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The development of computational FE system for creep damage analysis of weldment

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Abstract

A Finite Element Analysis (FEA) system was designed for the analysis of creep deformation and damage evolution in weldment. This project essentially consists of three parts which involves 1) transfer programme development, 2) numerical integration subroutine development, and 3) validation of complete FEA system. Firstly, the development of a user-friendly pre- and post- processing transfer programme and its assembly with the numerical solver was reported; its primary development was published before. This part includes file format understanding, specific parameter adding, and transfer algorithm design. Secondly, a numerical integration subroutine which developed for specific creep constitutive equations was introduced. This part includes the numerical method selection, accuracy control in finite element method, and its validation. Thirdly, because this project has not finished yet, a demonstration how this system works was assumed in future work. For this part, a circumferentially notched bar with low Cr alloy material case was purposed to prove the capability of transfer programme and integration subroutine.

1. Introduction

Creep deformation and damage in weldment is a serious problem for high temperature industries. A weldment typically consists of four material zones such as parent metal, fine grain HAZ (FGHAZ), coarse grain HAZ (CGHAZ), and weld metal. The mis-match in mechanical properties among these zones and the influence on stress re-distribution leads to extremely complication in understanding the mechanisms of failure of a weldment.

Computational approach (finite element analysis based) has been used in research. However, due to the advanced nature of the creep damage constitutive equations, the analysis capability is not available from the standard FE. Only two ways can provide the computational means; one is to develop a User's Subroutine for existing commercial FEA software such as ABAQUS or ANSYS [1], the other is to develop an in-house numerical solver in junction with commercial pre- and post- processing software [2]. The second approach has its own advantages and merits.

Liu et al [3, 4] intend to develop an in-house solver which utilised current subroutines to fit his algorithm. However, for the solver development itself, there is a need of accurate and efficient integration which requires further research; in addition to the development of numerical solver, there is a gap between standard pre- and post-processing software and the need for creep damage analysis. Thus,

this project is part of the integral of the project of developing FEA software for creep deformation and damage analysis of weldments, and complements to the research work carried out or to be carried out by Liu et al [3, 4].

This research utilised the Femsys [5] as the pre- and post- processor, and reports the development of the data transfer software between Femsys and in-house numerical solver. Femsys was utilised by some researchers such as Hayhurst et al [6] and Becker, et al [7], and it is an important reason to choose Femsys in this research. The authors also reviewed the detail in previously publication [8], for example:

1. DAMAGE XX [9] is an early creep damage analysis solver developed at UMIST. The authors have noted that there are detailed publication on its development, however, it is understood that this software is of plane stress, plane strain, and axi-symmetrical version, written in Fortran 77 and the failed elements are removed from the stiffness matrix. Fourth order Runge-Kutta integration method was adopted. It has been an important tool for a number of researches and supporting the production of significant number of publication, these publications are not listed here for brevity. Femsys is used for pre- and post- processing.
2. DAMAGE XXX [10] is a new advanced version of DAMAGE XX, which was also developed at UMIST. This package not only adds a 3D finite element analysis function but also expands to parallel computation. Hayhurst et al. [11] report its validation via analysing creep failure in the HAZ zone of Cr-Mo-V cross-welds and its application. Femsys is used as pre- and post-processing software.
3. FE-DAMAGE is another in-house code developed at University of Nottingham. It has been used in research, for example, Becker et al. [6] used the FE-DAMAGE program to present four different creep damage results (e.g. uniaxial problem, biaxial perforated plate problem, tri-axial notched bar problem and multi-material cross-weld problem in his paper). Femsys is also used as the pre- and post- processing software.

Creep damage problem is complicated and dynamically developing, and there is not readily available analysis capability in most of the commercial analysis software. There is still a need, to certain degree, to develop and then use in-house software in research community. Tan et al. [8] reviewed the current situation of computational tools in 2012. This paper also introduced the detail of numerical integration subroutines development such as integration method selection, time step control. Even the concept is following previously researchers [9, 10, 12, 13], all the technique skills details are authors own work [8, 14].

2. Data transfer interface development

Following the research on data structure of Femsy [5, 15], because Femsys is a general pre- and post-processor, the file format cannot fit to every in-house software. Therefore, some gaps will influence the file transfer progress such as 1) In creep damage analysis, a lot of special creep material parameters such as A, B, C, h, H*, Kc, and v will participate in calculation; however, the both of them cannot obtain from Femsys; 2) Which integration method will be chosen and been included in the input data

In order to solve these problems which mentioned above, a series of subroutines were coded. After that, these subroutines were assembled, and the software running flowchart shows below.

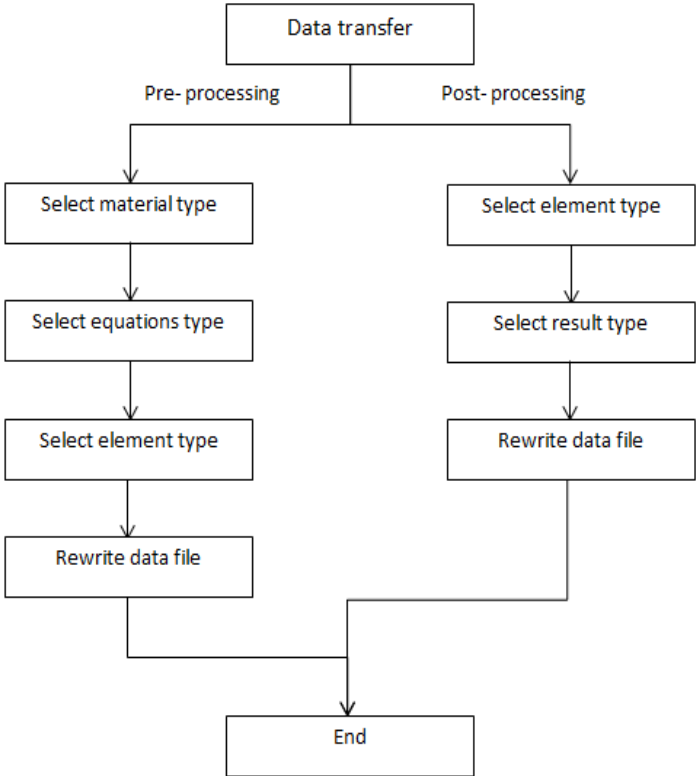


Figure 1. Flowchart of interface programme [16]

In pre-processing transfer, node coordinate system was completely adopted. Element definition will be rewrite depend on which element type had been chosen. Constraint and load should be rewrite to fit solver’s format. The information of material’s parameter and constitutive equations type must be added. In post-processing transfer, the specific result head set required be added, and all the result format will be rewrite to fit Femsys format.

A notched bar case was used to verify the tranfer programme; however, the damage value is assumed because creep damage FE package is unavailiable yet. The damage was assumed to appere on the centre of notched part.

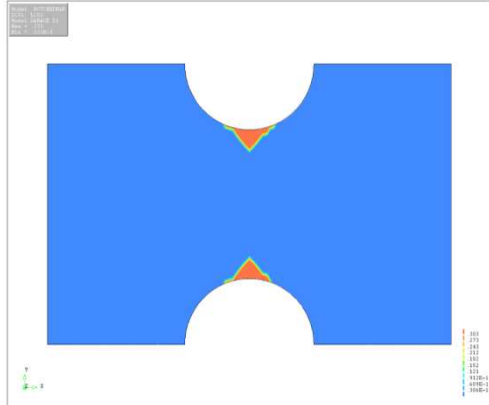
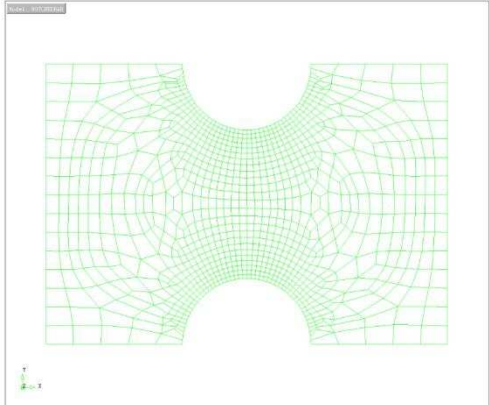


Figure 2 left) Mesh model of notched bar; right) assumed damage on notched bar

3. Numerical integration subroutines development

The Kachanov–Rabotnov–Hayhurst (KRH) constitutive equations were utilised in this research [15]. Its uni-axial form can be expressed as:

$$\dot{\varepsilon} = A \sinh\left(\frac{B\sigma(1-H)}{(1-\varphi)(1-\omega)}\right) \quad (1-1)$$

$$\dot{H} = \frac{h}{\sigma} \left(1 - \frac{H}{H^*}\right) \dot{\varepsilon} \quad (1-2)$$

$$\dot{\varphi} = \frac{K_c}{3} (1 - \varphi)^4 \quad (1-3)$$

$$\dot{\omega} = C \dot{\varepsilon}^* \quad (1-4)$$

The KRH constitutive equations multi-axial form can be expressed:

$$\dot{\varepsilon}_{ij} = \frac{3S_{ij}}{2\sigma_e} A \sinh\left(\frac{B\sigma_e(1-H)}{(1-\varphi)(1-\omega)}\right) \quad (2-1)$$

$$\dot{H} = \frac{h}{\sigma_e} \left(1 - \frac{H}{H^*}\right) \dot{\varepsilon}_e \quad (2-2)$$

$$\dot{\varphi} = \frac{K_c}{3} (1 - \varphi)^4 \quad (2-3)$$

$$\dot{\omega} = CN \dot{\varepsilon}_e^* \left(\frac{\sigma_1}{\sigma_e}\right)^v \quad (2-4)$$

The uni-axial form can be used to investigate which integration method is better, such as Euler's method and Runge-Kutta method. The multi-axial form is used in the real FE software to compute the strain increment and three kinds of damage parameter. Such constitutive equations adopt a set of stress deviator components to compute the strain deviator components; however, the existing FE subroutine normally output stress components as the result and utilise strain components to redistribute the stress. This must be noticed in software development.

3.1 Integration method selection

Two different integration methods were advised by previous researchers [10], the Euler's method and Runge-Kutta Method (RKM) were compared to make sense the benefit of each integration method. The author designed the comparison procedure: (1) setting the result of Euler's method as the baseline; (2) comparing the result of RKM within different tolerance control value; (3) comparing Euler's method and RKM.

Two programmes were prepared, one is for constitutive equations integration within Euler's method via call self-coded subroutine, and the other is for integration within RKM via call NAG subroutine D02BJF [17]. A simple uni-axial creep under stress of 40 MPa is used for test, the component is deemed failed if the damage parameter reaches 0.33 which is the criterion used here. To solve this set of constitutive equations within NAG routine D02BJF [17], the terminated time should be predicted for prepared this numerical experiment because this routine was suggested from one specific time to another specific time.

3.1.1 Result based on Euler's method

In order to make sense the most exactly lifetime, a simple Euler's method programme had been coded. The programme was tested using different time increment such as 1, 0.1, 0.01, 0.001, 0.0001 hour respectively.

The Table I show the terminated time, strain, and absolute damage value depending on the size of time interval. The time interval 0.0001 is the most accurate between the five different intervals. Even from mathematic aspect, the interval 0.0001 is the best selection; however, from the physics aspect, 0.0001 hours equal to 0.36 second, and this is a too short time interval. Therefore, the author selects the time interval 0.01 hour as the master accuracy control parameter. Following that, the lifetime value can be observed from table 1 is 104032.27 hours.

TABLE I result of Euler's method

Time interval (s)	Terminated time (h)	Ω (damage value)	ϵ_f (fracture strain)
1	104034.0000	0.333435236633273	0.179875512020971
0.1	104032.4000	0.333339889351067	0.179824075821904
0.01	104032.2700	0.333333868058920	0.179820827565906
0.001	104032.2580	0.333333386466599	0.179820567765346
0.0001	104032.2577	0.333333316847831	0.179820530208621

3.1.2 Result based on Runge-Kutta method

Because of the nature of NAG subroutine, the variable TOL was designed as the accuracy control parameter, where the TOL is a positive tolerance for controlling the error in integration. Give the duration from t=0 to t=104032.27 to NAG routine, and record the results of seven different TOL value ranging from 0.1E-01 to 0.1E-07 as shown in the following Table II.

TABLE II result of RK method

TOL	ϵ_f (fracture strain)	Ω (damage value)
0.1E-01	0.136548062074	0.253119148370
0.1E-02	0.178172199475	0.330277813609
0.1E-03	0.179803968745	0.333302624373
0.1E-04	0.179819797001	0.333331965213
0.1E-05	0.179820066343	0.333332464492
0.1E-06	0.179820072754	0.333332476375
0.1E-07	0.179820072807	0.333332476473

3.1.3 Errors analysis (accuracy)

The elastic strain under 40 MPa is $\epsilon = \frac{\sigma}{E} = \frac{40MPa}{200GPa} = 2 \times 10^{-4}$. The master curve (assuming accurate enough) creep strain at failure is 0.179820827565906 obtained with Euler's method at interval 0.01h; When TOL=0.1 $\times 10^{-3}$, strain at failure is 0.179803968745

The error in creep strain at is

$$\begin{aligned} \text{Error} &= |0.179803968745 - 0.179820827565906| \\ &= 1.6858820906 \times 10^{-5} \\ \text{error rate} &= \frac{1.6858820906 \times 10^{-5}}{2 \times 10^{-4}} = 8.42\% \end{aligned}$$

When $TOL=0.1 \times 10^{-7}$, strain at failure is 0.179820072807

The error in creep strain at failure is

$$\begin{aligned} \text{Error} &= |0.179820072807 - 0.179820827565906| \\ &= 7.54758906 \times 10^{-7} \\ \text{error rate} &= \frac{7.54758906 \times 10^{-7}}{2 \times 10^{-4}} = 0.37\% \end{aligned}$$

Similarly, the error rate in creep strain was calculated and all the results were shown in Table III.

From this Table, the $TOL=0.1 \times 10^{-7}$ is obviously satisfied the accuracy requirement, and the $TOL=0.1 \times 10^{-3}$ is too big than the expected value, say 1%, due to the high exponential or power law relationship between stress level and creep strain rate. It can be seen that when TOL value is 0.1E-05 is a very good choice.

TABLE III error rate

TOL	Percentage errors of strain at failure
0.1E-01	21636%
0.1E-02	824%
0.1E-03	8.43%
0.1E-04	0.51%
0.1E-05	0.38%
0.1E-06	0.37%
0.1E-07	0.37%

3.1.4 Efficiency analysis

In order to test the efficiency of this subroutine, 10,000 times calling was supposed, and the total calculation times following different TOL value were recorded and used for comparison. This constitutive equations subroutine offered the solutions of strain and damage value in each given durations. Once the subroutine running, an integration point would be solved in the finite element analysis processing. Basic that, a complete finite element analysis will call this subroutine over all the integration points and time iterations, typically in the order of thousands times thousands. This is the reason to call the subroutine 10,000 times.

The Euler's method was also tested for efficiency following the same experimental setting. The results are shown in Table IV and Table V.

TABLE IV RKM running time

Runge-Kutta Method Test	
TOL	Programme Running Time (s)
0.1	NONE
0.1×10^{-1}	10.2649
0.1×10^{-2}	15.2569
0.1×10^{-3}	15.7717
0.1×10^{-4}	15.8653
0.1×10^{-5}	16.1149
0.1×10^{-6}	16.4113
0.1×10^{-7}	17.0665

0.1×10^{-8} (Over Load)	1.56×10^{-2}
----------------------------------	-----------------------

TABLE V Euler's running time

Euler's method test	
Time interval	Programme running time (s)
1	1.5600100E-02
0.1	0.1716011
0.01	1.7628113
0.001	17.6593132
0.0001	175.64153

For a similar accuracy, the Euler's method will cost about 10% more computing time. This is demonstrated by the following. It can be seen from Table IV, when $TOL = 0.1 \times 10^{-5}$, the programme running time is 16.1149s. From Table VIII, when time interval is 0.001h, the programme running time is 17.6593132s. It can be defined a speed percentage like:

$$\text{percentage} = \frac{17.6593132 - 16.1149}{16.1149} = 9.58\%$$

As mentioned before, the accuracy of Euler's method at interval 0.001h can be derived as 0.13%; however, the absolute error is similar with R-K method at TOL of $0.1E-05$.

From the above discussion, it is clear that, based on the balance of accuracy and efficiency, the Euler method should not be used, and the TOL of $0.1E-04$ or $0.1E-05$ is a good choice for R-K method on the balance of accuracy and computing efficiency. It is also further noted that further reducing the value of TOL does increase the accuracy significantly without much increase of computing time.

It does not seem to show that Euler's method is the best; it is only the first attempt. The R-K method will be implemented and examined in real case where the stress re-distribution may affect the time step allowed which will be discussed next.

3.2 Time step control

Following previous researchers' step [9, 10, 12], a time step control concept will be adopted in this research. In order to guarantee the accuracy of integration result, make sure each integration step will not more than 0.1% of total strain, a result checking subroutine was designed and named 'time step control'. In the first integration step, the time increment will be set as big as possible such as a constant 50 (hours), and the checking criteria can be expressed as:

$$\frac{\Delta \varepsilon_e}{\varepsilon_e} < 0.001$$

Where $\Delta \varepsilon_e, \varepsilon_e$ are creep equivalent strain increment and creep equivalent strain respectively;

If the result is satisfied this criterion then the loops will go on; if not, the time increment will reduce half and re-do this loop until the result satisfied the criteria.

For the consequent steps, the time increment will follow the previous one, and was fitted in the criterion in each integration step.

4. Future Work

A number of researchers developed new constitutive equations or conducted FE application for weldments [18, 19, 20]. The future work will include 1) the development and implementation of time step control; 2) expansion of types of creep damage constitutive equations into library; 3) input data structure need to be expanded to accommodate for other types of constitutive equations and other type of elements; 4) real test of current integration subroutines, et al. Future progress will be reported in due course.

5. Conclusion

This paper reports to date progress in the developing computational system for creep deformation and damage analysis for weldments. It covered the requirement of computational tools of creep damage analysis, development of data transfer interface and constitutive equations' numerical integration scheme. The future work has been outlined.

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