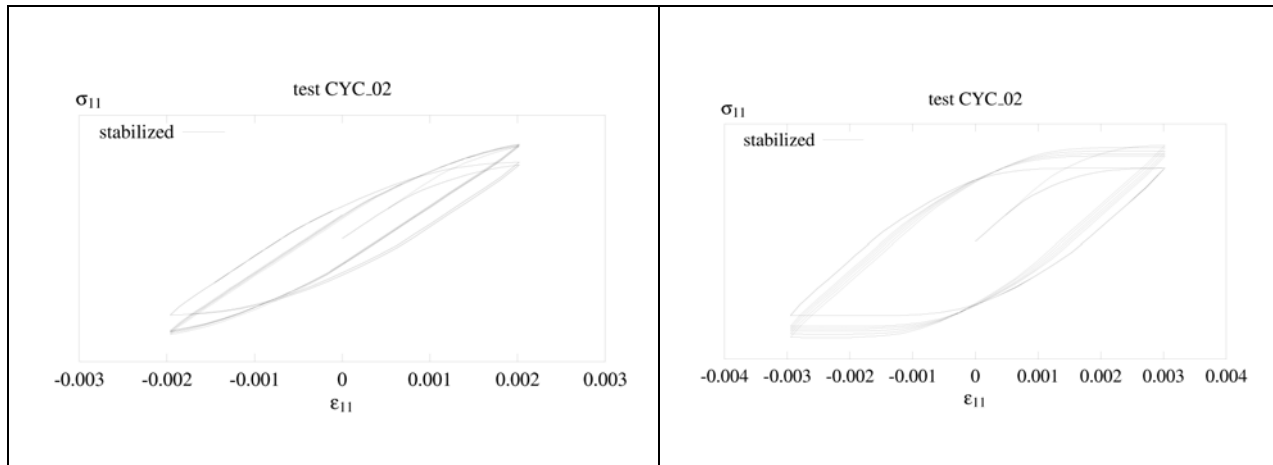


Figure 11: Evolution of the stress strain loops for the final optimized set of parameters

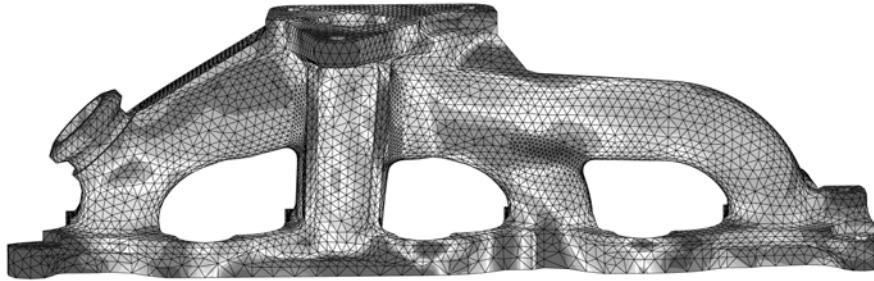


Figure 12: Stress range

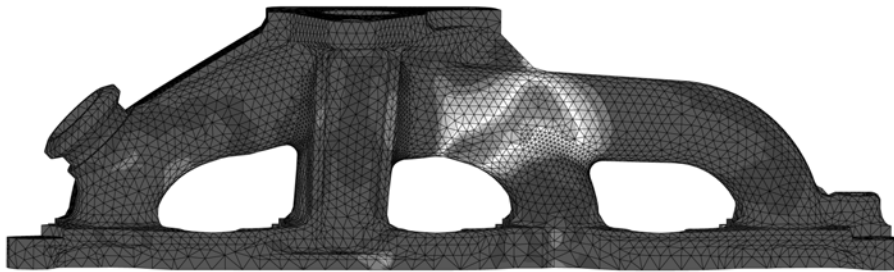


Figure 13: strain field at the end of the idle speed retention time