An Adaptive Multiscale Finite Element Method for Large Scale Simulations

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Final Report

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AN ADAPTIVE MULTISCALE GENERALIZED FINITE ELEMENT METHOD FOR
LARGE SCALE SIMULATIONS

FA9550-12-1-0379

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Abstract

Hypersonic vehicles are subjected to extreme acoustic, thermal and mechanical loading with strong spatial and temporal gradients and for extended periods of time. Long duration, 3-D simulations of non-linear response of these vehicles, is prohibitively expensive using available Finite Element Methods and algorithms. This report presents recent advances of a Generalized Finite Element Method (GFEM) for multiscale non-linear simulations. This method is able to handle complex non-linear problems such as those exhibiting softening in the load-displacement curve. Cohesive fracture models lead to this class of non-linear behavior, which are significantly more computationally expensive than in the case of linear elastic fracture mechanics. In this novel GFEM, scale-bridging enrichment functions are updated on the fly during the non-linear iterative solution process. Non-linear fine-scale solutions are embedded in the global scale using the partition of unity framework of the Generalized FEM. Damage information computed at fine-scale problems are also used at the coarse scale in order to avoid costly non-linear iterations at the global scale. This method enables high-fidelity non-linear simulation of representative aircraft panels using finite element meshes that are orders of magnitude coarser than those required by available finite element methods.

We also report on a technique to perform a near-orthogonalization of scale-bridging enrichments used in the multiscale GFEM. We show that, for any discretization error level, it leads to systems of equations that are orders of magnitude better conditioned than in available GFEMs. This so-called Stable Generalized FEM (SGFEM) requires minimal modifications of existing GFEM software and leads to optimal convergence rates, regardless of the presence of singular solutions due to cracks. We also show that the error within enrichment zones in the SGFEM is lower than in the GFEM. This is important for fracture mechanics problems since parameters such as stress intensity factors are extracted within these zones.
Generalized Finite Element Approximations

Generalized FEM approximation spaces (i.e., trial and test spaces) consist of three components – (a) patches or clouds, (b) a partition of unity, and (c) the patch or cloud approximation spaces. The main ideas of the GFEM are summarized in this section.

Consider the usual finite element partitioning $\Omega^h$ of a given domain $\Omega$, in which $\Omega^h$ is the union of individual finite elements $\Omega^e$, $e = 1, \ldots, \text{nel}$. The basic idea behind the GFEM is to hierarchically enrich a low-order standard FEM approximation space, $S_{FEM}$, with special functions tailored for the physics of the problem at hand. These functions belong to a space $S_{ENR}$ defined using the partition of unity property of Lagrangian finite element shape functions, i.e.,

$$\sum_{\alpha \in J^h} N^\alpha = 1,$$

where $\alpha, \alpha \in J^h = \{1, \ldots, n_G\}$, is the index of a node in a finite element mesh with $n_G$ nodes. Linear FEM shape functions are adopted in this work.

The test and trial GFEM space $S_{GFEM}$ are given by

$$S_{GFEM} = S_{FEM} + S_{ENR}$$

where

$$S_{FEM} = \sum_{\alpha \in J^h} N^\alpha d^\alpha \quad \text{and} \quad S_{ENR} = \sum_{\alpha \in J^h_{enr}} N^\alpha \chi_\alpha, \quad \chi_\alpha = \sum_{i} L^{\alpha i} d^{\alpha i}, \quad d^\alpha, d^{\alpha i} \in \mathbb{R}^3$$

Here, $i, i = 1, \ldots, n^\alpha_{enr}$, denotes the index of the enrichment function $L^{\alpha i}$ at node $\alpha$ and $n^\alpha_{enr}$ is the number of enrichments at node $\alpha$. Enrichments $L^{\alpha i}$, $i = 1, \ldots, n^\alpha_{enr}$, form a basis of the patch or cloud space $\chi_\alpha(\omega_\alpha)$ with $\omega_\alpha$ being the support of the FEM shape function $N^\alpha$.

The set $J^h_{enr} \subset J^h$ has the indexes of the nodes with enrichment functions. It is noted that each patch (node) may adopt a different basis, depending on the behavior of the solution of the problem over the node support.

Based on the above definitions, a GFEM shape function at a node $\alpha \in J^h_{enr}$ is given by

$$\phi^{\alpha i}(x) = N^{\alpha}(x)L^{\alpha i}(x) \quad \text{(no summation on } \alpha).$$

The definition of shape functions as described above provides great flexibility since enrichment functions are not limited to polynomials as in the standard FEM. For example, in the case of cohesive fracture problems considered in this study, Heaviside functions are adopted to represent discontinuities arbitrarily located in a finite element mesh. Furthermore, enrichment functions for multiscale and non-linear problems can be computed numerically as described next.
Bridging Scales with the Generalized Finite Element Method

The Generalized Finite Element Method with global-local enrichments (GFEM\textsuperscript{gl}) combines ideas from the classical global-local finite element method with the Generalized FEM described in the previous section. In contrast to available Generalized or eXtended FEMs, which use analytical enrichment functions, this method provides a framework that allows the enrichment of the GFEM solution space with functions obtained from the solution of local boundary value problems. The boundary conditions for local problems are obtained from the solution of the global problem discretized with a coarse finite element mesh. The local problems can be accurately solved using an adaptive GFEM, and therefore the GFEM\textsuperscript{gl} can be applied to problems with limited \textit{a priori} knowledge about the solution like those involving 3-D complex fractures, multiscale or non-linear phenomena. In this method, the patch or cloud approximation spaces are built with the aid of local boundary value problems defined in a neighborhood $\Omega_L$ of a crack or other local feature of interest. Global-local enrichment functions can be built for many classes of problems. Here we report on a three-dimensional formulation developed for propagating non-linear cohesive fractures. Further details can be found in [12, 14]. It is noted that the GFEM developed in project FA9550-09-1-0401 assumed linear behavior for propagating fractures or non-linear but stationary fractures. In contrast, the GFEM described here can handle the case of propagating non-linear fractures with load-displacement curves exhibiting softening. This creates several challenges for a multiscale method since it requires algorithms able to deal with load-dependent discretization spaces while avoiding mapping of solutions between spaces.

Model boundary value problem

Let a domain $\Omega_G$ with discontinuity surfaces $\Gamma^\text{coh}$ be occupied by a body to be open, and bounded by a smooth boundary $\Gamma_G$ that involves $\Gamma^u_G$ and $\Gamma^t_G$ for prescribed displacement $\bar{u}$ and traction $\bar{t}$, respectively. Figure

The body can be characterized by a single variable, the displacement field $u_G: \Omega_G \rightarrow \mathbb{R}^{n_{\text{dim}}}$ (with $n_{\text{dim}} = 3$ for three dimensions) which weakly satisfies equilibrium in a Hilbert space $H^1$ as

$$
\int_{\Omega_G} \nabla^s (\delta u_G) : \sigma (u_G) \, \mathrm{d}V + \int_{\Gamma^\text{coh}} \delta [u_G] \cdot t_{\text{coh}} ([u_G]) \, \mathrm{d}S + \eta \int_{\Gamma^t_G} \delta u_G \cdot u_G \, \mathrm{d}S
= \int_{\Omega_G} \delta u_G \cdot b \, \mathrm{d}V + \int_{\Gamma^u_G} \delta u_G \cdot \bar{u} \, \mathrm{d}S + \eta \int_{\Gamma^t_G} \delta u_G \cdot \bar{t} \, \mathrm{d}S
$$

for all $\delta u_G \in H^1$. Here, we use notations $\sigma$ for the Cauchy stress tensor, $b$ for the volumetric body force, $\eta$ for the penalty parameter, and $[u_G]$ for the jump of displacement on $\Gamma^\text{coh}$, respectively.

The constitutive relation between the cohesive traction, $t_{\text{coh}}$, and the displacement jump, $[u_G]$, is in general highly non-linear. Global-local enrichments able to approximate this behavior are presented next.
Global boundary value problem

Local boundary value problem

Figure 1: GFEM\textsuperscript{pl} framework for two-scale simulations of propagating cohesive fractures. Numerically computed solutions of the extracted local boundary value problem are used to enrich global shape functions while solutions of the original global boundary value problem provide boundary conditions for the local problem, thus defining two interdependent problems at different scales.

Fine-scale non-linear local problem

Let \( u^{k-1}_G \in S^{k-1}_G(\Omega_G) \) be a GFEM approximation of the solution \( u_G \) of Problem (5) at the \((k-1)\)th load/displacement step. Hereafter a load and/or displacement step is denoted simply by load step. The definitions of a global problem to compute \( u^{k-1}_G \) and the solution space \( S^{k-1}_G \) are provided later. Global-local enrichments are used in the definition of \( S^{k-1}_G \). These functions are the solution of non-linear local problems as described next.

Let a sub-domain \( \Omega_L \subset \Omega_G \) containing, for simplicity, the entire pre-defined crack path as illustrated in Figure 1. Prescribed displacements \( \vec{u}^k \) and tractions \( \vec{t}^k \) at the \( k \)th solution step are prescribed on \( \Gamma_L \cap \Gamma^u_G \) and \( \Gamma_L \cap \Gamma^t_G \), respectively, where \( \Gamma_L \) denotes the boundary of \( \Omega_L \). The boundary conditions prescribed on \( \Gamma_L \setminus (\Gamma_L \cap (\Gamma^u_G \cup \Gamma^t_G)) \) are provided by an estimate, \( u^{k,0}_G \), of the global solution at the \( k \)th load step and defined as

\[
  u^{k,0}_G := \frac{k}{k-1} u^{k-1}_G. \tag{6}
\]

Solution \( u^{k,0}_G \) is used as boundary conditions on the portion of \( \Gamma_L \) that does not intersect with the boundary of the global domain \( \Omega_G \). This is a key aspect of the method.

Using the above definitions, the weak statement of the non-linear local problem at the \( k \)th
load step reads: Find \( \boldsymbol{u}_L^k \in \mathcal{S}_L^k(\Omega_L) \subset H^1(\Omega_L) \) such that for all \( \delta \boldsymbol{u}_L^k \in \mathcal{S}_L^k(\Omega_L) \),

\[
\int_{\Omega_L} \nabla^k (\delta \boldsymbol{u}_L^k) : \sigma(\boldsymbol{u}_L^k) \, dV + \int_{\Gamma_{coh}} \delta \cdot \Gamma_{coh}(\delta \mathbb{U}_L^k) \cdot \mathbb{T}_{coh}(\mathbb{U}_L^k) \, dS + \eta \int_{\Gamma_L \cap \Gamma_G^a} \delta \boldsymbol{u}_L^k \cdot \mathbb{U}_L^k \, dS
+ \kappa \int_{\Gamma_L \setminus (\Gamma_L \cap \Gamma_G^u \cup \Gamma_G^t)} \delta \boldsymbol{u}_L^k \cdot \mathbb{U}_L^k \, dS = \int_{\Omega_L} \delta \boldsymbol{u}_L^k \cdot \mathbb{b} \, dV + \int_{\Gamma_L \cap \Gamma_G^a} \delta \boldsymbol{u}_L^k \cdot \mathbb{t} \, dS
+ \eta \int_{\Gamma_L \cap \Gamma_G^a} \delta \boldsymbol{u}_L^k \cdot \mathbb{U}_L^k \, dS + \kappa \int_{\Gamma_L \setminus (\Gamma_L \cap \Gamma_G^u \cup \Gamma_G^t)} \delta \boldsymbol{u}_L^k \cdot [\mathbb{t}(\mathbb{U}_G^k, 0) + \kappa \mathbb{U}_G^k, 0] \, dS
\] (7)

for the penalty parameter \( \eta \) and the spring constant \( \kappa \) defined on \( \Gamma_L \cap \Gamma_G^a \) and \( \Gamma_L \setminus (\Gamma_L \cap (\Gamma_G^u \cup \Gamma_G^t)) \), respectively. The local solution space \( \mathcal{S}_L^k(\Omega_L) \) is defined using the standard GFEM shape functions. Much finer meshes are typically used at local than in the global problem as illustrated in Figure 2. This figures shows the application of the GFEM\(_{gl}\) to a three-point bending test. This problem was used in [12] to validate the proposed multiscale method.

Figure 2: Model problem used to illustrate the non-linear GFEM\(_{gl}\). The solution computed on the coarse global mesh provides boundary conditions for the extracted local domain in a neighborhood of non-linear cohesive fracture. A fine mesh is required to resolve fine-scale features in the local problem, whereas a coarse mesh is used to capture smooth structural behavior in the global problem. Red spheres denote nodes enriched by local solutions in the global mesh and nodes enriched by Heaviside functions in the local mesh, respectively. It is noted that the local mesh does not match the global one at the local domain boundary.

Global-Local Enrichment Functions for Cohesive Fractures

The local solution \( \boldsymbol{u}_L^k \) defined in the previous section is used to build the following GFEM shape function for the approximation of global solution \( \boldsymbol{u}_G \) of Problem (5)

\[
\phi_{\alpha, k} = N_{\alpha}^k \boldsymbol{u}_L^k,
\] (8)
where the partition of unity function, \( N^\alpha \), is provided by a coarse global FE mesh for \( \Omega_G \) and \( u^k_L \) has the role of an enrichment or basis function for the patch space \( \chi_\alpha(\omega_\alpha) \). Hereafter, \( u^k_L \) is denoted a global-local enrichment function at the \( k^{th} \) load step. The corresponding global GFEM space is given by hierarchically augmenting the standard FEM solution space \( S_{FEM}^k \) with an enrichment space \( S_{ENR}^k \) containing shape function \( \phi^\alpha_k \), i.e.,

\[
S_G^k = S_{FEM} + S_{ENR}^k = S_{FEM} + \{ N^\alpha u^{gL,k}_\alpha \text{ (no summation on } \alpha), \alpha \in J^{gl} \}
\]

where \( J^{gl} \) has the indexes of nodes (patches) enriched with global-local functions. A node \( \alpha \) can belong to set \( J^{gl} \) only if \( \omega_\alpha \subset \Omega_L \). Vector \( u^{gL,k}_\alpha \) belongs to \( \chi_\alpha(\omega_\alpha) \) and is given by

\[
u^{gL,k}_\alpha = \begin{cases} u^k_L <u> \\ v^k_L <v> \\ w^k_L <w> \end{cases}
\]

where \( u^k_L <u> \), \( v^k_L <v> \), \( w^k_L <w> \) are the components of the local solution \( u^k_L \) vector in the global Cartesian coordinate directions and \( u^k_L, v^k_L, w^k_L \in \mathbb{R} \) are global degrees of freedom. Equation (10) implies that G-L enrichments lead to only three additional DOFs per global node, regardless of the size of the local problem used in the computation of \( u^k_L \).

The global GFEM space \( S_G^k \) defined above can be used to discretize the non-linear global problem (5) and find a global approximation \( u^G_k \in S_G^k(\Omega_G) \) at the \( k^{th} \) load step. The methodology is illustrated in Figure 2. The global solution provides boundary conditions for fine-scale problems while their solutions are used as enrichment functions for the coarse-scale problem through the partition of unity framework of the GFEM. Figure 3 shows the load-displacement curves computed with the GFEM\(^{gl} \) and reference numerical and experimental data [12]. It is noted that the GFEM\(^{gl} \) model has about 10 times fewer degrees of freedom than in the case of available adaptive methods.

It is noted that the solution space \( S_G^k \) is adaptive: It changes at every load step in order to approximate the non-linear response of the problem while keeping the global mesh unchanged. This change must be properly handled when solving the non-linear equations using, for example, Newton-Rhapson algorithms. In particular, the vector with global DOFs \( d_G^{k-1} \) computed at the previous load step is not a robust choice for the initialization of the Newton-Rhapson non-linear iterations at load step \( k \): The global vectors \( d_G^{k} \) and \( d_G^{k-1} \) represent coefficients of different sets of GFEM shape functions. Even though the global GFEM mesh does not change, the solution space does. An efficient and robust algorithm to deal with this issue is presented in [12]. It is based on the solution of a linear problem using a secant material stiffness instead of the tangent stiffness. Further details can be found in [12, 14].
**Stable Generalized Finite Element Method**

In this section, we report on a technique to perform a near-orthogonalization of enrichments used in the Generalized FEM. The technique involves modifications to enrichments for the *GFEM* in order to create functions that are near orthogonal to the finite element partition of unity. This so-called Stable *GFEM* (*SGFEM*) was originally proposed by Babuška and Banerjee [BB12]. They have shown that the conditioning of the *SGFEM* is not worse than that of the standard FEM. In this project, extensions of the *SGFEM* to three-dimensional fracture problems were developed in collaboration with Prof. Ivo Babuška from University of Texas at Austin and Prof. Uday Banerjee from Syracuse University. This collaboration is at no cost to the AFOSR. A summary of the method is presented below. Details on this 3-D *SGFEM* are described in [10, 8].

In the *SGFEM*, the enrichment functions employed in *GFEM* are locally modified to construct the patch approximation spaces \( \tilde{\chi}_\alpha \), \( \alpha \in J^h_{\text{enr}} \). The modified *SGFEM* enrichment functions \( \tilde{L}^{\alpha_i}(x) \in \tilde{\chi}_\alpha(\omega_\alpha) \) are given by

\[
\tilde{L}^{\alpha_i}(x) = L^{\alpha_i}(x) - I_{\omega_\alpha}(L^{\alpha_i})(x) \quad \text{and} \quad \tilde{\chi}_\alpha = \text{span}\{\tilde{L}^{\alpha_i}\}_{i=1}^{n^\alpha}
\]

where \( I_{\omega_\alpha}(L^{\alpha_i}) \) is the piecewise tri-linear finite element interpolant of the enrichment function \( L^{\alpha_i} \) on the patch \( \omega_\alpha \). The interpolant \( I_{\omega_\alpha}(L^{\alpha_i})(\xi) \) at master coordinate \( \xi \) of a finite element \( \tau \) with nodes \( \mathcal{J}(\tau) \) and belonging to patch \( \omega_\alpha \) is given by

\[
I_{\omega_\alpha}(L^{\alpha_i})(\xi) = \sum_{\beta \in \mathcal{J}(\tau)} L^{\alpha_i}(x_\beta) N^{\beta}(\xi)
\]
where vector $\mathbf{x}_\beta$ has the coordinates of node $\beta$ of element $\tau$ and $N^\beta$ is the piecewise trilinear FE shape function for node $\beta$. Further details can be found in [10]. The global enrichment space associated with $\tilde{Z}_\alpha$ is denoted by $\tilde{S}_{ENR}$. Therefore, the $SGFEM$ trial space $S_{SGFEM}$ is given by

$$S_{SGFEM} = S_{FEM} + \tilde{S}_{ENR}. \quad (13)$$

The $SGFEM$ shape functions $\tilde{\phi}^{\alpha i}(x)$ belonging to $\tilde{S}_{ENR}$ are constructed using the same framework as in the $GFEM$ and are given by

$$\tilde{\phi}^{\alpha i}(x) = N^\alpha(x) \tilde{L}^{\alpha i}(x). \quad (14)$$

Figure 4 illustrates the computation of $SGFEM$ enrichment functions and shape functions in $S_{ENR}$ in a 2-D setting.

**Figure 4:** Figure illustrating the computation of an $SGFEM$ enrichment function in 2-D. The picture on the left shows the construction of a $GFEM$ shape function. The center picture features the original enrichment function, $L^{\alpha i}$, at the top, the piecewise bi-linear finite element interpolant of which is in the middle, $I_{0\alpha i}(L^{\alpha i})$, and the modified $SGFEM$ enrichment function, $\tilde{L}^{\alpha i}$, is shown at the bottom. The picture on the right shows the construction of an $SGFEM$ shape function, $\tilde{\phi}^{\alpha i}$.

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**References**


**Publications and Presentations**


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**AFRL Collaborator**

Dr. Thomas Eason, AFRL, Air Vehicles Directorate, WPAFB, OH, Phone 937-255-3240, e-mail thomas.eason.3@us.af.mil

**Transitions**

The multiscale Generalized FEM and Stable GFEM developed and analyzed in this project are implemented in *ISET*—a GFEM research software developed by the PI at the University of Illinois at Urbana-Champaign. *ISET* is currently used by researchers at AFRL Structural
Sciences Center (SSC) for the modeling of vibratory damage with reduced-order models and the GFEM as reported in [OH14, ODE15].

**Impact in the Research Community**

The research results of this project have attracted considerable attention from the computational mathematics and mechanics research community. An evidence of this impact is the various keynote lectures at international conferences and invited research lectures at prestigious universities delivered by the PI.
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Carlos Armando Duarte

Program Manager
The AFOSR Program Manager currently assigned to the award
Dr. Jean-Luc Cambier

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**Archival Publications (published) during reporting period:**


elastic fracture mechanics using the stable generalized finite element method. Computational Mechanics, 2015. Accepted for publication.

**Changes in research objectives (if any):**

**Change in AFOSR Program Manager, if any:**

The Program Officer at the start of this project was Dr. Fariba Fahroo. The current Program Officer of the Computational Mathematics Program is Dr. Jean-Luc Cambier.

**Extensions granted or milestones slipped, if any:**

**AFOSR LRIR Number**

**LRIR Title**

**Reporting Period**

**Laboratory Task Manager**

**Program Officer**

**Research Objectives**

**Technical Summary**

**Funding Summary by Cost Category (by FY, $k)**

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**Appendix Documents**

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