Three-dimensional crack analyses under thermal stress field by XFEM using only the Heaviside step function

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Received: 26 February 2020; Revised: 27 April 2020; Accepted: 13 July 2020

Abstract
A three-dimensional crack analysis method based on XFEM using only the Heaviside step function was applied to heat transfer and subsequent thermal stress analyses of cracked structures. The proposed method employs tip elements to discretize the weak form governing equations using the approximation function with discontinuity. Two kinds of XFEM analysis software, which perform steady-state or transient heat transfer analysis and thermal stress analysis to evaluate J-integrals and stress intensity factors, were developed. As the XFEM model for the stress analysis is consistent with the heat transfer analysis model, nodal temperature data can be directly imported for stress analysis as thermal load data. The developed codes were verified by solving some benchmark crack problems, including both mechanical and thermal loading cases, and comparing the results with those of conventional methods and a reference. It was shown that the developed codes provide appropriate results for practical thermal stress analysis of cracked structures considering temperature-dependent material properties.

Keywords: XFEM, Heat transfer analysis, Stress analysis, Thermal stress, Stress intensity factor, Domain integral method, J-integral, M-integral

1. Introduction

The extended finite element method (XFEM) (Belytschko and Black, 1999; Moës et al., 1999; Sukumar et al., 2000; Mohammadi, 2012; Belytschko et al., 2014; Zhang et al., 2014) using enriched finite element interpolation functions satisfying the partition of unity condition has been applied to various crack and crack propagation analyses (Gravouil et al., 2002; Nagashima and Miura, 2008, 2009) because crack geometry can be modelled independently of the finite element mesh. The standard XFEM models crack geometry implicitly by the signed distance function based on the level set method (Sethian, 1999; Moës et al., 2002) and uses interpolation functions enriched with an asymptotic bases and the Heaviside step function for a neighboring crack tip and crack, respectively (Moës et al., 2002). Asymptotic basis functions, which can reproduce the displacement field around a crack tip in a two-dimensional homogeneous isotropic linear elastic body, are usually used. Regarding cracks in orthotropic materials and heterogeneous interface cracks, although the authors (Nagashima et al., 2003) employed a conventional asymptotic basis for isotropic cracks, the asymptotic basis functions, which can reconstruct the corresponding displacement field, should be used strictly. Actually, Sukumar et al. (2004) used asymptotic bases for the displacement field of a bi-material isotropic interface crack. Moreover, Ashari and Mohammadi (2011) used asymptotic bases for the displacement field of bi-material orthotropic interface crack. In contrast, the range of enriched nodes regarding asymptotic bases around a crack tip is arbitrary, and two kinds of methods were proposed (Béchet et al., 2005). One is the topological enrichment method, which enriches only a set of nodes included in the element containing a crack tip, and another is the geometrical enrichment method, which enriches a set of appropriate nodes within the domain, including a crack tip. Strictly, all of the nodes in an element construction, including a crack tip, should be enriched with asymptotic bases to reconstruct the asymptotic displacement function. An element that does not satisfy the above condition exactly is referred to as a blending element (Chessa et al., 2003). Because a blending element cannot reconstruct an asymptotic solution and may have an adverse effect on the convergence rate, a strategy for solving this
problem has been proposed (Fries, 2008; Shibanuma and Utsunomiya, 2009). In addition, because a cohesive crack (Camanno et al., 2003; Anderson, 2005) generally has no stress singularity around its crack tip, enrichment with an asymptotic displacement function around a crack tip is not appropriate. Zi and Belytschko (2003) proposed a two-dimensional triangular crack tip element enriched with only the Heaviside step function. In summary, as mentioned above, it is not so easy to determine enriched nodes by selecting an appropriate asymptotic basis function and enrichment domain and avoiding blending problems.

One practical way to apply XFEM to cracks in various materials including isotropic, orthotropic, homogeneous and non-homogeneous materials, the same as in conventional FEM, is to use only the Heaviside step function without asymptotic basis functions. This method may lose some of the benefits of XFEM discussed above, but the blending problem never occurs. Consequently, because a stress singularity does not arise at a crack tip, this approach can be used to model cohesive cracks. Actually, Zi and Belytschko (2003) performed cohesive crack analyses using tip elements enriched with only the Heaviside step function. In addition, the authors (Nagashima and Sawada, 2014, 2016) proposed a quasi-three-dimensional XFEM analysis method in conjunction with a bi-linear type cohesive zone mode (Camanno et al., 2003), which uses three-dimensional pentahedral elements obtained by extruding triangular tip elements in the thickness direction. Moreover, Higuchi et al. (2017) applied this method to analyze damage propagation in carbon fiber reinforced plastic (CFRP) laminates.

Currently, to evaluate structural integrity, crack analyses under a thermal-stress field are often required in practical engineering. Thermal stress analysis using a general-purpose finite element code usually requires the finite element models to have the same mesh divisions for both the heat transfer and thermal stress analyses, and then both kinds of analysis are performed in succession. If XFEM analysis adopts the same procedure, XFEM models for both heat transfer and stress analysis are preferred to be compatible. Therefore, it is convenient when enriched nodes for both models are consistent. Compatible approximated functions of XFEM for heat transfer and stress analyses make it possible to use the nodal temperature obtained by heat transfer analyses directly to perform subsequent stress analyses.

This paper presents an XFEM analysis method using three-dimensional eight-node hexahedral elements enriched with only the Heaviside step function as a part of study to use XFEM for general purposes. Because enrichment with only the Heaviside step function can avoid blending problems and does not require selection of an asymptotic basis function dependent on the material, XFEM can be applied to crack problems of various materials, such as those that are homogeneous, inhomogeneous, isotropic, or orthotropic. XFEM has previously been applied to heat transfer and thermal stress analyses (Duflot, 2008; Ghaffari et al., 2016; Esmati et al., 2018). To date, an enrichment method using only the Heaviside step function has not been applied to heat transfer and subsequent thermal stress analyses. Therefore, the proposed method should be verified before being applied to practical cracked structure problems. Moreover, the same enrichment functions for both heat transfer and stress analysis make it possible to transfer nodal temperature data from the heat transfer analysis to the thermal stress analysis.

However, this method requires special treatment for the tip element. In fact, partitioning of the tip element is indispensable to discretize the weak form governing equations for numerical integration because the approximation function has discontinuity. Moreover, an enriched approximation function should be appropriately assigned to each subdivided domain. A convenient method for composing two-dimensional triangular elements was proposed (Zi and Belytschko), and three-dimensional pentahedral tip elements can be easily obtained by extruding triangular tip elements in the thickness direction (Nagashima and Sawada, 2014, 2016). In contrast, formulation of three-dimensional hexahedral tip elements requires tallying all the types of cutting patterns and setting appropriate enriched interpolation functions corresponding to each pattern.

This paper proposes a three-dimensional planar crack analysis method using eight-node hexahedral elements enriched with only the Heaviside step function. The proposed method provides not only stress analysis for mechanical loading but also steady and unsteady heat transfer analysis and subsequent thermal stress analysis. The proposed method has the limitation that the planar crack surface should exactly coincide with the hexahedral surface; however, it can be applied to solve many practical crack problems. Moreover, it is important to evaluate the stress intensity factors at a crack tip precisely. Therefore, this paper considers the evaluation of stress intensity factors under a thermal stress field with a temperature-dependent thermal expansion coefficient by the domain integral method.

The remainder of this paper is organized as follows. Section 2 presents the analysis method based on a level set XFEM using hexahedral elements enriched with only the Heaviside function. Section 3 outlines the codes developed to implement the proposed method. In Section 4 presents numerical internal and external crack analyses under mechanical
and thermal loads, as well as a practical thermal stress analysis of a suddenly cooled cracked plate for verification. Finally, a summary is provided in Section 5.

2. Analysis method

2.1 Governing equations

2.1.1 Heat transfer analysis

The initial and boundary-value problem for a temperature field $T(x_i,t)$ for an elastic body $V$ in three-dimensional Cartesian coordinates $x_i$ $(i=1,2,3)$ at a time $t$, as shown Fig. 1(a), is considered (Huebner, 2001). If temperature, heat flux, convection, and radiation boundary conditions are given on $S_1$, $S_2$, $S_3$, and $S_4$, respectively, temperature boundary condition is expressed as follows:

\[ T = \bar{T} \quad \text{on } S_1 \quad (1) \]

where $\bar{T}$ is the specified temperature. The heat flux, convection, and radiation boundary conditions are expressed as follows:

\[ q = \begin{cases} -\bar{q}_s & \text{on } S_2 \\ \frac{h}{\bar{T} - \bar{T}_\infty} & \text{on } S_3 \\ \sigma \varepsilon F(T - \bar{T}_s) & \text{on } S_4 \end{cases} \quad (2) \]

where $q$ is the outward heat flux in a direction normal to the surface; $\bar{q}_s$ is a specified inflow heat flux; $h$ is a convection coefficient; $\bar{T}_\infty$ is the ambient temperature; and $\sigma$, $\varepsilon$, and $F$ are the Stephan–Boltzmann constant, emission rate, and emission shape coefficient, respectively.

The governing equation and the heat flux, convection, and radiation boundary conditions can be described as follows:

\[ \int_V \left( \lambda_{ij}(T) \frac{\partial T}{\partial x_i} \frac{\partial T}{\partial x_j} + \rho C_p(T) \frac{\partial T}{\partial t} T^* \right) dV = \int_{S_2} \left[ \bar{q} T^* dS - \int_{S_3} h(T - \bar{T}_s) T^* dS - \int_{S_4} \sigma \varepsilon F(T - \bar{T}_s) T^* dS \right] \quad (3) \]

where $\lambda_{ij}$ is the heat conduction tensor, $\bar{Q}$ is the heat generation per unit volume, $\rho$ is the mass density, $C_p$ is the specific heat, and $T^*$ is an arbitrary weight function. In addition, temperature dependency of $\lambda_{ij}$ and $C_p$ are considered in Eq. (3).

2.1.2 Thermal stress analysis

The boundary-value problem for a stress field $\sigma_{ij}$, a strain field $\varepsilon_{ij}$, and a displacement field $u_i$ for the three-dimensional deformed body shown in Fig. 1(b) is considered. If the geometrical and mechanical boundary conditions are given on $S_u$ and $S_s$, respectively, the boundary conditions are expressed as follows:

\[ u_i = \bar{u}_i \quad \text{on } S_u \quad (4) \]

\[ t_i = \bar{t}_i \quad \text{on } S_s \quad (5) \]

where $\bar{u}_i$ and $\bar{t}_i$ are the specified displacement and traction components, respectively. Here, the principle of virtual work for the infinitesimal deformation problem can be described as follows:
\[
\iiint_{V} \sigma_{ij} \varepsilon_{ij}^m dV = \iiint_{S} \bar{b}_{ij} u_{ij} dV + \iint_{S} \bar{r}_{ij} u_{ij} dS
\]  
(6)

where \( \bar{b}_{ij} \) is the specified body force per unit volume. This paper uses the linear elastic constitutive considering the thermal strain as follows:

\[
\sigma_{ij} = C_{ijkl} e_{ij}^{m} = C_{ijkl} (\varepsilon_{ij} - \varepsilon_{ij}^{th}) 
\]  
(7)

where \( \varepsilon_{ij}^{m} \) and \( \varepsilon_{ij}^{th} \) are the mechanical and thermal strain fields, respectively. Here, the thermal strain field can be defined using temperature-dependent expansion coefficient \( \alpha(T) \) as follows:

\[
\varepsilon_{ij}^{th} = \{\alpha(T)(T - T_0) - \alpha(T_i)(T_i - T_0)\} \delta_{ij} 
\]  
(8)

where \( T_0 \) is the temperature of zero thermal strain and \( T_i \) is the initial temperature.

Fig. 1 Solution domain.

2.2 Approximation of field variable by XFEM

2.2.1 Geometry expression by the level set method (Moës et al., 2002)

XFEM analysis presented in this paper expresses crack geometry implicitly by the level set method. Namely, crack surface is defined as a set of triangular patches in a three-dimensional space, as shown in Fig. 2. Here, two kind of functions \( \phi \) and \( \psi \), which are the signed distance function regarding crack surface and front, respectively, are defined as follows:

\[
\phi(x) = \min_{x \in S_{EXT}} \|x - x_s\| \text{sign}(n_s \cdot (x - x_s)) 
\]
\[
\psi(x) = \min_{x \in \Gamma} \|x - x_s\| \text{sign}(n_c \cdot (x - x_s)) 
\]
(9.1)  
(9.2)

where \( S \), \( \Gamma \), and \( S_{EXT} \) are the crack surface expressed by the triangular patches, the crack front, and the extension of the crack surface, respectively; \( n_s \) is the outward normal vector of the patch; and \( n_c \) is perpendicular to \( n_s \) and \( \Gamma \).
2.2.2 Classification of element

XFEM analyses performed in the present study discretize a three-dimensional domain using eight-node hexahedral elements. Each element is classified into numerous patterns according to the level set values of $\phi$ and $\psi$ at eight nodes of the element. More specifically, each node is classified into three states (positive, negative, or zero) depending on the nodal level set value $\phi$ and consequently, each element can be simply estimated as $3^8 = 6,561$ patterns. To execute such a large classification volume is not impossible, but it has not been finished yet. Therefore, only a plain crack, where the surface of the crack coincides with that of the element, is treated in this study. The assumption limits the analysis to only two kinds of classification patterns by $\phi$ as shown in Fig. 3. One is the element having a bottom surface that coincides with the surface crack $[\phi_i \geq 0, (i = 1, \cdots, 8)]$. Another is the element having a top surface that coincides with the surface crack $[\phi_i \leq 0, (i = 1, \cdots, 8)]$. The cut plane of both elements is a quadrilateral. Moreover, the quadrilateral can be classified into 14 patterns using the nodal value of $\psi$, which may be positive, negative, or zero, as shown in Fig. 4. Namely, according to the combination of nodal values of $\psi$ at four nodes, the quadrilateral is classified into cut elements, such as $b$, $e$, $g$, and $j$; tip elements, such as $c$, $h$, $k$, $l$, and $m$; and ligament elements, such as $a$, $d$, $f$, and $i$.

![Fig. 2 Three-dimensional crack modelling by the level set method.](image)

![Fig. 3 Classification of hexahedral elements according to nodal values of signed distance function: $\phi$.](image)
2.2.3 Nodal enrichment and element partition

Using the aforementioned classification procedure of the elements using the values of the signed distance functions $\phi$ and $\psi$, the node of the element can be enriched and the element can be partitioned into several pentahedrons if required. Here, as an example, nodal enrichment and element partition of tip element P3N1 are shown in Fig. 4(c), the bottom surface of which coincides with the crack surface, as shown in Fig. 5. Two kinds of enrichment case are shown. Fig. 5(a) shows the case of enrichment with asymptotic bases, and Fig. 5(b) shows the case of enrichment with the Heaviside function.

In both Fig. 5(a) and (b), node 1, the $\psi$ value of which is negative, is enriched, and therefore $\psi$ is zero at points A and B. Then, points C and D are set as natural coordinates $r_1$ and $r_2$ and have the same values of A and B, respectively. Finally, the elements are divided into four pentahedrons. One is pentahedron N1 (1AB-5CD) having the crack surface and the other three are pentahedrons P1 (34B-78D), P2 (3BA-7DC), and P3 (23A-67C) having no crack surfaces. Pentahedrons obtained by partitioning a hexahedron are used only for integration of the hexahedral elements. Although the vertex of the pentahedron is not used for nodes in the sense of finite elements, the interpolation function for pentahedral elements is utilized in the present formulation. Regarding other patterns, such as tip elements $h$, $k$, $l$, and $m$, the same method can be adopted.
2.2.4 Approximation function

Temperature and displacement fields are approximated using an eight-node hexahedral element enriched with only the Heaviside step function. Here, the approximation function for the tip element, including a crack front, is shown. Regarding the pattern P3N1 shown in Fig. 5(b), the approximated temperature and displacement fields $T^h$ and $u^h$ can be expressed as follows:

$$T^h(x) = \sum_{i=1}^{8} N_i^{\text{HEXA}}(x)T_i + N_1^{\text{PENTA,N1}}(x)a_i : N1$$

(10)

$$u^h(x) = \sum_{i=1}^{8} N_i^{\text{HEXA}}(x)u_i + N_1^{\text{PENTA,N1}}(x)b_i : N1$$

(11)

where $N_i^{\text{HEXA}}$ and $N_1^{\text{PENTA,N1}}$ are interpolation functions for eight-node hexahedral and six-node pentahedrons, respectively; $a_i$ is a nodal degree of freedom allocated to node 1 for the temperature field; and $b_i$ is nodal degrees of freedom allocated to node 1 for the displacement field.

In the case of using asymptotic basis functions for enrichment, as shown in Fig. 5(a), the approximated displacement field $u^h$ is expressed as follows:

$$u^h(x) = \sum_{i=1}^{8} N_i^{\text{HEXA}}(x)u_i + \sum_{k=1}^{4} \gamma_k(x)c_k$$

(12)

where $c_k$ is a degree of freedom allocated to the enriched node and $\gamma_k (k=1,2,3,4)$ are asymptotic bases for the displacement field around a crack tip and expressed using the polar coordinate system $r, \theta$, the origin of which is the evaluation point on the crack front, as follows (Moës et al., 2002):

$$\gamma_1 = \sqrt{r} \cos \frac{\theta}{2},\gamma_2 = \sqrt{r} \sin \frac{\theta}{2},\gamma_3 = \sqrt{r} \sin \theta,\gamma_4 = \sqrt{r} \cos \frac{\theta}{2} \sin \theta$$

(13)

2.3 Discretized equations

The analyzed domain is divided into eight-node hexahedral finite elements, and then the governing Eqs. (3) and (6), which are expressed as the method of the weighted residual for heat transfer analysis and the principle of virtual work for stress analysis, are discretized. Two-point Gauss integration is adopted to integrate the equations numerically for normal and cut elements because field variables have no discontinuity within the elements. In contrast, for multiple divided pentahedrons, numerical integration by a combination of integration for triangular elements and Gauss integration is used, as shown in Fig. 6, which illustrates integration method schematically for a tip element with pattern P3N1 located above and below the crack surface. In this method, P1*, P2*, and P3* are the pentahedrons in the ligament side above the crack surface, and N1* is the pentahedron in the crack side above the crack surface. Conversely, P1, P2, and P3* are the pentahedrons in the ligament side below the crack surface, and N1* is the pentahedron in the crack side below the crack surface.
2.3.1 Heat transfer analysis

The governing equations for heat transfer analysis shown in Eq. (3) can be discretized through the aforementioned approximated temperature field shown in Eq. (10) as follows:

$$\mathbf{M}_H(T)\dot{T} + \mathbf{K}_H(T)T = \mathbf{F}_H(t)$$  \hspace{1cm} (14)

where \(\mathbf{M}_H, \mathbf{K}_H, \mathbf{F}_H, T\) are the thermal capacity matrix, the heat conduction matrix, the heat flux vector, and the nodal temperature vector, respectively. Eq. (14) is a nonlinear equation because it considers temperature dependency of the specific heat, the thermal conductivity, and the heat radiation. In addition, it is dependent on time for transient problems. The full implicit method is used as a time integration scheme for the temperature, and the Newton–Raphson method is employed to solve the nonlinear equation for temperature.

2.3.2 Thermal stress analysis

The governing equations for stress analysis shown in Eq. (6) are discretized through the aforementioned approximated temperature and displacement fields shown in Eqs. (10) and (11) as follows:

$$\mathbf{K}_S(T)U = \mathbf{F}_S^{m} + \mathbf{F}_S^{th}(T)$$  \hspace{1cm} (15)

where \(\mathbf{K}_S\) and \(U\) are the stiffness matrix and the nodal displacement vector, respectively. Because Eq. (15) considers the temperature dependency on material properties, such as Young’s modulus, the stiffness matrix \(\mathbf{K}_S\) is a function of the temperature. In addition, to consider the thermal load induced by the thermal strain depending on the temperature, not only load vector \(\mathbf{F}_S^{m}\) for the mechanical load but also the thermal load vector \(\mathbf{F}_S^{th}(T)\), which is dependent on the temperature, is employed.

2.4 \(J\)-integral and \(M\)-integral by the domain integral method

2.4.1 \(J\)-integral

The section-averaged \(J\)-integral, which is referred to as \(J_{ave}\), at an arbitrary point on the crack front of a three-dimensional planar crack can be expressed in the domain integral form when the body force is neglected as follows (Shih et al., 1986):
\[
\bar{J} = \iiint_V \left( \sigma_{ij} \frac{\partial \bar{u}_i}{\partial x_j} + \sigma_{ij} \frac{\partial q}{\partial x_j} - w \frac{\partial q}{\partial x_j} + \sigma_{ij} \frac{\partial \varepsilon_{ij}^m}{\partial x_k} q \right) dV \tag{16.1}
\]

\[
w = \int_0^1 \sigma_{ij} d \varepsilon_{ij} = \frac{1}{2} \sigma_{ij} \varepsilon_{ij}^m = \frac{1}{2} \sigma_{ij} \left( \varepsilon_{ij}^m - \varepsilon_{ij}^{m_0} \right) \tag{16.2}
\]

\[
J_{ave} = \bar{J} \int q dl \tag{16.3}
\]

where \( V, l, \) and \( w \) are the integral domain, the length along the crack front, and the strain energy density function, respectively, and \( q \) is an arbitrary continuous weight function, which is unity at the crack tip and decreases to zero at the boundary of the integral domain \( V \). In addition, \( \bar{x}_i \) is the local Cartesian system, the origin of which is the evaluation point of the \( J \)-integral shown in Fig. 7, and \( \bar{\sigma}_{ij}, \bar{\varepsilon}_{ij}, \) and \( \bar{u}_i \) are the stress, strain, and displacement components, respectively, expressed by the local Cartesian coordinate system \( \bar{x}_i \). In the present method, a parallelepiped with the edges having lengths \( L_1, L_2, \) and \( L_3 \) in the \( \bar{x}_1, \bar{x}_2, \bar{x}_3 \) directions is used for the integration domain (Sukumar et al., 2000; Nagashima and Miura, 2008, 2009).

After substitution of Eq. (8) into (16.1), the following equation can be obtained:

\[
\bar{J} = \iiint_V \left[ \sigma_{ij} \frac{\partial \bar{u}_i}{\partial x_j} + \sigma_{ij} \frac{\partial q}{\partial x_j} - w \frac{\partial q}{\partial x_j} + \left\{ \alpha(T) + \frac{d \alpha}{dT} (T - T_0) \right\} \frac{\partial T}{\partial x_j} \bar{\sigma}_{ij} q \right] dV \tag{17}
\]

![Fig. 7 Rectangular parallelepiped for domain integral.](image)

### 2.4.2 Mode separation by \( M \)-integral

Regarding mixed mode crack problems of a homogeneous isotropic linear elastic material, the stress intensity factor can be separated by the \( M \)-integral method (Yau and Wang, 1984). The domain integral equations for the \( M \)-integral are expressed as follows:

\[
\frac{2(1 - \nu^2)}{E} (K_I^{max} + K_{II}^{max}) + \frac{K_{III}^{max}}{G} \int q dl
\]

\[
= \iiint_V \left( \sigma_{ij}^{max} \frac{\partial \bar{u}_i}{\partial x_j} + \sigma_{ij}^{max} \frac{\partial q}{\partial x_j} - \sigma_{ij}^{max} \varepsilon_{ij}^{m_0} \frac{\partial q}{\partial x_j} + \left\{ \alpha(T) + \frac{d \alpha}{dT} (T - T_0) \right\} \frac{\partial T}{\partial x_j} \bar{\sigma}_{ij}^{max} q \right) dV \tag{18}
\]

where \( E \) and \( G \) are Young’s modulus and the shear modulus at the evaluation point of stress intensity factors, respectively, and the superscript aux for the stress and strain components represents the auxiliary solution.

After calculation of the right-hand side of Eq. (18) using three kinds of auxiliary solutions obtained by analytical displacement and stress fields around a crack tip of isotropic linear elastic material for pure modes I, II, and III, the stress intensity factors \( K_I, K_{II}, \) and \( K_{III} \) can be evaluated.
3. Analysis system

Based on XFEM using only the Heaviside step function, the formulation of which is shown in Section 2, a three-dimensional heat transfer analysis code referred to as NLXFEM3Dheat and a three-dimensional stress analysis code referred to as NLXFEM3Dstruct were developed. The specifications of the developed in-house codes are shown in Tables 1 and 2. The main features of NLXFEM3Dheat are as follows:

- Uses an approximation function for the temperature field based on XFEM enriched with only the Heaviside step function
- Capable of both steady-state and transient heat transfer analysis
- Considers the temperature-dependent thermal properties, including the heat conductance and specific heat
- Considers heat flux, heat convection, and heat radiation boundary conditions
- Employs a fully implicit method for time integration
- Uses a quasi-Newton method for iterative solution of nonlinear equations

The main features of NLXFEM3Dstruct are as follows:

- Uses an approximation function for the displacement field based on the XFEM enriched with only the Heaviside step function
- Considers temperature-dependent mechanical properties, including Young’s modulus, Poisson’s ratio, and thermal expansion
- Considers thermal load due to the thermal strain
- Capable of elastic and elastic-plastic analyses
- Performs J-integral evaluation by the domain integral method
- Provides mode separation of $K_I$, $K_{II}$, and $K_{III}$ for homogeneous isotropic linear elastic materials by the domain form of the $M$-integral.

Because both codes employ implicit methods and therefore require the solving of simultaneous linear equations, they use the direct sparse solver, referred to as Pardiso, that is included in Intel MKL (2020).

Input and output files for both of the in-house codes are shown in Fig. 8. These codes require finite element model files ($H.dat$, $S.dat$), which can be prepared by existing FEM preprocessors, and crack geometry, which is modelled by a set of triangular patch definition file (crk) as input. Nodal enrichment is automatically set within the codes. Numerical results, including nodal displacement, element stress, J-integrals, and stress intensity factors, and data for visualization used by the commercial visualization software GLview Inova (2020) are output to results files ($H.out$, $S.out$) and visualization files ($H.vtf$, $S.vtf$), respectively. In addition, analytical processes are recorded in log files ($H.log$, $S.log$). The same crack geometry definition file (crk) can be used for both the heat transfer and stress analysis codes. In addition, nodal temperatures obtained by heat transfer analysis are output to the temperature file (tmp) and can be directly input to the stress analysis code.

| Code | NLXFEM3Dheat |
|------|--------------|
| Latest version | 1.181129 |
| Development language | ANSI-C |
| Discretization method | eXtended Finite Element Method |
| Analysis type | Steady state/Transient Heat transfer Analysis |
| Element type | 8-node hexahedral element |
| Material type | Isotropic (Temperature dependent) |
| Boundary conditions | Specified temperature, Specified heat flow, Convective heat transfer, Radiant heat transfer |
| Enrichment type | Heaviside function |
| Method use to solve the system equation | Direct method: Skyline method, Pardiso (Intel Math Kernel Library) |

| Code | NLXFEM3Dstruct |
|------|----------------|
| Latest version | 1.191210 |
| Development language | ANSI-C |
| Discretization method | eXtended Finite Element Method |
| Analysis type | Elastic Static Analysis, Elastic-plastic Static Analysis |
| Element type | 8-node hexahedral element, 8-node interface element considering cohesive zone model |
| Material type | Isotropic |
| Enrichment type | Heaviside function |
| Method use to solve the system equation | Direct method: Skyline method, Pardiso (Intel Math Kernel Library) |
| Evaluation J-integral and SIF | Domain Integral Method |
4. Numerical analysis

4.1 Stress analysis of a circular internal crack

Stress analyses of an elastic body (Poisson’s ratio 0.3), including an internal circular crack under uniform tensile and shear load as shown in Fig. 9, were performed by XFEM. Stress intensity factors at the crack front were evaluated and compared with the theoretical values. The analyzed domain was a cube with an edge length of \( L \), and the radius of the circular internal crack was \( a \). In the actual analyses, Young’s modulus, the length \( L \), and the radius \( a \) were set to 206 GPa, 100 mm, and 10 mm, respectively, and eight-node hexahedral elements were employed. The finite element models (226,981 nodes and 216,000 elements) are shown in Fig. 10. XFEM analyses used both the model \( H \) enriched with only the Heaviside step function and the model \( HA \) enriched with the Heaviside step function and asymptotic basis, and the distribution of enriched nodes on the center plane is shown in Fig. 11(a) and (b). Stress intensity factors \( K_I \), \( K_{II} \), and \( K_{III} \) were evaluated through the \( M \)-integral method by the domain integral method and they are compared with the theoretical values.

As mentioned in Section 2, a parallelepiped is employed independently of finite elements to perform domain integral in XFEM analysis. If the edge length of an eight-node hexahedral element is \( h \) next to the evaluation point for stress intensity factors, the edge lengths \( L_1 \), \( L_2 \), and \( L_3 \) of the parallelepiped in the local 1, 2, and 3 directions are set to \( 6h \), \( 3h \), and \( 6h \), respectively. These sizes correspond to the third integration contours used in the domain integral method for the conventional FEM. In addition, Newton-Cotes integration is adopted to perform numerical integration of the parallelepiped domain, and \( 40 \times 40 \times 40 \) integration points are employed in this calculation.

Stress intensity factors \( K_I \), \( K_{II} \), and \( K_{III} \) under uniform tensile load \( \sigma \) can be expressed in non-dimensional form as follows:

\[
F_i = \frac{K_i}{\sigma \sqrt{\pi a}}, F_{II} = \frac{K_{II}}{\sigma \sqrt{\pi a}}, F_{III} = \frac{K_{III}}{\sigma \sqrt{\pi a}}
\]

The reference solutions for a circular internal crack within an infinite body under uniform tensile load (Murakami, 1987) are \( F_I=2/\pi \) and \( F_{II}=F_{III}=0 \). Distributions of non-dimensional stress intensity factors along the circular crack front obtained by both XFEM enriched with only the Heaviside function and XFEM enriched with both the Heaviside function and asymptotic bases are shown in Fig. 12 and compared with those obtained by the reference solution. Both kinds of XFEM analyses give almost the same results compatible with the reference solution; however, slight fluctuations can be seen for XFEM enriched with both the Heaviside function and asymptotic bases.

Stress intensity factors \( K_I \), \( K_{II} \), and \( K_{III} \) under uniform shear load \( \tau \) can be expressed in non-dimensional form as follows:

\[
F_i = \frac{K_i}{\tau \sqrt{\pi a}}, F_{II} = \frac{K_{II}}{\tau \sqrt{\pi a}}, F_{III} = \frac{K_{III}}{\tau \sqrt{\pi a}}
\]

The reference solutions for a circular internal crack in infinite body under uniform shear load (Murakami, 1987) are
In these equations, $\theta$ is the location angle along the circular crack front. Distribution of non-dimensional stress intensity factors along the circular crack front obtained by both XFEM enriched with only the Heaviside function and XFEM enriched with both the Heaviside function and asymptotic basis are shown in Fig. 13 and compared with those obtained by the reference solution. Both kinds of XFEM analyses give almost same results consistent with the reference solution.

Fig. 9 Penny-shaped crack under uniform tensile and shear loads.

Fig. 10 Finite element model for cube with penny-shaped crack (full model).

Fig. 11 Distributed enrichment nodes for the penny-shaped crack models.
4.2 Stress analysis of a plate with a semi-elliptical surface crack under uniform tensile load

4.2.1 Analysis model

Stress analyses were performed on an elastic plate with Young’s modulus of 206 GPa and Poisson’s ratio 0.3 with a semi-elliptical surface crack under uniform tensile load $\sigma$, as shown in Fig. 14. In the analyses, the height $L$, width $W$, and thickness $t$ of the plate were 1,000 mm, 1,000 mm, and 50 mm, respectively, and the length $2c$ and depth $a$ of the crack were 200 mm and 20 mm, respectively. Due to model symmetry, quarter models using eight-node hexahedral elements were employed. The procedure to enforce symmetric boundary conditions for the XFEM model is described in detail in Nagashima and Miura (2008). The FEM model (26,908 nodes and 24,030 elements) and XFEM model (412,776 nodes and 390,625 elements) used for comparison are shown in Fig. 15(a) and (b), respectively. Although the total number of nodes for the FEM and XFEM models is quite different, both models have almost the same mesh size of 2.5 mm near the crack front. XFEM analyses use both the model $H$ enriched with only the Heaviside step function and the model $HA$ enriched with the Heaviside step function and asymptotic bases, and the distribution of enriched nodes on the center plane are shown in Fig. 16(a) and (b).
4.2.2 Results and Discussion

Stress analyses under uniform tensile loading were performed and the stress intensity factors along the crack front were evaluated. The results were compared with those obtained by FEM analysis and the reference solution by Raju and Newman (1979). In the evaluation of stress intensity factors by the domain integral method, the third contour integral was employed by FEM and the corresponding size of parallelepiped was used by XFEM. The distributions of non-dimensional stress intensity factor $F_1$ obtained by the analyses are shown in Fig. 17, where the horizontal axis $\theta$ is the eccentric angle. In the evaluation, the stress intensity factors at the free surface were not evaluated, because their physical meaning is not clear. The results by XFEM almost agree with those by FEM and the reference solution except in area of the free surface, where the eccentric angle is less than 15 degrees. For the free surface, XFEM using only the Heaviside step function gives results close to those obtained with FEM; however, XFEM using the Heaviside step function and asymptotic bases provides slightly different results. The evaluation method of stress intensity factors by the domain integral method requires more consideration.
4.3 Thermal stress analysis of a plate with a rectangular surface crack

Thermal stress analyses of a plate with a rectangular surface crack, as shown in Fig. 18, were performed. In the analyses, the height $L$, width $W$, and thickness $t$ of the plate were 200 mm, 100 mm, and 10 mm, respectively, and the crack length $a$ was 50 mm; the stress intensity factors at the crack front were evaluated. FEM and XFEM models using eight-node hexahedral elements were employed for heat transfer and stress analyses. The crack was modelled using double nodes by FEM and the Heaviside enriched nodes by XFEM. The numbers of nodes and elements for the FEM model, which is shown in Fig. 18, were 462 and 200, respectively. The material is assumed to be ferrite steel, and the material properties used in the heat transfer and stress analyses are shown in Table 3. In the analyses, temperature-dependent heat conduction, specific heat, Young’s modulus, and thermal expansion were considered. First, steady-state heat transfer analyses were performed with $T_L$ and $T_R$, which are the temperature at the left and right surface of the plate, respectively, set to 0 and 300 °C. Next, stress analyses using the nodal temperature data obtained by the heat transfer analyses were performed, and the stress intensity factors $K_I$ at the crack front were evaluated.

4.3.1 Temperature-independent case

In the temperature-independent case, heat transfer analyses using the material properties shown in Table 3 at 20 °C were followed by stress analysis to evaluate the stress intensity factors $K_I$ at the crack front by FEM and XFEM. To confirm the path independency of $K_I$ by the domain integral method, the relations between the contour integral path and the calculated $K_I$ by FEM and XFEM are shown in Fig. 19. In the FEM model, the set of hexahedral elements, including the evaluation point (node) for $J$-integral or SIF on the crack front, is defined as “Set 1”. Next, the element set that surrounds “Set 1” is defined as “Set 2”. In the same way, “Set 3”, “Set 4”, and additional sets can be defined in succession. In the domain integration method, “Path 1” represents the integration domain of “Set 1” and “Path 2” represents the integration domain of the union of “Set 1” and “Set 2”. Moreover, “Path 3” and additional paths can be defined in the same way. In contrast, in an XFEM model, a rectangular parallelepiped is employed. “Path 1” represents the parallelepiped, the size of which is almost same as “Path 1” for an FEM model. In the same way, “Path 2” and additional paths can be defined. As shown, after the third integration, path independency for both analyses can almost be obtained. The $K_I$ values obtained by FEM and XFEM showed differences of 0.24%, and 0.80%, respectively, compared with the reference (Shih et al., 1986) ($K_I=2,986$ MPa mm$^{0.5}$ for plane strain).

4.3.2 Temperature-dependent case

Similar analyses were performed for a temperature-dependent case by FEM and XFEM, and the stress intensity factor $K_I$ at the crack front was evaluated. The path independency of $K_I$ using the domain integral method by FEM and XFEM is shown in Fig. 20(a) and (b), respectively. It is shown that path independency in the FEM analysis can be clearly obtained after the third integration; however, the path independency for XFEM is not so clear in this analysis. Therefore, to confirm the path independency for FEM and XFEM, cases when the gradient of the thermal expansion $da/dT$ in Eqs. (17) and (18) are not considered were also evaluated. The results are shown and compared with the
analysis results with \( \frac{d\alpha}{dT} \) in Fig. 21. As shown in Fig.21(b), the path independency is apparently lost without the \( \frac{d\alpha}{dT} \) term. Therefore, this term is indispensable to perform appropriate domain integration in the temperature-dependent case.

![FEM model diagram]

Fig. 18 Edge-cracked plate subjected to thermal field.

### Table 3 Material properties.

| Temperature \(^{\circ}\)C | Young Modulus \(\text{MPa}\) | Expansion \(\alpha\) \(/^{\circ}\)C | Conductivity \(\lambda\) \(\text{W/m/}^{\circ}\text{C}\) | Density \(\rho\) \(\text{g/cm}^3\) | Specific heat \(C_p\) \(\text{J/kg}^{\circ}\text{C}\) |
|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| 0               | 205,000         | 11.22 x 10^{-6} | 37.7            | 7,800           | 447.12          |
| 20              | 204,000         | 11.22 x 10^{-6} | 37.7            | 7,800           | 447.12          |
| 50              | 203,000         | 11.45 x 10^{-6} | 38.6            | 7,800           | 460.35          |
| 100             | 200,000         | 11.79 x 10^{-6} | 39.9            | 7,800           | 483.95          |
| 150             | 197,000         | 12.14 x 10^{-6} | 40.5            | 7,800           | 503.62          |
| 200             | 193,000         | 12.47 x 10^{-6} | 40.5            | 7,800           | 523.95          |
| 250             | 189,000         | 12.78 x 10^{-6} | 40.2            | 7,800           | 547.12          |
| 300             | 185,000         | 13.08 x 10^{-6} | 39.5            | 7,800           | 567.09          |

Fig. 19 Path independency of \(K_I\) obtained by FEM and XFEM using constant material properties.
Fig. 20 Path independency of $K_I$ obtained by FEM and XFEM using temperature-dependent material properties.

Fig. 21 Path independency of $K_I$ obtained by FEM and XFEM with and without gradient-of-thermal-expansion terms.

4.4 Transient thermal stress analysis of a plate with a semi-elliptical surface crack

Thermal stress analyses of a plate with a semi-elliptical surface crack subject to sudden cooling were performed by the transient heat transfer and subsequent stress analyses, as shown in Fig. 22. In the analyses, the height, width, and thickness of the plate were 2,000 mm, 2,000 mm, and 100 mm, respectively, and the crack length and depth were 40 mm and 10 mm, respectively. The initial temperature of the plate was 150 °C, and the ambient temperature linearly decreased from 150 °C to 20 °C in 60 s and held at 20 °C for an additional 540 s (600 s total cooling time). The convective heat transfer coefficient was 20,000 W/m²/K. The material properties were as same as used in the analysis discussed in Section 4.3. Both conventional FEM and XFEM enriched with only the Heaviside function were employed to solve these problems and evaluate the history of temperatures at representative points on the $x_1$-$x_2$ plane, as shown in Fig. 22(c), and stress intensity factors at the deepest point of the crack by performing transient heat transfer and thermal stress analyses. The FEM (129,800 nodes and 121,336 elements) and XFEM (156,716 nodes and 148,200 elements) models are shown in Fig. 23. The temperature histories at points ($x_1$=$x_3$=0, $x_2$=0.0, 10.0, 48.0, 100.0) obtained by the heat transfer analysis and stress intensity factors at points ($x_1$=$x_3$=0, $x_2$=10.0) using FEM and XFEM are shown in Figs. 24(a) and (b), respectively. XFEM gives almost same results for both the history of the temperature and stress intensity factor as those given by FEM. In addition, these results obtained by the in-house FEM and XFEM codes agree well with those obtained by the commercial FEM code Abaqus.
Fig. 22 Edge cracked plate subjected to thermal field.

Fig. 23 Finite element models (quarter models).

Fig. 24 Comparison of numerical results by FEM, XFEM, and commercial FEM code.
5. Conclusions

A three-dimensional eight-node hexahedral tip element enriched with only the Heaviside step function was formulated, and in-house codes using such elements were developed to perform heat transfer and subsequent stress analyses. The developed codes can consider temperature-dependent material properties so as to solve practical thermal stress problems. In addition, the $J$-integral and stress intensity factor at the crack tip can be evaluated by the domain integral method. Because the XFEM model for the stress analysis is consistent with the heat transfer analysis model, nodal temperature data can be directly imported for stress analysis as thermal load data. The developed codes were applied to solve several benchmark problems and the results, including stress intensity factors, were compared with those obtained by conventional FEM and a reference solution. If a fine mesh is used, XFEM enriched with only the Heaviside step function gives almost same result as XFEM enriched with the Heaviside step function and asymptotic bases. When evaluating the $J$-integral and stress intensity factors by the domain integral method, needless to say, the path independency is important. Even for crack problems under a thermal stress field, where the thermal expansion coefficient is temperature-dependent, path independency can be maintained by including the gradient of the thermal expansion in the domain integration equations. Finally, a thermal stress analysis of a cracked plate was performed, and the results were verified through comparison of the history of the temperature and stress intensity factor with those obtained by the in-house and commercial FEM codes.

The crack geometry that can be modelled by the proposed method using XFEM is limited to a planar crack with a surface that coincides with the element surface. Even with this limitation, many practical crack problems are expected to be solvable. However, for more general application, modelling of an arbitrary non-planar crack is indispensable. Classification of tip elements into many additional patterns and their element partition is required; therefore, further work should be done.

Acknowledgments

The present study was supported by JSPS KAKENHI JP18K11341.

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