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Practical guidance on the application of R-K integration method in finite element analysis of creep damage problem

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Abstract—A practical user guidance of Runge-Kutta (R-K) integration method with the context of non-linear time dependent finite element analysis (FEA) was proposed in this paper. Following the literature review of different integration method within the finite element analysis framework, detailed numerical experiments were conducted to find out the right balance between computing accuracy and efficiency. It contributes to knowledge to the numerical analysis software development in general and specific to computational creep damage mechanics.

Key words—integration method, creep damage, finite element analysis

I. INTRODUCTION

In general finite element analysis software, the complete processing progress can be divided into three stages. The first stage is pre-processing where topology of a FEA model, boundary condition, and type of problem (where the solution method need to be specified) is defined. The second stage is a numerical problem solving, for example, the stress and strain will be calculated and other field variables will be updated. The third stage is post-processing where the numerical results obtained in second stage will be presented and analysed by users, typically with interaction with graphic presentation. There is readily available commercial software for the pre- and post-processing now, such as FEMSYS or GID [1, 2].

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. [3] reviewed the current situation of computational tools in 2012 and reported, for example, 1) DAMAGE XX [4] is an early creep damage analysis solver, for 2D problem, developed at and used by the researchers at UMIST, and DAMAGE XXX [5] is a new advanced version for 3D problem; 2) FE-DAMAGE is another in-house code developed at University of Nottingham; 3) HTΣ is a Chinese package used for creep damage analysis which proposed by Tu [6]; 4) A Japanese in-house code was mentioned by Haigihara [7].

The nature of creep damage analysis is of time dependant and the field variables such as stress, strain, and creep damage variables need to be updated where an integration scheme needs to be implemented. Liu et al. [8] proposed some detailed algorithms to build an in-house FE package.

From literature review [6, 9], it seems that the fourth-order R-K method is a good choice due to its computing efficiency and accuracy. This paper reports an investigation about the balance between accuracy and efficiency in its use to integrate creep damage constitutive equations. It contributes to knowledge to the numerical analysis software development in general and specific to computational creep damage mechanics.

II. INTEGRATION METHOD

A. Euler’s method

The Euler method is a first-order numerical procedure for solving ordinary differential equations with a given initial value [10]. The Euler method required extremely small time steps to ensure the convergence of iterations and accuracy of calculations in creep fracture problem [11]. The method has advantages of brevity and simplicity in concept and programming. Unfortunately, this scheme is only conditionally stable and the stability condition is rather stringent. In creep fracture problem, high concentration of creep strain exists near the crack tip; the use of Euler method for creep damage simulation is quite uneconomic.

It can be found from literature that this method was adopted by an in-house code was developed by Tsing Hua University [11]. It is understood that DAMAGE XX has incorporated it as one of the integration methods while the user has to make
decision on which one to use.

B. Runge-Kutta method

Actually, in order to improve the efficiency of Euler’s method, a new numerical method was suggested. A standard way to determine whether the Runge–Kutta values are sufficiently accurate is to re-compute the value at the end of each interval with the step size cut in half. This method is also called “step doubling” [5]. If this makes a change of negligibly magnitude, the results are accepted; if not, the step is halved again until the results are satisfactory.

It is generally understood that R-K method is more accurate and efficient in comparison with forward Euler method, and thus its application has been reported. For instance, DAMAGE and efficient in comparison with forward Euler method, a new numerical method was suggested. A standard way to determine whether the Runge–Kutta values are obtained; the algebraic manipulation of these numbers leads to numerical rounding errors.

IV. SPECIFIC CONSTITUTIVE EQUATIONS

The KRH uni-axial constitutive equations [12] were used in the test:
\[
\dot{\varepsilon} = A \sinh \left( \frac{B \sigma (1 - H)}{(1 - \varphi) (1 - \omega)} \right) \quad (4.1)
\]
\[
H = \frac{h}{\sigma} \left( \frac{1 - \frac{H}{H^*}}{\varphi} \right) \quad (4.2)
\]
\[
\dot{\varphi} = \frac{K}{3} (1 - \varphi)^4 \quad (4.3)
\]
\[
\omega = C \dot{\varepsilon}^* \quad (4.4)
\]

The KRH multi-axial constitutive equations can be expressed:
\[
\varepsilon_{ij} = \frac{3s_{ij}}{2\sigma_e} \sinh \left( \frac{B \sigma_e (1 - H)}{(1 - \varphi)(1 - \omega)} \right) \quad (4.5)
\]
\[
H = \frac{h}{\sigma_e} \left( 1 - \frac{H}{H^*} \right) \dot{\varepsilon}_e \quad (4.6)
\]
\[
\dot{\varphi} = \frac{K}{3} (1 - \varphi)^4 \quad (4.7)
\]
\[
\omega = C \dot{\varepsilon}^* \left( \frac{\dot{\varepsilon}_e}{\sigma_e} \right)^v \quad (4.8)
\]

Where \( A = 2.1618 \times 10^{-9} \text{MPa}^{-1} \), \( B = 0.20524 \text{MPa}^{-1} \), \( C = 1.8537 \), \( h = 2.4326 \times 10^{15} \text{MPa} \), \( H^* = 0.5929 \), \( K_c = 9.2273 \times 10^{-5} \text{MPa}^{-3} \), \( v = 2.8 \).

V. NAG ROUTINE

D02BHF (NAG) [13] integrates a system of first-order ordinary differential equations solution using Runge-Kutta-Merson method. This subroutine can be adopted in the FEA software of creep damage analysis development, and a detailed instruction on how to use it was published by the company [13]. Basically, this routine can be written as:

SUBROUTINE D02BHF (X, XEND, N, Y, TOL, IRELAB, HMAX, FCN, G, W, IFAIL)

INTEGER N, IRELAB, IFAIL
REAL X, XEND, Y(N), TOL, HMAX, G, W(N, 7)
EXTERNAL FCN, G

D02BHF aims to solve ordinary differential equation using Runge-Kutta-Merson method, until a user-specified function of the solution is zero; therefore, it cannot be adopted completely. The variables which mentioned above should be re-identified in creep damage analysis application area.

1. X – real
   The X means the start moment t1
2. XEND – real
   The XEND means the finish moment t2
3. N – integer
   The N means the number of constitutive equations
4. Y(N) - real array
   The Y(N) means the arrays which store the data of strain, damage, hardness….. respectively
5. TOL – real
   The TOL means the tolerance for controlling the time steps
6. IRELAB – integer
   The IRELAB means the type of error control, in here, normally set as 1.
7. HMAX – real
   HMAX means the original user-defined time step
8. FCN – subroutine
The FCN means the constitutive equations statement
9. G – real function
The G was originally developed for terminate this
programme when the specific function equal to zero. This
function would not be used in creep damage analysis because
all constitutive equations should not be expected to appear a
solution equal to zero. The G was suggested to set as the
default G=Y(1).
10. W(N,7) – real array
11. IFAIL – integer
IFAIL means the routine error feedback, and must be set to
0, -1 or 1.

VI. NUMERICAL EXPERIMENT
This case is uni-axial creep under stress of 40 MPa. 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, the terminated
time should be predicted for prepared this numerical
experiment because this routine was suggested from one
specific time to another specific time.

A. Result based on Euler’s method
In order to make sense the most exactly lifetime, a simple
Euler’s method programme had been coded. And the code was
tested using different time increment such as 1, 0.1, 0.01,
0.001, 0.0001 hour respectively.
Three Tables were listed to show the detail of the results.
The Table I shows the terminated time and omega depending
on the size of time interval. The time interval 0.0001 is the
most accurate between the five different intervals. Table II and
Table III displayed the specific creep strain value, H which is
the primary creep state variable (strain hardening), and φ
which is the precipitate coarsening state variable.
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 I is 104032.27
hours.

<table>
<thead>
<tr>
<th>Time interval (s)</th>
<th>Terminated time (h)</th>
<th>ω</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>104034.0000</td>
<td>0.333435236633273</td>
</tr>
<tr>
<td>0.1</td>
<td>104032.4000</td>
<td>0.33339889351067</td>
</tr>
<tr>
<td>0.01</td>
<td>104032.2700</td>
<td>0.33333868058920</td>
</tr>
<tr>
<td>0.001</td>
<td>104032.2580</td>
<td>0.33333386466599</td>
</tr>
<tr>
<td>0.0001</td>
<td>104032.2577</td>
<td>0.33333316847831</td>
</tr>
</tbody>
</table>

B. Result based on Runge-Kutta method
Because of the nature of NAG subroutine, the variable TOL
was designed as the accuracy control parameter. 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 IV.
Tables IV and V show the detailed results. And a
comparison will be processed with previous results which
based on Euler’s method to looking for the most accurate
value of TOL, strain and damage value.

<table>
<thead>
<tr>
<th>TOL</th>
<th>εf</th>
<th>ω</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1E-01</td>
<td>0.136548062074</td>
<td>0.253119148370</td>
</tr>
<tr>
<td>0.1E-02</td>
<td>0.178172199475</td>
<td>0.33027813609</td>
</tr>
<tr>
<td>0.1E-03</td>
<td>0.179803968745</td>
<td>0.333302624373</td>
</tr>
<tr>
<td>0.1E-04</td>
<td>0.179819797001</td>
<td>0.33331965213</td>
</tr>
<tr>
<td>0.1E-05</td>
<td>0.17982006343</td>
<td>0.33332464492</td>
</tr>
<tr>
<td>0.1E-06</td>
<td>0.179820072574</td>
<td>0.33332476375</td>
</tr>
<tr>
<td>0.1E-07</td>
<td>0.179820072807</td>
<td>0.33332476473</td>
</tr>
</tbody>
</table>

C. Errors Analysis (ACCURACY)
The elastic strain under 40 MPA is $\varepsilon = \frac{\sigma}{E} = \frac{40\text{MPa}}{200\text{GPa}} = 2 \times 10^{-4}$, and an error in the calculated creep strain will
eventually affect the stress updating. The master curve
(assuming accurate enough) creep strain at failure is
0.179820827565906 obtained with Euler’s method at interval
0.01h;
1. When TOL=0.1x10^-3, strain at failure is
0.179803968745
The error in creep strain at is
\[
\text{Error} = |0.179803968745 - 0.179820827565906| = 1.685882096 \times 10^{-5}
\]
\[
\text{error rate} = \frac{1.685882096 \times 10^{-5}}{2 \times 10^{-4}} = 8.42%
\]
2. When \( TOL=0.1 \times 10^{-7} \), strain at failure is 0.179820072807

The error in creep strain at failure is
\[
Error = |0.179820072807 - 0.179820827565906| = 7.54758906 \times 10^{-7}
\]
\[
error\ rate = \frac{7.54758906 \times 10^{-7}}{2 \times 10^{-4}} = 0.37\%
\]

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

From this table, the TOL=0.1×10^{-7} is obviously satisfied the accuracy requirement, and the TOL=0.1×10^{-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>
<thead>
<tr>
<th>TOL</th>
<th>Percentage errors of strain at failure</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1E-01</td>
<td>21636%</td>
</tr>
<tr>
<td>0.1E-02</td>
<td>824%</td>
</tr>
<tr>
<td>0.1E-03</td>
<td>8.43%</td>
</tr>
<tr>
<td>0.1E-04</td>
<td>0.51%</td>
</tr>
<tr>
<td>0.1E-05</td>
<td>0.38%</td>
</tr>
<tr>
<td>0.1E-06</td>
<td>0.37%</td>
</tr>
<tr>
<td>0.1E-07</td>
<td>0.37%</td>
</tr>
</tbody>
</table>

D. Efficiency Analysis

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.

A problem occurred here is running this subroutine once, and the running time cannot be present by computer because the value is too small. 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.

The Euler’s method was also tested for efficiency following the same experimental setting. The results are shown in Table VII and Table VIII.

It can be seen that, from Table VII, when TOL = 0.1×10^{-6}, 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:

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, nor costs that much more time.

<table>
<thead>
<tr>
<th>Runge-Kutta Method Test</th>
<th>Programme Running Time (s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>TOL</td>
<td></td>
</tr>
<tr>
<td>0.1</td>
<td>NONE</td>
</tr>
<tr>
<td>0.1×10^{-1}</td>
<td>10.2649</td>
</tr>
<tr>
<td>0.1×10^{-2}</td>
<td>15.2569</td>
</tr>
<tr>
<td>0.1×10^{-3}</td>
<td>15.7717</td>
</tr>
<tr>
<td>0.1×10^{-4}</td>
<td>15.8653</td>
</tr>
<tr>
<td>0.1×10^{-5}</td>
<td>16.1149</td>
</tr>
<tr>
<td>0.1×10^{-6}</td>
<td>16.4113</td>
</tr>
<tr>
<td>0.1×10^{-7}</td>
<td>17.0665</td>
</tr>
<tr>
<td>0.1×10^{-8} (Over Load)</td>
<td>1.56×10^{-2}</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Euler’s method test</th>
<th>Programme running time (s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Time interval</td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>1.5600100E-02</td>
</tr>
<tr>
<td>0.1</td>
<td>0.1716011</td>
</tr>
<tr>
<td>0.01</td>
<td>1.7628113</td>
</tr>
<tr>
<td>0.001</td>
<td>17.6593132</td>
</tr>
<tr>
<td>0.0001</td>
<td>175.64153</td>
</tr>
</tbody>
</table>

VII. Conclusion

This paper reviewed the position which the creep constitutive equations in the finite element analysis method. An advance numerical method, Runge-Kutta method was suggested by Hyhurst, and a Chinese scholar also follows this approach. The more efficient NAG routine was adopted in this research to help the creep FE software development. A specific computational experiment was been written detailed, and highlight the way to find a satisfied TOL value.

References

Basic format for books:


