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SHORT COMMUNICATION

An exact reanalysis algorithm using incremental Cholesky factorization and its application to crack growth modeling

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SUMMARY

In this paper, an exact reanalysis algorithm based on an incremental Cholesky factorization is presented, which can solve a linear system of equations when a small portion of the coefficient matrix is modified. The efficiency of the proposed algorithm is demonstrated by modeling quasi-static crack growth in the extended finite element method. The example presented shows that a 60% to 70% reduction in computational time is achievable by using the reanalysis approach for solving crack growth problems. It is shown that the reanalysis approach has increasing benefits as the mesh density increases. Copyright © 2012 John Wiley & Sons, Ltd.

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1. INTRODUCTION

The extended finite element method (XFEM) [1] is an elegant solution to many of the challenges associated with the numerical simulation of crack propagation. Crack growth is often modeled as a quasi-static problem. In this methodology, only a small portion of the stiffness matrix will change as crack growth occurs. Once Heaviside terms are added to the stiffness matrix to model the discontinuity because of a crack, they will remain unchanged in future iterations of crack growth. At each iteration of crack growth, the previous crack tip components will need to be modified to account for the changing crack tip position. The objective of this paper is to maximize recycling computational resources during crack growth simulation by using this property. For the first iteration of the quasi-static solution procedure, the Cholesky factorization of the full stiffness matrix is calculated. In subsequent iterations, only the changed portion of the stiffness matrix is calculated (i.e., the new Heaviside and crack tip enrichment components). The existing Cholesky factorization is directly modified using row-add and row-delete operations. This solution procedure significantly reduces the cost of assembling the stiffness matrix and solving the system of matrix equations in the XFEM framework.

Reanalysis algorithms [2, 3] have been developed primarily for use in the fields of design and optimization to efficiently solve problems where small perturbations to the finite element domain are made. These methods can be classified as either being exact or approximate [4]. The exact methods are generally based on the Sherman–Morrison [5] inversion formula and consider cases where

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the modified elements affect a small number of degrees of freedom. The approximate methods are typically iteration based [3, 4, 6] and are used when the modified elements affect a large number of degrees of freedom. We directly modify an existing Cholesky factorization for reanalysis [7–13]. In the event that a Cholesky factorization is not possible, an alternative reanalysis algorithm may be used to achieve similar computational improvements.

The remaining part of the paper is organized as follows. First, the extended finite element method is reviewed and the crack growth model is introduced in Section 2. Next, the details of the exact reanalysis method used here are discussed in Section 3. Finally, in Section 4, a quasi-static crack growth problem is used as a test problem to evaluate the effectiveness of the proposed reanalysis method with respect to computational time and level of mesh refinement.

2. EXTENDED FINITE ELEMENT METHOD

The extended finite element method [1] (XFEM) allows discontinuities to be represented independent of the finite element mesh. Arbitrarily oriented discontinuities can be modeled independent of the finite element mesh by enriching all elements cut by a discontinuity using enrichment functions satisfying the discontinuous behavior and additional nodal degrees of freedom. The displacement approximation for an isotropic linear elastic material with a crack takes the form

$$\mathbf{u}^{\mathrm{h}}(\mathbf{x}) = \sum_{\mathrm{I}\in\Omega} \mathrm{N}_{\mathrm{I}}(\mathbf{x}) \left[\mathbf{u}_{\mathrm{I}} + \sum_{\mathrm{I}\in\Omega_{\mathrm{H}}} \mathrm{H}_{\mathrm{I}}(\mathbf{x})\mathbf{a}_{\mathrm{I}} + \sum_{\mathrm{I}\in\Omega_{\mathrm{T}}} \sum_{\alpha=1}^{4} \Phi_{\mathrm{I},\alpha}(\mathbf{x})\mathbf{b}_{\mathrm{I}}^{\alpha} \right], \tag{1}$$

where Ω_{H} is the domain cut by the crack, Ω_{T} is the domain containing the crack tip, $\mathrm{H}(\mathbf{x})$ is the shifted Heaviside enrichment and $\Phi_{\alpha}(\mathbf{x})$ is the shifted crack tip enrichment. The global stiffness matrix is symmetric and follows

$$\mathbf{K} = \begin{bmatrix} \mathbf{K}_{\mathrm{uu}} & \mathbf{K}_{\mathrm{au}}^{\mathrm{T}} & \mathbf{K}_{\mathrm{bu}}^{\mathrm{T}} \\ \mathbf{K}_{\mathrm{au}} & \mathbf{K}_{\mathrm{aa}} & \mathbf{K}_{\mathrm{ba}}^{\mathrm{T}} \\ \mathbf{K}_{\mathrm{bu}} & \mathbf{K}_{\mathrm{ba}} & \mathbf{K}_{\mathrm{bb}} \end{bmatrix}, \tag{2}$$

where subscript ‘u’ refers to the traditional finite element stiffness values, subscript ‘a’ refers to the Heaviside enrichment values and subscript ‘b’ refers to the crack tip enrichment values.

The direction of crack growth is found from the maximum circumferential stress criterion [14], which predicts that the crack will grow in the direction where $\sigma_{\theta\theta}$ is maximum. Here, a fixed increment of crack growth Δa is considered. The stress intensity factors needed for the maximum circumferential stress criterion are calculated using the domain form of the interaction integrals [15, 16].

3. EXACT REANALYSIS BY MODIFICATION OF CHOLESKY FACTORIZATION

It can be noticed from Equations (1) and (2) that the stiffness component associated with the traditional finite element approximation is not a function of the crack location, which implies that the $\mathbf{K}_{\mathrm{uu}}$ component of the stiffness matrix will be constant at each iteration of crack growth. This implies that the changing portion of the stiffness matrix is limited to the enriched portion, which will be small compared with the unenriched portion. Furthermore, it can also be noticed that while the Heaviside enrichment terms $\mathbf{K}_{\mathrm{aa}}$ are functions of the crack location within an element, that once a Heaviside enrichment or coupling to the classical FE approximation is introduced its value will not change in any future iterations. The stiffness components $\mathbf{K}_{\mathrm{uu}}$, $\mathbf{K}_{\mathrm{ua}}$, and $\mathbf{K}_{\mathrm{aa}}$ will be constant for future iterations of crack growth. An example of the nodes whose corresponding stiffness components need to be updated to account for crack growth is shown in Figure 1.

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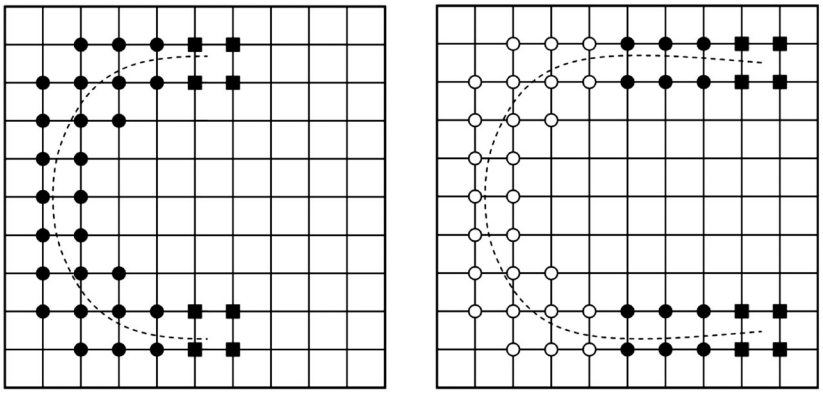

Figure 1. Finite element mesh with enriched nodes. (A) Initial crack geometry and (B) first iteration of crack growth. Circles denote nodes enriched with the Heaviside function and squares denote nodes enriched with the crack tip enrichment function. Filled circles and squares denote new enriched nodes for the current iteration while open circles and squares denote previously enriched nodes.

Once the boundary conditions have been applied, the stiffness matrix becomes positive definite and it is possible to compute the Cholesky factorization for the XFEM stiffness matrix as

$$\mathbf{K} = \begin{bmatrix} \mathbf{K}_{uu} & \mathbf{K}_{au}^{T} & \mathbf{K}_{bu}^{T} \\ \mathbf{K}_{au} & \mathbf{K}_{aa} & \mathbf{K}_{ba}^{T} \\ \mathbf{K}_{bu} & \mathbf{K}_{ba} & \mathbf{K}_{bb} \end{bmatrix} = \begin{bmatrix} \mathbf{L}_{uu} & & \\ \mathbf{L}_{au} & \mathbf{L}_{aa} & \\ \mathbf{L}_{bu} & \mathbf{L}_{ba} & \mathbf{L}_{bb} \end{bmatrix} \begin{bmatrix} \mathbf{D}_{uu} & & \\ & \mathbf{D}_{aa} & \\ & & \mathbf{D}_{bb} \end{bmatrix} \begin{bmatrix} \mathbf{L}_{uu}^{T} & \mathbf{L}_{au}^{T} & \mathbf{L}_{bu}^{T} \\ & \mathbf{L}_{aa}^{T} & \mathbf{L}_{ba}^{T} \\ & & \mathbf{L}_{bb}^{T} \end{bmatrix} = \mathbf{L}\mathbf{D}\mathbf{L}^{T}. \tag{3}$$

Because the XFEM stiffness matrix is largely constant and slowly evolving (i.e., additional Heaviside and changing crack tip stiffness components), it would be computationally attractive if the Cholesky factorized matrices, $\mathbf{L}$ and $\mathbf{D}$, are directly updated. The modification of the initial Cholesky factorization through sparse row-add and row-delete operations [7, 10–13] requires fewer floating-point operations for subsequent iterations of crack growth.

Suppose that the i-th row and column of $\mathbf{K}$ is equal to the i-th row/column of the identity matrix. This i-th row has no effect on the Cholesky factorization of the rest of the matrix. We refer to replacing this i-th row/column of $\mathbf{K}$ with a nontrivial row/column as a 'row-addition.' It can be computed with the solution of a system of equations where the matrix $\mathbf{L}$ is upper triangular and a rank-one downdate, as described below. A 'row-deletion' does the opposite, by replacing a nontrivial row/column of $\mathbf{K}$ with the corresponding row/column of the identity matrix.

To find the fill-reducing ordering for this matrix, the connectivity of all possible elements is used to create a matrix $\mathbf{K}_s$ with unity in all matrix locations that would contain information if all possible Heaviside and crack tip nodes were active. The nonzero pattern of $\mathbf{K}_s$ is a superset of any $\mathbf{K}$ that would be seen in the subsequent numerical factorizations computed during crack propagation, and thus the nonzero pattern of its Cholesky factor $\mathbf{L}_s$ will also be a superset of any Cholesky factor $\mathbf{L}$ seen later. A fill-reducing ordering is obtained for $\mathbf{K}_s$ from the approximate minimum degree ordering (AMD) algorithm [17–19]. Finding an optimal fill-reducing ordering for an arbitrary matrix is computationally impossible, and thus AMD is a heuristic, as are all fill-reducing algorithms. However, because AMD is applied to the entire $\mathbf{K}_s$ matrix, it will limit the fill-in in the matrix $\mathbf{L}_s$, and thus it will also limit the upper bound of any fill-in in any Cholesky factor $\mathbf{L}$ computed later. This strategy ensures that the size of the stiffness matrix is constant for each iteration of crack growth, even if the number of active degrees of freedom for each crack growth iteration is non-constant. This preallocation approach did not significantly impact the amount of memory needed to

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store the current Cholesky factor $\mathbf{L}$ when compared with the amount of memory needed to store $\mathbf{L}$ without preallocation.

After applying the fill-reducing ordering, the permuted stiffness matrix is referred to as $\mathbf{K}_\mathrm{p}$. The fill-reducing ordering is applied to reduce the fill-in of subsequent iterations of crack growth as the active enriched nodes evolve. For elements that are initially intersected by the crack, the corresponding enriched degrees of freedom are set active, while all other nodes are defined inactive. Any rows or columns of $\mathbf{K}$, and subsequently $\mathbf{K}_\mathrm{p}$, corresponding to an inactive enriched degree of freedom have rows and columns, which are set to zero, except for their diagonal component, which is unity. To update the Cholesky factorization, only the modified components of the updated stiffness matrix $\bar{\mathbf{K}}$ (e.g., new Heaviside and crack tip components) are needed. Before updating the previous Cholesky factorization, the fill-reducing ordering is applied to $\bar{\mathbf{K}}$ yielding $\bar{\mathbf{K}}_\mathrm{p}$. Consider the stiffness matrix at the initial iteration of crack growth, given as

$$\mathbf{L}\mathbf{D}\mathbf{L}^\mathrm{T}=\begin{bmatrix}\mathbf{L}_{11} & & \\ 0 & 1 & \\ \mathbf{L}_{31} & 0 & \mathbf{L}_{33}\end{bmatrix}\begin{bmatrix}\mathbf{D}_{11} & & \\ & 1 & \\ & & \mathbf{D}_{33}\end{bmatrix}\begin{bmatrix}\mathbf{L}_{11}^\mathrm{T} & 0 & \mathbf{L}_{31}^\mathrm{T} \\ & 1 & 0 \\ & & \mathbf{L}_{33}^\mathrm{T}\end{bmatrix}=\begin{bmatrix}\mathbf{K}_{11} & 0 & \mathbf{K}_{31}^\mathrm{T} \\ 0^\mathrm{T} & 1 & 0^\mathrm{T} \\ \mathbf{K}_{31} & 0 & \mathbf{K}_{33}\end{bmatrix}=\mathbf{K}_\mathrm{p}, \tag{4}$$

where the identity row denotes an inactive enriched degree of freedom and $\mathbf{K}_\mathrm{p}$ is the XFEM stiffness matrix permuted to a fill-reducing ordering. After crack growth has occurred and the previously inactive degree of freedom becomes active, the new stiffness matrix $\bar{\mathbf{K}}_\mathrm{p}$ is given as

$$\begin{aligned}\bar{\mathbf{L}}\bar{\mathbf{D}}\bar{\mathbf{L}}^\mathrm{T} &= \begin{bmatrix}\mathbf{L}_{11} & & \\ \bar{\mathbf{l}}_{12}^\mathrm{T} & 1 & \\ \mathbf{L}_{31} & \bar{\mathbf{l}}_{32} & \mathbf{L}_{33}\end{bmatrix}\begin{bmatrix}\mathbf{D}_{11} & & \\ & \bar{\mathbf{d}}_{22} & \\ & & \mathbf{D}_{33}\end{bmatrix}\begin{bmatrix}\mathbf{L}_{11}^\mathrm{T} & \bar{\mathbf{l}}_{12} & \mathbf{L}_{31}^\mathrm{T} \\ & 1 & \bar{\mathbf{l}}_{32}^\mathrm{T} \\ & & \mathbf{L}_{33}^\mathrm{T}\end{bmatrix} \\ &= \begin{bmatrix}\mathbf{K}_{11} & \bar{\mathbf{k}}_{12} & \mathbf{K}_{31}^\mathrm{T} \\ \bar{\mathbf{k}}_{12}^\mathrm{T} & \bar{\mathbf{k}}_{22} & \bar{\mathbf{k}}_{32}^\mathrm{T} \\ \mathbf{K}_{31} & \bar{\mathbf{k}}_{32} & \mathbf{K}_{33}\end{bmatrix}=\bar{\mathbf{K}}_\mathrm{p}.\end{aligned} \tag{5}$$

The modification of the initial $\mathbf{L}\mathbf{D}\mathbf{L}^\mathrm{T}$ to add a new enriched degree of freedom to the Cholesky factorization is detailed by Davis and Hager [12].

Crack tip stiffness components will need to be modified after each iteration of crack growth; therefore, it is necessary to also consider the case of a row-delete operation to remove old entries into the stiffness matrix associated with the crack tip enrichment function. In this case from the previous iteration the stiffness matrix and corresponding factorization are given as

$$\begin{aligned}\mathbf{L}\mathbf{D}\mathbf{L}^\mathrm{T} &= \begin{bmatrix}\mathbf{L}_{11} & & \\ \mathbf{l}_{12}^\mathrm{T} & 1 & \\ \mathbf{L}_{31} & \mathbf{l}_{32} & \mathbf{L}_{33}\end{bmatrix}\begin{bmatrix}\mathbf{D}_{11} & & \\ & 1 & \\ & & \mathbf{D}_{33}\end{bmatrix}\begin{bmatrix}\mathbf{L}_{11}^\mathrm{T} & \mathbf{l}_{12} & \mathbf{L}_{31}^\mathrm{T} \\ & 1 & \mathbf{l}_{32}^\mathrm{T} \\ & & \mathbf{L}_{33}^\mathrm{T}\end{bmatrix} \\ &= \begin{bmatrix}\mathbf{K}_{11} & \mathbf{k}_{12} & \mathbf{K}_{31}^\mathrm{T} \\ \mathbf{k}_{12}^\mathrm{T} & 1 & \mathbf{k}_{32}^\mathrm{T} \\ \mathbf{K}_{31} & \mathbf{k}_{32} & \mathbf{K}_{33}\end{bmatrix}=\mathbf{K}_\mathrm{p},\end{aligned} \tag{6}$$

where the second row and column correspond to an enriched crack tip entry in the XFEM stiffness matrix. The corresponding stiffness matrix and factorization with the old crack tip component removed is given as

$$\bar{\mathbf{L}}\bar{\mathbf{D}}\bar{\mathbf{L}}^\mathrm{T}=\begin{bmatrix}\mathbf{L}_{11} & & \\ 0 & 1 & \\ \mathbf{L}_{31} & 0 & \bar{\mathbf{L}}_{33}\end{bmatrix}\begin{bmatrix}\mathbf{D}_{11} & & \\ & 1 & \\ & & \mathbf{y}\mathbf{D}_{33}\end{bmatrix}\begin{bmatrix}\mathbf{L}_{11}^\mathrm{T} & 0 & \mathbf{L}_{31}^\mathrm{T} \\ & 1 & 0 \\ & & \bar{\mathbf{L}}_{33}^\mathrm{T}\end{bmatrix}=\begin{bmatrix}\mathbf{K}_{11} & 0 & \mathbf{K}_{31}^\mathrm{T} \\ 0^\mathrm{T} & 1 & 0^\mathrm{T} \\ \mathbf{K}_{31} & 0 & \mathbf{K}_{33}\end{bmatrix}=\bar{\mathbf{K}}_\mathrm{p}. \tag{7}$$

The modification of the initial $\mathbf{L}\mathbf{D}\mathbf{L}^\mathrm{T}$ to remove a crack tip enriched degree of freedom from the Cholesky factorization is detailed by Davis and Hager [12].

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The new stiffness components associated with the crack tip enrichment function are added using the row-add operation previously discussed. For more details on the row-add and row-delete algorithms, readers are referred to the work of Davis and Hager [12, 13] including proofs of optimal convergence. Our implementation was accomplished based on the creation of a MEX file which created a link between a MATLAB (Matthew J. Pais, Gainesville, FL) XFEM code [20] and CHOLMOD [9]. The proposed reanalysis algorithm for crack growth can be summarized as follows:

1. Calculate the superset matrix $\mathbf{K}_s$ for the initial quasi-static iteration.
2. Find the fill-reducing permutation of $\mathbf{K}_s$ with AMD.
3. Calculate **L** and **D** from the initial **K** using the fill-reducing ordering permutation.
4. Solve for the traditional and enriched degrees of freedom.
5. Calculate K_I, K_{II}, and ΔK. Grow the crack.
6. Calculate the new portions of $\bar{\mathbf{K}}$ from prior crack growth.
7. Use row-delete to remove prior crack tip **K** components from **L** and **D**.
8. Use row-add to add new Heaviside and crack tip $\bar{\mathbf{K}}$ components to **L** and **D**. 9. Repeat steps 3–7.

For a Cholesky factorization there are two steps: a symbolic step that finds the structure of the Cholesky factorization and a numerical step that finds its values.The difference between the native MATLAB backslash and CHOLMOD implementations is that the MATLAB backslash operation does not retain the symbolic factorization that is required to enable the row add/delete operations. Therefore, the symbolic factorization must be repeated in addition to the numerical work for each iteration of crack growth, which results in additional computational overhead compared with the CHOLMOD implementation where only the numerical work must be completed at each iteration. The MATLAB interface for CHOMOD adds additional work however. A MATLAB function cannot modify its inputs, thus to create a modified version of **L** and entirely new copy must be made. This copy of **L** dominates the time taken. However, even with this constraint, we still obtain substantial improvements over the time taken to compute the Cholesky factorization from scratch.

4. NUMERICAL RESULTS

The first step in evaluating the proposed reanalysis algorithm is to consider a simple geometry that will allow us to both assess the savings from the proposed algorithm and to study the effect that increasing or decreasing the mesh density locally around the crack tip has on the proposed reanalysis algorithm. To perform this study, an edge crack of initial length 0.25 m in a finite plate of size 2 m × 2 m under unit uniaxial tension with 30 increments of 0.05 m crack growth was considered as shown in Figure 2. Because the loading is pure Mode I, the crack propagates horizontally following the dashed line. The material properties were elastic modulus $E = 1$ Pa and Poisson's ratio $v = 0.3$. To study the effect of repeated iterations of crack growth, a structured mesh of square plane strain elements with characteristic length 0.05 m was used, which was sufficient to achieve convergence in the Modes I and II stress intensity factors for this geometry.

The savings is both the stiffness matrix assembly time and the time to factoring the global stiffness matrix or updating an existing factorization and then solving the resulting system of equations. The normalized times were calculated as the reanalysis algorithm divided by the traditional approach as a function of crack growth iteration as shown in Figure 3. The traditional approach is considered to be calculating or factoring and solving **K** at each iteration from scratch. We assume the performance of factoring and solving a given system of equations between CHOLMOD and the native *backslash* function within MATLAB to be comparable. It can be noticed from Figure 3 that the general trend for assembly is increased savings with additional iterations. This can be explained as having a larger crack increases the bandwidth of **K**, while only calculating the new enriched elements is approximately constant for the case of a fixed Δa. The increased fill-in as the number of enriched element increases subtly increases the cost of updating the existing Cholesky factorization as the number of crack growth iterations increases. Figure 4 shows that the savings increases proportional to the number of elements.

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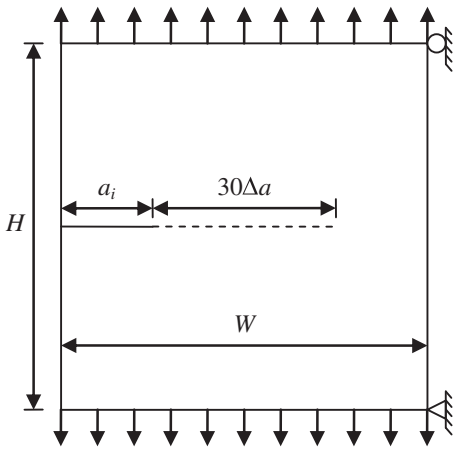

Figure 2. Edge crack in a finite plate geometry used to test quasi-static crack growth with the reanalysis algorithm.

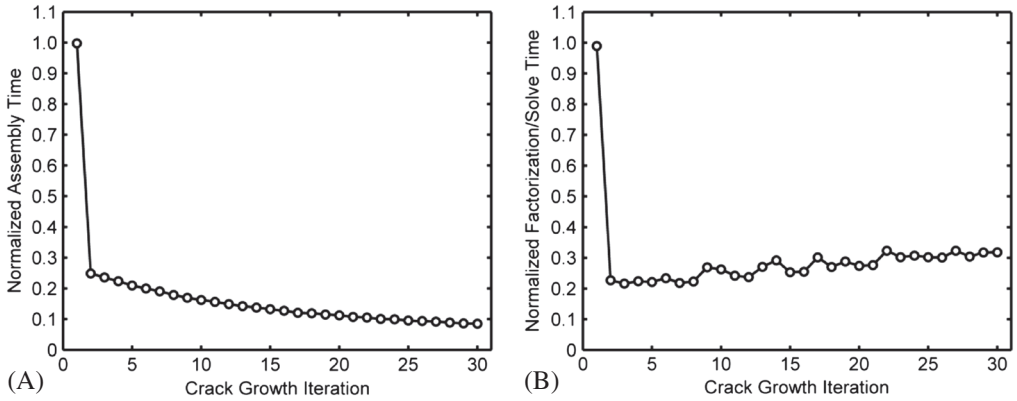

Figure 3. Normalized computational time for stiffness matrix assembly (A) and factorization and solving of system of linear equation (B) as a function of number of iterations.

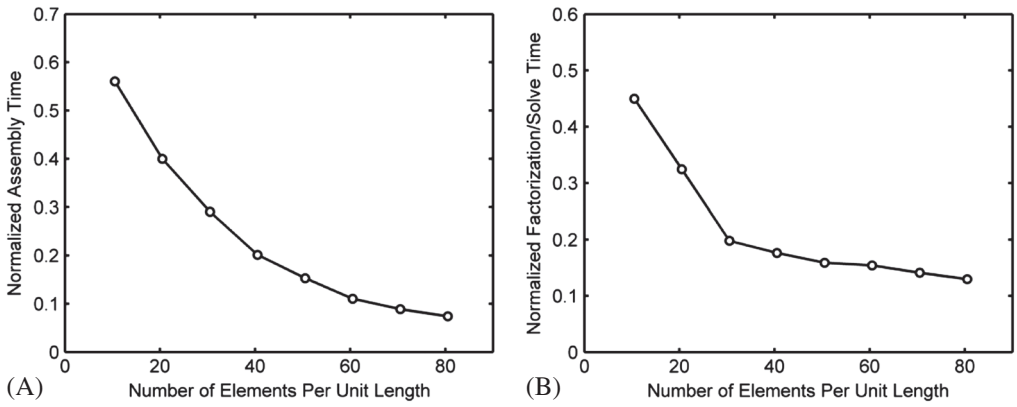

Figure 4. Normalized computational time for stiffness matrix assembly (A) and factorization and solving of system of linear equation (B) as a function of mesh density.

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5. CONCLUSIONS

The XFEM allows for discontinuities in solid bodies to be represented independent of the finite element mesh through the use of enrichment functions and additional nodal degrees of freedom. For the crack tip enrichment functions, only a localized portion of the stiffness matrix is modified as a result of crack growth. An exact reanalysis algorithm is presented based on the direct modification of a sparse Cholesky factorization through the use of row modification operations. It has been shown that there is a reduced computational cost for each iteration of crack growth based on locally updating a Cholesky factorization instead of simply factoring and solving the resulting system of linear equations. A study of the effect on mesh density was performed and it was found that while savings can be achieved over the full range of mesh densities, the largest savings were achieved when the mesh had an increased level of refinement.

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