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FINAL REPORT ON SUPPORT FOR XFEM COMPONENT INTEGRITY ANALYSIS: TASK 1 LITERATURE SURVEY

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Final Report
On

Support for XFEM Component Integrity Analysis: Task 1 Literature Survey

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TABLE OF CONTENTS

1 INTRODUCTION

Historically, simulating cracks and crack growth using conventional Finite Element Methods/Analysis (FEM/FEA) has proven difficult and time consuming especially for modeling realistic multi-directional crack growth. More recently, methods that allow for realistic crack growth to be modeled using straight forward techniques have been developed. Specifically, the extended finite element method (XFEM) [1] is a FEA tool that allows for mesh-independent analysis of discontinuities and singularities and can be used to simulate crack growth in complex geometries in a simplified manner [2]. The Abaqus commercial FEA software [3] implementation of XFEM is potentially a powerful tool for representing cracks and simulating crack growth in industry relevant models. With the right choice of elements and meshing parameters, XFEM has proven capable of simulating critical and fatigue crack growth rates in complex systems, with results that closely match classic numerical and experimental results [4]. In some cases, XFEM results have shown to be extremely reliable, and have been used in developing industry standards regarding flaw proximity analyses [5], [6], [7]. Researchers have also investigated the Abaqus implementation of XFEM to calculate stress intensity factors for pre-existing cracks and found good agreement with stress intensity factors generated with traditional FEA meshes [8]. While the use of crack-conforming meshes and procedural re-meshing allow for crack growth simulations with traditional finite element analysis, it is the ability of XFEM to accomplish such simulations without these cumbersome procedures that make XFEM particularly useful.

To better appreciate the capabilities and limitations associated with XFEM, it is best to understand how the various numerical methods are derived from continuum mechanics. With this basic understanding the identified four major crack growth numerical techniques can be compared: (1) traditional Hybrid FEM approach (independent analysis with explicit crack-tip singularity, post-processor for stress intensity factor (SIF) and increment crack growth, update new model mesh, repeat) (2) Finite Element Alternating Method (3) XFEM and (4) Peridynamics. Each of the four numerical methods have been used to evaluate crack growth applications with each having advantages and disadvantages.

2 FRACTURE AT THE CONTINUUM LEVEL

The mechanical behavior of solids may be understood on the basis of the atomistic structure of the material and the forces which cause the coherence of individual atoms or molecules. The macroscopic strength expressed as the maximum stress that can be sustained by a structural member of this material is influenced only to a small extent by theoretical atomic or molecule bond forces, as discussed by Sommer [9]. Instead, the characteristics of imperfections, their number and distribution determine the actual resistance of a material against failure. Since information about these microscopic quantities is generally not readily available and cannot directly be used to determine the actual behavior of a structure, the concept of continuum mechanics has been introduced as a first approximation to the real problem. The state of a continuous body can be described in terms of stresses, strains and displacements. Between those quantities mathematical relations exist, for example, in the form of differential equations. These relations already define the mathematical model, which also includes the boundary conditions of a particular problem. Since exact solutions are available only for a very limited number of mathematical problems, in general numerical models must be set up and solved [10].

3 NUMERICAL METHODS TO SOLVE CRACK PROBLEMS

Figure 1 is intended to provide a simple hierarchical flow from fundamental solid mechanics equations of motion as they develop into the key numerical methods in use today. While there are many particular details, the general idea may be illustrated with a simple elastic example. Equations of the theory of elasticity need to be solved in a given domain for finding an equilibrium configuration of a deformable elastic body [11]. This is a strong form of the problem. At the same time, the total mechanical energy (strain energy of the body + potential energy of externally applied forces) is at a minimum in an equilibrium state, which means that certain functionals need to be minimized with respect to the unknown field of displacements for finding the solution [12]. This is a weak form (one among many possibilities) of the problem. Both formulations are mathematically equivalent but allow for different numerical methods to find approximate solutions.

Solving the strong form (governing differential equations) is not always efficient and there are not always classical solutions to a particular problem. This is true especially in the case of complex domains and/or different material interfaces. Moreover, incorporating boundary conditions is always a daunting task when solving strong forms of equations directly as the requirement on continuity of field variables is much stronger.

From these fundamental equations, key numerical methods have been developed. As detailed in the following sections, the key numerical methods highlighted in red in Figure 1 will be explored to gain an understanding of the identified four major crack growth numerical techniques: (1) traditional Hybrid FEM approach (independent analysis with explicit crack-tip singularity, post-processor for stress intensity factor (SIF) and increment crack growth, update new model mesh, repeat) (2) Finite Element Alternating Method (3) XFEM and (4) Peridynamics. From a conceptual overview of these techniques, Figure 2 shows the key mesh features (refinement and special meshing requirements) for each of these techniques.

These key numerical methods are explored in greater detail in the following sections.

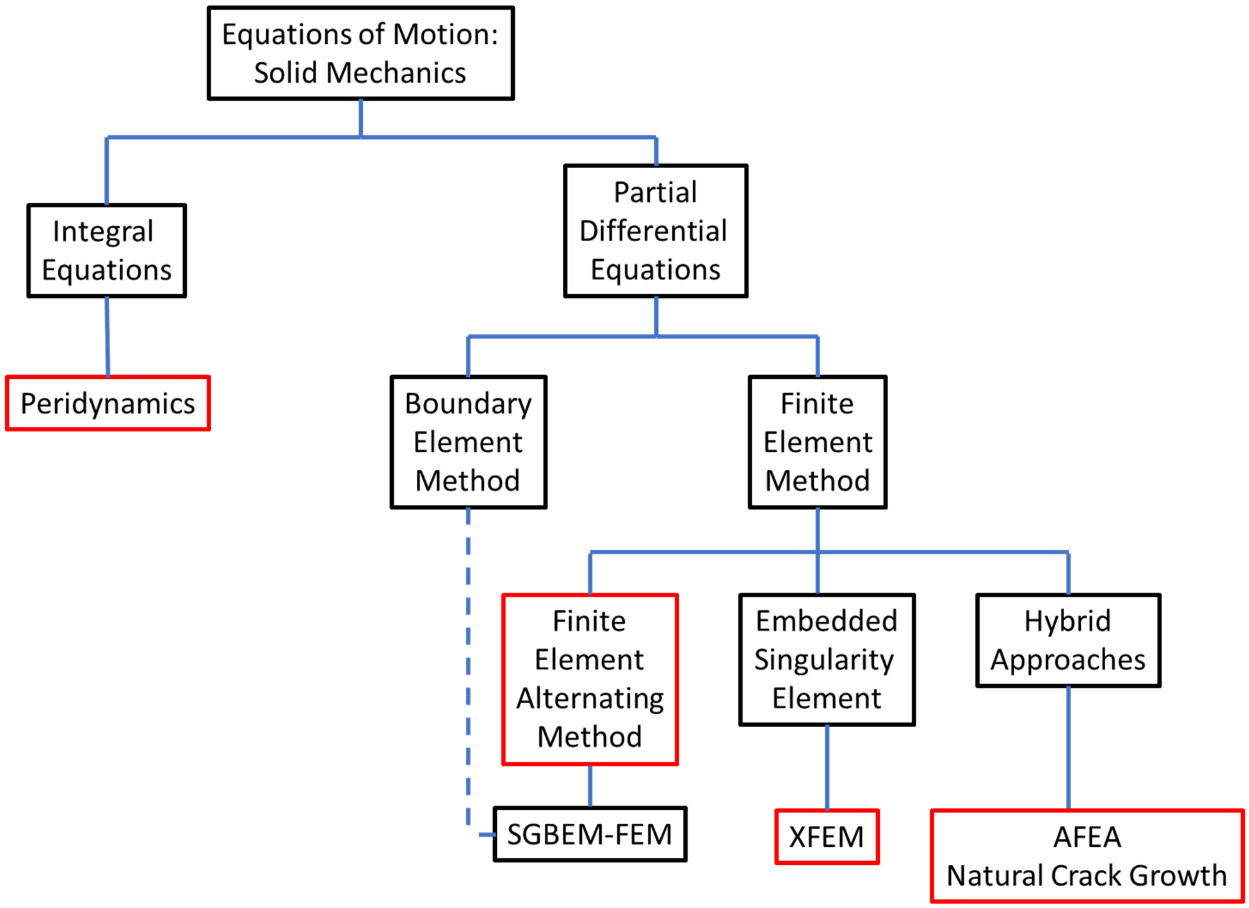
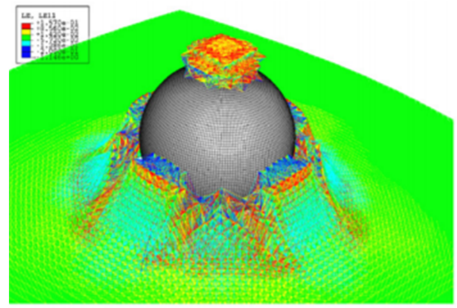


Figure 1 Hierarchical Flow of Fracture Mechanics Numerical Methods Development from Solid Mechanics Equations of Motion

Peridynamics

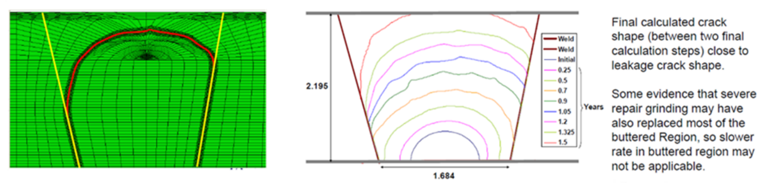
- Molecular Dynamics at continuum-level
- No explicit crack tip mesh required. (failure included in material model)
- Local mesh in damaged region are essentially interconnected truss-like elements for bond-based formulation.



Taken from Macek [13]

Finite Element Method (basis for Hybrid approach)

- Requires explicit modeling of singularity with normal mesh refinement.

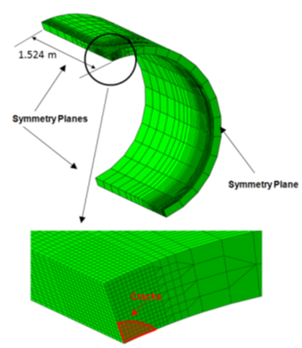


AFEA mesh at 1.325 years

Taken from Shim [14]

Finite Element Alternating Method

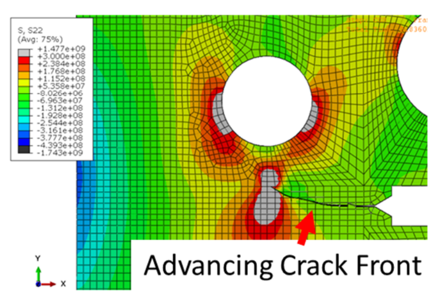
- No explicit modeling of crack in FEM portion. (coarse FEA mesh has been shown to be accurate)
- Crack-location and analytical crack solution is specified outside of FEA solution.



Based on Brust [15]

Extended Finite Element Method (XFEM)

- No specialized crack mesh required in FEA mesh.
- Initial crack location specified at beginning of analysis.
- Increased mesh refinement is typically required.



Based on Miranda [16]

Figure 2 Meshing Features for Key Fracture Mechanics Numerical Methods

3.1 Integral Equation Formulation - Peridynamics

Peridynamics [17] has been developed within the last twenty years based on integral equations using the strong- form of the equations of motion. Since the integral equations remain valid in the presence of discontinuities such as cracks, the method has the potential to model fracture and damage with great generality and without the complications of mathematical singularities that plague conventional continuum finite element approaches [18].

In its original formulation, linear-elastic bond-based peridynamics modeled fracture by equating the critical energy release rate of the continuum with the one from peridynamic theory, which leads finally to a critical stretch between the particles as fracture criterion which can be implemented with ease. Peridynamic models need no additional external criteria for the initiation and propagation of cracks as failure of the material is invoked through the material response in the theory. However, the extension to nonlinear materials and complex mixed-mode fracture has required additional research developments which are still ongoing. Nonetheless, this approach has been applied to some numerical simulation of discontinuous damage problems in recent years including stress corrosion cracking [19].

It should be noted that the calculation efficiency of peridynamics is much lower than that of FEM because of the non-local theory (i.e. every peridynamic particle is interacting with all particles within its neighborhood). Currently, the only known commercial FEA solver to incorporate peridynamics is LS-DYNA [20], which has implemented the bond-based formulation which limits the response to linear elasticity and its applications to brittle materials. From the author's perspective, this promising technology should be monitored for future usage especially when the approach is combined with traditional FEA to allow for direct specification of boundary conditions.

3.2 Partial Differential Equation Formulations

In order to overcome the above difficulties on performance and boundary condition specifications, weak formulations based on partial differential equations have generally been preferred for structural analyses. They reduce the continuity requirements on the approximation functions thereby allowing the use of easy-to-construct and implement polynomials. This is one of the main reasons for the popularity of weak formulations despite many disadvantages they

pose when applied to some class of problems, like non-symmetric matrix systems [10]. In weak forms, boundary conditions come naturally and hence, implementing them is easy. The typical finite element method formulation is a weak form based on the partial differential equations of motion.

Weak forms rarely give perfectly accurate solutions because of the reduction in the requirements of smoothness and weak imposition of Neumann boundary conditions. The weak formulation relaxes the continuity requirements for the approximate displacements since derivatives are passed from the approximate solution to the weighting function. This approach does not have any inaccuracy issues aside from the approximate nature of the solution itself. Weak forms still give relatively accurate results with the mesh refinement and are extremely good for engineering simulations, and solutions can be obtained even if there is no classical solution such as in the case of problems with complex domains and different materials, contact etc. Improving the accuracy of a solution in weak formulations depends upon the type of problem being solved. Often, mesh refinement and/or higher order shape functions will suffice.

The calculation of fracture mechanics parameters (such as the stress intensity factors of Modes I, II and III), for arbitrary non-planar three-dimensional surface and internal cracks, remains an important task in the structural integrity assessment and damage tolerance analyses [21]. In spite of its wide-spread popularity, the traditional finite element method, with simple polynomial interpolations, is unsuitable for modeling cracks and their propagation, partially due to the high-inefficiency of approximating stress and strain-singularities using polynomial FEM shape functions. In order to overcome this difficulty for prior known singularity stress fields, embedded-singularity elements by Tong [22], and singular quarter-point elements by Barsoum [23], among others, were developed in the 1970s, in order to capture the crack-tip/crack-front singular field. Many such related developments were summarized in Atluri [10] and they are now widely available in many commercial FEM software, such as Abaqus [3]. However, the need for constant remeshing makes the automatic fatigue-crack-propagation analyses with FEM extremely difficult.

3.2.1 XFEM – Extended Finite Element Method

The XFEM (Extended Finite Element Method), which was put forward first in [1], has become widely used in the past two decades. In actuality, XFEM differs very little in theory from the embedded-singularity elements developed in the 1970s and cited above. Both the XFEM of the 2000s, and the embedded-singularity elements of the 1970s, use crack-tip singular fields to enrich the approximation functions. Both of them use weak-form variational principles to develop FEM equations using path-independent/domain-independent integrals as in [24] among other techniques to extract and evaluate the stress intensity factors from the computed displacement solutions converted to strain and stress solutions using constitutive models. Moreover, for both the XFEM and the much earlier embedded-singularity elements, singular enrichment is confined only to the elements which are immediately adjacent to the crack-tip/crack-front. Therefore, as seen in most XFEM, an extremely fine and good-quality mesh is still necessary to capture the high gradients of the stress field, at locations close to the crack tips/crack fronts.

XFEM is intrinsically a mesh-independent method. In the context of fracture mechanics, this means that the crack can cut through any element so that the mesh does not need to conform to the crack position. Consequentially, this can lead to a tremendous reduction of the model creation time. Nevertheless, XFEM remains a finite element method for which the size of the mesh plays a crucial role in the accuracy of the solution.

One of main reasons why very fine meshes are required is that Abaqus does not allow one to put a crack front right at the interface of an element – the crack front must cut through the enriched elements and the calculations are performed based on the nodal values of those cut elements. The finer the mesh, the less variations among those nodal values and hence, better consistency at the crack front. In Emc^2 previous work [4] for the US Department of Transportation (where XFEM was used for approximately two thousand calculations), for a pipe, elliptical surface crack, the element size in the crack and enriched region was around 0.33 mm to ensure accuracy – which is quite fine. However, the convenience of being able to develop meshes for complicated geometries for crack growth modeling is a big advantage of XFEM approaches. Moreover, crack growth within one mesh is possible as new meshes do not have to be developed for each crack growth location. With Abaqus one can also use a fine hex element

region for the crack growth portion (often requiring hundreds of thousands of elements for accuracy) and coarser simpler elements (for instance easy to mesh tetrahedral elements) away from this region that are tied to the crack elements using the automatic Abaqus Lagrange constraint 'tie' process, further making this possibility convenient for crack growth in complex geometries such as control rod drive mechanism (CRDM) heads.

In a recent 2018 publication [25], researchers utilized an XFEM-based representative model that improved estimation of primary water stress corrosion cracking (PWSCC) crack growth of CRDM nozzle tubes by considering both residual stress of the CRDM nozzle *and* primary water contact conditions. This proposed XFEM workflow utilized Abaqus user-subroutine coding to demonstrate more feasible PWSCC growth, which starts from the surface and moves to the interior of the CRDM nozzle tubes due to continuous contact with primary water. The simulation shows good agreement with reported PWSCC incidents. Additionally, the effects of weld parameters and mesh density (number of beads, circumferential mesh density and number of mesh layers) on XFEM crack propagation were also studied. It was found that although the number of weld element layers did not significantly affect the weld residual stress (WRS) distribution, it resulted in a distinguishable difference in crack propagation geometry. Hence, mesh specification was found to play a crucial role.

Beginning in the Abaqus 2019 release, a simplified fatigue capability was introduced to model fatigue growth under static loading using, among other features, XFEM. This is meant as a way to simplify fatigue models and allows for fatigue growth using the standard Paris Law without modeling cycles directly, only the loading state at the maximum linear elastic strain energy release rate, G_{max}. This relationship can be exploited for use in PWSCC (or other time-dependent) modeling where PWSCC growth uses the maximum stress intensity factor, K_{max}, to determine the crack growth rate with the fact that the simplified fatigue is only calculating G under the "fully loaded" condition. This means that there is a direct relationship between the crack growth rate of an Abaqus simplified fatigue model and PWSCC growth. Initial scoping work for modeling PWSCC of Alloy 182 SMA weld material in a compact tension specimen has shown that the complete workflow can now be completed using built-in features of Abaqus. A full description of this work will be provided in the Task 2 (Sensitivity Studies) Report for this project.

3.2.2 Finite Element Alternating Methods

In a fundamentally different mathematical way, after the derivation of analytical solutions for embedded elliptical cracks whose faces are subjected to arbitrary normal and shear tractions, the first modern paper on a Finite Element (Schwartz-Neumann) Alternating Method (FEAM) was published in [26]. The FEAM uses the Schwartz-Neumann alternation between a relatively coarse mesh finite element solution for an uncracked structure and the analytical solution for an infinite body containing the crack. The success of this method is mostly due to the work of [27], in which the analytical solutions for an embedded elliptical crack, the faces of which are subjected to arbitrary normal and shear tractions, are derived. Subsequent 3D and 2D variants of the finite element alternating methods were successfully developed and applied to perform structural integrity and damage tolerance analysis of many practical engineering structures, including PWSCC crack growth in the nuclear industry [28] [29].

An interesting extension to this work is to use a general boundary element method to replace the analytical solution in the infinite body. In the SGBEM-FEM alternating method [30], a finite element analysis is carried out on the uncracked body using the externally applied loading and next a boundary element analysis is performed by reversing the stresses found on the crack location from the finite element analysis, and the residual stresses on the boundary of the finite body are determined. The steps are repeated until convergence is achieved where the residual stresses on the boundaries and traction on the crack surfaces are close to zero. This approach allows for a general flaw shape (non-planar curvilinear defects) and the potential for non-planar crack extension. Unfortunately, no directly reported information is available regarding computational requirements and modeling difficulty for alternating method techniques.

3.2.3 Hybrid Methods

The Advanced Finite Element Analysis (AFEA) has been developed and used to model the 'natural crack growth' in simple geometries such as pipe components. AFEA consists of calculating stress intensity factors at numerous points along the crack, growing the crack at each point, development of a new automatic finite element mesh to produce the next crack size and shape, calculating the stress intensity factor along the crack front, and growing the crack further until instability occurs. The AFEA process requires an automated finite element mesh generator

and the entire process is managed with a controlling script (e.g. Python). The script develops a mesh for the current crack size, produces a finite element model based input file, submits the finite element job, extracts results (especially stress intensity factors along the crack front), grows the crack at points along the crack, develops next mesh, and so on until the crack grows to instability. This growth process typically requires hundreds of ‘spider’ crack meshes to be developed and often takes significant solution time (often a day with a couple hundred solutions if the mesh generator is rapid) to model crack growth to a through-wall crack and growth of the through-wall crack. Because each solution is elastic (e.g. PWSCC is currently characterized by the elastic stress intensity factor) the solution time is manageable. The AFEA process can only be automated for relatively simple geometries such as pipes or plates where automatic crack meshes can be easily developed. Emc^2 uses a code called PipeFracCAE for this purpose. Other commercial software packages for this task are available from Quest Integrity (FEACrack) [31] and Zentech (ZENCRACK) [32].

Advanced finite element analyses (AFEA) have successfully been conducted by both the United States Nuclear Regulatory Commission (US NRC) and the nuclear industry for long circumferential indications found at the Wolf Creek power plant [33], for an axial crack found in the V.C. Summer hot leg dissimilar metal weld [34], and for cracking in CRDM tubes [35][*]. In these assessments, PWSCC occurs in the nozzle to piping Alloy 82/182 dissimilar metal welds. PWSCC occurs due to a combination of four factors (i) tensile weld residual stresses (WRS) at the nozzle inner diameter, (ii) water chemistry, (iii) a material that is susceptible to corrosion (i.e. Alloy 82/182 weld metal), and (iv) high temperature (usually greater than 300C). The ability of AFEA to handle the elastic stress intensity factor that PWSCC is characterized by along with a mapped welding residual stress as an elastic field was key in developing this for production-capable assessments.

In 2019, a variation of the hybrid method has been proposed by Shi [36]. In this approach, a non-conforming, non-focused finite element mesh with enrichment functions was utilized to extract stationary-crack stress-intensity factor solutions using the built-in Abaqus XFEM capability. Abaqus python programming was then used to evaluate a postulated circumferential

[*] For the CRDM PWSCC analysis the AFEA process required tweaking of each individual mesh since the geometry is complex. Natural crack growth for the inlay problem, which results in ‘bubble’ shaped cracks, has been performed using a similar approach.

PWSCC crack in feeder pipe dissimilar metal welds. The comparison of XFEM natural crack growth predictions with the typical advanced finite element analyses (focused-mesh AFEA) approach shows good agreement in terms of crack progression from surface crack to through-wall crack and the crack growth rate. The advantages of this new approach would be significantly reduced model build-up efforts for the finite-element based crack growth modeling as only one-mesh is required (only updates to the location of the stationary crack is required). It also makes 3D arbitrary crack modeling possible. Additional work remains with this method to ensure that reasonable stress intensity factor solution values can be obtained with reasonable mesh densities and element distortion metrics.

4 SUMMARY OF KEY FINDINGS

The XFEM method, wherein 'enriched' shape functions are included in the formulation, now permits crack solutions for stress intensity factors within codes where this method is included as an option. In theory, XFEM permits one to model crack growth without using a focused 'spider web' type mesh often required using conventional elements. This is convenient, especially for complicated geometries where the AFEA type meshers (PipeFracCAE, for instance) are not available. XFEM method, which is an automated extension of the original embedded singular (often hybrid method) element approaches in the 1970s, requires a fine mesh. The finite element alternating method, which Emc^2 often uses, does not suffer from this limitation as coarse meshes can be used, except that complicated crack shapes, i.e. natural crack growth, is not possible and the crack must grow as a partial ellipse, although through-wall crack growth is also possible.

In a rather remarkable finding, even though the XFEM was developed to reduce the computational effort required to simulate crack propagation, none of the studies reviewed do actually compare computation times between XFEM and the other available technologies. One would expect the computation time would decrease, especially with the introduction of XFEM. The works considered in this review are inconclusive in this regard, mainly because computation times (with processor speeds) are rarely stated. In order to choose between the various computational techniques for modelling crack propagation, a systematic evaluation of a common problem should be evaluated utilizing the various techniques.

5 CONCLUSIONS

To summarize the conclusions of the Literature Review:

General XFEM Implementation

- Advantage:
  - With the right choice of elements and meshing parameters, XFEM has proven capable of simulating critical and subcritical (fatigue and PWSCC) crack growth rates in complex systems within a self-contained integrated workflow.
    - No specialized crack tip meshing required.
    - No remeshing required.
- Disadvantage:
  - Requires more refined (2D quadrilateral or 3D hexahedral) and higher-quality mesh than standard FEA models.

Built-in Abaqus XFEM Implementation

- Advantage:
  - Built-in into general commercial FEA package with all necessary pre- and post-processing capabilities.
- Disadvantages:
  - Extremely fine and high-quality mesh is required.
    - Abaqus does not allow one to put a crack front right at the interface of an element – the crack front must cut through the enriched elements and the calculations are performed based on the nodal values of those cut elements. The finer the mesh, the less variations among those nodal values and hence, better consistency at the crack front.
    - In the case of unstructured or relatively coarse meshes, it becomes extremely challenging to maintain a smooth, continuous three-dimensional crack front during nonplanar crack propagation with the Abaqus XFEM method. New in Abaqus 2020, improvements are made to utilize the nonlocal stress/strain fields ahead of the crack tip to improve the computed crack propagation direction. The effectiveness of this improvement will need to be investigated.
  - Subcritical (fatigue and environment) crack growth relations are typically provided in terms of the stress intensity factor, *K*. However, Abaqus provides the relationship strictly in terms of the strain energy release rate, *G*. As a result, an Excel-based tool will be developed to convert between these parameters and as well as for common unit conversions.

XFEM requires special coding into each finite element solver separately. In addition to Abaqus (/Standard solver with /CAE pre- and post-processing), XFEM has also been coded as a core implementation in such DOE-sponsored research codes such as INL's Grizzly and commercial finite element software codes as Ansys and VirFac Crack/Morfeo. Implementation details will

likely vary within and between each code. As an example for the former, Ansys offers both ‘phantom node’ vs “singularity-based’ XFEM methods for stationary crack evaluation. For the latter, Abaqus supports distributed pressure on the crack face while Ansys does not support this option.

To provide additional capability for both research and commercial usage, user element and associated subroutines have been coded to further develop capabilities in the basic XFEM methods, level sets and discontinuity abstractions. This work has been primarily performed in Abaqus but other codes have similar capabilities for method development and structural evaluations.

As another approach, ‘Morfeo/Crack for Abaqus’ utilizes the built-in XFEM capability in Abaqus/Standard along with the user interface of Abaqus/CAE. After initial model setup in Abaqus/CAE, this method is based on calling Abaqus/Standard at each propagation step. Between each step, it reads the Abaqus solution, recovers an XFEM solution, accurately computes the stationary-crack stress intensity factors which determine the crack advance and updates the Abaqus input file with the new crack position.

Regardless of final implementation chosen, significant benchmarking of results for a given problem class is recommended. With that stated, general modeling recommendations associated with the built-in Abaqus XFEM implementation should serve as a reasonable starting point.

Based on the available literature studied, XFEM is capable of accurately predicting stress intensity factors and calculating crack extension rates for simple handbook geometries. To address the capabilities for more complex geometries, a systematic approach as outlined in the next section should be undertaken to ensure that this capability is reliable and allow analyses to be completed in a more efficient manner.

6 RECOMMENDATIONS FOR TASK 2 (SENSITIVITY STUDIES)

With the right choice of mesh and analysis parameters, XFEM is capable of simulating critical and sub-critical crack growth in complex systems, with results that closely match classic numerical and experimental results, including PWSCC behavior. Using capabilities already integrated into Abaqus 2020, a method to model PWSCC crack growth using XFEM techniques is being developed [37]. This method shows that reasonable stress intensity factors and crack growth rates for both applied load and residual stress configurations, using subcritical and noncyclic driving forces, are possible. Further, the mesh (mesh density, mesh distortion and usage of tie constraints for mesh coarsening transition) and model control parameters will aid in more complex assessments. For this first work, PWSCC of Alloy 182 SMA weld material has been modeled in a compact tension specimen [38]. All crack extension should be planar.

Next a modified compact tension (CT) specimen that contains an additional hole in the standard CT specimen will be considered. The presence of the additional hole will perturb the crack path, resulting in a curvilinear crack growth. This referenced work ([16] and [39]) also includes experimental work which adds additional credibility to the problem. Additionally, XFEM modelers [40] have studied this problem and provided modeling parameters using their Abaqus XFEM implementation.

The last sensitivity model should include a model that has previously been solved with other techniques such that direct comparisons of preparation and computational resource requirements can be made. This can be achieved by performing a built-in Abaqus XFEM crack growth solution along with a previous AFEA evaluation. The V.C. Summer hot leg dissimilar metal v-groove weld axial crack evaluation documented in [41] or an axial flaw in a hillside CRDM nozzle ([42] and [43]) would provide valuable insight into these questions.

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