A general approach for solving three-dimensional transient nonlinear inverse heat conduction problems in irregular complex structures

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\textbf{A B S T R A C T}

A novel general approach is proposed for solving three-dimensional transient nonlinear inverse heat conduction problems in irregular complex structures. The complex-variable-differentiation method (CVDM) is introduced into the commercial finite element method (FEM) software ABAQUS, for solving three-dimensional inverse heat conduction problems for the first time. First, the complex variable finite elements are set up, and the complex variable FEM is innovatively developed through the user element subroutine (UEL) in ABAQUS. Then, the key parameters in the Levenberg-Marquardt algorithm for solving inverse problems—sensitivity matrix coefficients—are accurately evaluated by utilizing the CVDM and ABAQUS standard solvers with the UEL. Finally, several numerical tests are carried out to verify the performances of the new approach for solving the three-dimensional transient nonlinear inverse heat conduction problem in an irregular complex structure.

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1. Introduction

Inverse heat conduction problems (IHCPs) have attracted many researchers’ interests, and a lot of innovative work [1–14] has been implemented, attributed to their promising potentials in various engineering applications. The objective of the IHCP is to determine thermal-physical parameters, initial conditions, internal heat sources, boundary conditions or geometrical parameters, when part of temperatures or heat flux is known [11–14]. Inverse problems are ill-posed that small errors or change of input conditions could cause oscillations and large errors of solutions. These make the solving of inverse problems very challenging.

To solve inverse heat conduction problems, many innovative methods have been being proposed [15–25]. These methods can be generally classified into two categories: the stochastic and the gradient [20]. The gradient methods are known for both high accuracy and efficiency, in which the accurate evaluation of sensitivity matrix coefficients is a key issue. In the recent years, the authors’ group have focused on the accurate calculation of sensitivity coefficients in gradient methods; a complex-variable-differentiation method (CVDM) [26] was introduced into inverse heat transfer problems to calculate the sensitivity matrix coefficients, and satisfactory results have been obtained [12,20,27–29]. Numerical tests showed that the CVDM is very promising that accurate sensitivity matrix coefficients could be calculated even for highly nonlinear inverse problems [30–32]. However, the previous work cannot combine the CVDM with any commercial software, which limits the engineering application scope of the CVDM. It will be desirable to implement CVDM into typical commercial software, such as the nonlinear finite element method (FEM) software ABAQUS that possesses high accuracy, efficiency and adaptivity to irregular complex structures in engineering applications.

To employ the FEM software ABAQUS for heat conduction analysis in complex structures, a gradient method that was based on the central difference scheme for sensitivity analysis was developed and excellent results were obtained [29]. However, the algorithm was not always effective to solve the nonlinear inverse heat conduction problem, because the central difference would not be always accurate for sensitivity analysis for solving nonlinear inverse problems. To overcome the above-mentioned problem, the CVDM is introduced into the FEM commercial software ABAQUS in the present work, for solving 3D inverse heat conduction problems, by which sensitivity matrix coefficients are calculated. Then, the efficient Levenberg-Marquardt (LM) algorithm [20] is applied to solve inverse heat conduction problems, attributed to its good inversion performances.

There are two main challenges to implement the CVDM with ABAQUS and the LM algorithm for solving inverse heat conduction
problems. First, ABAQUS is a real-valued FEM which could not directly provide complex value operations. Second, data exchange has to be efficiently carried out between intermediate results and input/output files. For the first problem, complex elements are first set up, and a user element subroutine (UEL) is used to develop a small imaginary part, or heat convective coefficient, W·m⁻²·°C⁻¹. In the present work, the inversion approach is developed by Fortran codes, and the batch file is used to call ABAQUS with Python scripts with high efficiency and accuracy, which could be accurate with 9 decimals. When the ABAQUS analysis is completed, the results are extracted by ABAQUS CAE through Python scripts and output by ABAQUS with a small imaginary part, or heat convective coefficient, W·m⁻²·°C⁻¹. A user element subroutine (UEL) is used to develop a small imaginary part, or heat convective coefficient, W·m⁻²·°C⁻¹. In the present work, the inversion approach is developed by Fortran codes, and the batch file is used to call ABAQUS with Python scripts with high efficiency and accuracy, which could be accurate with 9 decimals.

In the present work, the inversion approach is developed by Fortran codes, and the batch file is used to call ABAQUS with Python scripts. In this way, a series of processes, such as modeling, meshing and analysis, can be performed by employing ABAQUS with UEL, and then inverse heat conduction problems can be solved.

2. Three-dimensional transient nonlinear heat conduction problem

The energy equation for the three-dimensional (3D) transient nonlinear heat conduction problem could be written as follows [34]:

\[
\rho(T)c(T) \frac{\partial T}{\partial t} = \frac{\partial}{\partial x} \left[ \lambda(T) \frac{\partial T}{\partial x} \right] + \frac{\partial}{\partial y} \left[ \lambda(T) \frac{\partial T}{\partial y} \right] + \frac{\partial}{\partial z} \left[ \lambda(T) \frac{\partial T}{\partial z} \right] + \rho(T)Q
\]

with the initial condition

\[
T(x, y, z, t=0) = T(x, y, z)
\]

The boundary conditions are:

\[
T = T_1 \quad \text{(boundary of } \Gamma_1)\]

\[
\lambda(T) \frac{\partial T}{\partial n} + \lambda(T) \frac{\partial T}{\partial y} + \lambda(T) \frac{\partial T}{\partial z} = q \quad \text{(boundary of } \Gamma_2)
\]

where \(\lambda(T)\) is the thermal conductivity, W·m⁻¹·°C⁻¹, and \(\rho(T)\) is the density, kg·m⁻³.

\[
\lambda(T) \frac{\partial T}{\partial n} + \lambda(T) \frac{\partial T}{\partial y} + \lambda(T) \frac{\partial T}{\partial z} = h(T_1 - T) \quad \text{(boundary of } \Gamma_3)
\]

3. Traditional finite element method for solving heat conduction problems

To determine the transient distributed temperatures, the basic equation of finite element can be obtained by a difference algorithm. The equations for solving the transient heat conduction problem by using FEM can be summarized as:

\[
[C] \{\partial T/\partial t\} + [K]\{T\} = \{P\}
\]

where \([C]\) is the heat capacity matrix, \([\partial T/\partial t]\) is a vector which contains the derivatives of temperature with respect to time, \([K]\) is the heat conduction matrix, \(\{T\}\) is the vector of temperature, and \([P]\) is the vector of thermal load.

Employing an interpolation formula, one could obtain:

\[
\theta(\partial T/\partial t)_{t,A,M} + (1 - \theta)(\partial T/\partial t)_{t,A,M_{+1}} = (T_{t,A,M} - T_{t,A,M-1})/\Delta t
\]

where \(\theta\) is the weighted coefficient that determines the difference scheme. For example, the Euler method will be used with \(\theta = 0\) and the central difference method is adopted with \(\theta = 1/2\). In the present work, we choose \(\theta = 1\), which is the backward difference. Given \(\theta = 1\), Eq. (8) becomes

\[
\frac{[C]}{\Delta t} + [K]\{T\}_{t,A,M} = \{P\}_{t,A,M} + \frac{[C]}{\Delta t}\{T\}_t
\]
For each step, the heat capacity matrix [C], conduction matrix [K], temperature vector (T), and load vector (P) are known, while the temperature vector (T) is unknown. By representing $C + [K]$, (T) is determined at time $t > 0$. With $K$, T and P, it follows that

$$KT = P$$ (10)

4. Levenberg-Marquardt algorithm

In the present inverse heat conduction problem, the boundary conditions are unknown and need to be inverted. Other conditions are kept the same as in the direct conduction problem. The additional information required is the temperature measurement, which is measured data or calculated by the direct heat conduction problem.

4.1. Objective function

The inverse problem can be constructed as a problem of minimization of the following objective function:

$$F(s_1, s_2, ..., s_N) = \frac{1}{M} \sum_{i=1}^{M} \left( T_i^a - T_i(s_1, s_2, ..., s_N) \right)^2$$ (11)

where $M$ is the number of measured temperatures, $N$ is the number of parameters to be inverted. The vector $s = (s_1, s_2, ..., s_N)$ is made up of the inverted parameters, and $s_i$ is the $i$th inverted parameter. $T_i^a$ and $T_i$ are the measured and calculated temperatures, respectively, $i = 1, 2, ..., M$.

The inverted parameter vector is updated by:

$$s_i^{n+1} = s_i^n + \delta^p$$ (12)

where $p$ is the iteration number, $k = 1, 2, ..., N$, and $\delta$ is determined by the following equation [20]:

$$\left[ J^T + \mu \text{diag}(J^T) \right] \delta = J^T [T_i^a - T_i(s)]$$ (13)

where $J$ is the sensitivity coefficient matrix as shown in Eq. (14), diag represents diagonal elements, $\mu$ is the damping factor which is adjusted at each iteration. The newly proposed approach in Ref. [20] is adopted to determine the damping factor at each iteration, which would relate the damping factor directly to the dimensionless objective function.

$$J = \begin{bmatrix}
\frac{\partial f_1(s)}{\partial s_1} & \frac{\partial f_1(s)}{\partial s_2} & ... & \frac{\partial f_1(s)}{\partial s_N} \\
\frac{\partial f_2(s)}{\partial s_1} & \frac{\partial f_2(s)}{\partial s_2} & ... & \frac{\partial f_2(s)}{\partial s_N} \\
\vdots & \vdots & \ddots & \vdots \\
\frac{\partial f_N(s)}{\partial s_1} & \frac{\partial f_N(s)}{\partial s_2} & ... & \frac{\partial f_N(s)}{\partial s_N}
\end{bmatrix}$$ (14)

4.2. The complex-variable-differentiation method (CVDM)

The CVDM proposed by Lyness and Moler [26] is employed to determine the sensitivity coefficient matrix. In CVDM, the variable $X$ of a real function $f(X)$ is replaced by the complex variable $X + ih$, with the imaginary part $h$ being very small. The function $f(X + ih)$ can be expanded in a Taylor series as:

$$f(X + ih) = f(X) + ihf'(X) - \frac{h^2}{2}f''(X) + o(h^3)$$ (15)

Since $h$ is very small, the derivative of $f(X)$ is:

$$f'(X) = \frac{\text{Im}(f(X + ih))}{h}$$ (16)

It has been validated that the CVDM was with high accuracy for calculating the sensitivity coefficients, either for linear or nonlinear inverse problems [12,20,27–29,31]. However, the CVDM could not be combined with any commercial software in the previous work, which limit its engineering applications.

5. FEM in ABAQUS with CVDM

To use the CVDM in ABAQUS, the traditional FEM in ABAQUS should be in complex form. From Eqs. (15) and (16), it can be seen that only the imaginary part of the inverted parameter needs a small value, and the calculation process of complex-variable FEM is the same as that in the traditional FEM calculation process. Then, Eq. (10) could be written as:

$$\bar{K} \bar{T} = \bar{P}$$ (17)

In Eq. (17), $\bar{K}$, $\bar{P}$ and $\bar{T}$ have the same forms as the real $K$, $P$ and $T$. Thus, for each step, $K^$, $P^$ are known and $T^$ is not known. The complex temperature vector is as the following form

$$T^ = T_{re} + T_{im} i$$ (18)

In Eqs. (17) and (18), $\bar{K}$ and $\bar{P}$ have the same form as $\bar{T}$. Starting the complex variable FEM by replacing the variable s with the complex variable, the following equation can be obtained from Eq. (16):

$$\frac{\partial T_{re}}{\partial s} = \frac{T_{im}}{h}$$ (19)

Thus, the sensitivity coefficient can be calculated. ABAQUS is a real-valued FEM, which does not have a provision for complex operations. Therefore, a user element subroutine (UEL) [33] could be used to implement the complex variable FEM within ABAQUS.

As shown in Fig. 1, two sets of nodes (one real set and one imaginary set) are defined for each element. They are different and a little difficult than those in two-dimensional problems [35]. For heat conduction problem, every node has one degree of freedom. We represent the real temperature $T_{re}$ for the real node and the imaginary perturbation $T_{im}$ for the imaginary node. Thus, the complex element has 2n degrees of freedom, if the degrees of freedom in the traditional element is n. Since any complex number $a + bi$ can be represented in matrix form as $\begin{bmatrix} a & -b \\ b & a \end{bmatrix}$, Eq. (17) can be expressed as:

$$\begin{bmatrix} \text{Real Nodes} \\ \text{Imaginary Nodes} \end{bmatrix}$$

Fig. 1. Sketch of the complex variable element.
where the imaginary parts $K_{\text{Im}}$ and $P_{\text{Im}}$ are generated by adding a small value ($10^{-30}$ to $10^{-20}$) to the inverted parameter, using the UEL and carrying out direct calculation in complex-variable FEM, not just specified given values. Equation (20) is a system equation, and the unknown temperatures and sensitivity coefficients can be obtained by solving this equation.

6. Computational procedure

The iteration is stopped until the objective function or the difference between $F^{p+1}$ and $F^p$ is within a specified tolerance [18].

$$F(s_1, s_2, \ldots, s_N) \leq \zeta \text{ or } |F^{p+1} - F^p| \leq \zeta$$

(21)

where $\zeta$ is a small positive number.

The inversion procedure is summarized as follows.

Start the program with an initial guess $s^0$ for the inverted parameters, and set $p = 1$. Then perform the steps below.

Step 1: Calculate transient temperature filed and sensitivity coefficients by ABAQUS with UEL based on the guessed values of $s^0$.

Step 2: Calculate the objective function by Eq. (11).

Step 3: Check the convergence criterion Eq. (21). Stop the iteration if the convergence criterion is achieved. Otherwise, continue the following procedure.

Step 4: Solve Eq. (13) to obtain $\delta$ based on the sensitivity coefficients which have been calculated in Step 1.

Step 5: Update the initial guess $s^0$ by Eq. (12), and update $p$ by $p + 1$. Then, return to Step 1.

The flowchart of the computational procedure is shown in Fig. 2.

7. Numerical examples

To verify the performances of the proposed method, numerical examples for direct and inverse heat conduction problems are given.

7.1. Example 1: Direct heat conduction problem solved by ABAQUS with UEL

Considering a complex three-dimensional structure, the initial temperature is $0^\circ C$ and the time is 200 s. The geometry and boundary conditions are shown in Figs. 3 and 4, respectively. The left side of the pipe is specified with a temperature of $1000^\circ C$ and the right is at $0^\circ C$. The top of the three small pipes (from left to right) are specified with temperatures of $60^\circ C$, $120^\circ C$ and $180^\circ C$, respectively. The inner surfaces of the four pipes are subjected to the convective boundary conditions. For the three small pipes, the convective heat transfer coefficients and fluid temperatures are:

$$h_1 = 367 \text{ W m}^{-2} \text{C}^{-1}, T_1 = 672 \text{ C},$$

$$h_2 = 291 \text{ W m}^{-2} \text{C}^{-1}, T_2 = 834 \text{ C},$$

$$h_3 = 197 \text{ W m}^{-2} \text{C}^{-1}, T_3 = 1134 \text{ C},$$

For the inner surface of the main pipe, $h_4 = 174 \text{ W m}^{-2} \text{C}^{-1}, T_4 = 200 \text{ C}$. The heat flux on the outer surface is $50,000 \text{ W m}^{-2}$.

The density and specific heat of the pipe are $7800 \text{ kg m}^{-3}$ and $611.5 \text{ J kg}^{-1} \text{C}^{-1}$, respectively. The temperature-dependent thermal conductivities are shown in Table 1.

Fig. 5 shows the ABAQUS meshes with 35,931 nodes and 23,256 elements, which have been verified by the mesh independence. Figs. 6–8 give the transient temperatures using traditional ABAQUS and ABAQUS with UEL, and Fig. 9 shows the comparison of computed temperatures at positions A, B and C. It can be seen from Figs. 6–8 that the transient temperature field of the inner face increases with time and the temperature of three small pipes increases faster than the main pipe; it is because the ambient temperature of the three
small pipes is higher than the main pipe. As showing in Figs. 6–9, the computed temperatures using the ABAQUS with UEL are in excellent agreement with those using the traditional ABAQUS. It is verified that the results of the present complex variable FEM are accurate for solving the direct heat conduction problem.

### 7.2. Example 2: Inverse heat conduction problem for the complex structure

#### 7.2.1. Simultaneously identification of boundary conditions

In the inverse analysis, the Dirichlet, Neumann and Robin boundary conditions, i.e., five temperatures, the heat flux on the outer surface, and the heat convective coefficients at four representative positions are assumed unknown and need to be identified, but everything else is kept the same as in the direct problem. As shown in Fig. 3, three positions (D, E and F) are chosen as measurement points, and the measurement is implemented every 5 s. Therefore, there are 120 measurements.

Figs. 10–12 show the convergence curves of the boundary conditions, and it can be seen that the convergence could be achieved. The inverted parameters could nearly reach its stability after 5 iterations, and they converge after 10 iterations, which shows the high efficiency of the identification. In addition, the final optimal objective function is $2.4938 \times 10^{-7}$, which indicates the high accuracy of the identification; this validates both high efficiency and high accuracy of the present method for solving the inverse heat conduction problem.

#### 7.2.2. Effects of initial guessed values

The stability for identifying the boundary conditions of the complex structure is tested. The heat flux on the outer surface and the heat convective coefficients at four representative positions are assumed unknown, but everything else is kept the same as in the direct problem. To investigate the effects of initial guessed values, five sets of initial guessed values are tested and Table 2 lists the inversion results. It can be seen from Table 2 that convergence can be achieved for each set of initial guessed values, which shows initial guessed values have a weak effect on inversion results. In
addition, it can be seen that the larger of the deviation values between initial guessed values and real values, the more of the iteration number. It is demonstrated that the present method has good stability, if the initial guessed values do not deviate too much from real values.

7.2.3. Effects of measurement errors

In the above examples, the temperature measurements are exact and the measurement errors are not considered. However, in actual applications, there must be measurement errors. The effect of random measurement errors on the accuracy of the inversion results is therefore examined. In order to quantitatively investigate the effect of measurement errors on inversion results, the relative errors are defined as

$$E_{rel} = \frac{|s_{estimated} - s_{exact}|}{s_{exact}} \times 100\%$$

where $s_{exact}$ and $s_{estimated}$ represent the exact and the recovered values, respectively. An error term is added to the exact temperature to account for the random measurement error [20,36]:

$$T_{measured} = T_{exact} \left(1 + \frac{\zeta}{2.576}\right)$$

where $\zeta$ is the random measurement error, and $\gamma$ is a random number between $-1$ and 1.

Three random measurement errors are considered, i.e., $\zeta = 0\%$, $\zeta = 3\%$ and $\zeta = 5\%$, respectively, and the random numbers applied to the exact measurement are the same for each $\zeta$. Table 3 lists the inversion results of the boundary conditions and the relative

![Fig. 6. Temperature contours at 5 s: (a) Traditional ABAQUS; (b) ABAQUS with UEL.](image)

![Fig. 7. Temperature contours at 100 s: (a) Traditional ABAQUS; (b) ABAQUS with UEL.](image)
Fig. 8. Temperature contours at 200 s: (a) Traditional ABAQUS; (b) ABAQUS with UEL.

Fig. 9. Comparison of computed temperatures at points A, B and C.

Fig. 10. Convergence curves of the Dirichlet boundary conditions.

Fig. 11. Convergence curve of the Neumann boundary condition.

Fig. 12. Convergence curves of the Robin boundary conditions.
errors with different measurement errors. It can be seen from Table 3 that the present method can reflect the effect of measurement errors on inversion results. That is, the identification error increases as the measurement error increases. In addition, the relative error $E_{rel}$ in the example is mostly less than the measurement error, which means that the new inverse analysis method is less affected by the measurement errors and has good robustness.

8. Conclusions

In the present work, the CVDM is introduced into the FEM commercial software ABAQUS to solve three-dimensional transient nonlinear inverse heat conduction problems in irregular complex structures for the first time. The Levenberg-Marquardt method is employed for solving the inverse problem, attributed to its outstanding inversion performances. The sensitivity matrix coefficients are accurately calculated by the newly developing complex variable FEM though ABAQUS with UEL, using the CVDM. Numerical examples are given to validate the new approach and main conclusions are as follows:

1. The newly developed complex variable FEM in ABAQUS with UEL is accurate for solving the direct three-dimensional transient nonlinear heat conduction problem, which provides the basis for solving the inverse problem.
2. The present inverse approach could accurately identify multiple parameters with high efficiency.
3. The present approach has a good stability, provided that the guessed values do not deviate too much from real values. In addition, satisfactory results can be still obtained when there is a certain error in the measurement data.
4. The present work provides a general method for solving three-dimensional transient nonlinear inverse heat conduction problems in irregular complex structures, which has strong potentials in engineering applications.

Declaration of Competing Interest

None declared.

Acknowledgments

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References


### Table 2

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### Table 3

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