AUTOMATIC MATERIAL MODELLING

FOR FINITE ELEMENT ANALYSIS

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1 INTRODUCTION

Up to now, there has been an accelerating rate at which various structural materials were developed to assist the objective of industrial designers. In various industrial fields, materials are often used under severe operating conditions such as cyclic loading, high temperature, high pressure and high irradiation. For the reliable evaluation of deformation behaviours of these materials, thermo-inelastic analyses are indispensable. A variety of theoretical models, which describe a wide range of viscoplastic behaviours of materials have been proposed and discussed in the literature [N. Ohno, 1990]. Viscoplastic constitutive equations derived from these theories involve many parameters, which significantly influence the behaviours of the constitutive equations. Appropriate parameters must be determined accordingly such that the accurate behaviours of materials can be expressed.

Every constitutive model has its own method for the parameter identification. The advance of computer hardware has increased the popularity of an approach where all the parameters are identified simultaneously and, most commonly, optimisation methods are used to find the parameter set by adjusting them until they provide the best agreement between the measured data and the computed model response by the fact that this approach is applicable to a wide range of constitutive models [Y. Bard, 1974]. Out of them, continuous evolutionary algorithms (CEAs), previously proposed by the authors [T. Furukawa, 1996], have demonstrated their capability to yield good approximate solutions efficiently for parameter identification of inelastic constitutive equations [T. Furukawa and G. Yagawa, 1997]. In order to use this approach, one however needs to put a great deal of effort on the implementation of a model of concern.

In this paper, we hence present the generalised material modelling and, further, an automatic modelling system for finite element analysis. Thanks to the generalisation, the system requires only the minimum inputs under user-friendly environment. The next section refers to the overview of conventional constitutive models, and a general formulation for constitutive modelling and identification are represented in the third section. The fourth section deals with the developed system and conclusions are summarised in the final section.

2 FORMULATION

Inelastic constitutive equations describe stress-strain relationship of material behaviours in inelastic range and are, in a general sense, given by

$$\mathbf{F} = \hat{\boldsymbol{\sigma}}(\boldsymbol{\varepsilon}; \mathbf{x}), \tag{1}$$

where σ , ε and x represent the stress, strain and parameters respectively. Note here that we only will present formulations for strain control partly because the strain control test is more popular than the stress control test and partly because the stress control formulation can be given by exchanging the stress and strain. Such constitutive models can be typically classified into two types: models having only observable variables, i.e., stress and strain, and those having variables describing material internal behaviours as well as observable variables [J.L. Chaboche and G. Rousselier, 1983]. One simple model for the former is Ramberg-Osgood model, which is given by

$$\varepsilon = \frac{\sigma}{E} + a(\frac{\sigma}{b})^n, \qquad (2)$$

where a, b and n are parameters to be identified. A typical example of the latter may be Chaboches model [J.L. Chaboche, 1989], based on the unified theory:

$$\varepsilon = \varepsilon^e + \varepsilon^{vp}, \tag{3a}$$

$$\dot{\varepsilon}^{vp} = \left\langle \frac{|\sigma - \chi| - R}{K} \right\rangle^n \operatorname{sgn}(\sigma - \chi), \qquad (3b)$$

$$\dot{\chi} = H\dot{\varepsilon}^{\nu p} - D\chi \left| \dot{\varepsilon}^{\nu p} \right|, \qquad (3c)$$

$$\dot{R} = h \left| \dot{\varepsilon}^{\nu p} \right| - dR \left| \dot{\varepsilon}^{\nu p} \right|, \tag{3d}$$

where χ and R represent material internal variables, describing the yield stress and the drag stress respectively. ε^{e} and ε^{vp} are elastic and viscoplastic strains, and $\mathbf{x} = [K, n, H, D, h, d, E]$ are parameters to be determined.

3 GENERALISATION

3.1 Modelling

The difficulty of general formulation can be easily understood by having a look at the various description of models as described in the last section. The models however can be generalised in terms of mathematical considerations. The first equation to be constructed deals with the static stress-strain relationship, and is given by

$$\boldsymbol{\sigma} = \hat{\boldsymbol{\sigma}}(\boldsymbol{\varepsilon}, \boldsymbol{\xi}; \mathbf{a}) \tag{4}$$

where $\boldsymbol{\xi}$ is the set of internal variables including the viscoplastic strain, back stress and drag stress, and **a** is the set of material parameters. The internal evolution with respect to time is then given by the state space equations:

$$\dot{\boldsymbol{\xi}} = \hat{\boldsymbol{\xi}}(\boldsymbol{\sigma}, \boldsymbol{\xi}; \mathbf{a}) \tag{5}$$

covering viscoplastic constitutive models. The model thus consists of Eq. (4), and also Eq. (5) if internal variables are considered additionally. Ramberg-Osgood model, for example,

consists of Eq. (4), and Chaboche model is defined by Eqs. (4) and (5) with internal variables ε^{vp} , χ and R.

3.2 Simulation

The definition of these equations allows simulation by giving the initial conditions of the internal variables:

$$\boldsymbol{\xi}(0) = \boldsymbol{\xi}_0 \tag{6}$$

As the initial condition of the strain is known beforehand, the initial condition of the stress can be then calculated by Eq. (4):

$$\sigma(0) = \hat{\sigma}(\varepsilon_0, \boldsymbol{\xi}_0; \mathbf{a}) \tag{7}$$

The rate of change of the internal variables is given by Eq. (5):

$$\dot{\boldsymbol{\xi}}(k-1) = \dot{\boldsymbol{\xi}}(\boldsymbol{\sigma}(k-1), \boldsymbol{\xi}(k-1); \mathbf{a})$$
⁽⁸⁾

The increments of the internal variables and the strain of the viscoplastic model are thus given by

$$\Delta \boldsymbol{\xi}(k-1) = \Delta t \cdot \boldsymbol{\dot{\xi}}(k-1) . \tag{9}$$

and the integration derives the next state of the internal variables can be derived as

$$\xi(k) = \xi(k-1) + \Delta \xi(k-1).$$
(10)

As the strain $\varepsilon(k)$ is given, the next state of the observable variable can also be derived by $\sigma(k) = \hat{\sigma}(\varepsilon(k) \ \xi(k) \cdot \mathbf{a})$ (11)

$$O(k) = O(\mathcal{E}(k), \zeta(k), \mathbf{a})$$
(11)

Continuous simulation is conducted by iterating these processes. Consequently, parameters necessary for simulation are strain rate $\dot{\varepsilon}(k-1)$ and time increment Δt .



Figure 2. Cyclic tests.

The variable which control the strain evolution, $\dot{\varepsilon}(k-1)$ for viscoplastic models, is dependent on the type of experiment to be simulated, which includes the monotonic test and

the cyclic test each with $\varepsilon_0 = 0$ most popularly. The general description of the variables for these tests is at least necessary, and Figures 1 and 2 show the monotonic and cyclic tests respectively. One of the parameters common in both the tests is the maximum absolute value of strain ε_{max} , and let the number of iterations until the strain reaches ε_{max} from zero be p_{sim} . If q cycles are simulated in the cyclic test, the strain rate is given by

$$\dot{\varepsilon}(k) = \begin{cases} 4np_{sim} \le k < (4n+1)p_{sim} \\ \dot{\varepsilon}_c & \text{for} \\ -\dot{\varepsilon}_c & \text{for} \\ -\dot{\varepsilon}_c & \text{for} \\ (4n+3)p_{sim} \le k < (4n+3)p_{sim} \\ 4n+1)p_{sim} \le k < (4n+3)p_{sim} \end{cases}$$
(12)

where n = 1, 2, ..., q. Note that the monotonic test is treated as the first quarter of the cyclic test, and it is, thus, also given by Eq. (3) in the case of n = 0, i.e., $0 \le k < p_{sim}$. The strain interval for one iteration is given by

$$\Delta \varepsilon_c = \frac{\varepsilon_{\max}}{p_{sim}} \tag{13}$$

and this derives the time increment Δt :

$$\Delta t = \frac{\Delta \varepsilon_c}{\dot{\varepsilon}_c} \tag{14}$$

The monotonic and cyclic tests can be conclusively governed by only four parameters, i.e., the maximum absolute value of strain ε_{max} , the number of iterations p_{sim} , strain rate $\dot{\varepsilon}_c$ and the number of cycles q.

3.3 Identification

As the majority of experimental data are taken with a constant increment, we here suppose that there are m experiments, each having m_j stress-strain data, $[\sigma_i^{j*}, \varepsilon_i^{j*}]$, $\forall i \in \{1, 2..., m^j\}$, $\forall j \in \{1, 2..., m\}$, with constant increment:

$$\Delta \varepsilon_{\exp}^{j} = \varepsilon_{i}^{j} * - \varepsilon_{i-1}^{j} *$$
⁽¹⁵⁾

and there are r^{j} experimental data between the strains of 0 and \mathcal{E}_{max}^{j} excluding the initial condition:

$$\boldsymbol{\varepsilon}_{\max}^{j} = \boldsymbol{r}^{j} \cdot \Delta \boldsymbol{\varepsilon}_{\exp}^{j} \tag{16}$$

Parameters which are to be identified may include material parameters **a** and initial conditions ξ_0 . By expressing the unknown and known parameters separately in vector form as $\mathbf{a} = [\mathbf{a}', \mathbf{a}^*]$ and $\xi'_0 = [\xi'_0, \xi^*_0]$, we first define parameters to be identified as $\mathbf{x} = [\mathbf{a}', \xi'_0]$. In accordance with the model description in the last subsection, the identification problem is formulated as:

$$\min_{\mathbf{x}} \sum_{j=1}^{m} \sum_{i=0}^{m_j} w_{ij} \left\| \boldsymbol{\sigma}_i^j \ast - \hat{\boldsymbol{\sigma}}(\boldsymbol{\varepsilon}_i^j \ast, \boldsymbol{\xi}(k); \mathbf{a}) \right\|^2 \tag{17}$$

subject to the parameter space constraints:

$$\mathbf{x}_{\min} \le \mathbf{x} \le \mathbf{x}_{\max} \,, \tag{18}$$

where W_{ij} is the weighting factor. As seen in the formulation, it is required that strain $\varepsilon(k)$ coincide with each experimental data ε_i^{j*} :

$$\varepsilon(k) = \varepsilon_i^j *, \tag{19}$$

As simulation increment $\Delta \varepsilon_c^j(k)$ is very small comparatively to experimental step $\Delta \varepsilon_{exp}^j$, this means that k at which the experimental data are compared has to be the multiplication of i_j .

If p_{id}^{j} iterations take place until the simulation reaches ε_{i}^{*} from $\varepsilon_{i-1}^{j}^{*}$, k th iteration of simulation can be hence related to *i* th stress-strain data by

$$k = p_{id}^{j} \cdot i \tag{20}$$

The strain increment for simulation and the number of simulations can be derived respectively as

$$\Delta \varepsilon_c^{\ j} = \frac{\Delta \varepsilon_{\exp}^{\ j}}{p_{id}^{\ j}} \tag{21}$$

$$p_{sim}^{j} = p_{id}^{j} \cdot r^{j} \tag{22}$$

The parameters defined in Eqs. (21) and (22) allows the simulation of plastic models compatible with experimental data, and the simulation of viscoplastic models can be also achieved by calculating time increment Δt in terms of Eq. (14).

Parameters necessary for identification include the model, known initial conditions and material parameters, search space for unknown initial conditions and material parameters, the number of experiments, experimental conditions, stress-strain data and the number of iterations of each experiment, weights for optimisation criteria and parameters for CEA.



Figure 3. System overview.

Figure 4. Main window.

4 AUTOMATED SYSTEM

4.1 System configuration

Figure 3 illustrates the schematic diagram of the developed system, and the main window of the system is shown in Figure 4. The system consists of Control Manager and Computation subsystems. In Control Manager subsystem, the user can control the system, construct a model of concern, input parameters, execute simulation with parameters all specified, and see the result of computation. Meanwhile, Computation subsystem computes the processes of simulation and identification. While Control Manager subsystem is programmed in JAVA so as to take the advantage of its capability for graphical user interface, Computation subsystem is programmed in C due to its fast computation.

The execution of the system first shows a window with a menu bar, which includes the menus of Model, Window, Execute and System, and Input Window by default. The modelling is first conducted in Model menu if the model of concern has not been generated yet or needs to be modified. The generated model and other parameters are then inputted for identification. After the process of identification, and the results of the process is visualised.

4.2 Modelling

The modelling process is shown in Figure 5. Because the computation part is written in C, the model is provided as part of a function of C file, and is created with the submenu of New or edited with Open if the model file exists. If New is selected in the submenu, the number of state variables and the number of parameters to be identified are sequentially asked for input. An alphabet or word is then assigned to each variable or parameter in order that the user can easily understand their values. If Open is selected, we only need to input the model file name. Input of these values then runs the model editor with a help window to be shown.



Figure 5. Modelling process.

Figure 6. Modelling window.

Figure 6 shows the window where the user edit the model. The window consists of two parts and the user writes Eq. (4) in one part and Eq. (5) in the other. When the edition is over, the interface compiles the program to check its grammar by pressing Compile button and terminates the modelling if the compilation is succeeded. Otherwise, the user goes back to the edition. The 'model' file can be saved at anytime during the edition as a file with suffix "*.mod.c".

4.3 Identification

The parameters in the current system include all of those explained in the formulation

except for weighting factor W_i , which will be implemented in the next version. In addition to the model file, the files that have to be prepared beforehand for identification are those describing experiments wherein two files, experimental data file (*.dat) and experimental condition file (*.dat.con), represent each experiment. While the data file includes the set of stress-strain data, conditions under which the experiment took place are written in the condition file.

In the input of model-related parameters for identification, only known parameters are specified, the search space being inputted for the unknown parameters. In order to do so, the user is first asked to select 'Known' or 'Unknown' for each parameter and further fills in value(s). Meanwhile, experimental data files to be used for identification can be added by pressing 'Add' and deleted by pressing 'Delete'. Finally, the identification can be executed by choosing 'Start' in 'Execute' menu. Transition of the identification and the resultant stress-strain curve can be then investigated after the execution, and they are illustrated in Figure 7.

Generalisation of inelastic constitutive modelling for automated parameter identification and the parameter identification system, developed by the authors, has been presented in the paper. The generalisation and the modeller developed accordingly has allowed the user to model a wide range of constitutive equations. In addition, the user can identify parameters very easily thanks to the user-friendly graphical user interface. For further studies, the system is being updated such that it automatically extracts a model file with parameters identified for commercially available finite element analysis packages. While the automation of the input of geometrical information is much studied, material models have been manually implemented into the finite element code, and this update will greatly improve the finite element analysis.

5 CONCLUSIONS

An automated system for parameter identification of inelastic constitutive models, which is based on CEAs, have been presented. The greatest advantages of the system are its applicability to a variety of inelastic constitutive equations, reliable and stable acquaintance of a good approximate solution and user-friendliness of interface. Currently ongoing work includes the structurisation of the program, simplification of a modelling process, further userfriendliness as software. With the completion of these assignments, the program will be distributed on the Internet as free software.

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Figure 7. Results of identification.