Finite Elements in Analysis and Design 125 (2017) 24–40

Contents lists available at ScienceDirect

Finite Elements in Analysis and Design

journal homepage: www.elsevier.com/locate/finel

Conforming to interface structured adaptive mesh refinement: New technique for the automated modeling of materials with complex microstructures

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ARTICLE INFO

Keywords:
CISAMR
FEM
Mesh generation
Adaptive refinement
Material interface
Complex microstructure

ABSTRACT

This manuscript introduces a new method named Conforming to Interface Structured Adaptive Mesh Refinement (CISAMR) for the automated finite element modeling of problems with complex morphologies. The CISAMR transforms a simple structured mesh of quadrilateral elements into a conforming hybrid mesh composed of quadrilateral and triangular elements with low aspect ratios using a non-iterative algorithm. The automated construction of the mesh begins with implementing a customized Structured Adaptive Mesh Refinement (SAMR) algorithm to achieve the desired element size along materials interfaces. A new *r*-adaptivity algorithm is then employed to move selected nodes of nonconforming elements to intersection points of their edges with the interface, followed by the diagonal sub-triangulation of all elements deformed during this process into conforming sub-triangles. CISAMR does not require relocating the nodes of the background mesh or creating any new node away from materials interfaces after the completion of the SAMR phase. Further, this method can easily handle special cases such as intersecting boundaries/interfaces, while ensuring that aspect ratios of resulting sub-elements are lower than three. A comprehensive discussion is provided on different aspects of the implementation of CISAMR, followed by several example problems to show its application for modeling materials with complex microstructures.

1. Introduction

The finite element method (FEM) is one of the most popular numerical techniques for simulating a wide range of problems in physics and engineering. However, creating appropriate conforming finite element (FE) meshes has been a long-standing challenge for modeling problems with complex morphologies. Significant research has been carried out to develop robust algorithms for generating conforming meshes with proper element aspect ratios [1–3]. Amongst methods used in this field we can mention the Delaunay triangulation algorithms [4], advancing front [5], and Quadtree/Octree based techniques [6–8].

The Delaunay triangulation method aims at satisfying the criterion that no mesh node must be placed inside the circumcircle of a triangle, or the circumsphere of a tetrahedron [4]. Hence, the location of each node in a Delaunay mesh depends on locations of all its neighboring nodes, resulting in a non-linear system of equations that must be solved iteratively; thereby making this technique computationally expensive for discretizing large-scale problems. Advancing front techniques have been developed to facilitate progressive refinement around points, surfaces, and sharp corners [9,10,5]. In this method, new triangular/tetrahedral elements are created in an active front emanating from specified regions in the domain, which are progressively advanced to discretize the entire domain.

Quadtree/octree based approaches recursively subdivide quadrilateral and hexahedral background elements to reach a desirable level of refinement [11,6–8]. Grid points are then relocated to the interface to create a conforming mesh comprising heavily distorted elements. The element aspect ratios are improved through subsequent iterative mesh smoothing. Yerry et al. [11] employed a Laplacian smoothing technique, which relocates interior mesh nodes to the average coordinates of all its neighboring nodes, by iteratively solving a non-linear system of equations. An optimization based boundary smoothing was introduced by Baehmann et al. [7] to enable a better representation of boundaries and interfaces. Although more computationally expensive, this optimization based smoothing scheme requires less iterations for the con-

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http://dx.doi.org/10.1016/j.finel.2016.11.003
Received 19 August 2016; Received in revised form 18 October 2016; Accepted 15 November 2016

struction of a high quality conforming mesh.

Octree-based techniques have been implemented in conjunction with iso-contouring for modeling materials with multiple interfaces [12–14]. The Marching Cubes algorithm visits each hexahedral cell and performs triangulation based on sign configurations of its vertices [12], but has limitations that could lead to the creation of elements with bad aspect ratios or inaccurate representation of sharp corners of the interface. The Dual Contouring method, which performs the sub-triangulation using special minimizer points, can be employed to address these limitations [13,14]. Liang et al. [14] combined the Octree method with Dual Contouring to generate high quality triangular and tetrahedral meshes. Zhang et al. [13,15] have used a similar approach to obtain triangular, quadrilateral, tetrahedral, and hexahedral meshes for problems involving two or more materials interfaces. However, implementing this method could be computationally demanding, as it requires locating normal vectors to materials interfaces and performing several calculations to locate minimizer points. Further, subsequent mesh smoothing might be inevitable to obtain elements with acceptable aspect ratios [15].

Despite the development of such sophisticated mesh generation algorithms, the complexity and labor cost associated with creating conforming meshes are still major barriers toward modeling problems with complex morphologies. This challenge is further magnified in problems such as design optimization [16] and uncertainty quantification [17], which require the construction of multiple FE models throughout the simulation. The implementation of techniques such as the *hp*-adaptive refinement [18–20] and the Arbitrary Eulerian–Lagrangian (ALE) [21,22] could alleviate the labor cost and computational burden associated with the mesh generation process. However, maintaining elements with proper shapes and good aspect ratios, while minimizing the geometric discretization error, remain to be challenging tasks in such methods.

To obviate the difficulties associated with the construction of conforming meshes in the standard FEM, one can implement alternative numerical techniques such as the Boundary Element Method (BEM) [23,24] and Meshfree Methods (MMs) [25–28]. Despite successful application to simulate certain problems, at lower computational cost and higher accuracy compared to FE analyses in some cases, such methods lack the flexibility of the FEM for the treatment of a wide range of governing equations. For example, the application of the BEM is limited to problems for which Green's functions can be evaluated analytically [29].

FE-based methods such as CutFEM [30], eXtended/Generalized FEM (X/GFEM) [31–34], Interface-enriched Generalized FEM (IGFEM) [35,36], and Hierarchical Interface-enriched FEM (HIFEM) [37,38] have also been introduced, which eliminate the requirement for using meshes that conform to the problem geometry. This is often achieved by using appropriate enrichment functions for approximating the field in nonconforming elements to capture weak (gradient) discontinuities along materials interfaces. Although such methods are often categorized as mesh-independent techniques, it is often necessary to subdivide the elements cut by materials interfaces into smaller conforming sub-elements for numerical quadrature and/or evaluating the enrichment functions [39,36]. Further, additional treatments are often necessary to avoid the construction of stiffness matrices with high condition numbers, and for accurate approximation of the gradient (e.g., stress concentrations) along the interface [40,41,37]. The Conformal Decomposition FEM (CDFEM) [42,43] also subdivides the elements cut by the interface into smaller conforming sub-elements, although unlike X/GFEM does not use enrichment functions to capture weak discontinuities. Instead, it replaces the nonconforming background elements with the resulting conforming sub-elements and approximates the field using the standard FEM. However, the arbitrary aspect ratios of such elements could lead to significant errors in approximating local phenomena governed by the gradient field, such as the stress and damage initiation, as well as resulting in a high condition number for the stiffness matrix.

In this manuscript, we introduce a Conforming to Interface Structured Adaptive Mesh Refinement (CISAMR) technique for the automated modeling of problems with complex morphologies. CISAMR transforms a structured mesh into a high quality conforming mesh composed of quadrilateral and triangular elements with low aspect ratios. What distinguishes this technique from existing methods in the literature is the ability to control the aspect ratios of resulting elements for all possible case scenarios, including materials interfaces that are in close proximity, intersecting with one another, or located in the vicinity of the domain boundaries using a non-iterative algorithm. To achieve this, CISAMR integrates customized versions of three techniques, namely the Structured Adaptive Mesh Refinement (SAMR) [44–46] of the background mesh, *r*-adaptivity [47] of the nodes of elements cut by materials interfaces, and sub-triangulation of these elements to create an appropriate conforming mesh.

While the computational cost associated with creating a conforming mesh in CISAMR is comparable to the process of creating integration (children) sub-elements in enriched FE-based methods, CISAMR ensures that aspect ratios of these children elements are lower than three. Thus, a high quality conforming mesh is generated without the need for an iterative smoothing process, which is used in several of mesh generation algorithms [6–8,15]. Further, CISAMR does not relocate the nodes of the background mesh away from materials interface; thereby preserves the main structure of this grid. This enables handling multiple non-intersecting and even intersecting materials interfaces using a non-iterative algorithm. Moreover, although not addressed in the numerical examples presented in this work, CISAMR highly facilitates the simulation of moving boundary problems, as the background mesh is modified locally to adapt to the interface/boundary morphology. Therefore, similar to X/GFEM [48,49], mapping the solution using an L_2-projection scheme between the current and updated meshes is limited to the elements cut by the interface. This feature not only reduces the computational cost but also improves the accuracy by mapping super-convergent nodal values of the solution for majority of the nodes. It must be noted that although the focus of this article is on introducing the CISAMR algorithm for modeling 2D problems, there is no inherent limitation for expanding this method to 3D. However, the computational geometry aspects involved in the implementation of 3D CISAMR, including compatibility of sub-element surfaces, are out of the scope of the current manuscript.

The remainder of this article is structured as follows: In Section 2 we present the governing equations for simulating linear elasticity and continuum damage problems. The CISAMR algorithm is introduced in Section 3, followed by discussing required considerations for the treatment of special cases such as intersecting materials interfaces in Section 4. Different algorithmic aspects of the CISAMR implementation, together with a detailed comparison with other mesh generation algorithms and mesh-independent methods such as IGFEM and X/GFEM are provided in Section 5. Four numerical examples are provided in Section 6 to shed light on the accuracy and convergence of CISAMR and demonstrate its application for modeling materials with complex microstructures. Final concluding remarks are presented in Section 7.