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| 1. REPORT DATE (DD-MM-YYYY)<br>08-12-2021                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         |                   | 2. REPORT TYPE<br>Final Report |                                                       | 3. DATES COVERED (From - To)<br>13-Jul-2018 - 8-Jul-2021 |                                                       |
| 4. TITLE AND SUBTITLE<br>Final Report: The shifted interface method for solid mechanics:<br>An embedded domain approach                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           |                   |                                | 5a. CONTRACT NUMBER<br>W911NF-18-1-0308               |                                                          |                                                       |
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| 6. AUTHORS                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        |                   |                                | 5d. PROJECT NUMBER                                    |                                                          |                                                       |
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| 7. PERFORMING ORGANIZATION NAMES AND ADDRESSES<br>Duke University<br>C/O Office of Research Support<br>2200 W. Main St., Ste. 710<br>Durham, NC 27705 -4677                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |                   |                                | 8. PERFORMING ORGANIZATION REPORT NUMBER              |                                                          |                                                       |
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| 13. SUPPLEMENTARY NOTES<br>The views, opinions and/or findings contained in this report are those of the author(s) and should not be construed as an official Department of the Army position, policy or decision, unless so designated by other documentation.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   |                   |                                |                                                       |                                                          |                                                       |
| 14. ABSTRACT                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      |                   |                                |                                                       |                                                          |                                                       |
| 15. SUBJECT TERMS                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |                   |                                |                                                       |                                                          |                                                       |
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| a. REPORT<br>UU                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   | b. ABSTRACT<br>UU | c. THIS PAGE<br>UU             |                                                       |                                                          | 19b. TELEPHONE NUMBER<br>919-660-5075                 |

# RPPR Final Report

## as of 09-Dec-2021

Agency Code: 21XD

Proposal Number: 71733MA

Agreement Number: W911NF-18-1-0308

### INVESTIGATOR(S):

**Name:** Guglielmo Scovazzi  
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Country: USA

DUNS Number: 044387793

EIN: 560532129

**Report Date:** 08-Oct-2021

Date Received: 08-Dec-2021

**Final Report** for Period Beginning 13-Jul-2018 and Ending 08-Jul-2021

**Title:** The shifted interface method for solid mechanics: An embedded domain approach

**Begin Performance Period:** 13-Jul-2018

**End Performance Period:** 08-Jul-2021

**Report Term:** 0-Other

Submitted By: Guglielmo Scovazzi

Email: guglielmo.scovazzi@duke.edu

Phone: (919) 660-5075

**Distribution Statement:** 1-Approved for public release; distribution is unlimited.

**STEM Degrees:** 2

**STEM Participants:**

**Major Goals:** The major goal of this project is the development of an advanced immersed boundary method for solid mechanics, based on the Shifted Boundary Method. The key applications is the simulation of the very complex geometries that emerge from additive manufacturing/topology optimization tools, and/or imaging of rocks and related geologic formations of interest in some of the Army/ARO applied research directorates.

Historically, embedded domain discretizations have been confined to the realm of fluid mechanics applications. They have shown considerable impact, especially when the complex geometrical shapes pose severe challenges to conformal mesh generation. The imposition of boundary conditions is more challenging in the case of embedded/immersed methods than in the case of conformal method (i.e., methods in which the computational grid conforms to the domain boundary).

In recent work, the PI and his research group have developed a new embedded finite element method, named Shifted Boundary Method (or SB method). This new approach overcomes the difficulty on matrix conditioning and algorithmic stability that the occurrence of small cut cells produced in standard embedded methods. This without creating complicated data structures and limiting in general computational complexity to a minimum. The key feature of the SB method is the idea of shifting the location where boundary conditions are applied from the true to the surrogate boundary, and to appropriately modify the shifted boundary conditions, enforced weakly, in order to preserve optimal convergence rates of the numerical solution. This process yields a method that is simple, robust, and efficient. Previously, the PI's research team successfully applied the SB method to the Poisson, Stokes, linear advection-diffusion, and Navier-Stokes equations. In the case of Poisson and linear advection-diffusion equations, proofs of stability and convergence were also derived. Typically, embedded methods are of finite volume type if fluid problems are the target.

Although one would expect that embedded finite element methods could naturally apply to solid mechanics calculations, the existing literature is scarce if non-existing on the subject. From a certain perspective, it may seem strange, at first sight, to consider an embedded method for solid mechanics, but there can be many benefits. If we look at modern manufacturing techniques, like additive manufacturing (e.g., 3D-printing and related techniques), the geometric complexity of the final shapes is considerably higher than in more standard forging, milling, drilling processes. This geometric complexity is intrinsic in additive manufacturing processes, in which materials are added layer upon layer rather than removed from a bulk block with very specific tools. As a consequence, existing mesh generators may be severely challenged. Additionally, if one would like to simulate the actual process of manufacturing, with the purpose of computing residual stresses and improving/optimizing the overall production cycle, then thermo-chemo- mechanical simulations of solid with advancing interfaces are required, a task for which

## RPPR Final Report as of 09-Dec-2021

embedded methods seem a natural choice.

All these challenges have been addressed in this project. The PI and his team at Duke University have successfully developed and implemented an immersed/embedded algorithm that effectively tackles all the above issues.

**Accomplishments:** The PI and his team accomplished most of the proposed tasks in this project. In particular:

1. It was developed a shifted boundary immersed algorithm for solid mechanics
2. The numerical analysis of stability and error convergence was developed
3. Very challenging three-dimensional test were successfully performed and documented, using geometry descriptions from CAD and reconstructions of geometry from images.
4. Preliminary results in nonlinear mechanics are under development
5. The method was extended to fracture mechanics, which is a development beyond the planned tasks, despite the original project plan was quite challenging. Preliminary results are included. The PI is grateful to all his domestic and international collaborators for that.

**Training Opportunities:** The funding helped training 2 Ph.D. students who graduated during the course of the project, and two more students that just started their graduate curriculum at Duke University.

**Results Dissemination:** The PI and his team published a total of 10 papers in top archival journals and 2 Ph.D. theses (see the products section of this report). Multiple presentations were given at national and international conferences and seminar series (about 20). The computational software developed in the PI's team is available to interested parties at ARO and ARL through the freeBSD license.

**Honors and Awards:** The PI was named Distinguished Lecturer at POSTECH (Pohang University of Science and Technology, South Korea).

**Protocol Activity Status:**

**Technology Transfer:** Nothing to Report

### PARTICIPANTS:

**Participant Type:** PD/PI

**Participant:** Guglielmo Scovazzi

**Person Months Worked:** 1.00

Project Contribution:

National Academy Member: N

**Funding Support:**

**Participant Type:** Postdoctoral (scholar, fellow or other postdoctoral position)

**Participant:** Nabil Atallah

**Person Months Worked:** 12.00

Project Contribution:

National Academy Member: N

**Funding Support:**

**Participant Type:** Graduate Student (research assistant)

**Participant:** Kangan Li

**Person Months Worked:** 12.00

Project Contribution:

National Academy Member: N

**Funding Support:**

**RPPR Final Report**  
as of 09-Dec-2021

**ARTICLES:**

**Publication Type:** Journal Article      Peer Reviewed: Y      **Publication Status:** 1-Published

**Journal:** Journal of Computational Physics

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Publication Identifier: 10.1016/j.jcp.2018.04.052

Volume: 369

Issue:

First Page #: 45

Date Submitted: 2/12/19 12:00AM

Date Published: 9/1/18 4:00AM

Publication Location:

**Article Title:** The shifted boundary method for hyperbolic systems: Embedded domain computations of linear waves and shallow water flows

**Authors:** T. Song, A. Main, G. Scovazzi, M. Ricchiuto

**Keywords:** Embedded boundary conditions Wave equation Shallow water flows Finite elements Approximate boundary methods

**Abstract:** We propose a new computational approach for embedded boundary simulations of hyperbolic systems and, in particular, the linear wave equations and the nonlinear shallow water equations. The proposed approach belongs to the class of surrogate/approximate boundary algorithms and is based on the idea of shifting the location where boundary conditions are applied from the true to a surrogate boundary. Accordingly, boundary conditions, enforced weakly, are appropriately modified to preserve optimal error convergence rates. This framework is applied here in the setting of a stabilized finite element method, even though other spatial discretization techniques could have been employed. Accuracy, stability and robustness of the proposed method are tested by means of an extensive set of computational experiments for the acoustic wave propagation equations and shallow water equations. Comparisons with standard weak boundary conditions imposed on body-fitted grids, which conform to the geometry of

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**Publication Type:** Journal Article      Peer Reviewed: Y      **Publication Status:** 1-Published

**Journal:** Computer Methods in Applied Mechanics and Engineering

Publication Identifier Type: DOI

Publication Identifier: 10.1016/j.cma.2018.12.040

Volume: 347

Issue:

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Date Submitted: 8/29/19 12:00AM

Date Published: 4/1/19 12:00AM

Publication Location:

**Article Title:** A reduced basis approach for PDEs on parametrized geometries based on the shifted boundary finite element method and application to a Stokes flow

**Authors:** Efthymios N. Karatzas, Giovanni Stabile, Leo Nouveau, Guglielmo Scovazzi, Gianluigi Rozza

**Keywords:** shifted boundary method, embedded finite element methods

**Abstract:** We propose a model order reduction technique integrating the Shifted Boundary Method (SBM) with a POD-Galerkin strategy. This approach allows to deal with complex parametrized domains in an efficient and straightforward way. The impact of the proposed approach is threefold. First, problems involving parametrizations of complex geometrical shapes and/or large domain deformations can be efficiently solved at full-order by means of the SBM. This unfitted boundary method permits to avoid remeshing and the tedious handling of cut cells by introducing an approximate surrogate boundary. Second, the computational effort is reduced by the development of a Reduced Order Model (ROM) technique based on a POD-Galerkin approach. Third, the SBM provides a smooth mapping from the true to the surrogate domain, and for this reason, the stability and performance of the reduced order basis are enhanced. This feature is the net result of the combination of the proposed ROM approach and the SBM. Similar

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**Journal:** Journal of Computational Physics

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Publication Identifier: 10.1016/j.jcp.2019.108898

Volume: 398

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Date Submitted: 10/8/20 12:00AM

Date Published: 8/1/19 8:00PM

Publication Location:

**Article Title:** High-order gradients with the shifted boundary method: An embedded enriched mixed formulation for elliptic PDEs

**Authors:** L. Nouveau, M. Ricchiuto, G. Scovazzi

**Keywords:** Darcy flow Embedded boundary Finite element method High-order approximation Stabilized methods Computational fluid dynamics

**Abstract:** We propose an extension of the embedded boundary method known as “shifted boundary method” to elliptic diffusion equations in mixed form (e.g., Darcy flow, heat diffusion problems with rough coefficients, etc.). Our aim is to obtain an improved formulation that, for linear finite elements, is at least second-order accurate for both flux and primary variable, when either Dirichlet or Neumann boundary conditions are applied. Following previous work of Nishikawa and Mazaheri in the context of residual distribution methods, we consider the mixed form of the diffusion equation (i.e., with Darcy-type operators), and introduce an enrichment of the primary variable. This enrichment is obtained exploiting the relation between the primary variable and the flux variable, which is explicitly available at nodes in the mixed formulation. The proposed enrichment mimics a formally quadratic pressure approximation, although only nodal unknowns are stored, similar to a linear finite element ...

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**Publication Type:** Journal Article      Peer Reviewed: Y      **Publication Status:** 1-Published

**Journal:** Computer Methods in Applied Mechanics and Engineering

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Volume: 370

Issue: 113273

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Date Published: 10/1/20 12:00PM

Publication Location:

**Article Title:** A Reduced-Order Shifted Boundary Method for Parametrized incompressible Navier-Stokes equations

**Authors:** Efthymios N. Karatzas, Giovanni Stabile, Leo Nouveau, Guglielmo Scovazzi, Gianluigi Rozza

**Keywords:** shifted boundary method, reduced order modeling, proper orthogonal decomposition

**Abstract:** We investigate a projection-based reduced-order model of the steady incompressible Navier-Stokes equations for moderate Reynolds numbers. In particular, we construct an “embedded” reduced basis space, by applying proper orthogonal decomposition to the Shifted Boundary Method, a high-fidelity embedded method recently developed. We focus on the geometrical parametrization through level-set geometries, using a fixed Cartesian background geometry and the associated mesh. This approach avoids both remeshing and the development of a reference domain formulation, as typically done in fitted mesh finite element formulations. Two-dimensional computational examples for one and three-parameter dimensions are presented to validate the convergence and the efficacy of the proposed approach.

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**Publication Type:** Journal Article      Peer Reviewed: Y      **Publication Status:** 1-Published

**Journal:** IUTAM Symposium on Model Order Reduction of Coupled Systems, Stuttgart, Germany, May 22–25, 2018 pp 111-125

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Date Published: 7/20/19 8:00AM

Publication Location:

**Article Title:** A Reduced Order Approach for the Embedded Shifted Boundary FEM and a Heat Exchange System on Parametrized Geometries

**Authors:** Efthymios N. Karatzas Giovanni Stabile Nabil Atallah Guglielmo Scovazzi Gianluigi Rozza

**Keywords:** Shifted boundary method, embedded methods, reduced order modeling

**Abstract:** A model order reduction technique is combined with an embedded boundary finite element method with a POD-Galerkin strategy. The proposed methodology is applied to parametrized heat transfer problems and we rely on a sufficiently refined shape-regular background mesh to account for parametrized geometries. In particular, the employed embedded boundary element method is the Shifted Boundary Method (SBM), recently proposed in Main and Scovazzi, J Comput Phys [17]. This approach is based on the idea of shifting the location of true boundary conditions to a surrogate boundary, with the goal of avoiding cut cells near the boundary of the computational domain. This combination of methodologies has multiple advantages. In the first place, since the Shifted Boundary Method always relies on the same background mesh, there is no need to update the discretized parametric domain. Secondly, we avoid the treatment of cut cell elements, which usually need particular attention. Thirdly, since the whole

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Publication Identifier: <https://doi.org/10.1002/nme.6231>

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Publication Location:

**Article Title:** The Shifted Interface Method; A Flexible Approach to Embedded Interface Computations

**Authors:** Kangan Li; Nabil M. Atallah; G. Alex Main

**Keywords:** Embedded interface, small cut-cell problem, surrogate interface, approximate jump conditions, finite element method

**Abstract:** We propose a new embedded finite element method to simulate partial differential equations over domains with internal interfaces. Our approach belongs to the family of surrogate/approximate interface methods and relies on the idea of shifting the location and value of jump interface conditions. This choice has the goal of preserving optimal convergence rates while avoiding small cut cells and related problematic issues, typical of traditional embedded methods. The proposed approach is accurate, robust, efficient, and simple to implement. We apply this concept to internal interface computations in the context of the mixed Poisson problem, also known as the Darcy flow problem. An extensive set of numerical tests is provided to demonstrate the performance of the proposed approach.

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Volume: 358

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Date Submitted: 10/8/20 12:00AM

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Publication Location:

**Article Title:** Analysis of the Shifted Boundary Method for the Stokes Problem

**Authors:** Nabil M. Atallah, Claudio Canuto, Guglielmo Scovazzi

**Keywords:** Embedded methods; immersed boundary method; small cut-cell problem; approximate domain boundaries; weak boundary conditions; finite element method.

**Abstract:** The analysis of stability and accuracy of the shifted boundary method is developed for the Stokes flow equations. The key feature of the shifted boundary method, an embedded finite element method, is the shifting of the location where boundary conditions are applied from the true to a surrogate boundary, and an appropriate modification (shifting) of the value of the boundary conditions. An inf-sup condition is proved for the variational formulation associated to the shifted boundary method and we derive, by way of Strang's second lemma, an optimal error estimate in the natural SBM norm. We also derive an L2-error estimate for the velocity field, by means of an extension of the Aubin-Nitsche approach to embedded, non-consistent, mixed finite element methods.

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**Journal:** Journal of Computational Physics

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Volume:

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Date Submitted: 10/8/20 12:00AM

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Publication Location:

**Article Title:** A weighted Shifted Boundary Method for free surface flow problems

**Authors:** Oriol Colomés, Alex G. Main, Léo Nouveau, Guglielmo Scovazzi

**Keywords:** Immersed boundaryUnfitted finite element methodApproximate boundaryFree-surface flowsComputational fluid dynamicsShifted Boundary Method

**Abstract:** The Shifted Boundary Method (SBM) was recently introduced for the Poisson, linear advection/diffusion, Stokes, Navier-Stokes, acoustics, and shallow-water equations and belongs to the class of unfitted (or immersed, or embedded) finite element methods. By reformulating the original boundary value problem over a surrogate (approximate) computational domain, the SBM avoids integration over cut cells and the associated problematic issues regarding numerical stability and matrix conditioning. Accuracy is maintained by modifying the original boundary conditions using Taylor expansions. Hence the name of the method, that shifts the location and values of the boundary conditions. In this article, we extend the SBM to the simulation of incompressible Navier-Stokes flows with moving free-surfaces, by appropriately weighting its variational form with the elemental volume fraction of active fluid. This approach prevents spurious pressure oscillations in time, which would otherwise be produced if

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Publication Location:

**Article Title:** The shifted boundary method for solid mechanics

**Authors:** Nabil M. Atallah, Claudio Canuto, Guglielmo Scovazzi

**Keywords:** approximate boundary conditions, complex geometry, imaging-to-computing, shifted boundary method, solid mechanics, unfitted finite elements

**Abstract:** We propose a new embedded/immersed framework for computational solid mechanics, aimed at vastly speeding up the cycle of design and analysis in complex geometry. In many problems of interest, our approach bypasses the complexities associated with the generation of CAD representations and sub-sequent body-fitted meshing, since it only requires relatively simple representations of the surface geometries to be simulated, such as collections of disconnected triangles in three dimensions, widely used in computer graphics. Our approach avoids the complex treatment of cut elements, by resorting to an approximate boundary representation and a special (shifted) treatment of the boundary conditions to maintain optimal accuracy. Natural applications of the proposed approach are problems in biomechanics and geomechanics, in which the geometry to be simulated is obtained from imaging techniques. Similarly, our computational framework can easily treat geometries that are the result of topology optimization

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Publication Location:

**Article Title:** The second-generation Shifted Boundary Method and its numerical analysis

**Authors:** Nabil M. Atallah, Claudio Canuto, Guglielmo Scovazzi

**Keywords:** Shifted Boundary Method; Immersed boundary method; Small cut-cell problem; Approximate domain boundaries; Weak boundary conditions; Unfitted finite element methods

**Abstract:** Recently, the Shifted Boundary Method (SBM) was proposed within the class of unfitted (or immersed, or embedded) finite element methods. By reformulating the original boundary value problem over a surrogate (approximate) computational domain, the SBM avoids integration over cut cells and the associated problematic issues regarding numerical stability and matrix conditioning. Accuracy is maintained by modifying the original boundary conditions using Taylor expansions. Hence the name of the method, that shifts the location and values of the boundary conditions. In this article, we present enhanced variational SBM formulations for the Poisson and Stokes problems with improved flexibility and robustness. These simplified variational forms allow to relax some of the assumptions required by the mathematical proofs of stability and convergence of earlier implementations. First, we show that these new SBM implementations can be proved asymptotically stable and convergent even without the ...

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Publication Location:

**Article Title:** The shifted fracture method

**Authors:** Kangan Li, Nabil M. Atallah, Antonio Rodríguez-Ferran, Dakshina M. Valiveti, Guglielmo Scovazzi

**Keywords:** approximate boundary conditions, embedded methods, extended finite element method, fracture mechanics, shifted boundary method, shifted interface method

**Abstract:** We propose a new framework for fracture mechanics, based on the idea of an approximate fracture geometry representation combined with approximate interface conditions. Our approach evolves from the shifted interface method, and introduces the concept of an approximate fracture surface composed of the full edges/faces of an underlying grid that are geometrically close to the true fracture geometry. The original interface conditions are then modified on the surrogate fracture geometry, by way of Taylor expansions. The shifted fracture method does not require cut cell computations or complex data structures, since the behavior of the true fracture is mimicked with standard integrals on the approximate fracture surface. Furthermore, the energetics of the true fracture are represented within the accuracy of the underlying polynomial finite element approximation and independently of the grid topology. The computational framework is presented here in its generality and then applied in the s

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Acknowledged Federal Support: Y

### DISSERTATIONS:

**Publication Type:** Thesis or Dissertation

**Institution:** Duke University

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Completion Date: 5/1/20 10:55PM

**Title:** THE SECOND GENERATION SHIFTED BOUNDARY METHOD AND ITS APPLICATIONS TO POROUS MEDIA FLOW AND SOLID MECHANICS

**Authors:** Nabil Atallah

Acknowledged Federal Support: N

**Publication Type:** Thesis or Dissertation

**Institution:** Duke University

Date Received: 07-Dec-2021

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**Title:** The Shifted Interface/Boundary Method for Embedded Domain Computations

**Authors:** Kangan Li

Acknowledged Federal Support: N

# **RPPR Final Report**

as of 09-Dec-2021

## **Partners**

,

We initiated a collaboration with Professor Antonio Rodriguez-Ferran at the Barcelona Tech University (Universitat F

I certify that the information in the report is complete and accurate:

Signature: Guglielmo Scovazzi

Signature Date: 12/8/21 4:59PM

# Final Report: Award W911NF-18-1-0308

## The shifted interface method solid mechanics: An embedded domain approach.

### Summary

We developed a new embedded/immersed framework for computational solid mechanics, aimed at vastly speeding up the cycle of design and analysis in complex geometry. In many problems of interest, our approach bypasses the complexities associated with the generation of CAD representations and subsequent body-fitted meshing, since it only requires relatively simple representations of the surface geometries to be simulated, such as collections of disconnected triangles in three dimensions, widely used in computer graphics. Our approach avoids the complex treatment of cut elements, by resorting to an approximate boundary representation and a special (shifted) treatment of the boundary conditions to maintain optimal accuracy. Natural applications of the proposed approach are problems in biomechanics and geomechanics, in which the geometry to be simulated is obtained from imaging techniques. Similarly, our computational framework can easily treat geometries that are the result of topology optimization methods and are realized with additive manufacturing technologies. We developed a full analysis of stability and convergence of the method, and we complemented it with an extensive set of computational experiments in two and three dimensions, for progressively more complex geometries.

We also extended the proposed framework to some problems in fracture mechanics, based on the idea of an approximate fracture geometry representation combined with approximate interface conditions. This approach evolves from the shifted interface method, and introduces the concept of an approximate fracture surface composed of the full edges/faces of an underlying grid that are geometrically close to the true fracture geometry. The original interface conditions are then modified on the surrogate fracture geometry, by way of Taylor expansions. The shifted fracture method does not require cut cell computations or complex data structures, since the behavior of the true fracture is mimicked with standard integrals on the approximate fracture surface. Furthermore, the energetics of the true fracture are represented within the accuracy of the underlying polynomial finite element approximation and independently of the grid topology. This computational framework was applied in the specific context of cohesive zone models, with extensive numerical experiments.

### 1. Introduction and overview

Geometrical complexity plays a dominant role in many problems of interest in computational solid mechanics. For the longest time, the finite element method has been the standard computational paradigm for complex geometry simulations. Finite element methods rely on CAD (Computer Aided Design) representations of the geometry and on the generation of computational grids adapted to these representations (body-fitted meshing).

More recently, IGA (Iso-Geometric Analysis) [19, 45] has been presented as an alternative paradigm, in which NURBS or T-Spline functions are used to build discrete approximation spaces directly on the CAD representation, somewhat avoiding the costly operation of generating body-fitted grids in complex geometry.

In the last decade, a variety of new embedded/immersed geometry approaches [54, 60, 100, 109, 119] have been proposed to further speed up design and analysis in complex geometry. These approaches started from the realization that the generation of CAD geometrical representations can still be a costly phase in the overall design and analysis process, especially if the geometry is obtained from the pixels/voxels that are the result of two/three-dimensional image reconstruction techniques. These approaches rapidly spread their area of application to problems in which CAD representations are more easily available, and showed great promise when combined with topology optimization [13, 30, 99].

Our approach falls in the broad category of embedded/immersed methods for solid mechanics just mentioned, and addresses some of the long standing problems that have somewhat limited the broader application of such techniques in the engineering practice. Specifically, common embedded strategies for the enforcement of boundary conditions revolve around 1) the use of exact cut-cell geometry representations to construct the solution space and 2) the Nitsche's method [90] for consistent weak boundary enforcement [59]. For body-fitted approaches, employing Nitsche's method does not adversely affect the conditioning of the system matrix. However, in the case of embedded finite elements, due to the arbitrariness of the size of the cut elements, naïve approaches suffer from numerical instabilities and poor matrix conditioning problems. A number of approaches have addressed this issue in recent years [29, 31, 120, 121], but the geometric construction of the partial elements cut by the embedded boundary typically remains a complex and computationally intensive process. Similarly, the construction of appropriately accurate quadrature formulas to integrate the variational equations on cut cell is challenging, and typically relies on the use of sub-triangulations (an approach that somewhat defeats the purpose of immersed methods) or the development of complex quadrature formulas directly in physical space (since there it is not possible to define the parent domain of a cut element of general shape).

In this project, we propose a new immersed geometry approach to solid mechanics, based on the Shifted Boundary Method (SBM) [9, 76, 77, 92, 134], in which the complex geometry to be simulated is immersed in a pre-existing grid, and boundary conditions are enforced on a surrogate boundary (the red segmented curve, in Fig. 1a), which lies in proximity of the true boundary (the blue curve, in Fig. 1a). This strategy has the advantage of bypassing the labor-intensive phase of CAD/mesh generation, since a simple representation of the surface geometry using collections of disconnected triangles in three dimensions (e.g., the stereolithography STL format, common in computer graphics) is sufficient to setup computations.

One surprising aspect of the proposed approach is that the geometric representations of boundaries may not even need to be water tight on a fine scale, as long as their resolution is finer than the resolution of the grids utilized in simulations. More details on this aspect will be presented in the section of this article on numerical experiments.

The definition of the surrogate domain in the shifted boundary method, however, poses the challenge of devising effective strategies for the imposition of boundary conditions of optimal accuracy. To this end, Taylor extrapolations of the numerical solution are introduced on the surrogate boundary to correct the boundary conditions and account for the discrepancy of location between the surrogate and true boundary. Numerical results for the Poisson and Stokes problems [76]

showed optimal convergence rates and adequate conditioning of the algebraic systems of equations. Afterwards, the SBM was extended to the advection/diffusion equation and the laminar and turbulent incompressible Navier-Stokes equations [77] in addition to hyperbolic systems such as wave propagation problems in acoustics and shallow water flows [134]. The authors of [92] proposed a number of strategies to increase the accuracy of the method in elliptic problems and the authors of [9] presented a complete numerical analysis of the SBM for the Stokes problem (the analysis of the Poisson problem was already presented in [76]).

The general tradeoff of the SBM is that integration and data management of cut cells is completely avoided, at the expense of variational formulations that include additional terms with respect to the corresponding cutFEMs, Immersogeometric (Immersed IGA) and Finite Cell Methods. We believe that this tradeoff is a more efficient option when considering very complex geometries, including the case of non water-tight descriptions.

In fact, to modify an existing body-fitted finite element method into a SBM, all that is needed is: 1) a preprocessing phase in which the surrogate boundary is defined, as well as its (vector) distance  $\mathbf{d}$  from the true boundary (a step that can be achieved using either modified closed-point projection techniques, level-set approaches, or variational methods [20]); and 2) the modification of the boundary conditions of the original body-fitted variational formulation using Taylor expansions of the solution along  $\mathbf{d}$ . These two steps are usually much less complex to implement than the data structures for the geometrical description of volumes/boundaries of cut cells and the corresponding numerical integration strategies.

When considering solid mechanics problems, the enforcement of Neumann conditions becomes crucial, since traction (or traction-free) boundary conditions are quite common on the majority of the boundary surfaces defining the geometry. This is in contrast to the case of fluid mechanics problems, where Neumann conditions are applied at inflow/outflow boundaries that do not typically require to be embedded/immersed. Unfortunately, if a displacement-based, irreducible formulation of the SBM is used in combination with piecewise linear finite element spaces, it is not possible to accurately enforce traction boundary conditions, as they require a Taylor extrapolation of the derivative of the stress, that is, the second derivative of the displacement.

In this project, we propose instead to circumvent this issue by resorting to a mixed strain-displacement formulation, defined only on the layer of elements neighboring the surrogate (approximate) boundary, as a way to reconstruct second-order derivatives of the displacements in a stable, accurate and robust way. The mixed formulation on this layer of elements is then weakly (i.e., variationally) coupled to the rest of the computational domain, where a standard primal (displacement) formulation is applied. The net result is an improved formulation that maintains the bulk cost of the base primal formulation, but allows for an accurate imposition of immersed traction boundary conditions.

The literature of immersed/embedded computational methods for interfaces or fracture mechanics is vast (X-FEMs [85, 86], partition of unity methods [72, 81, 140], method of universal meshes [110, 112] and its mathematical analysis [111], etc.), as it is vast the literature of immersed methods [101, 102] on equations other than the ones of solid mechanics (immersed finite differences/volumes/elements for heat conduction, Stokes flow, fluid/structure interaction, etc.). We prefer not to even attempt the presentation of a full account of previous works on these areas, which we feel peripheral to the present contribution. We refer an interested reader to [9, 44, 76, 77, 134] where an introduction of the SBM in a broader context is presented, although references to the massive amount of existing work may still lack completeness.

In this project, we also made preliminary steps to extend the Shifted Boundary/Interface Method to fracture mechanics. Specifically, we developed the Shifted Fracture Method (SFM), a new computational framework for fracture mechanics. The SFM is based on the idea of approximating the fracture interface conditions on an approximate fracture geometry (the surrogate fracture) that coincides with the edges/faces of the grid that are closest, in some sense, to the true fracture geometry.

It is important to realize that shifting only the location of the interface conditions would produce a computational method analogous to the node-release technique [32, 33, 133, 143], with the consequent drawback of mesh dependency of the numerical results.

Instead, by shifting also the value of the fracture interface conditions, the SFM is not affected by such mesh dependencies, and its variational formulation automatically incorporates the projection of the surrogate surface area onto the true surface area, which is instrumental in the representation of the correct energy released by the fracture.

In order to put into perspective the SFM, we attempt to present a brief - and certainly not comprehensive - account of the earlier and most recent contributions to computational fracture mechanics. Some of the earliest computational strategies to simulate fracture propagation problems involve the node-release technique [32, 33, 133, 143] and the element deletion approach [133]. In the node release technique, the fracture is numerically represented by duplicating displacement degrees-of-freedom along the edges/faces of the computational grid in two/three dimensions, and applying appropriate cohesive zone models on the numerical crack faces. The propagation of the fracture cannot then follow an arbitrary direction, but must follow along the edges/faces of the computational grid. With this strategy, the surface area of the fracture is incorrectly captured, and consequently, large errors in fracture release energy may occur. To correct these issues, adaptive mesh refinement can be used to allow the grid to align with the theoretical direction of propagation of the fracture, and alleviate the problem of incorrect fracture surface representations. The drawback of these techniques is the added complexities of managing remeshing data structures as the fracture propagates and the need to transfer information from the old mesh to the new mesh at each adaptive refinement.

More recently, Lew and collaborators developed the Universal Meshes algorithm [108, 112], in which a base computational grid is locally adapted as the fracture propagates through the domain. This approach avoids mesh dependencies by mesh adaptation, and has been implemented also in the context of higher-order discretizations [41, 42].

Mesh dependencies in the behavior of the fracture are also observed when considering element-deletion techniques [133], and more generally fracture damage modeling techniques [16, 113]. There, a damage model is introduced to reduce the stiffness of elements that lie in proximity of a fracture. In their simplest implementation in conjunction with piecewise-linear finite element approximations of the displacements, also element damage models do not correctly capture the energy released in the fracture [95, 117, 118]. Part of the limitations of element deletion techniques is due to the piecewise-constant approximation of the stresses (or strains), which is not sufficient to prevent large mesh dependencies in the numerical solution. In a recent development, the authors of [14, 35–37, 39, 40, 43, 68] proposed a new breed of damage models based on mixed formulations of the equations of elasticity, which allow higher-order stresses approximations and avoid the mesh dependencies of earlier contributions. The numerical results are certainly promising and somewhat “resuscitate” methods that have in the simplicity of implementation their strong point.

Over the past two decades, the computational fracture mechanics community explored ideas

aimed at circumventing the limitation of node-release techniques. The literature is vast, and a full account is possibly beyond the scope of this project. Nonetheless, it is important to mention a number of essential contributions.

By relating the loss of ellipticity of the partial differential equations governing the classical continuum model to the development of strong discontinuities, Simo *et al.* [130] proposed a general localized failure framework that was later expanded by Armero and Garikipati [5].

Embedded Finite Element Methods (EFEMs) were proposed by several groups [5, 22, 56, 69, 74, 93, 94, 97], and rely on the idea of augmenting the finite element shape functions with appropriate enrichments that can be used to approximate the kinematics of the crack. These methods are typically distinguished in approaches with strong discontinuities (introducing displacement jumps) [5, 56, 69, 74, 93, 94, 96] or with weak discontinuity (introducing strain jumps) [22, 97, 132]. The latter approach is more applicable in the case in which an obvious jump in strains occurs, such as in shear bands of metals and soils. Weak enrichment EFEMs enrich the strains with incompatible modes, and result in non-conforming finite elements, in which, typically, the surface of the fracture is approximated as a globally discontinuous geometric object. Weak enrichment EFEMs typically require a length scale parameter to define the width of the strain jump and as yet have been unable to overcome mesh dependencies [131]. In strong enrichment EFEMs, by means of appropriately constructed enhanced shape functions, elements can properly capture the highly localized modes that prelude failure. Recent developments in this area are found in [4, 6, 57, 72, 73].

Later, the eXtended FEM (or XFEM) [21, 48, 85] and the Generalized FEM (GFEM) [23, 49–51] were introduced to have a more general description of the kinematic fields in proximity of the fracture, allowing the enrichments to be much more general than in the earlier EFEM. From a general perspective, XFEMs/GFEMs can be considered as Partition of Unity FEMs [12, 81], in which the standard finite element basis is locally enriched to represent the displacement and stress fields in close proximity of the fracture. A large body of literature has since been developed, and here we would like to point out the contributions in the realm of cohesive-zone models [84, 140, 141], which are the focus of the present project.

On a completely different area of development, new damage models were developed using variational principles to control and drive the evolution of cracks. These approaches follow under the name of gradient damage models [79, 103, 104], phase-field models [25, 26, 82, 83], and have provided very important tools to numerically simulate crack nucleation, branching and merging. These methods are based on a diffuse representation of the fracture, and the introduction of a damage variable that controls the evolution of fractures. By relying on gradient information, phase-field and gradient damage models are intrinsically nonlocal models, although they rely on a classical partial differential equation description of the fields representing the fracture process. For this reason, they are simpler to implement than nonlocal damage models of the integral type [18, 105], as they do not require the computation of a nonlocal state variable as the weighted average of a local state variable in a neighborhood of each point of the computational domain.

An alternative nonlocal approach to fracture is Peridynamics (PD) [58, 75, 123, 125, 126], in which the equations of continua are reformulated as an integro-differential equation. At the price of an increased computational cost, PD offers a more general and comprehensive approach to fracture, and has found various implementations, including meshfree/meshless algorithms [124], which had already been proposed as a tool to study crack propagation problems [24, 106, 107]. PD shares with phase-field algorithms the ability to more easily attack crack branching and nucleation, although the technical reasons are different.

We would like now to make a few comments on two of the approaches to fracture mentioned above, namely XFEM and phase-field models. As previously mentioned, The XFEM represents the fracture as a sharp interface that can cut across finite elements, and obviates to the severe grid-dependence issues associated with earlier models. It is however of difficult implementation in three-dimensions, since it requires special data structures and special integration procedures that are hard to implement. At the same time the numerical stability and the algebraic system of equations associated with XFEM variational formulation may be affected by the presence of small-cut elements, and a number of stabilization approaches have been proposed [3, 47, 61, 65, 86].

Phase-field models, instead, resort to an energetic principle for the characterization of the numerical fracture, and are of easier implementation in the three-dimensional case. However, they introduce a diffuse representation of the fracture itself, and they may be, for this reason, less efficient in the numerical representation of the fracture away from the crack tip. In addition, the location of the crack is not directly given in a phase-field model, but this might be important in studying problems in which other physics are coupled to the propagation of fracture, such as the case of fractured porous media with flow coupling, etc. An approach that blends a phase-field model and a sharp crack representation was presented in [87–89].

The SFM approach described here evolves from the Shifted Interface Method [71, 76], an approximate domain approach, in which interfaces are approximated by the set of closest edges on the grid, and interface conditions are appropriately modified (shifted), using Taylor expansions, to achieve a prescribed level of accuracy. Here, we describe how these ideas can be used in general, and more specifically in the context of cohesive zone models. The description of the crack relies on the definition of a distance (vector) between the location of the true crack (or a sufficiently accurate estimate of it), and the location of the surrogate crack. The SFM does not require cut cell computations or complex data structures, since the behavior of the true fracture is mimicked with standard integrals on the approximate fracture, which preserves the energetics of the true fracture to a high degree of accuracy. In fact, the SFM adopts the same integration quadratures and data structures utilized in common node-release techniques. In this sense, the SFM stands as an interesting alternative to both node-release techniques and XFEM/GFEM approaches, in that it has the computational data structure of a node-release technique but the accuracy of a XFEM/GFEM.

## 2. Static linear elasticity

The equations of linear isotropic elastostatics describe the deformation of a solid medium under prescribed external loading. In what follows, we will consider a mixed formulation in terms of displacement and strain variables, with the purpose of developing a sufficiently general framework for the imposition of Dirichlet and, particularly, Neumann boundary conditions.

### 2.1. Governing equations

Let  $\Omega$  be a connected open set in  $\mathbb{R}^{n_d}$  with Lipschitz boundary ( $n_d = 2, 3$  indicates the number of spatial dimensions), and consider the following displacement/strain mixed form of the linear elastostatics equations:

$$-\nabla \cdot \boldsymbol{\sigma}(\boldsymbol{\varepsilon}) = \mathbf{b} \ , \quad (1a)$$

where  $\boldsymbol{\sigma}$  is the stress tensor,  $\mathbf{b}$  is the body force,  $\nabla$  and  $\nabla \cdot$  are the gradient and divergence operators, respectively, and

$$\boldsymbol{\varepsilon} = \nabla^s \mathbf{u} \quad (1b)$$

is the strain tensor defined as the symmetric gradient of the displacement field  $\mathbf{u}$ , namely  $\nabla^s \mathbf{u} = 1/2 (\nabla \mathbf{u} + \nabla^t \mathbf{u})$  (with  $(\cdot)^t$  the transpose, or adjoint, operator). For elastic materials, the underlying stress-strain constitutive law is

$$\boldsymbol{\sigma}(\boldsymbol{\varepsilon}) = \mathbf{C} \boldsymbol{\varepsilon} , \quad (2)$$

where  $\mathbf{C} = [\mathbf{C}_{ijkl}]$  is the fourth-order elastic stiffness tensor. Equivalently,  $\boldsymbol{\sigma}(\nabla^s \mathbf{u}) = \mathbf{C} \nabla^s \mathbf{u} = 1/2 \mathbf{C} (\nabla \mathbf{u} + \nabla^t \mathbf{u})$ . We recall some general notation and properties that will be useful in what follows, such as an extended Voigt notation for the second order and fourth order tensors. The standard Voigt notation relies on the fact that the stress tensor  $\boldsymbol{\sigma}$  and strain tensor  $\boldsymbol{\varepsilon}$  are symmetric, and, consequently, the fourth order elasticity tensor  $\mathbf{C}$  possesses some major and minor symmetries. In particular, the stress and strain tensors are represented as six-component vectors, and the elasticity tensor is represented as a symmetric six-by-six matrix. For the purpose of the derivations to follow, we prefer instead to have the redundant extended Voigt notation in which second-order tensors are represented as nine-component vectors and the elasticity tensor is represented as a nine-by-nine symmetric matrix, with real eigenvalues. The ellipticity condition [55] on the elasticity equations implies that all eigenvalues of the elasticity matrix are positive, namely  $\chi : (\mathbf{C} \chi) \geq \rho_0(\mathbf{x}) \chi : \chi > 0$  for any symmetric  $\chi \neq \mathbf{0}$  and some positive scalar  $\rho_0(\mathbf{x})$ , which may depend on the position  $\mathbf{x}$  but is independent of  $\chi$ . From the discussion outlined so far,  $\mathbf{C}$  is represented by a symmetric positive definite matrix, and its square root can be defined as the fourth-order tensor associated to the square root of its matrix in the extended Voigt notation. We will indicate this, with a slight abuse of notation, by  $\mathbf{C} = \mathbf{C}^{1/2} \mathbf{C}^{1/2}$ . Indicating with  $\rho_c(\mathbf{x})$  the spectral radius (largest eigenvalue) of the extended Voigt matrix representation of  $\mathbf{C}(\mathbf{x})$ , we have that  $\rho_0(\mathbf{x}) \chi : \chi \leq \chi : (\mathbf{C} \chi) \leq \rho_c(\mathbf{x}) \chi : \chi$ . In what follows, we will omit the dependency on  $\mathbf{x}$  and write, more simply,  $\rho_0$  and  $\rho_c$ . Further, we assume that  $\mathbf{C}$  is bounded and uniformly positive definite in  $\Omega$  (i.e.,  $\rho_{\min} := \inf_{\mathbf{x} \in \Omega} \rho_0(\mathbf{x}) > 0$  and  $\rho_{\max} := \sup_{\mathbf{x} \in \Omega} \rho_c(\mathbf{x}) < \infty$ ).

For isotropic materials,  $\mathbf{C}$  collapses to

$$\mathbf{C}_{ijkl} = \lambda \delta_{ij} \delta_{kl} + \mu (\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}) . \quad (3)$$

Here  $\lambda$  and  $\mu$  are the Lamé coefficients, which are related to the Young's modulus  $E$ , the Poisson ratio  $\nu$ , the bulk modulus  $\kappa$ , and the shear modulus  $G$  by:

$$\lambda = \frac{E\nu}{(1+\nu)(1-2\nu)} , \quad \mu = G = \frac{E}{2(1+\nu)} , \quad \kappa = \lambda + 2\mu/3 . \quad (4)$$

Classical results in isotropic elasticity imply that  $\rho_0 = \min(\mu, 3\kappa)$  and  $\rho_c = \max(2\mu, 3\kappa)$ . Assuming that the boundary  $\Gamma = \partial\Omega$  is partitioned as  $\overline{\Gamma_D} \cup \overline{\Gamma_N}$  with  $\Gamma_D \cap \Gamma_N = \emptyset$ , displacement boundary conditions

$$\mathbf{u}|_{\Gamma_D} = \mathbf{u}_D(\mathbf{x}) \quad (5)$$

are enforced on  $\Gamma_D$  and traction boundary conditions

$$\boldsymbol{\sigma}(\boldsymbol{\varepsilon}) \mathbf{n}_{|\Gamma_N} = (\mathbf{C} \boldsymbol{\varepsilon}) \mathbf{n}_{|\Gamma_N} = \mathbf{t}_N(\mathbf{x}) \quad (6)$$

are enforced on  $\Gamma_N$ , where  $\mathbf{t}_N$  is the normal traction and  $\mathbf{n}$  is the outward-pointing normal to the boundary  $\Gamma_N$ .

## 2.2. General notation

Let us denote by  $L^2(\Omega)$  the space of square integrable functions over the set  $\Omega \subset \mathbb{R}^{n_d}$ . Here and in the following,  $(v, w)_\omega = \int_\omega v w$  denotes the  $L^2$ -inner product on a subset  $\omega \subseteq \tilde{\Omega}_h$ , and  $\langle v, w \rangle_\gamma = \int_\gamma v w$  denotes the  $L^2$ -inner product on a subset  $\gamma \subseteq \tilde{\Gamma}_h$ . Let  $H^m(\Omega) = W^{m,p}(\Omega)$  indicate the Sobolev spaces of index of regularity  $m \geq 0$  and index of summability  $p = 2$ , equipped with the (scaled) norm

$$\|v\|_{H^m(\Omega)} = \left( \|v\|_{L^2(\Omega)}^2 + \sum_{k=1}^m \|l(\Omega)^k \mathbf{D}^k v\|_{L^2(\Omega)}^2 \right)^{1/2}, \quad (7)$$

where  $\mathbf{D}^k$  is the  $k$ th-order spatial derivative operator and  $l(\Omega) = (\text{meas}_{n_d}(\Omega))^{1/n_d}$  is a characteristic length of the domain  $\Omega$  (introduced here to maintain dimensional consistency in the definitions of the Sobolev norms). Note that  $H^0(\Omega) = L^2(\Omega)$ . As usual, we use a simplified notation for norms and semi-norms, i.e., we set  $\|v\|_{m;\Omega} = \|v\|_{H^m(\Omega)}$  and  $|v|_{k;\Omega} = \|\mathbf{D}^k v\|_{0;\Omega} = \|\mathbf{D}^k v\|_{L^2(\Omega)}$ . Furthermore, we indicate by  $H^{1/2}(\Gamma)$  the fractional trace space associated with  $H^1(\Omega)$ , and by  $H^{-1/2}(\Gamma)$  and  $H^{-1}(\Omega)$  the duals (spaces) of  $H^{1/2}(\Gamma)$  and  $H^1(\Omega)$ , respectively.

## 3. The shifted boundary method

### 3.1. The true domain, the surrogate domain and maps

Consider a closed domain  $\mathcal{D}$  such that  $\text{clos}(\Omega) \subseteq \mathcal{D}$  and we introduce a family of admissible and shape-regular triangulations of  $\mathcal{D}$ . Then, we restrict each triangulation  $\mathcal{T}_h$  by selecting those elements that are contained in  $\text{clos}(\Omega)$ , i.e., we form

$$\tilde{\mathcal{T}}_h := \{T \in \mathcal{T}_h : T \subset \text{clos}(\Omega)\}.$$

This identifies the *surrogate domain*

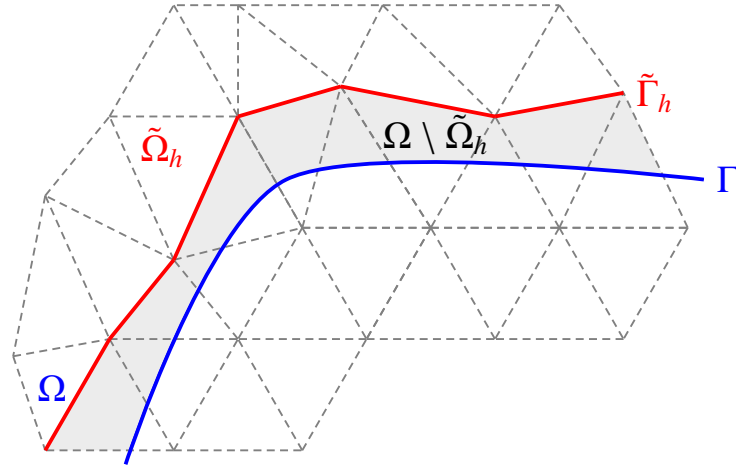
$$\tilde{\Omega}_h := \text{int}\left(\bigcup_{T \in \tilde{\mathcal{T}}_h} T\right) \subseteq \Omega,$$

with *surrogate boundary*  $\tilde{\Gamma}_h := \partial\tilde{\Omega}_h$  and outward-oriented unit normal vector  $\tilde{\mathbf{n}}$  to  $\tilde{\Gamma}_h$ . Obviously,  $\tilde{\mathcal{T}}_h$  is an admissible and shape-regular triangulation of  $\tilde{\Omega}_h$  (see Figure 1a). We now select a mapping

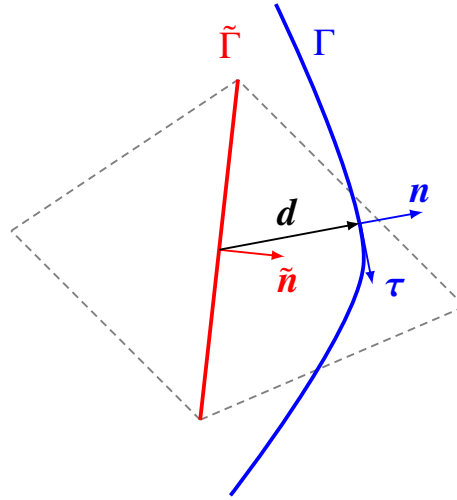
$$\mathbf{M}_h : \tilde{\Gamma}_h \rightarrow \Gamma, \quad (8a)$$

$$\tilde{\mathbf{x}} \mapsto \mathbf{x}, \quad (8b)$$

as defined in [8, Section 2.1] which associates to any point  $\tilde{\mathbf{x}} \in \tilde{\Gamma}_h$  on the surrogate boundary a point  $\mathbf{x} = \mathbf{M}_h(\tilde{\mathbf{x}})$  on the physical boundary  $\Gamma$ . Through  $\mathbf{M}_h$ , a distance vector function  $\mathbf{d}_{\mathbf{M}_h}$  can be



(a) The true domain  $\Omega$ , the surrogate domain  $\tilde{\Omega}_h \subset \Omega$ , the true boundary  $\Gamma$ , and the surrogate boundary  $\tilde{\Gamma}_h$ .



(b) The distance vector  $d$ , the true normal  $n$ , the true tangent  $\tau$ , and the surrogate normal  $\tilde{n}$ .

Figure 1: The surrogate domain, its boundary, and the distance vector  $d$ .

defined as

$$\mathbf{d}_{M_h}(\tilde{\mathbf{x}}) = \mathbf{x} - \tilde{\mathbf{x}} = [\mathbf{M} - \mathbf{I}](\tilde{\mathbf{x}}). \quad (9)$$

For the sake of simplicity, we set  $\mathbf{d} = \mathbf{d}_{M_h}$  where  $\mathbf{d} = \|\mathbf{d}\|\mathbf{v}$  and  $\mathbf{v}$  is a unit vector.

**Remark 1.** *There are other strategies in the definition of the map  $\mathbf{M}_h$  and, correspondingly, the distance vector  $\mathbf{d}$ . Among them is a level set description of the true boundary, in which  $\mathbf{d}$  is defined by means of a distance function.*

In case the boundary  $\Gamma$  is partitioned into a Dirichlet boundary  $\Gamma_D$  and a Neumann boundary  $\Gamma_N$  with  $\Gamma = \overline{\Gamma_D} \cup \overline{\Gamma_N}$  and  $\Gamma_D \cap \Gamma_N = \emptyset$ , we need to identify whether a surrogate edge  $\tilde{E} \subset \tilde{\Gamma}_h$  is associated with  $\Gamma_D$  or  $\Gamma_N$ . To that end, we partition  $\tilde{\Gamma}_h$  as  $\tilde{\Gamma}_{D,h} \cup \tilde{\Gamma}_{N,h}$  with  $\tilde{\Gamma}_{D,h} \cap \tilde{\Gamma}_{N,h} = \emptyset$  using again a map  $\mathbf{M}_h$ , such that

$$\tilde{\Gamma}_{D,h} = \{\tilde{E} \subseteq \tilde{\Gamma}_h : \mathbf{M}_h(\tilde{E}) \subseteq \Gamma_D\} \quad (10)$$

and  $\tilde{\Gamma}_{N,h} = \tilde{\Gamma}_h \setminus \tilde{\Gamma}_{D,h}$ .

We indicate by  $h_T$  ( $h_T^i$ , resp.) the circumscribed diameter (inscribed diameter, resp.) of an element  $T \in \tilde{\mathcal{T}}_h$  and by  $h$  ( $h^i$ , resp.) the piecewise constant function in  $\tilde{\Omega}_h$  such that  $h|_T = h_T$  ( $h|_T = h_T^i$ , resp.) for all  $T \in \tilde{\mathcal{T}}_h$ . We also introduce the following mesh parameters

$$h_\tau := (h_T h_T^i)^{1/2}, \quad (11a)$$

$$h_{\tilde{\Gamma}_h} := \max_{T \in \tilde{\mathcal{T}}_h : T \cap \tilde{\Gamma}_h \neq \emptyset} h_T, \quad (11b)$$

$$h_{\tilde{\Omega}_h} := \max_{T \in \tilde{\mathcal{T}}_h} h_T, \quad (11c)$$

$$h_\perp := \frac{\text{meas}_{n_d}(T)}{\text{meas}_{n_d-1}(\tilde{E})} \quad \forall \tilde{E} \in \tilde{\Gamma}_h, \quad T \cap \tilde{E} \neq \emptyset, \quad T \in \tilde{\mathcal{T}}_h. \quad (11d)$$

With regard to the numerical analysis of the SBM, presented in Section 4, besides the shape-regularity of the grids, we assume there exist constants  $C_r, \xi_1, \xi_2 \in \mathbb{R}^+$  such that  $(1/\sqrt{C_r})h \leq h_\tau \leq h$  and  $\xi_1 h \leq h_\perp \leq \xi_2 h$ . With slight abuse of notation, we will assume  $h, h_\tau$  and  $h_\perp$  are interchangeable.

### 3.1.1. Boundaries with edges, corners, or multiple boundary conditions

We describe now in more detail the treatment of boundaries with edges or corners, as they are of importance in practical engineering applications. Let us assume that the boundary  $\Gamma$  of the original domain  $\Omega$  is partitioned into  $M$  subsets  $\Gamma_m, m = 1, \dots, M$ , hereafter termed *sidesets*, with the following properties:

1. Each  $\Gamma_m$  is relatively closed in  $\Gamma$ , and satisfies  $\cup_m \Gamma_m = \Gamma$ ,  $\text{int } \Gamma_m \cap \text{int } \Gamma_n = \emptyset$  for  $m \neq n$ .
2. Each  $\Gamma_m$  is “smooth”, in the sense that the normal unit vector  $\mathbf{n}_m$  (pointing outward) exists at each  $\mathbf{x} \in \Gamma_m$  and varies in a continuous manner.
3. The assigned boundary condition data is a smooth function on each  $\Gamma_m$ .

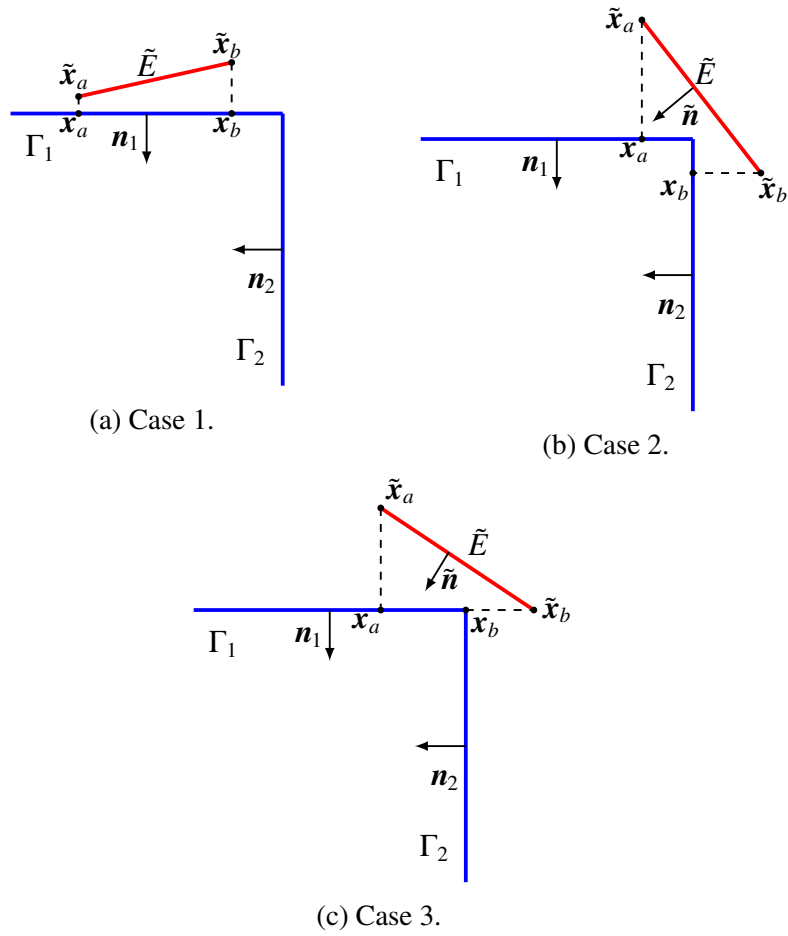


Figure 2: Cases involved in the strategy for assigning a sideset to the surrogate edge  $\tilde{E}$ .

We aim at associating a unique sideset to each edge (in two dimensions) or face (in three dimensions) of the triangulation  $\tilde{\mathcal{T}}_h$  that is sitting on the surrogate boundary  $\tilde{\Gamma}$ . All the information needed to define the transported boundary data on the edge/face will be drawn from the associated sideset.

Consider the case of an edge (in two dimensions)  $\tilde{E} \subset \tilde{\Gamma}_h$  (the three-dimensional case can be handled similarly) with  $\tilde{\mathbf{n}}$  as its unit normal vector. Let  $\tilde{\mathbf{x}}_a, \tilde{\mathbf{x}}_b$  be the endpoints of  $\tilde{E}$  and  $\mathbf{x}_a, \mathbf{x}_b$  be their respective closest-point projections upon  $\Gamma$ . Finally, let  $L$  be the set of sidesets that  $\mathbf{x}_a$  and  $\mathbf{x}_b$  belong to. To associate a unique sideset  $\Gamma_{m(\tilde{E})}$  to  $\tilde{E}$ , the following cases arise:

- (i) If  $\mathbf{x}_a$  and  $\mathbf{x}_b$  belong to the same unique sideset, say  $\Gamma_1$ , then the set  $L$  will have a single element, namely  $\Gamma_1$ , and thus  $\tilde{E}$  is associated with it (Figure 2a).
- (ii) If  $\mathbf{x}_a$  and  $\mathbf{x}_b$  belong to different, unique sidesets, say  $\Gamma_1$  and  $\Gamma_2$  respectively, then the set  $L$  will consist of  $\Gamma_1$  and  $\Gamma_2$  (Figure 2b). In such a case, we associate  $\tilde{E}$  with the sideset  $\Gamma_m$  in  $L$  such that

$$\Gamma_m = \arg \max_{\Gamma_s \in L} f(\Gamma_s) \quad (12)$$

where  $f(\Gamma_s) = \sum_{i=a,b} \tilde{\mathbf{n}} \cdot \mathbf{n}_{\Gamma_s}(\mathbf{x}_i)$ .

- (iii) If  $\mathbf{x}_a$  (or  $\mathbf{x}_b$ ) belongs to the intersection of two sidesets, say  $\Gamma_1$  and  $\Gamma_2$ , then both such sidesets are added to set  $L$ . At this point, we refer to case (ii) for associating  $\tilde{E}$  with a sideset (Figure 2c).

At last, we define the mapping  $\mathbf{M}_h$  on  $\tilde{E}$  by setting

$$\mathbf{M}_h(\tilde{\mathbf{x}}) := \text{the closest-point projection of } \tilde{\mathbf{x}} \text{ upon } \Gamma_{m(\tilde{E})}, \quad \forall \tilde{\mathbf{x}} \in \tilde{E}. \quad (13)$$

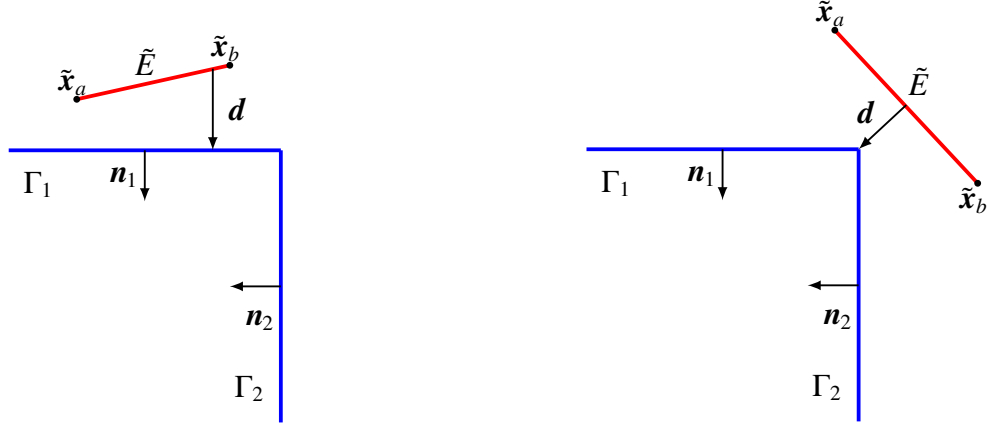
**Remark 2.** *i)* According to the given definition,  $\mathbf{M}_h$  may be multi-valued at the intersection of two edges. However, this has no effect at all since  $\mathbf{M}_h$  appears in the boundary integrals which are computed edge-wise. *ii)* If  $\mathbf{M}_h(\tilde{\mathbf{x}})$  falls in the interior of a sideset  $\Gamma_m$  and coincides with the closest-point projection of  $\tilde{\mathbf{x}}$  upon the whole  $\Gamma$ , then the vector  $\mathbf{d}$  is aligned with  $\mathbf{n}_m$  (Figure 3a). Otherwise, it may not be aligned (Figure 3b).

### 3.2. General strategy

The goal now is to discretize the linear elasticity equations (1a)–(1b) in  $\tilde{\Omega}_h$  rather than  $\Omega$ , with the challenge of appropriately imposing on  $\tilde{\Gamma}_h$  boundary conditions that would mimic (5) and (6). To this end, we resort to the idea introduced in [76] and perform a first-order Taylor expansion of  $\mathbf{u}$  and  $\mathbf{C}\boldsymbol{\varepsilon}$  at their respective surrogate boundaries in order to “shift” the boundary conditions from  $\Gamma$  to  $\tilde{\Gamma}_h$ . Thus, with the assumption that  $\mathbf{u}$  ( $\mathbf{C}\boldsymbol{\varepsilon}$ , resp.) is sufficiently smooth in the strip between  $\tilde{\Gamma}_{D,h}$  ( $\tilde{\Gamma}_{N,h}$ , resp.) and  $\Gamma_D$  ( $\Gamma_N$ , resp.), we can write

$$\mathbf{u}(\tilde{\mathbf{x}}) + (\nabla \mathbf{u} \mathbf{d})(\tilde{\mathbf{x}}) + (\mathbf{R}_D(\mathbf{u}, \mathbf{d}))(\tilde{\mathbf{x}}) = \mathbf{u}_D(\mathbf{M}_h(\tilde{\mathbf{x}})), \quad \text{on } \tilde{\Gamma}_{D,h}, \quad (14a)$$

$$((\mathbf{C}\boldsymbol{\varepsilon})(\tilde{\mathbf{x}}) + (\nabla(\mathbf{C}\boldsymbol{\varepsilon}) \mathbf{d})(\tilde{\mathbf{x}}) + (\mathbf{R}_N(\mathbf{C}\boldsymbol{\varepsilon}, \mathbf{d}))(\tilde{\mathbf{x}})) \mathbf{n}(\mathbf{M}_h(\tilde{\mathbf{x}})) = \mathbf{t}_N(\mathbf{M}_h(\tilde{\mathbf{x}})), \quad \text{on } \tilde{\Gamma}_{N,h}, \quad (14b)$$



(a) Distance vector  $\mathbf{d}$  aligned with  $\mathbf{n}_1$ .

(b) Distance vector  $\mathbf{d}$  not aligned with either  $\mathbf{n}_1$  or  $\mathbf{n}_2$ .

Figure 3: The distance vector  $\mathbf{d}$  and the normal vector  $\mathbf{n}$  to  $\Gamma$

where the remainders  $\mathbf{R}_D(\mathbf{u}, \mathbf{d})$  and  $\mathbf{R}_N(\mathbf{C}\boldsymbol{\varepsilon}, \mathbf{d})$  satisfy

$$\|\mathbf{R}_D(\mathbf{u}, \mathbf{d})\| = o(\|\mathbf{d}\|), \quad \|\mathbf{R}_N(\mathbf{C}\boldsymbol{\varepsilon}, \mathbf{d})\| = o(\|\mathbf{d}\|) \quad \text{as} \quad \|\mathbf{d}\| \rightarrow 0. \quad (15)$$

Introducing the functions  $\bar{\mathbf{u}}_D(\tilde{\mathbf{x}}) := \mathbf{u}_D(\mathbf{M}_h(\tilde{\mathbf{x}}))$  on  $\tilde{\Gamma}_{D,h}$ ,  $\bar{\mathbf{t}}_N(\tilde{\mathbf{x}}) := \mathbf{t}_N(\mathbf{M}_h(\tilde{\mathbf{x}}))$  on  $\tilde{\Gamma}_{N,h}$ , and  $\bar{\mathbf{n}}(\tilde{\mathbf{x}}) := \mathbf{n}(\mathbf{M}_h(\tilde{\mathbf{x}}))$  on  $\tilde{\Gamma}_{N,h}$  we have

$$\mathbf{u} + \nabla \mathbf{u} \mathbf{d} - \bar{\mathbf{u}}_D + \mathbf{R}_D(\mathbf{u}, \mathbf{d}) = \mathbf{S}_{D,h} \mathbf{u} - \bar{\mathbf{u}}_D + \mathbf{R}_{D,h} \mathbf{u} = \mathbf{0}, \quad \text{on } \tilde{\Gamma}_{D,h}, \quad (16a)$$

$$(\mathbf{C}\boldsymbol{\varepsilon} + \nabla(\mathbf{C}\boldsymbol{\varepsilon}) \mathbf{d}) \bar{\mathbf{n}} - \bar{\mathbf{t}}_N + \mathbf{R}_N(\mathbf{C}\boldsymbol{\varepsilon}, \mathbf{d}) \bar{\mathbf{n}} = \mathbf{S}_{N,h}(\mathbf{C}\boldsymbol{\varepsilon}) \bar{\mathbf{n}} - \bar{\mathbf{t}}_N + \mathbf{R}_{N,h}(\mathbf{C}\boldsymbol{\varepsilon}) \bar{\mathbf{n}} = \mathbf{0}, \quad \text{on } \tilde{\Gamma}_{N,h}. \quad (16b)$$

where we have introduced the boundary shift operators

$$\mathbf{S}_{D,h} \mathbf{u} := \mathbf{u} + \nabla \mathbf{u} \mathbf{d} \quad \text{on } \tilde{\Gamma}_{D,h}, \quad (17)$$

$$\mathbf{S}_{N,h}(\mathbf{C}\boldsymbol{\varepsilon}) := \mathbf{C}\boldsymbol{\varepsilon} + \nabla(\mathbf{C}\boldsymbol{\varepsilon}) \mathbf{d} \quad \text{on } \tilde{\Gamma}_{N,h}, \quad (18)$$

and  $\mathbf{R}_{D,h} \mathbf{u}$  ( $\mathbf{R}_{N,h}(\mathbf{C}\boldsymbol{\varepsilon})$ , resp.) is a short-hand notation for the Taylor expansion remainder  $\mathbf{R}_D(\mathbf{u}, \mathbf{d})$  ( $\mathbf{R}_N(\mathbf{C}\boldsymbol{\varepsilon}, \mathbf{d})$ , resp.). Neglecting the higher-order terms with respect to  $\|\mathbf{d}\|$  in (16), we obtain the final expression of the *shifted* boundary conditions

$$\mathbf{S}_{D,h} \mathbf{u} = \bar{\mathbf{u}}_D, \quad \text{on } \tilde{\Gamma}_{D,h}, \quad (19a)$$

$$\mathbf{S}_{N,h}(\mathbf{C}\boldsymbol{\varepsilon}) \bar{\mathbf{n}} = \bar{\mathbf{t}}_N, \quad \text{on } \tilde{\Gamma}_{N,h}. \quad (19b)$$

In what follows - for the sake of simplicity and whenever it does not cause confusion - we will omit the bar symbols from  $\bar{\mathbf{u}}_D$ ,  $\bar{\mathbf{t}}_N$  and  $\bar{\mathbf{n}}$ .

### 3.3. Preliminaries: A mixed shifted formulation for solid mechanics

In this section, we introduce a mixed variational formulation of solid mechanics. With some exceptions (see e.g., [35–38, 66, 67, 70, 91, 114, 115, 122, 128, 129, 135, 136] and references therein) mixed formulations of solid mechanics that adopt strain and displacements as variables are less common than irreducible (primal) formulations, which rely only on displacement unknowns.

The motivation for a mixed formulation in the context of the shifted boundary method is the ease of implementation of Neumann boundary conditions of the type (19b). The price to be paid with mixed formulations is an increase in the overall computational cost, although, at the same time, the stresses and strains are typically captured with higher accuracy and incompressibility constraints can be treated more robustly.

In Section 3.4, we will show that the computational cost of our approach for accurately imposing Neumann boundary conditions can be drastically reduced by applying a mixed variational formulation *only* over a small layer of elements near the boundary. This specific version of the shifted boundary approach becomes comparable in computational cost to an irreducible (primal) formulation, as shown in the numerical performance tests discussed in Section 5.1.

Our first step is then to describe a general mixed form of the shifted boundary method that applies to the entire surrogate domain  $\tilde{\Omega}_h$ . Note that other choices of mixed formulations are applicable for the same purpose [35–38, 66, 67, 70, 114, 115, 122, 135, 136], and the discussion to follow in Section 3.4 is not confined to the specific mixed formulation considered here. Let  $V_{u,h}(\tilde{\Omega}_h)$  and  $V_{\varepsilon,h}(\tilde{\Omega}_h)$  be the discrete, globally continuous trial and test function spaces for the displacement  $\mathbf{u}$  and strain  $\varepsilon$ . Namely,

$$V_{u,h}(\tilde{\Omega}_h) = \{\mathbf{v} \in (C^0(\tilde{\Omega}_h))^{n_d} : \mathbf{v}|_T \in (\mathcal{P}^1(T))^{n_d}, \forall T \in \tilde{\mathcal{T}}_h\}, \quad (20a)$$

$$V_{\varepsilon,h}(\tilde{\Omega}_h) = \{\boldsymbol{\omega} \in (C^0(\tilde{\Omega}_h))^{n_d \times n_d} : \boldsymbol{\omega}|_T \in (\mathcal{P}^1(T))^{n_d \times n_d}, \boldsymbol{\omega} = \boldsymbol{\omega}^t, \forall T \in \tilde{\mathcal{T}}_h\}, \quad (20b)$$

where  $\mathcal{P}^1(T)$  is the space of linear polynomial functions over the element  $T$ .

Multiply the governing equation (1a)–(1b) by  $[\boldsymbol{\phi}^h, \mathbf{C}\boldsymbol{\psi}^h] \in V_{u,h}(\tilde{\Omega}_h) \times V_{\varepsilon,h}(\tilde{\Omega}_h)$ , integrate by parts the term  $(\nabla \cdot (\mathbf{C}\boldsymbol{\varepsilon}), \boldsymbol{\phi}^h)_{\tilde{\Omega}_h}$  and weakly enforce the Dirichlet boundary condition (19a) through the anti-symmetric form of Nitsche’s method, to obtain

$$\begin{aligned} 0 = & (\mathbf{C}\boldsymbol{\varepsilon}, \nabla^s \boldsymbol{\phi}^h)_{\tilde{\Omega}_h} - \langle (\mathbf{C}\boldsymbol{\varepsilon}) \tilde{\mathbf{n}}, \boldsymbol{\phi}^h \rangle_{\tilde{\Gamma}_{D,h}} - \langle (\mathbf{C}\boldsymbol{\varepsilon}) \tilde{\mathbf{n}}, \boldsymbol{\phi}^h \rangle_{\tilde{\Gamma}_{N,h}} - (\mathbf{b}, \boldsymbol{\phi}^h)_{\tilde{\Omega}_h} + (\boldsymbol{\varepsilon} - \nabla^s \mathbf{u}, \mathbf{C}\boldsymbol{\psi}^h)_{\tilde{\Omega}_h} \\ & + \langle S_{D,h} \mathbf{u} - \mathbf{u}_D, (\mathbf{C}\boldsymbol{\psi}^h) \tilde{\mathbf{n}} \rangle_{\tilde{\Gamma}_{D,h}} + \gamma \langle \rho_c h_{\perp}^{-1} (S_{D,h} \mathbf{u} - \mathbf{u}_D), S_{D,h} \boldsymbol{\phi}^h \rangle_{\tilde{\Gamma}_{D,h}}, \end{aligned} \quad (21)$$

where  $\gamma$  is a nondimensional positive constant, independent from the mesh size. In order to enforce the Neumann boundary condition on  $\tilde{\Gamma}_{N,h}$ , the unit normal vector  $\tilde{\mathbf{n}}$  in the term  $\langle (\mathbf{C}\boldsymbol{\varepsilon}) \tilde{\mathbf{n}}, \boldsymbol{\phi}^h \rangle_{\tilde{\Gamma}_{N,h}}$  can be decomposed as  $\tilde{\mathbf{n}} = (\tilde{\mathbf{n}} \cdot \mathbf{n}) \mathbf{n} + (\tilde{\mathbf{n}} \cdot \boldsymbol{\tau}^j) \boldsymbol{\tau}^j$ , where  $\boldsymbol{\tau}^j$  is a unit vector tangent to the true boundary surface (repeated index notation is implied). Substituting the traction condition (19b), adding and subtracting  $\langle (\mathbf{C}\boldsymbol{\varepsilon}) \mathbf{n}, (\tilde{\mathbf{n}} \cdot \mathbf{n}) \boldsymbol{\phi}^h \rangle_{\tilde{\Gamma}_{N,h}}$  then yields

$$\begin{aligned} 0 = & (\mathbf{C}\boldsymbol{\varepsilon}, \nabla^s \boldsymbol{\phi}^h)_{\tilde{\Omega}_h} - \langle (\mathbf{C}\boldsymbol{\varepsilon}) \tilde{\mathbf{n}}, \boldsymbol{\phi}^h \rangle_{\tilde{\Gamma}_h} - (\mathbf{b}, \boldsymbol{\phi}^h)_{\tilde{\Omega}_h} + (\boldsymbol{\varepsilon} - \nabla^s \mathbf{u}, \mathbf{C}\boldsymbol{\psi}^h)_{\tilde{\Omega}_h} \\ & + \langle (S_{N,h}(\mathbf{C}\boldsymbol{\varepsilon})) \mathbf{n} - \mathbf{t}_N, (\tilde{\mathbf{n}} \cdot \mathbf{n}) \boldsymbol{\phi}^h \rangle_{\tilde{\Gamma}_{N,h}} + \langle S_{D,h} \mathbf{u} - \mathbf{u}_D, (\mathbf{C}\boldsymbol{\psi}^h) \tilde{\mathbf{n}} \rangle_{\tilde{\Gamma}_{D,h}} \\ & + \gamma \langle \rho_c h_{\perp}^{-1} (S_{D,h} \mathbf{u} - \mathbf{u}_D), S_{D,h} \boldsymbol{\phi}^h \rangle_{\tilde{\Gamma}_{D,h}}. \end{aligned} \quad (22)$$

We also add a penalty term on the Neumann boundary,

$$\langle \tau_N \rho_c^{-1} ((S_{N,h}(\mathbf{C} \boldsymbol{\varepsilon})) \mathbf{n} - \mathbf{t}_N), (\tilde{\mathbf{n}} \cdot \mathbf{n})^2 (S_{N,h}(\mathbf{C} \boldsymbol{\psi}^h)) \mathbf{n} \rangle_{\tilde{\Gamma}_{N,h}}, \quad (23)$$

where  $\tau_N = c_N \bar{l}(\Omega)$ ,  $\bar{l}(\Omega)$  is the largest dimension of the bounding box of  $\Omega$ , and  $c_N$  is a nondimensional positive constant.

Observe that the chosen approximation spaces do not satisfy the inf-sup condition [27], a necessary and sufficient condition for stability of the numerical scheme. To circumvent this situation, we adopt a variational multiscale (VMS)[36, 63, 122] approach and add the term

$$\left( \tau_u \rho_c^{-1} (\nabla \cdot (\mathbf{C} \boldsymbol{\varepsilon}) + \mathbf{b}), \nabla \cdot (\mathbf{C} \boldsymbol{\psi}^h) \right)_{\tilde{\Omega}_h} - \left( \tau_\varepsilon (\boldsymbol{\varepsilon} - \nabla^s \mathbf{u}), \mathbf{C} (\boldsymbol{\psi}^h + \nabla^s \boldsymbol{\phi}^h) \right)_{\tilde{\Omega}_h} \quad (24)$$

to the discrete form of (22). In the numerical computations described in Section 5, we will take  $\gamma = 1$ ,  $\tau_\varepsilon = 1/2$ ,  $\tau_u = h_\tau \bar{l}(\Omega)$  and  $c_N = 1$ .

In summary, we obtain the SB variational formulation:

$$\text{Find } [\mathbf{u}^h, \boldsymbol{\varepsilon}^h] \in V_{u,h}(\tilde{\Omega}_h) \times V_{\varepsilon,h}(\tilde{\Omega}_h) \text{ such that, } \forall [\boldsymbol{\phi}^h, \boldsymbol{\psi}^h] \in V_{u,h}(\tilde{\Omega}_h) \times V_{\varepsilon,h}(\tilde{\Omega}_h),$$

$$\mathcal{B}_{\text{SBM}}^{[\tilde{\Omega}_h]}([\mathbf{u}^h, \boldsymbol{\varepsilon}^h]; [\boldsymbol{\phi}^h, \boldsymbol{\psi}^h]) = \mathcal{L}_{\text{SBM}}^{[\tilde{\Omega}_h]}([\boldsymbol{\phi}^h, \boldsymbol{\psi}^h]), \quad (25a)$$

where

$$\begin{aligned} \mathcal{B}_{\text{SBM}}^{[\tilde{\Omega}_h]}([\mathbf{u}, \boldsymbol{\varepsilon}]; [\boldsymbol{\phi}, \boldsymbol{\psi}]) &= \mathcal{B}_{\tilde{\Omega}_h}([\mathbf{u}, \boldsymbol{\varepsilon}]; [\boldsymbol{\phi}, \boldsymbol{\psi}]) + \mathcal{B}_{s;\tilde{\Omega}_h}([\mathbf{u}, \boldsymbol{\varepsilon}]; [\boldsymbol{\phi}, \boldsymbol{\psi}]) + \mathcal{B}_{\tilde{\Gamma}_{D,h}}([\mathbf{u}, \boldsymbol{\varepsilon}]; [\boldsymbol{\phi}, \boldsymbol{\psi}]) \\ &\quad + \mathcal{B}_{\tilde{\Gamma}_{N,h}}([\mathbf{u}, \boldsymbol{\varepsilon}]; [\boldsymbol{\phi}, \boldsymbol{\psi}]), \end{aligned} \quad (25b)$$

$$\mathcal{L}_{\text{SBM}}^{[\tilde{\Omega}_h]}([\boldsymbol{\phi}, \boldsymbol{\psi}]) = \mathcal{L}_{\tilde{\Omega}_h}([\boldsymbol{\phi}, \boldsymbol{\psi}]) + \mathcal{L}_{s;\tilde{\Omega}_h}([\boldsymbol{\phi}, \boldsymbol{\psi}]) + \mathcal{L}_{\tilde{\Gamma}_{D,h}}([\boldsymbol{\phi}, \boldsymbol{\psi}]) + \mathcal{L}_{\tilde{\Gamma}_{N,h}}([\boldsymbol{\phi}, \boldsymbol{\psi}]). \quad (25c)$$

with

$$\mathcal{B}_{\tilde{\Omega}_h}([\mathbf{u}, \boldsymbol{\varepsilon}]; [\boldsymbol{\phi}, \boldsymbol{\psi}]) = (\mathbf{C} \boldsymbol{\varepsilon}, \nabla^s \boldsymbol{\phi})_{\tilde{\Omega}_h} + (\boldsymbol{\varepsilon} - \nabla^s \mathbf{u}, \mathbf{C} \boldsymbol{\psi})_{\tilde{\Omega}_h}, \quad (25d)$$

$$\mathcal{B}_{s;\tilde{\Omega}_h}([\mathbf{u}, \boldsymbol{\varepsilon}]; [\boldsymbol{\phi}, \boldsymbol{\psi}]) = \left( \tau_u \rho_c^{-1} \nabla \cdot (\mathbf{C} \boldsymbol{\varepsilon}), \nabla \cdot (\mathbf{C} \boldsymbol{\psi}) \right)_{\tilde{\Omega}_h} - (\tau_\varepsilon (\boldsymbol{\varepsilon} - \nabla^s \mathbf{u}), \mathbf{C} (\boldsymbol{\psi} + \nabla^s \boldsymbol{\phi}))_{\tilde{\Omega}_h}, \quad (25e)$$

$$\mathcal{B}_{\tilde{\Gamma}_{D,h}}([\mathbf{u}, \boldsymbol{\varepsilon}]; [\boldsymbol{\phi}, \boldsymbol{\psi}]) = -\langle (\mathbf{C} \boldsymbol{\varepsilon}) \tilde{\mathbf{n}}, \boldsymbol{\phi} \rangle_{\tilde{\Gamma}_{D,h}} + \langle S_{D,h} \mathbf{u}, (\mathbf{C} \boldsymbol{\psi}) \tilde{\mathbf{n}} \rangle_{\tilde{\Gamma}_{D,h}} + \gamma \langle \rho_c h^{-1} S_{D,h} \mathbf{u}, S_{D,h} \boldsymbol{\phi} \rangle_{\tilde{\Gamma}_{D,h}}, \quad (25f)$$

$$\begin{aligned} \mathcal{B}_{\tilde{\Gamma}_{N,h}}([\mathbf{u}, \boldsymbol{\varepsilon}]; [\boldsymbol{\phi}, \boldsymbol{\psi}]) &= -\langle (\mathbf{C} \boldsymbol{\varepsilon}) \tilde{\mathbf{n}}, \boldsymbol{\phi} \rangle_{\tilde{\Gamma}_{N,h}} + \langle (S_{N,h}(\mathbf{C} \boldsymbol{\varepsilon})) \mathbf{n}, (\tilde{\mathbf{n}} \cdot \mathbf{n}) \boldsymbol{\phi} \rangle_{\tilde{\Gamma}_{N,h}} \\ &\quad + \langle \tau_N \rho_c^{-1} (S_{N,h}(\mathbf{C} \boldsymbol{\varepsilon})) \mathbf{n}, (\tilde{\mathbf{n}} \cdot \mathbf{n})^2 (S_{N,h}(\mathbf{C} \boldsymbol{\psi})) \mathbf{n} \rangle_{\tilde{\Gamma}_{N,h}}, \end{aligned} \quad (25g)$$

$$\mathcal{L}_{\tilde{\Omega}_h}([\boldsymbol{\phi}, \boldsymbol{\psi}]) = (\mathbf{b}, \boldsymbol{\phi})_{\tilde{\Omega}_h}, \quad (25h)$$

$$\mathcal{L}_{s;\tilde{\Omega}_h}([\boldsymbol{\phi}, \boldsymbol{\psi}]) = -\left( \tau_u \rho_c^{-1} \mathbf{b}, \nabla \cdot (\mathbf{C} \boldsymbol{\psi}) \right)_{\tilde{\Omega}_h}, \quad (25i)$$

$$\mathcal{L}_{\tilde{\Gamma}_{D,h}}([\boldsymbol{\phi}, \boldsymbol{\psi}]) = \langle \mathbf{u}_D, (\mathbf{C} \boldsymbol{\psi}) \tilde{\mathbf{n}} \rangle_{\tilde{\Gamma}_{D,h}} + \gamma \langle \rho_c h^{-1} \mathbf{u}_D, S_{D,h} \boldsymbol{\phi} \rangle_{\tilde{\Gamma}_{D,h}}, \quad (25j)$$

$$\mathcal{L}_{\tilde{\Gamma}_{N,h}}([\boldsymbol{\phi}, \boldsymbol{\psi}]) = \langle \mathbf{t}_N, (\tilde{\mathbf{n}} \cdot \mathbf{n}) \boldsymbol{\phi} \rangle_{\tilde{\Gamma}_{N,h}} + \langle \tau_N \rho_c^{-1} \mathbf{t}_N, (\tilde{\mathbf{n}} \cdot \mathbf{n})^2 (S_{N,h}(\mathbf{C} \boldsymbol{\psi})) \mathbf{n} \rangle_{\tilde{\Gamma}_{N,h}}. \quad (25k)$$

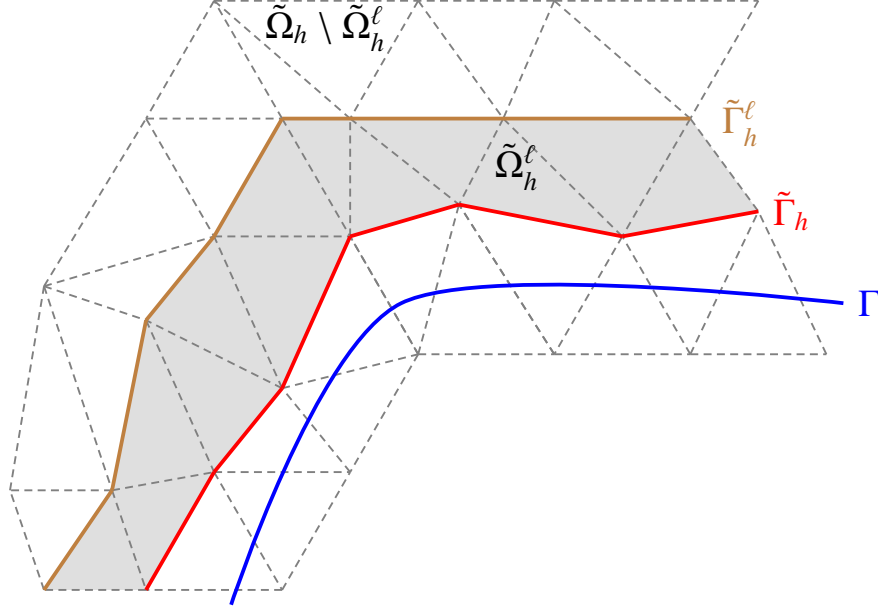


Figure 4: The true boundary  $\Gamma$  (blue), the surrogate boundary  $\tilde{\Gamma}_h$  (solid red), the set of elements with one node on the surrogate boundary  $\tilde{\Omega}_h^\ell$  (grey), the set of elements with no nodes on surrogate boundary  $\tilde{\Omega}_h \setminus \tilde{\Omega}_h^\ell$ , and the interface  $\tilde{\Gamma}_h^\ell$  (dashed red) between  $\tilde{\Omega}_h^\ell$  and  $\tilde{\Omega}_h \setminus \tilde{\Omega}_h^\ell$ .

### 3.4. The Shifted Boundary Method variational form

Solving the mixed form of the linear elasticity equations is often undesirable due to the increase in degrees of freedom and thus the associated computational cost. At the same time, a primal formulation with Neumann boundary conditions and  $\mathbf{u}^h \in V_{u,h}(\tilde{\Omega}_h)$  would lead to a first order accurate method. This can be clearly seen by replacing  $\boldsymbol{\sigma}(\nabla^s \mathbf{u}^h)$  for  $\boldsymbol{\sigma}(\boldsymbol{\varepsilon}^h)$  in (19b) whereby  $\nabla \boldsymbol{\sigma}(\nabla^s \mathbf{u}^h) = 0$ ,  $\forall \mathbf{u}^h \in V_{u,h}(\tilde{\Omega}_h)$ . This section introduces a strategy that significantly reduces the computational burden of solving the mixed system without jeopardizing the accuracy of our finite element displacement solution  $\mathbf{u}^h$ .

Recalling the definitions of  $\tilde{\Omega}_h$  and  $\tilde{\Gamma}_h$  in Section 3.1, we define  $\tilde{\Omega}_h^\ell$  as the set of elements  $\tilde{T} \subset \tilde{\Omega}_h$  with at least one node on  $\tilde{\Gamma}_h$  (see Figure 4), that is,

$$\tilde{\Omega}_h^\ell = \{\tilde{T} \subset \tilde{\Omega}_h : \tilde{T} \cap \tilde{\Gamma}_h \neq \emptyset\}. \quad (26)$$

The main idea is to restrict the mixed variational formulation (25a) to  $\tilde{\Omega}_h^\ell$ . In other words, (1) is restricted to  $\tilde{\Omega}_h^\ell$  while for the rest of the computational domain, namely  $\tilde{\Omega}_h \setminus \tilde{\Omega}_h^\ell$ , we solve the irreducible primal form the momentum equation  $-\nabla \cdot \boldsymbol{\sigma}(\nabla^s \mathbf{u}) = \mathbf{b}$ .

Overall, the governing equations in  $\tilde{\Omega}_h \setminus \tilde{\Omega}_h^\ell$  can thus be expressed as follows:

$$-\nabla \cdot \boldsymbol{\sigma}(\nabla^s \mathbf{u}) = \mathbf{b}, \quad \text{in } \tilde{\Omega}_h \setminus \tilde{\Omega}_h^\ell, \quad (27a)$$

$$\boldsymbol{\sigma}(\nabla^s \mathbf{u})^+ \mathbf{n}^+ + \boldsymbol{\sigma}(\boldsymbol{\varepsilon})^- \mathbf{n}^- = \mathbf{0}, \quad \text{on } \tilde{\Gamma}_h^\ell, \quad (27b)$$

where the "+" and "-" signs refer to the primal ( $\tilde{\Omega}_h \setminus \tilde{\Omega}_h^\ell$ ) and mixed ( $\tilde{\Omega}_h^\ell$ ) sides of the domain, respectively. Equation (27b) enforces continuity of the normal component of the stress across the interface  $\tilde{\Gamma}_h^\ell = \partial \tilde{\Omega}_h^\ell \setminus \tilde{\Gamma}_h$ . Obviously, the displacement field  $\mathbf{u}$  is continuous over  $\tilde{\Omega}_h$  and in particular

across  $\tilde{\Gamma}_h^\ell$ . Defining the discrete test functions as  $[\phi^h, \psi^h] \in V_{u,h}(\tilde{\Omega}_h) \times V_{\varepsilon,h}(\tilde{\Omega}_h^\ell)$ , multiplying (27a) by  $\phi^h|_{\tilde{\Omega}_h \setminus \tilde{\Omega}_h^\ell}$  and integrating by parts gives

$$\begin{aligned} (\sigma(\nabla^s \mathbf{u}), \nabla \phi^h)_{\tilde{\Omega}_h \setminus \tilde{\Omega}_h^\ell} - \langle \sigma(\nabla^s \mathbf{u})^+ \mathbf{n}^+, \phi^h \rangle_{\tilde{\Gamma}_h^\ell} = \\ (\mathbf{C} \nabla^s \mathbf{u}, \nabla \phi^h)_{\tilde{\Omega}_h \setminus \tilde{\Omega}_h^\ell} - \langle (\mathbf{C} \nabla^s \mathbf{u})^+ \mathbf{n}^+, \phi^h \rangle_{\tilde{\Gamma}_h^\ell} = (\mathbf{b}, \phi^h)_{\tilde{\Omega}_h \setminus \tilde{\Omega}_h^\ell}. \end{aligned} \quad (28)$$

Consider now the restriction of (1a) and (1b) to  $\tilde{\Omega}_h^\ell$ , multiplied by  $\phi^h|_{\tilde{\Omega}_h^\ell}$  and  $\psi^h$ , respectively. Following analogous derivations to the ones outlined in Section 3.3, we obtain

$$\mathcal{B}_{\text{SBM}}^{[\tilde{\Omega}_h^\ell]}([\mathbf{u}, \varepsilon]; [\phi^h, \psi^h]) - \langle (\mathbf{C} \varepsilon)^- \mathbf{n}^-, \phi^h \rangle_{\tilde{\Gamma}_h^\ell} = \mathcal{L}_{\text{SBM}}^{[\tilde{\Omega}_h^\ell]}([\phi^h, \psi^h]). \quad (29)$$

Adding (28) to (29) and enforcing (27b) gives the following final variational form:

$$\text{Find } [\mathbf{u}^h, \varepsilon^h] \in V_{u,h}(\tilde{\Omega}_h) \times V_{\varepsilon,h}(\tilde{\Omega}_h^\ell) \text{ such that, } \forall [\phi^h, \psi^h] \in V_{u,h}(\tilde{\Omega}_h) \times V_{\varepsilon,h}(\tilde{\Omega}_h^\ell),$$

$$\mathcal{B}_{\text{SBM}}([\mathbf{u}^h, \varepsilon^h]; [\phi^h, \psi^h]) = \mathcal{L}_{\text{SBM}}([\phi^h, \psi^h]), \quad (30a)$$

where

$$\mathcal{B}_{\text{SBM}}([\mathbf{u}, \varepsilon]; [\phi, \psi]) = (\mathbf{C} \nabla^s \mathbf{u}, \nabla \phi)_{\tilde{\Omega}_h \setminus \tilde{\Omega}_h^\ell} + \mathcal{B}_{\text{SBM}}^{[\tilde{\Omega}_h^\ell]}([\mathbf{u}, \varepsilon]; [\phi, \psi]), \quad (30b)$$

$$\mathcal{L}_{\text{SBM}}([\phi, \psi]) = (\mathbf{b}, \phi)_{\tilde{\Omega}_h \setminus \tilde{\Omega}_h^\ell} + \mathcal{L}_{\text{SBM}}^{[\tilde{\Omega}_h^\ell]}([\phi, \psi]). \quad (30c)$$

**Remark 3.** The formulation (30a) requires to solve the irreducible primal formulation over the major portion of the domain,  $\tilde{\Omega}_h \setminus \tilde{\Omega}_h^\ell$ , and to restrict the mixed variational formulation to a small layer of elements  $\tilde{\Omega}_h^\ell$  (one element deep) near the boundary  $\tilde{\Gamma}_h$ . Hence the mixed bilinear formulation can be understood as a gradient reconstruction technique, built to ensure optimal error convergence.

#### 4. Analysis of the SBM under Dirichlet boundary conditions

In atallah2021shifted, it was proved that, under suitable assumptions on the distance function  $\mathbf{d}$ , the bilinear form  $\mathcal{B}_{\text{SBM}}(\cdot; \cdot)$  is coercive for pure Dirichlet boundary conditions (i.e.,  $\tilde{\Gamma}_{N,h} = \emptyset$ ). This immediately implied the existence and uniqueness of the discrete solution of the SBM problem and was used to prove optimal convergence estimates in the natural (i.e., energy-type) SBM norm. We also proved an estimate of the  $L^2$ -norm of the displacement discretization error  $\mathbf{u} - \mathbf{u}_h$  based on the approach originally pursued in [8]. This is a summary of the main theoretical results that follow, and a reader less interested in the mathematical details can proceed directly to Section 5, where the numerical results are discussed.

#### 5. Numerical experiments

In this section, we conduct two- and three-dimensional numerical experiments. In the simulations presented next, unless otherwise specified, we set  $\gamma_{\text{bulk}} = \gamma_{\text{shear}} = 1$ ,  $\tau_\varepsilon = 1/2$ ,  $\tau_u = h \bar{l}(\Omega)$  and  $c_N = 1$ . These choices of parameters were already presented in Section 3.3. All the tests were

simulated on a cluster whose nodes are equipped with 24 Intel Xeon® E5-2670v3 2.3 GHz cores, connected by a Mellanox Switch X-2 Infiniband®. The algebraic system of equations is solved using the smoothed aggregation multigrid method in the ML Library, within the Trilinos Software Project [137] lead by Sandia National Laboratories.

### 5.1. Performance Assessment: Accuracy vs. computing time

To start, we present two accuracy tests, in two and three dimensions, respectively, in which the efficiency of the SBM is compared against a standard, body-fitted, FEM, relying on a primal displacement formulation with piecewise-linear interpolation spaces and strong boundary conditions. We compare only the time required to assemble and solve the algebraic systems of equations, and point the reader to Section 5.3 for a comparative analysis of the simulation setup time, required to acquire the geometrical information and build the appropriate data structures.

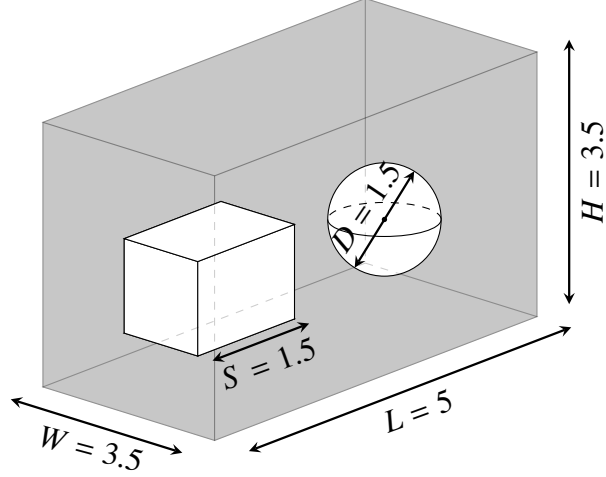
#### 5.1.1. Three-dimensional SBM performance test: A rectangular cuboid with holes

We consider here a three-dimensional non-convex domain with a boundary that includes smooth surfaces as well as sharp corners. As shown in Figure 5a, the linear isotropic elastostatics equations are computed in the domain  $\Omega = \Omega_1 \setminus (\Omega_2 \cup \Omega_3)$ , where  $\Omega_1$  is a rectangular cuboid centered at  $[0, 0, 0]$  of length  $L = 5$ , width  $W = 3.5$  and height  $H = 3.5$ ,  $\Omega_2$  is a cube of side of length  $S = 1.5$  and centered at  $[-1.25, 0, 0]$  and  $\Omega_3$  is a sphere centered at  $[1.25, 0, 0]$  with diameter  $D = 1.5$ . Consequently, we set  $\bar{l}(\Omega) = 5$  which is the longest dimension of the bounding box of  $\Omega$ . We consider the following manufactured solution

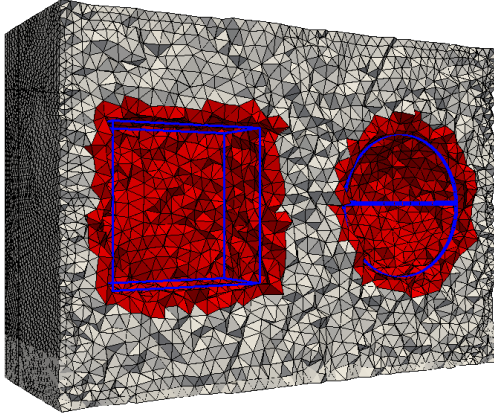
$$\mathbf{u} = \begin{Bmatrix} u_x \\ u_y \\ u_z \end{Bmatrix} = \frac{1}{10} \begin{Bmatrix} -\cos(\pi x) \sin(\pi y) \cos(\pi z) \\ \sin(\pi x/7) \sin(\pi y/3) \cos(\pi z/5) \\ \sin(\pi xyz/2) \end{Bmatrix}, \quad (31)$$

with a Young's modulus  $E = 200 \cdot 10^6$  MPa and a Poisson's ratio  $\nu = 0.3$ . We apply again the method of manufactured solutions to find an appropriate forcing  $\mathbf{b}$  in (1). Figure 5b depicts, on a coarse grid, the surrogate domain, the surrogate boundary, and the layer of elements  $\tilde{\Omega}_h^\ell$  attached to the surrogate boundary, used in the SBM formulation (30). In this test, the boundary  $\partial\Omega_2 \cup \partial\Omega_3$  are immersed while  $\partial\Omega_1$  is body-fitted. Dirichlet boundary conditions are strongly enforced on  $\partial\Omega_1$ , while Neumann boundary conditions are enforced on  $\partial\Omega_2 \cup \partial\Omega_3$  using the SBM approach. Also in this case, computations are performed on a single computing core, since both the SBM and the body-fitted FEM utilize the same procedures for parallelization, and a comparative study of parallel scalability is beyond the scope of this project.

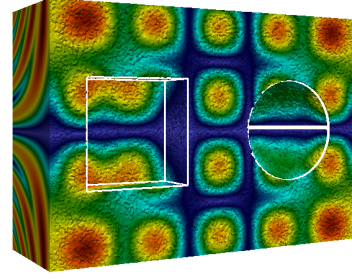
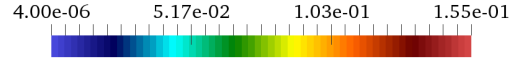
Figure 5d shows that optimal  $L_2$ -convergence rates for the displacement is obtained using formulation (30) despite the theoretical estimate of  $3/2$  in [11]. Note that, the SBM  $L_2$ -displacement error is lower than its body-fitted counterpart. This can be attributed to the slightly poorer mesh quality of the body-fitted meshes that are automatically generated to fit the boundaries. With respect to the corresponding SBM background grids, the body-fitted meshes have at least 1.5 times more elements with a ratio of the circumscribed/inscribed sphere diameters larger than two. This also seem to affect the overall computing time of the primal body-fitted FEM, as observed in Figure 5e: The SBM and body-fitted FEM have virtually the same rate and constant in the plot of the error versus computing time. This indicates that, for a desired level of accuracy, the SBM and the body-fitted FEM require the same computing time.



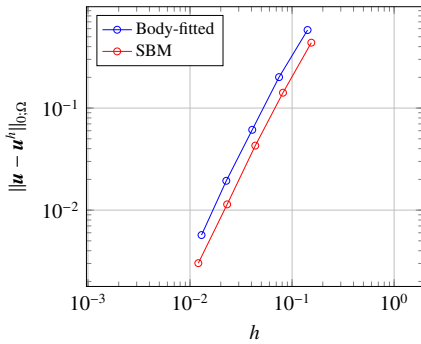
(a) Geometric setup of the problem (domain  $\Omega$  and dimensions).



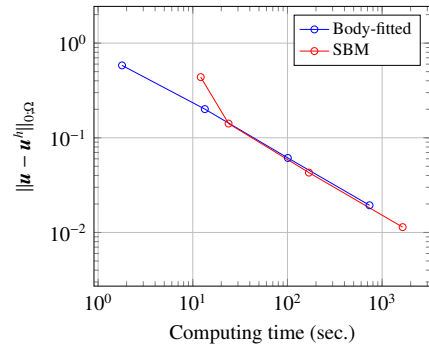
(b) Display of the surrogate domain  $\tilde{\Omega}_h$  (grey and red), the true boundary  $\Gamma$ , and the layer  $\tilde{\Omega}_h^\ell$  (red) for the SBM.



(c) Displacement magnitude.



(d)  $L^2$ -error convergence for the SBM formulation (30) and a body-fitted primal formulation.



(e)  $L^2$ -error vs. computing time for the SBM formulation (30) and a body-fitted primal formulation.

Figure 5: Three-dimensional test: Problem setup, displacement magnitude, convergence rates and computing times for the SBM formulation (30). Results with a primal body-fitted FEM with strong boundary conditions are plotted for reference.

This test, despite its simplicity, is very important for understanding the performance of the SBM formulation with respect to a standard FEM formulation in practical applications. In a body-fitted grid, some nodes must lie on the boundaries, and this constraint inevitably has an effect on the mesh quality, and ultimately the overall computational efficiency of the algebraic solve. This trend is more pronounced for grids of larger size, often required in practical large-scale simulations.

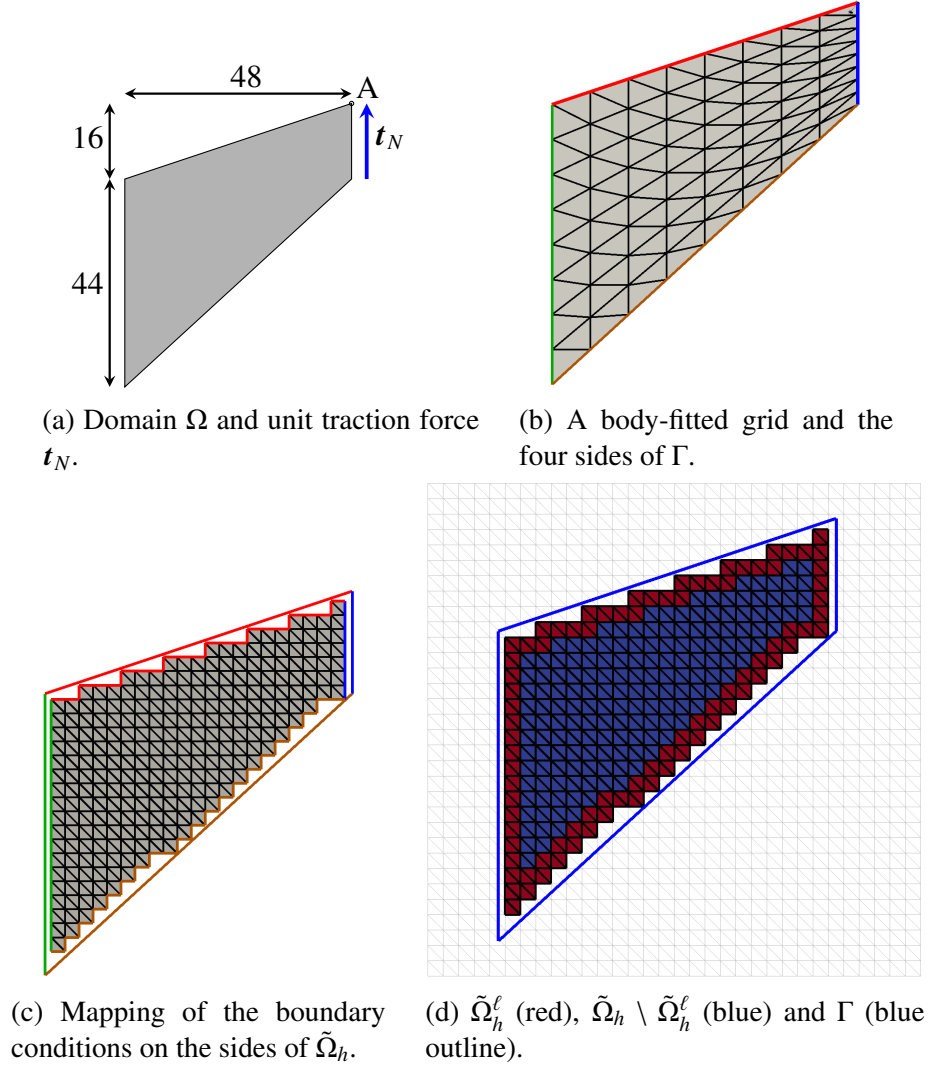
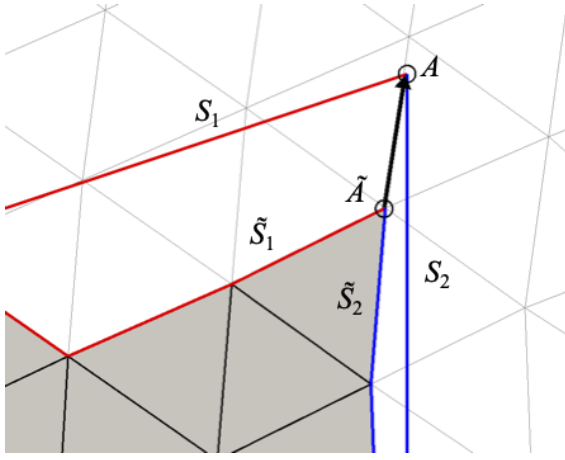
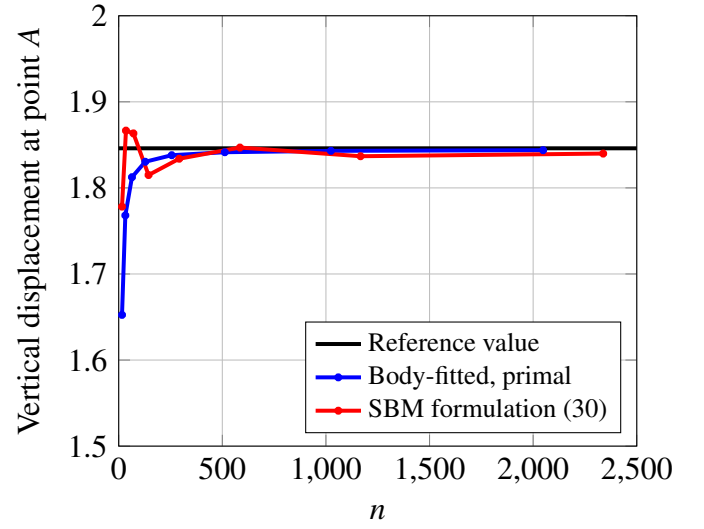


Figure 6: Setup of the Cook's membrane problem, with depiction of the true domain  $\Omega$  and surrogate domain  $\tilde{\Omega}_h$ , true boundary  $\Gamma$  and surrogate boundary  $\tilde{\Gamma}_h$ , the layer of  $\tilde{\Omega}_h^\ell$ , and the mapping between surrogate and true sides of the boundary.

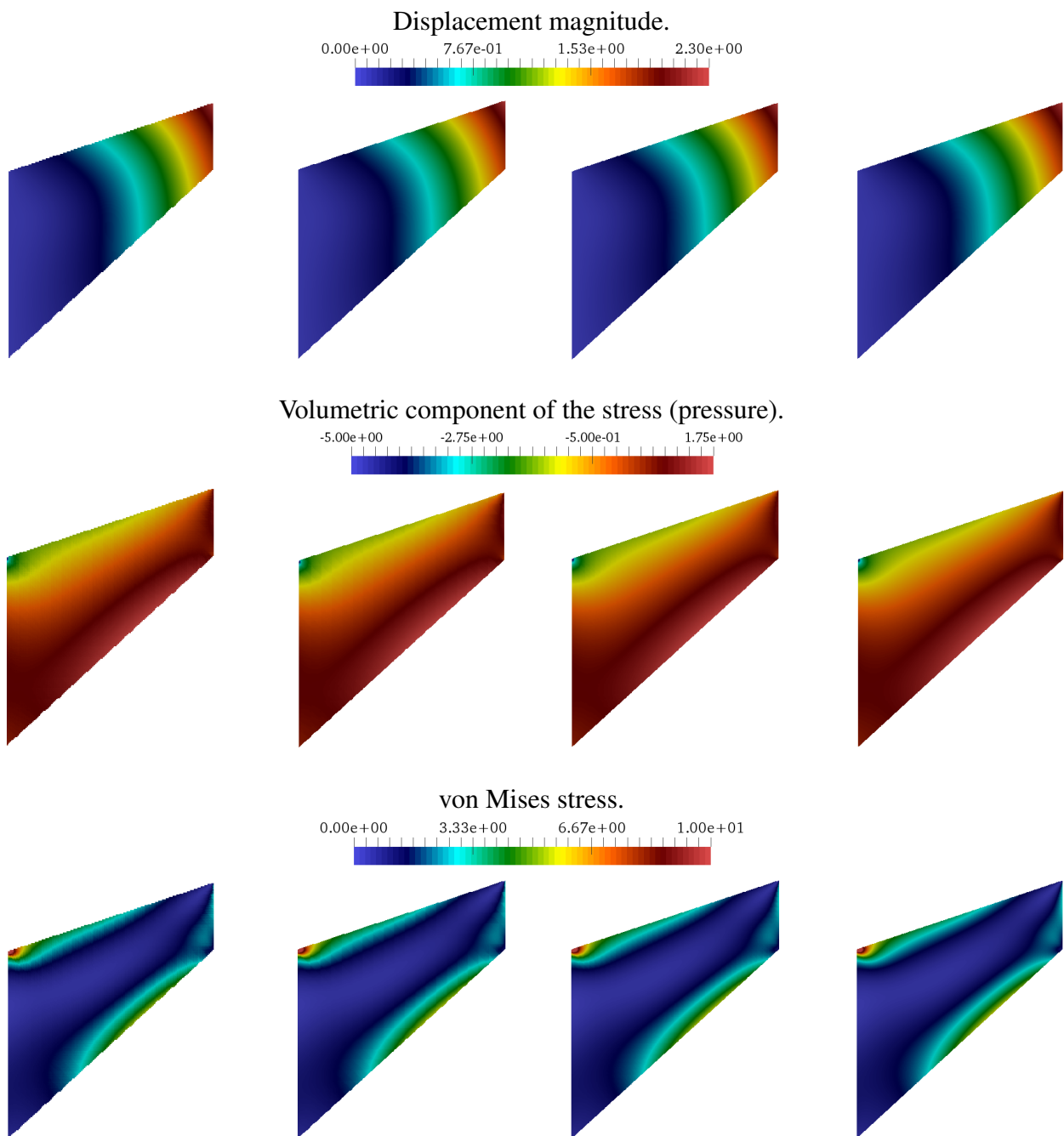


(a) Point A, at the top right corner of the Cook's membrane, and its corresponding surrogate node  $\tilde{A}$ , the sidesets  $S_1$ (red) and  $S_2$ (blue) on the true boundary and the corresponding surrogate sidesets  $\tilde{S}_1$  and  $\tilde{S}_2$  on the surrogate boundary.



(b) Vertical displacement at point A, where  $n$  is the total number of edges along  $S_1 \cup S_2$ , for the primal body-fitted formulation, or the total number of edges along  $\tilde{S}_1 \cup \tilde{S}_2$ , for the SBM formulation (30).

Figure 7: Left: Point A at the tip of the true boundary (top right corner) and the corresponding surrogate node  $\tilde{A}$ . Right: plots of the vertical displacement at point A for a primal body-fitted formulation and the enhanced SBM formulation (30). In the case of the SBM, the displacement at A is estimated from the displacement at  $\tilde{A}$  using (32).



37,842 active elements. 152,424 active elements. 613,084 active elements. 2,458,874 active elements.

Figure 8: Cook's membrane test, mesh refinement study: displacement magnitude, volumetric component of the stress, von Mises stress.

### 5.2. Two-dimensional Cook's membrane test

To test the SBM formulation (30) under a combined shear/bending behavior, we adapted the Cook's membrane test [36, 127] under a state of plane strain with Young's modulus  $E = 200 \cdot 10^9$  Pa and Poisson's ratio  $\nu = 0.3$ . The geometry is presented in Figure 6a and thus set  $\tilde{l}(\Omega) = 60$  which is the longest dimension of the bounding box of  $\Omega$ . A homogeneous Dirichlet boundary condition on the displacement is applied to the left side of the boundary (depicted in green, in Figure 6b), a unit tangential traction (Neumann) condition is applied on the right side (in blue, in Figure 6b) and traction-free (Neumann) boundary conditions are imposed on the top and bottom boundaries (in red and brown, in Figure 6b). Figure 6c depicts the surrogate domain  $\tilde{\Omega}_h$  and the layer of elements  $\tilde{\Omega}_h^\ell$ , for a coarse grid. Finally, Figure 6d displays how each of the sides of the true boundary maps to a corresponding sideset of the surrogate boundary (using again the color scheme green-red-blue-brown).

For the SBM simulations, we adopted eight levels of refinement of a structured grid of the type shown in Figure 6c. Similar refinements were considered for the body fitted FEM, for grids of the type depicted in Figure 6b.

The convergence of the tip displacement of the Cook's membrane (i.e., the displacement of point A in Figure 7a) is shown for the SBM formulation (30), the body-fitted formulation, and a reference solution computed on a very fine grid in Figure 7b.

While this computation is straightforward in the body-fitted case, the same cannot be said for a SBM formulation, due to the mismatch between the background mesh and the actual geometry. In the SBM case, we find the surrogate node  $\tilde{A}$  (corresponding to the tip node A) as the node lying at the intersection between the two sideset associated with the vertical traction and traction-free conditions (see Figure 7a), and then we extrapolate the solution's displacement from  $\tilde{A}$  to A according to the formula

$$u_y|_A = \frac{1}{n_A} \sum_{i=1}^{n_A} (u_y^{(i)} + \nabla u_y^{(i)} \mathbf{d})|_{\tilde{A}}, \quad (32)$$

where  $n_A$  is the total number of elements in  $\tilde{\Omega}_h$  attached to node  $\tilde{A}$ , and  $u_y^{(i)}|_{\tilde{A}}$  is the vertical displacement in element  $i$  evaluated at  $\tilde{A}$ . The results in Figure 7b show that the SBM formulation (30) is at least as accurate as its primal body-fitted counterpart for comparable mesh sizes.

Figure 8 shows the SBM numerical solution for the four finest level of refinement of the embedded grids. In particular, the first row of plots shows the magnitude of the displacement field, the second row of plots shows the Volumetric component of the stress (pressure), and the third row of plots shows the Frobenius norm of the deviator of the stress ( $J_2$ ), that is a non-normalized version of the von Mises stress. Both the displacement and stress fields are stable, smooth and free from spurious oscillations.

### 5.3. Three-dimensional, complex-geometry simulations

We consider next three tests with geometries that are progressively challenging for existing body-fitted mesh generation tools, and are representative of typical computational scenarios in the study of solid micro-structure, in biomedical design, and in geomechanics.

Table (1) shows the setup times for each of the three-dimensional tests. The SBM setup time includes the time it takes to: a) compute intersections between the STL surface that defines the

boundary and the background grid; b) generate the surrogate domain and boundaries; and c) calculate the distance vector  $\mathbf{d}$  along the surrogate boundary. To have a reference, the SBM setup time must be compared with the time it takes, in a body-fitted computation, to convert STL to CAD format, including geometry cleanup operations, and the time it takes to mesh the geometry.

| Geometry                      | No. elements | No. active elements | No. cores | No. true surface facets | setup time (s) |
|-------------------------------|--------------|---------------------|-----------|-------------------------|----------------|
| Sponge (Section (5.3.1))      | 11,498,942   | 5,758,480           | 288       | 138,078                 | 77             |
| Stent (Section (5.3.2))       | 66,023,424   | 10,303,826          | 600       | 46,484                  | 91             |
| Porous rock (Section (5.3.3)) | 5,229,000    | 3,458,639           | 240       | 112,629                 | 217            |

Table 1: Setup times for the three-dimensional tests.

Observe that the setup time for the porous rock problem is higher - in a relative sense - than the other problems. This is due to the fact that the rock surface is obtained from segmenting a CT-scan image, which contains several geometric artifacts. In particular, some disconnected pockets are present on the rock surface and need to be removed in a preprocessing phase. We point out that this initial geometry cleanup phase is completely automated and parallelized, as opposed to the typical geometry cleanup in body-fitted grids and/or CAD models, which requires the direct intervention of the user.

In any case, since all setup times fall below 4 minutes, it is fair to state that the setup phase for the SBM is smaller, by one to two orders of magnitude, than the typical, current setup times required by CAD and body-fitted grid generation tools.

For all tests described below, the material is isotropic elastic with bulk and shear moduli equal to 1 GPa and 100 MPa, respectively. The corresponding Poisson ratio is  $14/31 (\approx 0.452)$ .

All computational results were obtained using the SBM formulation (30). Note also that the stresses shown in the figures are obtained from the displacement gradients as piecewise constant elemental quantities.

#### 5.3.1. *Sponge-like solid*

In this section, we consider a domain with a sponge-like geometry [139], shown at the top left of Figure 9, as a representative of microstructures in porous media, weaved materials, and the like. The computational domain is the box  $\Omega = [-10, -10] \times [-10, -10] \times [-10, 6] \text{ mm}^3$  with the surrogate boundary is shown at the top right of Figure 9.

The displacement on the left side surface is set to  $\mathbf{u}^T = \{-0.04, 0.0, 0.0\} \text{ mm}$ , while the solid is clamped ( $\mathbf{u} = \mathbf{0}$ ) at the opposite surface (not seen). Traction-free boundary conditions are imposed elsewhere.

Numerical results, in terms of the magnitude of displacements, the volumetric stress, and von Mises stresses are shown in the three bottom rows of Figure 9. The smoothness of the computed fields indicates that the SBM can robustly address solid mechanics applications across very complex geometries and in scenarios beyond the hypotheses of applicability of the theoretical analysis discussed in Section 4.

### 5.3.2. Stent specimen

As a prototypical geometry from biomedical applications, we consider here the stent [1] shown in Figure 10. The computational domain is immersed in a hollow cylindrical mesh with the surrogate boundary shown at the top right of Figure 10.

The displacement on the right end surface (not seen in Figure 10) is set to

$$\mathbf{u} = \{2.5y \text{ mm}, -2.5x \text{ mm}, -0.5\text{mm}\}^T,$$

while the solid is clamped ( $\mathbf{u} = \mathbf{0}$ ) at the opposite surface. Traction-free boundary conditions are imposed elsewhere.

Numerical results, in terms of the magnitude of displacements, the volumetric stress, and von Mises stresses are shown in the three bottom rows of Figure 10, and are again characterized by a smooth behavior.

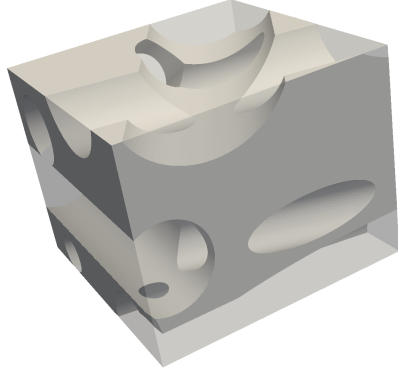
### 5.3.3. Porous rock

Finally, we consider a domain with a geometry that has been obtained via imaging techniques [2]. As shown at the top left of Figure 11, we consider a sample of a porous rock, that is the domain  $\Omega = [0, 0.3] \text{ mm} \times [0, 0.5] \text{ mm} \times [0.2, 0.47] \text{ mm}$ , that has been subdivided in voxels of size  $8.33 \cdot 10^{-3} \text{ mm} \times 8.33 \cdot 10^{-3} \text{ mm} \times 8.33 \cdot 10^{-3} \text{ mm}$ , by CT-scan techniques. The voxel representation of the sample has then been segmented, to represent the interface between the rocks and the voids in STL format (i.e., a set of disconnected triangular facets, which do not necessarily combine to form a water-tight surface).

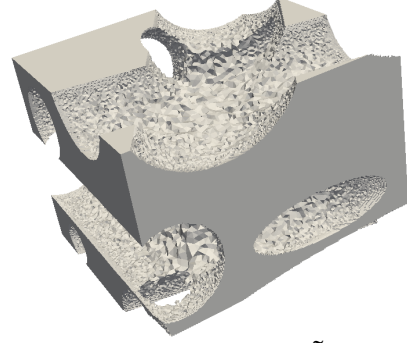
The displacement on the top side surface is set to  $\mathbf{u} = \{0.0\text{mm}, -5.4 \cdot 10^{-4}\text{mm}, 0.0\text{mm}\}^T$ , while the solid is clamped ( $\mathbf{u} = \mathbf{0}$ ) at the bottom surface. Traction-free boundary conditions are imposed elsewhere.

As apparent, the geometric features of this problem include a large number of fissures, holes and cracks which make body-fitted meshing very challenging, particularly since the (computational) interface rock/void is not water tight. It is in this situations that the power of an immersed/embedded solid mechanics method becomes clear, since the intersection of the interface solid/void with the background grid is an operation that is inherently parallelizable and much more robust and efficient than body-fitted mesh generation.

Numerical results are computed using the SBM formulation (30) over the surrogate domain shown at the top right of Figure 11. The three bottom rows of Figures 11 display the displacement magnitude, volumetric stress, and von Mises stress, respectively. Much like in the previous three-dimensional tests, the numerical solution is smooth and well-behaved, indicating that the SBM can serve as a valuable tool in the emerging imaging-to-computing field.



Geometry of the sponge-like domain  $\Omega$ .



Surrogate domain  $\tilde{\Omega}_h$ .

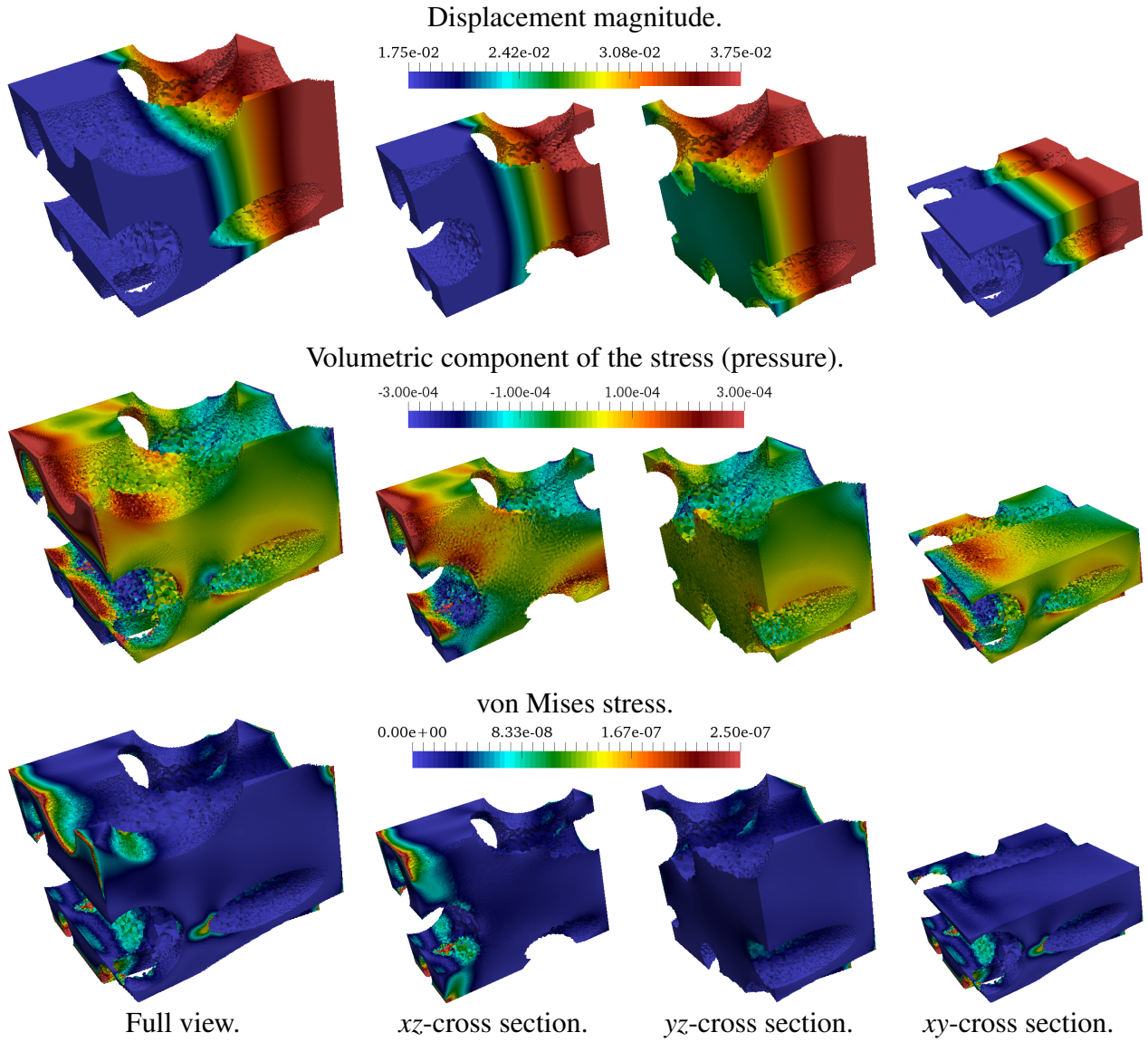
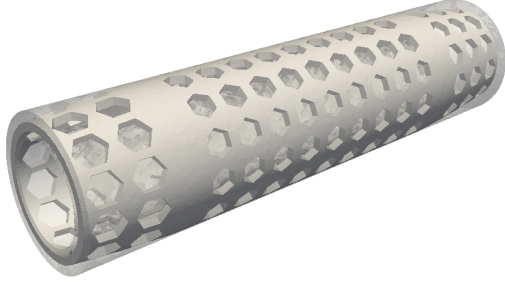
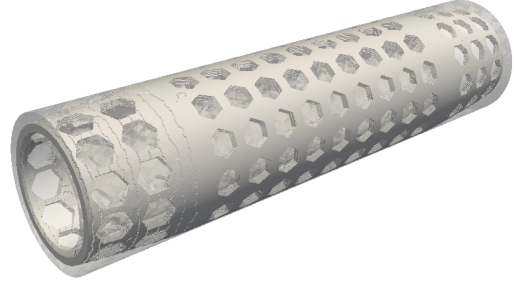


Figure 9: Sponge-like domain test. The geometry of the true domain  $\Omega$ , the surrogate domain  $\tilde{\Omega}_h$ , and contours of the displacement magnitude, the volumetric (pressure) stress and the von Mises stress, for various cross-sections (mid-planes).

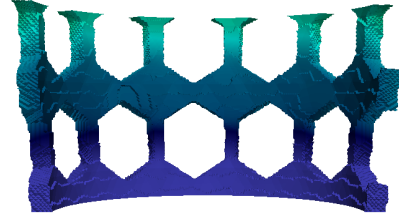
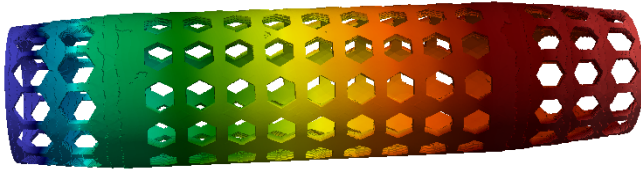
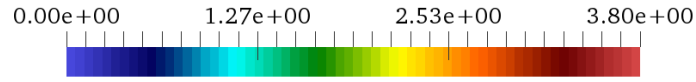


Geometry of the domain  $\Omega$ .

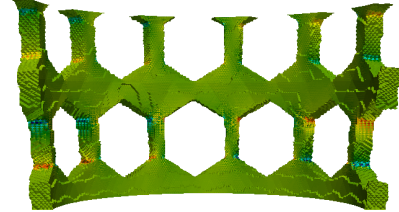
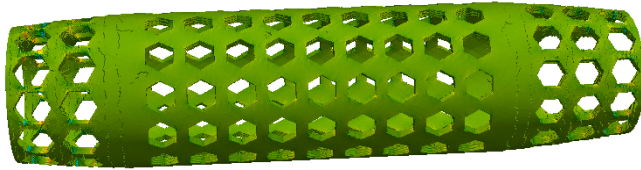
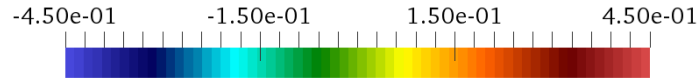


Surrogate domain  $\tilde{\Omega}_h$ .

Displacement magnitude.



Volumetric component of the stress (pressure).



von Mises stress.

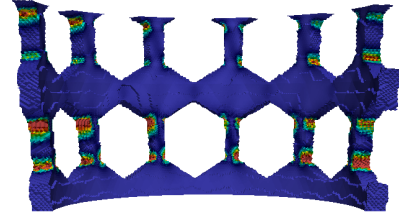
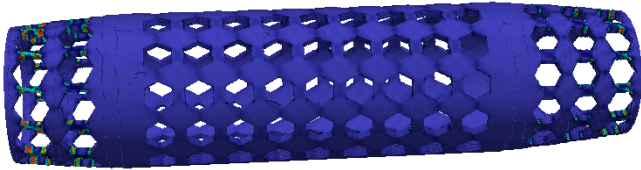
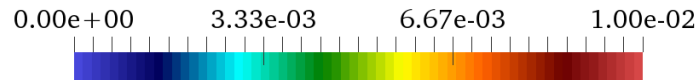
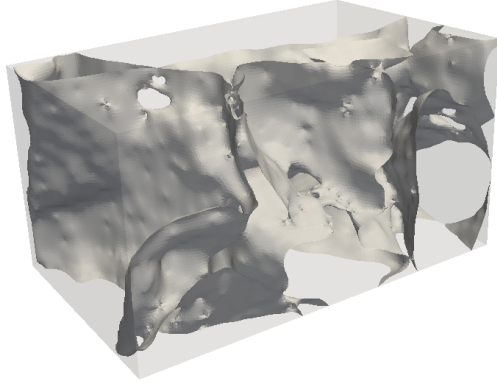
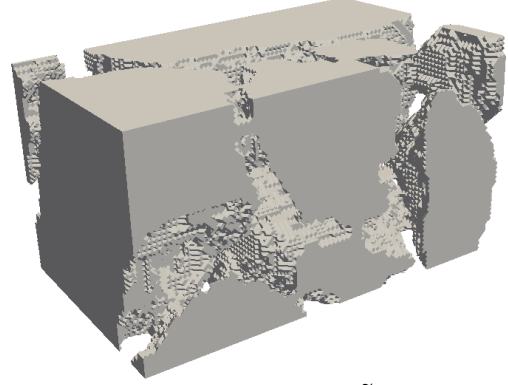


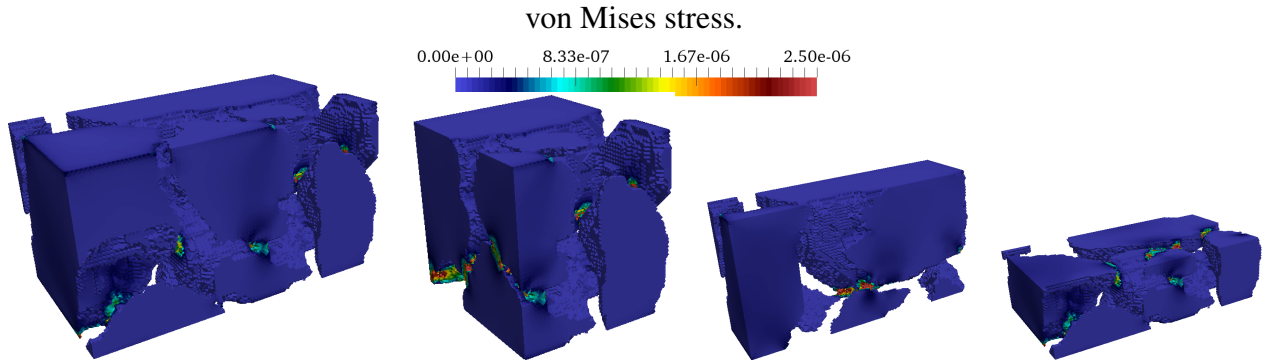
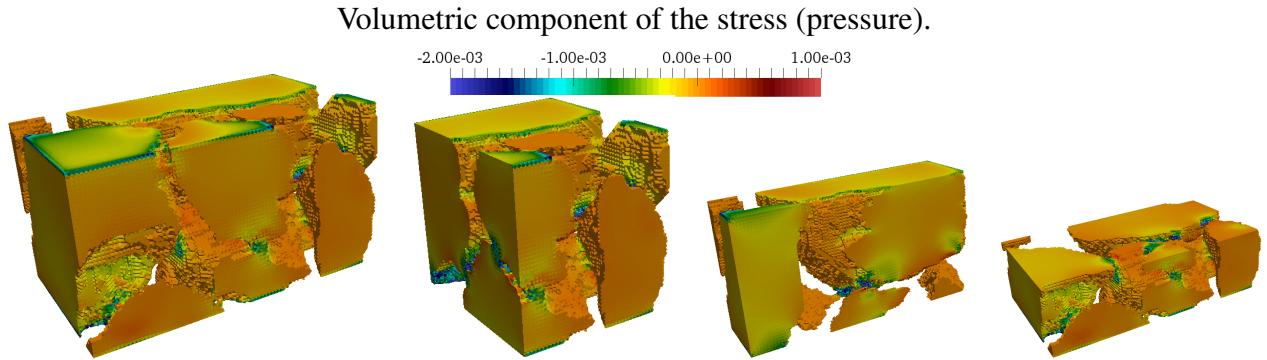
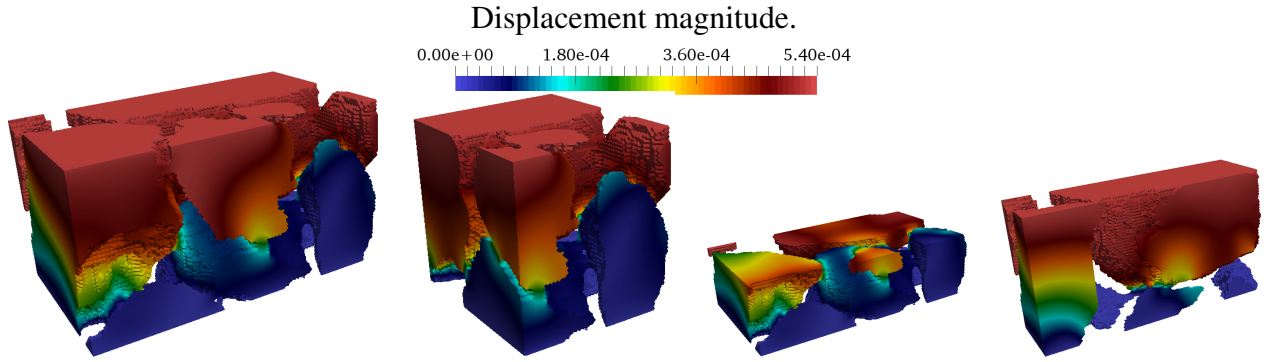
Figure 10: Stent domain test. The geometry of the true domain  $\Omega$ , the surrogate domain  $\tilde{\Omega}_h$ , and contours of the displacement magnitude, the volumetric (pressure) stress and the von Mises stress, and a close-up view on high-stress regions.



Geometry of the porous rock domain  $\Omega$ .



Surrogate domain  $\tilde{\Omega}_h$ .



Full view.

$xz$ -cross section.

$yz$ -cross section.

$xy$ -cross section.

Figure 11: Porous rock domain test. The geometry of the true domain  $\Omega$ , the surrogate domain  $\tilde{\Omega}_h$ , and contours of the displacement magnitude, the volumetric (pressure) stress and the von Mises stress, for various cross-sections (mid-planes).

## 6. The Shifted Fracture Approach

### 6.1. A cohesive approach to fracture propagation

We consider fracture propagation problems in linearly elastic solids under the assumption that a *cohesive law* governs the Fracture Process Zone (FPZ). This scenario is typical of cases in which linear elastic fracture mechanics (LEFM) is not applicable, that is when the FPZ at the crack tip is *not* small compared to the size of the crack and the size of the specimen [17]. Cohesive laws have been pioneered in the works of Dugdale [52], Barenblatt [15] and Hillerborg [62], and rely on traction-displacement relations on the portion of the crack faces inside the FPZ to propagate fractures.

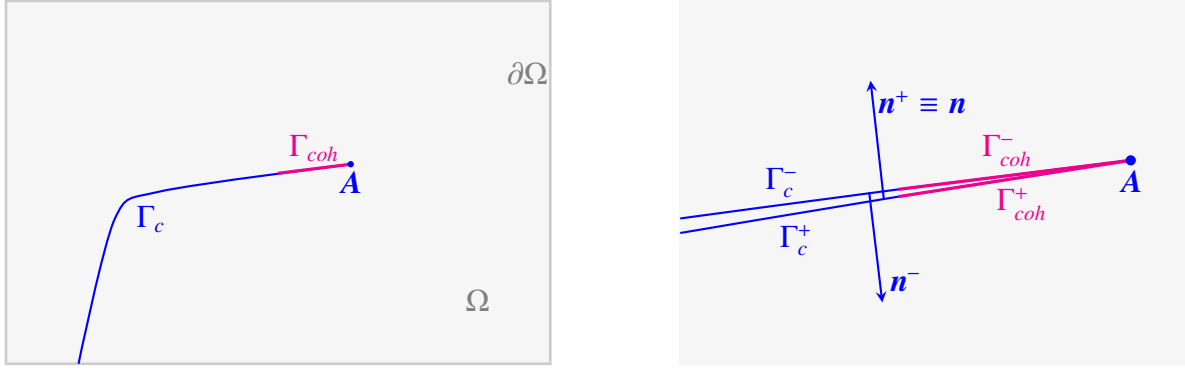


Figure 12: The (true) fracture path  $\Gamma_c$ , the cohesive zone  $\Gamma_{coh}$ , and the fracture tip  $A$ . A zoomed view in the vicinity of the crack tip is presented on the right.

Geometrically, a fracture can be described as an embedded interface as depicted in Figure 12. There,  $\Omega$  is a connected open set in  $\mathbb{R}^d$  with Lipschitz boundary  $\partial\Omega$  (where  $d = 2, 3$  indicates the number of spatial dimensions),  $\Gamma_c$  is the fracture interface,  $\Gamma_{coh}$  is the cohesive zone (the part of  $\Gamma_c$  where cohesive tractions are different from zero), and  $A$  is the crack tip.

We consider a cohesive zone model that is commonly adopted in many computational approaches to fracture mechanics (see, e.g., [84] for its application in the XFEM). In particular, we consider a generalized approach that encompasses Mode I and Mode II fracture propagation by means of a constitutive relation between an equivalent traction and an equivalent fracture opening [32, 46, 53, 78, 98, 138]. The discussion that follows should not be considered as restricted to the particular cohesive zone model chosen, but can easily be generalized to virtually any cohesive zone model.

Consider the crack faces (i.e., the opposite surfaces of the crack on  $\Gamma_c$  shown in the right panel of Figure 12) and their respective normals  $\mathbf{n}^+$  and  $\mathbf{n}^-$ , such that  $\mathbf{n}^+ = -\mathbf{n}^- = \mathbf{n}$ . A cohesive zone model relies on the definition of *cohesive tractions*  $\mathbf{t}^+$  and  $\mathbf{t}^-$  on the faces of the crack inside the cohesive zone  $\Gamma_{coh}$ . Outside the cohesive zone, that is over the set  $\Gamma_c \setminus \Gamma_{coh}$ , the cohesive tractions take the zero value. Hence, the cohesive zone model enforces the traction boundary condition

$$\mathbf{t} = \mathbf{t}_{coh}(\mathbf{w}) \quad \text{on } \Gamma_c, \quad (33)$$

with  $\mathbf{t}_{coh} = \mathbf{0}$  on  $\Gamma_c \setminus \Gamma_{coh}$ , where the *crack opening*  $\mathbf{w} = \mathbf{w}(\mathbf{u})$  along  $\Gamma_c$  is defined as

$$\mathbf{w}(\mathbf{u}) = \mathbf{u}^- - \mathbf{u}^+ = \llbracket \mathbf{u} \rrbracket, \quad (34)$$

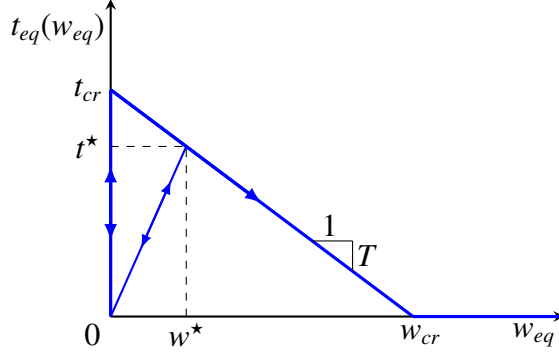


Figure 13: The cohesive law  $t_{eq}(w_{eq})$ .

in which  $[[\chi]] = \chi^- - \chi^+$  is the jump function. Note that the cohesive tractions must equilibrate, that is

$$\mathbf{t} \equiv \mathbf{t}^+ = \boldsymbol{\sigma}(\boldsymbol{\varepsilon})^+ \cdot \mathbf{n}^+ = -\boldsymbol{\sigma}(\boldsymbol{\varepsilon})^- \cdot \mathbf{n}^- = -\mathbf{t}^- \quad \text{on } \Gamma_c. \quad (35)$$

The traction  $\mathbf{t}_{coh}$  can be decomposed into a normal and tangential component, namely

$$\mathbf{t}_{coh} = t_n \mathbf{n} + t_s \boldsymbol{\tau}, \quad (36a)$$

$$t_n = \mathbf{t}_{coh} \cdot \mathbf{n}, \quad (36b)$$

$$t_s = \mathbf{t}_{coh} \cdot \boldsymbol{\tau}, \quad (36c)$$

where  $t_n$  is the component of the traction normal to the fracture surface and  $t_s$  is the component of the traction tangent to the fracture (the sliding component, along a unit vector  $\boldsymbol{\tau}$  that is given as a linear combination of the unit vectors  $\boldsymbol{\tau}_i$ , for  $i = 1, \dots, d-1$ ). Similarly, the crack opening  $\mathbf{w}(\mathbf{u})$  can be decomposed as

$$\mathbf{w}(\mathbf{u}) = w_n \mathbf{n} + w_s \boldsymbol{\tau}, \quad (37a)$$

$$w_n = \mathbf{w}(\mathbf{u}) \cdot \mathbf{n}, \quad (37b)$$

$$w_s = \mathbf{w}(\mathbf{u}) \cdot \boldsymbol{\tau}. \quad (37c)$$

In the generalized cohesive models described in [53, 98, 138], an equivalent crack opening  $w_{eq}$  is introduced, and defined as

$$w_{eq} = \sqrt{w_n^2 + \beta^2 w_s^2}, \quad (38)$$

where  $\beta$  is a model parameter. The normal and sliding component of the traction are then expressed as

$$t_n = t_{eq}(w_{eq}) \frac{w_n}{w_{eq}}, \quad (39a)$$

$$t_s = \beta^2 t_{eq}(w_{eq}) \frac{w_s}{w_{eq}}, \quad (39b)$$

where these expressions are motivated by considerations on the energetic consistency of the constitutive model. The complete specification of the cohesive zone model involves the definition of the function  $t_{eq}(w_{eq})$ , which in our case is given as [53, 138]

$$t_{eq}(w_{eq}) = \begin{cases} t_{cr} - Tw_{eq} & \text{for } 0 < w_{eq} = w^* < w_{cr}, \dot{w}^* > 0, \\ \frac{t^*}{w^*} w_{eq}, & \text{for } 0 \leq w_{eq} < w^* < w_{cr}, \dot{w}^* = 0, \\ 0, & \text{for } w_{eq} \geq w_{cr}, \end{cases} \quad (39c)$$

and is graphically depicted in Figure 13. The extent of the cohesive zone is implicitly defined by way of a critical crack opening parameter  $w_{cr}$ , used in the definition of the cohesive traction  $t_{coh}$ . The interpretation of the cohesive law function  $t_{eq}(w_{eq})$  is as follows: the traction force follows a rigid response until the value  $t_{cr}$  is reached (the vertical segment from the origin to the point  $(0, t_{cr})$  in Fig. 13), at which point the crack faces are allowed to separate ( $w_{eq} > 0$ ) and the cohesive traction follows the line  $t_{cr} - Tw_{eq}$  (i.e., the cohesive branch). Note also that  $T = t_{cr}/w_{cr} > 0$  is the magnitude of the (negative) slope of the linear profile of the cohesive traction law and that, by definition,  $t_{eq}(w_{eq}) \geq 0$ , which implies that the cohesive traction acts to close the fracture opening. In particular, the state  $w \geq w_{cr}$ , for which  $t_{eq}(w_{eq}) = 0$ , corresponds to points on  $\Gamma_c \setminus \Gamma_{coh}$ . Hence, the range of values  $0 < w < w_{cr}$ , for which  $t_{eq}(w_{eq}) > 0$ , implicitly defines  $\Gamma_{coh}$ . In the case in which unloading occurs in the cohesive zone, a history variable  $w^*$  tracks the largest (equivalent) crack opening achieved at a point on the crack surface, and the unloading/reloading occurs along the line  $(t^*/w^*)w_{eq}$ , which is also called the unloading/reloading branch (see again Fig. 13).

The boundary value problem associated with crack propagation involves the solution of (1) under the elastic constitutive law (2), the (outer) boundary conditions and the fracture interface conditions (33). We also define the fracture energy

$$G_F = \int_0^{w_{cr}} t_{eq}(w_{eq}) dw, \quad (40)$$

which collapses to  $G_F = t_{cr}w_{cr}/2$  for the model at hand.

**Remark 4.** A well-known drawback of the model presented here is its inability to prevent the interpenetration of the crack faces (i.e., a negative crack opening  $w$ ). Hence, the reader should not take this model too literally, but consider it instead as an example in the much broader realm of application of the shifted fracture approach.

**Remark 5.** Note that, for some cohesive zone models, the cohesive zone  $\Gamma_{coh}$  extends over the entire crack surface  $\Gamma_c$ , that is  $\Gamma_c \setminus \Gamma_{coh} = \emptyset$ . This is the case, for example, when the cohesive law has an exponential scaling, that is  $t_{eq}(w_{eq}) = t_{cr}e^{-w_{eq}/w_{cr}}$ . The discussion that follows on the shifted fracture approach can easily be adapted to this case, and other variations on this theme.

## 6.2. Variational equations

We consider now a general variational formulation in the context of the infinite-dimensional solution spaces

$$\mathcal{S}_u(\Omega \setminus \Gamma_c) = \left\{ \mathbf{v} \in \left( H^1(\Omega \setminus \Gamma_c) \right)^d : \mathbf{v}|_{\Gamma_D} = \mathbf{u}_D \right\}, \quad (41a)$$

$$\mathcal{S}_\varepsilon(\Omega \setminus \Gamma_c) = \left( H^1(\Omega \setminus \Gamma_c) \right)^{d \times d}, \quad (41b)$$

$$\mathcal{V}_u(\Omega \setminus \Gamma_c) = \left\{ \mathbf{v} \in \left( H^1(\Omega \setminus \Gamma_c) \right)^d : \mathbf{v}|_{\Gamma_D} = \mathbf{0} \right\}, \quad (41c)$$

$$\mathcal{V}_\varepsilon(\Omega \setminus \Gamma_c) = \mathcal{S}_\varepsilon(\Omega \setminus \Gamma_c), \quad (41d)$$

where  $H^k(\Omega \setminus \Gamma_c)$  is the Sobolev space of square-integrable functions with square-integrable weak derivatives up to order  $k$ , except at the interface  $\Gamma_c$ , that is, on the open set  $\Omega \setminus \Gamma_c$ . Here  $\mathcal{S}_u(\Omega \setminus \Gamma_c)$  and  $\mathcal{S}_\varepsilon(\Omega \setminus \Gamma_c)$  are the set of functions that represent the solution for displacements and strains, and  $\mathcal{V}_u(\Omega \setminus \Gamma_c)$  and  $\mathcal{V}_\varepsilon(\Omega \setminus \Gamma_c)$  are the corresponding test function spaces.

Multiplying (1a) and (1b) by  $\boldsymbol{\phi} \in \mathcal{V}_u(\Omega \setminus \Gamma_c)$  and  $\boldsymbol{\psi} \in \mathcal{V}_\varepsilon(\Omega \setminus \Gamma_c)$ , we obtain

$$-(\boldsymbol{\phi}, \nabla \cdot \boldsymbol{\sigma}(\boldsymbol{\varepsilon}))_{\Omega \setminus \Gamma_c} = (\boldsymbol{\phi}, \mathbf{b})_{\Omega \setminus \Gamma_c}, \quad (42a)$$

$$(\boldsymbol{\psi}, \boldsymbol{\varepsilon})_{\Omega \setminus \Gamma_c} = (\boldsymbol{\psi}, \nabla^s \mathbf{u})_{\Omega \setminus \Gamma_c}. \quad (42b)$$

Equation (35) can be recast in a form of wider applicability when considering the variational statements associated with cohesive zone models. Defining the  $\lambda$ -weighted average  $\llbracket \chi \rrbracket_\lambda = \lambda \chi^+ + (1 - \lambda) \chi^-$  of a quantity  $\chi$  for any  $\lambda \in [0, 1]$ , we can observe that (35) implies two important identities, namely

$$\llbracket \boldsymbol{\sigma}(\boldsymbol{\varepsilon}) \rrbracket \mathbf{n} = \mathbf{0} \quad \text{and} \quad \llbracket \boldsymbol{\sigma}(\boldsymbol{\varepsilon}) \rrbracket_\lambda \mathbf{n} = \mathbf{t}_{coh}. \quad (43)$$

Integrating by parts (42a) and accounting for the fact that the solution may not be smooth across  $\Gamma_c$  yields

$$(\nabla \boldsymbol{\phi}, \boldsymbol{\sigma}(\boldsymbol{\varepsilon}))_{\Omega \setminus \Gamma_c} - \langle \boldsymbol{\phi}, \boldsymbol{\sigma}(\boldsymbol{\varepsilon}) \mathbf{n} \rangle_{\partial \Omega} + \langle \llbracket \boldsymbol{\phi} \rrbracket, \llbracket \boldsymbol{\sigma}(\boldsymbol{\varepsilon}) \rrbracket_\lambda \mathbf{n} \rangle_{\Gamma_c} + \langle \llbracket \boldsymbol{\phi} \rrbracket_{1-\lambda}, \llbracket \boldsymbol{\sigma}(\boldsymbol{\varepsilon}) \rrbracket \mathbf{n} \rangle_{\Gamma_c} = (\boldsymbol{\phi}, \mathbf{b})_{\Omega \setminus \Gamma_c}, \quad (44)$$

where we have also used the identity  $\llbracket \boldsymbol{\sigma}(\boldsymbol{\varepsilon}) \boldsymbol{\phi} \rrbracket = \llbracket \boldsymbol{\sigma}(\boldsymbol{\varepsilon}) \rrbracket_\lambda \llbracket \boldsymbol{\phi} \rrbracket + \llbracket \boldsymbol{\sigma}(\boldsymbol{\varepsilon}) \rrbracket \llbracket \boldsymbol{\phi} \rrbracket_{1-\lambda}$  on  $\Gamma_c$ .

Without loss of generality, we assume that the Dirichlet boundary conditions are enforced strongly, which implies that  $\boldsymbol{\phi}|_{\Gamma_D} = \mathbf{0}$ . Thus, applying the Dirichlet boundary conditions (5), the Neumann boundary conditions (6), the cohesive law (39) on  $\Gamma_c$ , and recalling (43), equation (44) can be recast as

$$(\nabla \boldsymbol{\phi}, \boldsymbol{\sigma}(\boldsymbol{\varepsilon}))_{\Omega \setminus \Gamma_c} + \langle \llbracket \boldsymbol{\phi} \rrbracket, \mathbf{t}_{coh} \rangle_{\Gamma_c} = (\boldsymbol{\phi}, \mathbf{b})_{\Omega \setminus \Gamma_c} + \langle \boldsymbol{\phi}, \mathbf{t}_N \rangle_{\Gamma_N}. \quad (45)$$

Combining equation (42b) with (45), we have the final weak form as:

$$(\nabla \boldsymbol{\phi}, \boldsymbol{\sigma}(\boldsymbol{\varepsilon}))_{\Omega \setminus \Gamma_c} + (\boldsymbol{\psi}, \boldsymbol{\varepsilon} - \nabla^s \mathbf{u})_{\Omega \setminus \Gamma_c} + \langle \llbracket \boldsymbol{\phi} \rrbracket, \mathbf{t}_{coh} \rangle_{\Gamma_c} - (\boldsymbol{\phi}, \mathbf{b})_{\Omega \setminus \Gamma_c} - \langle \boldsymbol{\phi}, \mathbf{t}_N \rangle_{\Gamma_N} = 0. \quad (46)$$

**Remark 6** ((Euler-Lagrangian equations)). *Integrating (46) back by parts, we obtain*

$$\begin{aligned} & -(\boldsymbol{\phi}, \nabla \cdot \boldsymbol{\sigma}(\boldsymbol{\varepsilon}))_{\Omega \setminus \Gamma_c} + (\boldsymbol{\psi}, \boldsymbol{\varepsilon} - \nabla^s \mathbf{u})_{\Omega \setminus \Gamma_c} - \langle \llbracket \boldsymbol{\phi} \rrbracket, \llbracket \boldsymbol{\sigma}(\boldsymbol{\varepsilon}) \rrbracket_\lambda \mathbf{n} \rangle_{\Gamma_c} - \langle \llbracket \boldsymbol{\phi} \rrbracket_{1-\lambda}, \llbracket \boldsymbol{\sigma}(\boldsymbol{\varepsilon}) \rrbracket \mathbf{n} \rangle_{\Gamma_c} + \langle \llbracket \boldsymbol{\phi} \rrbracket, \mathbf{t}_{coh} \rangle_{\Gamma_c} \\ & - (\boldsymbol{\phi}, \mathbf{b})_{\Omega \setminus \Gamma_c} - \langle \boldsymbol{\phi}, \mathbf{t}_N \rangle_{\Gamma_N} = 0, \end{aligned} \quad (47)$$

which can be reformulated as

$$\begin{aligned} & -(\boldsymbol{\phi}, \nabla \cdot \boldsymbol{\sigma}(\boldsymbol{\varepsilon}) + \mathbf{b})_{\Omega \setminus \Gamma_c} + (\boldsymbol{\psi}, \boldsymbol{\varepsilon} - \nabla^s \mathbf{u})_{\Omega \setminus \Gamma_c} - \langle \llbracket \boldsymbol{\phi} \rrbracket_{1-\lambda}, \llbracket \boldsymbol{\sigma}(\boldsymbol{\varepsilon}) \rrbracket \mathbf{n} \rangle_{\Gamma_c} - \langle \llbracket \boldsymbol{\phi} \rrbracket, \llbracket \boldsymbol{\sigma}(\boldsymbol{\varepsilon}) \rrbracket_\lambda \mathbf{n} - \mathbf{t}_{coh} \rangle_{\Gamma_c} \\ & + \langle \boldsymbol{\phi}, \boldsymbol{\sigma}(\boldsymbol{\varepsilon}) \mathbf{n} - \mathbf{t}_N \rangle_{\Gamma_N} = 0, \end{aligned} \quad (48)$$

and corresponds to

$$-\nabla \cdot \boldsymbol{\sigma} - \mathbf{b} = \mathbf{0}, \quad \text{in } \Omega \setminus \Gamma_c, \quad (49a)$$

$$\boldsymbol{\varepsilon} - \nabla^s \mathbf{u} = \mathbf{0}, \quad \text{in } \Omega \setminus \Gamma_c, \quad (49b)$$

$$\boldsymbol{\sigma} \mathbf{n} - \mathbf{t}_N = \mathbf{0}, \quad \text{on } \Gamma_N, \quad (49c)$$

$$\llbracket \boldsymbol{\sigma} \rrbracket_\lambda \mathbf{n} - \mathbf{t}_{coh} = \mathbf{0}, \quad \text{on } \Gamma_c, \quad (49d)$$

$$\llbracket \boldsymbol{\sigma} \rrbracket \mathbf{n} = \mathbf{0}, \quad \text{on } \Gamma_c, \quad (49e)$$

which enforce the governing equations (1), the (outer) traction boundary conditions (6), the fracture interface conditions (33) and stress equilibration condition (35).

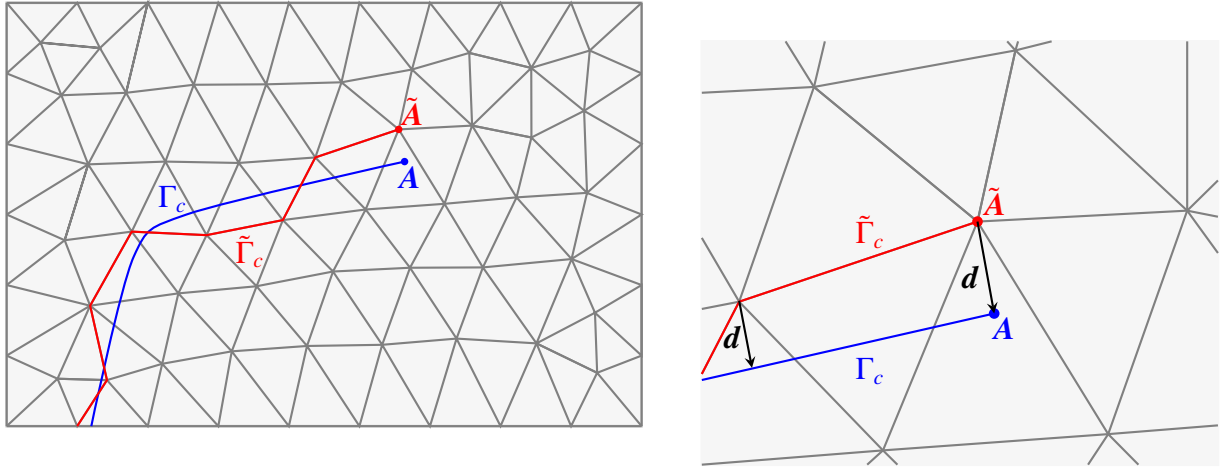


Figure 14: The fracture path  $\Gamma_c$ , the surrogate fracture path  $\tilde{\Gamma}_c$ , and the distance vector  $\mathbf{d}$  at two locations along  $\tilde{\Gamma}_c$ .

### 6.3. The true crack, the surrogate crack and maps

Consider a family  $\mathcal{T}_h$  of admissible and shape-regular triangulations of  $\Omega$ , and assume that each triangulation is cut by the crack  $\Gamma_c$ , depicted as a blue curve in Figure 14.

The key idea in the *Shifted Fracture Method* is to shift the location where the fracture cohesive conditions are applied from the true location of the fracture  $\Gamma_c$  to a surrogate location  $\tilde{\Gamma}_c$ , represented by the red segmented curve in Figure 14, and to appropriately modify the interface conditions.

There are many ways to define the surrogate fracture. One way is to consider the edges (or faces) in  $\mathcal{T}_h$  that are the closest to  $\Gamma_c$  in the sense of the closest point projection. We now define a mapping

$$\mathbf{M}_h : \tilde{\Gamma}_c \rightarrow \Gamma_c, \quad (50a)$$

$$\tilde{\mathbf{x}} \mapsto \mathbf{x}, \quad (50b)$$

using the closest point projection (see [7, 10] for more details).  $\mathbf{M}_h$  associates to any point  $\tilde{\mathbf{x}} \in \tilde{\Gamma}_c$  on the surrogate crack a point  $\mathbf{x} = \mathbf{M}_h(\tilde{\mathbf{x}})$  on the physical crack  $\Gamma_c$  and a corresponding distance

vector function  $\mathbf{d}_{M_h}$ , defined as

$$\mathbf{d}_{M_h}(\tilde{\mathbf{x}}) = \mathbf{x} - \tilde{\mathbf{x}} = [\mathbf{M} - \mathbf{I}](\tilde{\mathbf{x}}) . \quad (51)$$

For the sake of simplicity, we set  $\mathbf{d} = \mathbf{d}_{M_h}$  where  $\mathbf{d} = \|\mathbf{d}\|\mathbf{v}$  and  $\mathbf{v}$  is a unit vector.

**Remark 7.** *An alternative way of defining the map  $\mathbf{M}_h$ , and correspondingly the distance vector  $\mathbf{d}$ , is a level set description of the true crack, in which  $\mathbf{d}$  is defined by means of a distance function.*

#### 6.4. General strategy to shift cohesive zone conditions

The goal now is to discretize the linear elasticity equations (1a)–(1b) on  $\Omega$  with outer boundary conditions (5)–(6) on  $\Gamma$ , and to modify the fracture interface conditions (49d)–(49e) so that they are applied on  $\tilde{\Gamma}_c$  rather than  $\Gamma_c$ .

To this end, inspired by the ideas introduced in [76, 77], a first-order Taylor expansion of  $\mathbf{u}$  and  $\mathbf{C}\boldsymbol{\varepsilon}$  is performed at the surrogate crack  $\tilde{\Gamma}_c$ , in order to “shift” (49d) – (49e) from  $\Gamma_c$  to  $\tilde{\Gamma}_c$  (see for reference Figure 14). Thus,

$$\check{\mathbf{u}}(\tilde{\mathbf{x}}) := \mathbf{u}(\mathbf{M}_h(\tilde{\mathbf{x}})) = \mathbf{u}(\tilde{\mathbf{x}}) + (\nabla \mathbf{u} \mathbf{d})(\tilde{\mathbf{x}}) + \mathbf{R}_u(\tilde{\mathbf{x}}) , \quad \text{on } \tilde{\Gamma}_c , \quad (52a)$$

$$\check{\boldsymbol{\sigma}}(\tilde{\mathbf{x}}) := \boldsymbol{\sigma}(\mathbf{M}_h(\tilde{\mathbf{x}})) = \boldsymbol{\sigma}(\tilde{\mathbf{x}}) + (\nabla \boldsymbol{\sigma} \mathbf{d})(\tilde{\mathbf{x}}) + \mathbf{R}_\sigma(\tilde{\mathbf{x}}) , \quad \text{on } \tilde{\Gamma}_c , \quad (52b)$$

where we have defined the extension functions  $\check{\mathbf{u}}(\tilde{\mathbf{x}}) := \mathbf{u}(\mathbf{M}_h(\tilde{\mathbf{x}}))$  and  $\check{\boldsymbol{\sigma}}(\tilde{\mathbf{x}}) := \boldsymbol{\sigma}(\mathbf{M}_h(\tilde{\mathbf{x}}))$ , and the remainders  $\mathbf{R}_u$  and  $\mathbf{R}_\sigma$  satisfy

$$\|\mathbf{R}_u(\tilde{\mathbf{x}})\| = o(\|\mathbf{d}\|) \quad \text{and} \quad \|\mathbf{R}_\sigma(\tilde{\mathbf{x}})\| = o(\|\mathbf{d}\|) \quad \text{as} \quad \|\mathbf{d}\| \rightarrow 0 . \quad (53)$$

Neglecting the remainders  $\mathbf{R}_u$  and  $\mathbf{R}_\sigma$ , we have the approximation on  $\tilde{\Gamma}_c$

$$\check{\mathbf{u}}(\tilde{\mathbf{x}}) \approx \mathbf{S}(\mathbf{u})(\tilde{\mathbf{x}}) , \quad (54a)$$

$$\check{\boldsymbol{\sigma}}(\tilde{\mathbf{x}}) \approx \mathbf{S}(\boldsymbol{\sigma})(\tilde{\mathbf{x}}) , \quad (54b)$$

where we have introduced the shift operators:

$$\mathbf{S}(\mathbf{u})(\tilde{\mathbf{x}}) := \mathbf{u}(\tilde{\mathbf{x}}) + (\nabla \mathbf{u} \mathbf{d})(\tilde{\mathbf{x}}) , \quad (55a)$$

$$\mathbf{S}(\boldsymbol{\sigma})(\tilde{\mathbf{x}}) := \boldsymbol{\sigma}(\tilde{\mathbf{x}}) + (\nabla \boldsymbol{\sigma} \mathbf{d})(\tilde{\mathbf{x}}) . \quad (55b)$$

Our goal is to enforce the cohesive zone model on the surrogate cohesive crack  $\tilde{\Gamma}_c$  rather than on the true cohesive crack  $\Gamma_c$  (see again Figure 14). In order to maintain an optimal accuracy and avoid mesh dependencies, the cohesive zone model (33) also needs to be adapted appropriately. In particular, (33) can be used to express  $\check{\mathbf{t}}$  in terms of  $\check{\mathbf{u}}$  as

$$\check{\mathbf{t}} = \check{\boldsymbol{\sigma}} \check{\mathbf{n}} = \mathbf{t}_{coh}(\mathbf{w}(\check{\mathbf{u}})) , \quad \text{on } \tilde{\Gamma}_c , \quad (56a)$$

where  $\check{\mathbf{n}}(\tilde{\mathbf{x}}) := \mathbf{n}(\mathbf{M}_h(\tilde{\mathbf{x}}))$ . Approximating  $\check{\boldsymbol{\sigma}} \check{\mathbf{n}} \approx \mathbf{S}(\boldsymbol{\sigma}) \check{\mathbf{n}}$  and  $\mathbf{w}(\check{\mathbf{u}}) \approx \mathbf{w}(\mathbf{S}(\mathbf{u}))$ , we obtain the shifting of the cohesive zone model:

$$\mathbf{S}(\boldsymbol{\sigma}) \check{\mathbf{n}} \approx \mathbf{t}_{coh}(\mathbf{w}(\mathbf{S}(\mathbf{u}))) , \quad \text{on } \tilde{\Gamma}_c . \quad (56b)$$

In the next section we proceed to describe a viable variational discretization of the shifted cohesive zone model.

**Remark 8.** *The proposed approach is based on the validity of the Taylor expansion, which is a reasonable assumption in the context of cohesive zone models. In fact, cohesive zone models are designed to prevent the stress to become unbounded as the grid is refined. Note also that the finite element approximation of gradient quantities typically occurs from below, that is the stresses computed on coarse grids are typically lower than the true gradients. The combination of these two aspects offers a sufficient level of robustness in practical engineering computations for the algorithm to be detailed in what follows.*

**Remark 9.** *In principle, the Taylor expansion is not the only tool that can be used to shift the fracture conditions from  $\Gamma_c$  to  $\tilde{\Gamma}_c$ . Hence, depending on which shift operator is used, the approach described above defines a family of computational methods. In this sense, the Shifted Fracture Method can be interpreted as a framework, more than a single computational method.*

### 6.5. Shifted variational equations

The first step in the derivation of variational equations is the definition of  $\mathcal{S}_u^h(\Omega \setminus \tilde{\Gamma}_c)$  and  $\mathcal{S}_\varepsilon^h(\Omega \setminus \tilde{\Gamma}_c)$ , the discrete spaces of functions used to approximate the displacement  $\mathbf{u}$  and the strain  $\varepsilon$ :

$$\mathcal{S}_u^h(\Omega \setminus \tilde{\Gamma}_c) = \{\mathbf{v} \in (C^0(\Omega \setminus \tilde{\Gamma}_c))^d : \mathbf{v}|_{\Gamma_D} = \mathbf{u}_D, \mathbf{v}|_T \in (\mathcal{P}^1(T))^d, \forall T \in \mathcal{T}_h\}, \quad (57a)$$

$$\mathcal{S}_\varepsilon^h(\Omega \setminus \tilde{\Gamma}_c) = \{\boldsymbol{\omega} \in (C^0(\Omega \setminus \tilde{\Gamma}_c))^{d \times d} : \boldsymbol{\omega}|_T \in (\mathcal{P}^1(T))^{d \times d}, \boldsymbol{\omega} = \boldsymbol{\omega}^t, \forall T \in \mathcal{T}_h\}, \quad (57b)$$

where  $\mathcal{P}^1(T)$  is the space of linear polynomial functions over the element  $T$ . Essentially,  $\mathcal{S}_u^h(\Omega \setminus \tilde{\Gamma}_c)$  and  $\mathcal{S}_\varepsilon^h(\Omega \setminus \tilde{\Gamma}_c)$  are spaces of vector and symmetric tensor functions that are piecewise-linear and continuous everywhere except across the interface  $\tilde{\Gamma}_c$ , and are compatible with boundary conditions on  $\partial\Omega \setminus \Gamma_c$ . Analogously, we can define the test function spaces

$$\mathcal{V}_u^h(\Omega \setminus \tilde{\Gamma}_c) = \{\mathbf{v} \in (C^0(\Omega \setminus \tilde{\Gamma}_c))^d : \mathbf{v}|_{\Gamma_D} = \mathbf{0}, \mathbf{v}|_T \in (\mathcal{P}^1(T))^d, \forall T \in \mathcal{T}_h\}, \quad (57c)$$

$$\mathcal{V}_\varepsilon^h(\Omega \setminus \tilde{\Gamma}_c) = \mathcal{S}_\varepsilon^h(\Omega \setminus \tilde{\Gamma}_c). \quad (57d)$$

Instead of (42a), let us test the strong equations against  $\mathcal{V}_u^h(\Omega \setminus \tilde{\Gamma}_c)$  and  $\mathcal{V}_\varepsilon^h(\Omega \setminus \tilde{\Gamma}_c)$ , namely

$$-(\boldsymbol{\phi}, \nabla \cdot \boldsymbol{\sigma}(\boldsymbol{\varepsilon}))_{\Omega \setminus \tilde{\Gamma}_c} = (\boldsymbol{\phi}, \mathbf{b})_{\Omega \setminus \tilde{\Gamma}_c}, \quad (58a)$$

$$(\boldsymbol{\psi}, \boldsymbol{\varepsilon})_{\Omega \setminus \tilde{\Gamma}_c} = (\boldsymbol{\psi}, \nabla^s \mathbf{u})_{\Omega \setminus \tilde{\Gamma}_c}, \quad (58b)$$

where now the numerical solution may not be smooth across  $\tilde{\Gamma}_c$ . Integrating by parts (58a) and (58b) yields

$$(\nabla \boldsymbol{\phi}, \boldsymbol{\sigma}(\boldsymbol{\varepsilon}))_{\Omega \setminus \tilde{\Gamma}_c} + \langle \llbracket \boldsymbol{\phi} \rrbracket, \llbracket \boldsymbol{\sigma}(\boldsymbol{\varepsilon}) \rrbracket_\lambda \tilde{\mathbf{n}} \rangle_{\tilde{\Gamma}_c} + \langle \llbracket \boldsymbol{\phi} \rrbracket_{1-\lambda}, \llbracket \boldsymbol{\sigma}(\boldsymbol{\varepsilon}) \rrbracket \tilde{\mathbf{n}} \rangle_{\tilde{\Gamma}_c} = (\boldsymbol{\phi}, \mathbf{b})_{\Omega \setminus \tilde{\Gamma}_c} + \langle \boldsymbol{\phi}, \mathbf{t}_N \rangle_{\Gamma_N}, \quad (59)$$

where the two faces of the crack  $\tilde{\Gamma}_c$  are  $\tilde{\Gamma}_c^+$ , with outer normal  $\tilde{\mathbf{n}}^+$ , and  $\tilde{\Gamma}_c^-$ , with outer normal  $\tilde{\mathbf{n}}^-$ . We also define  $\tilde{\mathbf{n}} = \tilde{\mathbf{n}}^+$ .

We can now consider the terms  $\llbracket \sigma(\varepsilon) \rrbracket_\lambda \tilde{\mathbf{n}}$  and  $\llbracket \sigma(\varepsilon) \rrbracket \tilde{\mathbf{n}}$  in (59), and express them in terms of shifted fracture interface conditions. Starting from the term  $\llbracket \sigma(\varepsilon) \rrbracket_\lambda \tilde{\mathbf{n}}$ , we have

$$\begin{aligned} \llbracket \sigma(\varepsilon) \rrbracket_\lambda \tilde{\mathbf{n}} &= \llbracket \sigma(\varepsilon) \rrbracket_\lambda ((\tilde{\mathbf{n}} \cdot \mathbf{n})\mathbf{n} + (\tilde{\mathbf{n}} \cdot \boldsymbol{\tau})\boldsymbol{\tau}) \\ &= (\tilde{\mathbf{n}}(\tilde{\mathbf{x}}) \cdot \check{\mathbf{n}}(\tilde{\mathbf{x}})) \llbracket \sigma(\varepsilon(\tilde{\mathbf{x}})) \rrbracket_\lambda \check{\mathbf{n}}(\tilde{\mathbf{x}}) + (\tilde{\mathbf{n}}(\tilde{\mathbf{x}}) \cdot \check{\boldsymbol{\tau}}(\tilde{\mathbf{x}})) \llbracket \sigma(\varepsilon(\tilde{\mathbf{x}})) \rrbracket_\lambda \check{\boldsymbol{\tau}}(\tilde{\mathbf{x}}). \end{aligned} \quad (60)$$

Observing that  $\llbracket \sigma(\varepsilon(\tilde{\mathbf{x}})) \rrbracket_\lambda \check{\mathbf{n}}(\tilde{\mathbf{x}}) = \llbracket \sigma \check{\mathbf{n}} \rrbracket_\lambda = \llbracket (\check{\boldsymbol{\sigma}} - \nabla \sigma \mathbf{d}) \check{\mathbf{n}} \rrbracket_\lambda = \llbracket \check{\mathbf{t}} - (\nabla \sigma \mathbf{d}) \check{\mathbf{n}} \rrbracket_\lambda = \check{\mathbf{t}} - \llbracket (\nabla \sigma \mathbf{d}) \rrbracket_\lambda \check{\mathbf{n}}$ , since  $\check{\mathbf{t}}(\tilde{\mathbf{x}})$  and  $\check{\mathbf{n}}(\tilde{\mathbf{x}})$  are uniquely defined on  $\tilde{\Gamma}_c$ , and applying the Taylor expansion (52b), we obtain

$$\llbracket \sigma(\varepsilon) \rrbracket_\lambda \tilde{\mathbf{n}} = (\tilde{\mathbf{n}} \cdot \check{\mathbf{n}}) (\check{\mathbf{t}} - \llbracket (\nabla \sigma(\varepsilon) \mathbf{d}) \rrbracket_\lambda \check{\mathbf{n}}) + (\tilde{\mathbf{n}} \cdot \check{\boldsymbol{\tau}}) \llbracket \sigma(\varepsilon) \rrbracket_\lambda \check{\boldsymbol{\tau}}, \quad \text{on } \tilde{\Gamma}_c. \quad (61)$$

Hence, using (49d), (49e), (56a) and (56b),

$$\begin{aligned} \langle \llbracket \phi \rrbracket, \llbracket \sigma(\varepsilon) \rrbracket_\lambda \tilde{\mathbf{n}} \rangle_{\tilde{\Gamma}_c} &= \langle \llbracket \phi \rrbracket, (\tilde{\mathbf{n}} \cdot \check{\mathbf{n}}) (\check{\mathbf{t}} - \llbracket (\nabla \sigma(\varepsilon) \mathbf{d}) \rrbracket_\lambda \check{\mathbf{n}}) + (\tilde{\mathbf{n}} \cdot \check{\boldsymbol{\tau}}) \llbracket \sigma(\varepsilon) \rrbracket_\lambda \check{\boldsymbol{\tau}} \rangle_{\tilde{\Gamma}_c} \\ &= \langle \llbracket \phi \rrbracket, (\tilde{\mathbf{n}} \cdot \check{\mathbf{n}}) t_{coh}(\mathbf{w}(\mathbf{u} + \nabla \mathbf{u} \mathbf{d})) \rangle_{\tilde{\Gamma}_c} \\ &\quad - \langle \llbracket \phi \rrbracket, (\tilde{\mathbf{n}} \cdot \check{\mathbf{n}}) (\llbracket (\nabla \sigma(\varepsilon) \mathbf{d}) \rrbracket_\lambda \check{\mathbf{n}}) - (\tilde{\mathbf{n}} \cdot \check{\boldsymbol{\tau}}) \llbracket \sigma(\varepsilon) \rrbracket_\lambda \check{\boldsymbol{\tau}} \rangle_{\tilde{\Gamma}_c} \\ &= \langle \llbracket \phi \rrbracket, (\tilde{\mathbf{n}} \cdot \check{\mathbf{n}}) t_{coh}(\mathbf{w}(\mathbf{u} + \nabla \mathbf{u} \mathbf{d})) \rangle_{\tilde{\Gamma}_c} \\ &\quad + \langle \llbracket \phi \rrbracket, \llbracket \sigma(\varepsilon) \rrbracket_\lambda \tilde{\mathbf{n}} - \llbracket \sigma(\varepsilon) + \nabla \sigma(\varepsilon) \mathbf{d} \rrbracket_\lambda (\tilde{\mathbf{n}} \cdot \check{\mathbf{n}}) \check{\mathbf{n}} \rangle_{\tilde{\Gamma}_c}, \end{aligned} \quad (62)$$

where we have used again the decomposition of the normal  $\tilde{\mathbf{n}}$  in terms of its components along  $\check{\mathbf{n}}$  and  $\check{\boldsymbol{\tau}}$ . Similarly, applying to the term  $\langle \llbracket \phi \rrbracket_{1-\lambda}, \llbracket \sigma(\varepsilon) \rrbracket \tilde{\mathbf{n}} \rangle_{\tilde{\Gamma}_c}$  the first of (43), that is  $\llbracket \check{\sigma}(\varepsilon) \rrbracket \tilde{\mathbf{n}} = \mathbf{0}$ , yields

$$\begin{aligned} \langle \llbracket \phi \rrbracket_{1-\lambda}, \llbracket \sigma(\varepsilon) \rrbracket \tilde{\mathbf{n}} \rangle_{\tilde{\Gamma}_c} &= \langle \llbracket \phi \rrbracket_{1-\lambda}, (\tilde{\mathbf{n}} \cdot \check{\mathbf{n}}) \llbracket \check{\sigma}(\varepsilon) - \nabla \sigma(\varepsilon) \mathbf{d} \rrbracket \check{\mathbf{n}} + (\tilde{\mathbf{n}} \cdot \check{\boldsymbol{\tau}}) \llbracket \sigma(\varepsilon) \rrbracket \check{\boldsymbol{\tau}} \rangle_{\tilde{\Gamma}_c} \\ &= \langle \llbracket \phi \rrbracket_{1-\lambda}, -(\tilde{\mathbf{n}} \cdot \check{\mathbf{n}}) \llbracket \nabla \sigma(\varepsilon) \mathbf{d} \rrbracket \check{\mathbf{n}} + (\tilde{\mathbf{n}} \cdot \check{\boldsymbol{\tau}}) \llbracket \sigma(\varepsilon) \rrbracket \check{\boldsymbol{\tau}} \rangle_{\tilde{\Gamma}_c} \\ &= \langle \llbracket \phi \rrbracket_{1-\lambda}, \llbracket \sigma(\varepsilon) \rrbracket \tilde{\mathbf{n}} - (\tilde{\mathbf{n}} \cdot \check{\mathbf{n}}) \llbracket \sigma(\varepsilon) + \nabla \sigma(\varepsilon) \mathbf{d} \rrbracket \check{\mathbf{n}} \rangle_{\tilde{\Gamma}_c}. \end{aligned} \quad (63)$$

Substituting (62) and (63) into (59) and including the strain equation, we obtain

$$\begin{aligned} (\nabla \phi, \sigma(\varepsilon))_{\Omega \setminus \tilde{\Gamma}_c} + (\psi, \varepsilon - \nabla^s \mathbf{u})_{\Omega \setminus \tilde{\Gamma}_c} - (\phi, \mathbf{b})_{\Omega \setminus \tilde{\Gamma}_c} - \langle \phi, \mathbf{t}_N \rangle_{\Gamma_N} + \langle \llbracket \phi \rrbracket, (\tilde{\mathbf{n}} \cdot \mathbf{n}) t_{coh}(\mathbf{w}(\mathbf{u} + \nabla \mathbf{u} \mathbf{d})) \rangle_{\tilde{\Gamma}_c} \\ + \langle \llbracket \phi \rrbracket, \llbracket \sigma(\varepsilon) \rrbracket_\lambda \tilde{\mathbf{n}} - \llbracket \sigma(\varepsilon) + \nabla \sigma(\varepsilon) \mathbf{d} \rrbracket_\lambda (\tilde{\mathbf{n}} \cdot \mathbf{n}) \mathbf{n} \rangle_{\tilde{\Gamma}_c} \\ + \langle \llbracket \phi \rrbracket_{1-\lambda}, \llbracket \sigma(\varepsilon) \rrbracket \tilde{\mathbf{n}} - (\tilde{\mathbf{n}} \cdot \mathbf{n}) \llbracket \sigma(\varepsilon) + \nabla \sigma(\varepsilon) \mathbf{d} \rrbracket \mathbf{n} \rangle_{\tilde{\Gamma}_c} = 0, \end{aligned} \quad (64)$$

where we have omitted the symbol  $(\check{\cdot})$  over  $\mathbf{n}$ , for the sake of simplicity, and it is understood that all the fracture interface integrals are taken over  $\tilde{\Gamma}_c$ . In what follows, we will omit  $(\check{\cdot})$  over  $\mathbf{n}$  whenever it does not cause confusion. We then obtain the final variational problem

Find  $[\mathbf{u}, \varepsilon] \in \mathcal{S}_u^h(\Omega \setminus \tilde{\Gamma}_c) \times \mathcal{S}_\varepsilon^h(\Omega \setminus \tilde{\Gamma}_c)$  such that,  $\forall [\phi, \psi] \in \mathcal{V}_u^h(\Omega \setminus \tilde{\Gamma}_c) \times \mathcal{V}_\varepsilon^h(\Omega \setminus \tilde{\Gamma}_c)$ ,

$$\mathcal{B}_{\text{SFM}}^{[\Omega \setminus \tilde{\Gamma}_c]}([\mathbf{u}, \varepsilon]; [\phi, \psi]) - \mathcal{L}_{\text{SFM}}^{[\Omega \setminus \tilde{\Gamma}_c]}([\phi, \psi]) = \langle \phi, \mathbf{t}_N \rangle_{\Gamma_N}, \quad (65a)$$

where

$$\begin{aligned} \mathcal{B}_{\text{SFM}}^{[\Omega \setminus \tilde{\Gamma}_c]}([\mathbf{u}, \varepsilon]; [\phi, \psi]) - \mathcal{L}_{\text{SFM}}^{[\Omega \setminus \tilde{\Gamma}_c]}([\phi, \psi]) - (\phi, \mathbf{b})_{\Omega \setminus \tilde{\Gamma}_c} &= (\nabla \phi, \sigma(\varepsilon))_{\Omega \setminus \tilde{\Gamma}_c} + (\psi, \varepsilon - \nabla^s \mathbf{u})_{\Omega \setminus \tilde{\Gamma}_c} \\ &\quad + \langle \llbracket \phi \rrbracket, t_{coh}(\mathbf{w}(\mathbf{S}(\mathbf{u}))) \rangle_{\tilde{\Gamma}_c} \end{aligned}$$

$$\begin{aligned}
& + \langle \llbracket \boldsymbol{\phi} \rrbracket, \llbracket \boldsymbol{\sigma}(\boldsymbol{\varepsilon}) \rrbracket_\lambda \tilde{\mathbf{n}} - \llbracket \mathbf{S}(\boldsymbol{\sigma}(\boldsymbol{\varepsilon})) \rrbracket_\lambda (\tilde{\mathbf{n}} \cdot \mathbf{n}) \mathbf{n} \rangle_{\tilde{\Gamma}_c} \\
& + \langle \llbracket \boldsymbol{\phi} \rrbracket_{1-\lambda}, \llbracket \boldsymbol{\sigma}(\boldsymbol{\varepsilon}) \rrbracket \tilde{\mathbf{n}} - (\tilde{\mathbf{n}} \cdot \mathbf{n}) \llbracket \mathbf{S}(\boldsymbol{\sigma}(\boldsymbol{\varepsilon})) \rrbracket \mathbf{n} \rangle_{\tilde{\Gamma}_c} .
\end{aligned} \tag{65b}$$

**Remark 10.** *The reason why we have left the term  $\langle \boldsymbol{\phi}, \mathbf{t}_N \rangle_{\Gamma_N}$  out of the bilinear form will be apparent in Section 3.4, and we ask the reader to be patient in the meantime.*

### 6.6. Shifted Euler-Lagrangian equations

Integrating the first term of equation (64) by parts and accounting for potential discontinuities across the surrogate cohesive crack  $\tilde{\Gamma}_c$ , we have

$$\begin{aligned}
& (\boldsymbol{\phi}, -\nabla \cdot \boldsymbol{\sigma}(\boldsymbol{\varepsilon}) - \mathbf{b})_{\Omega \setminus \tilde{\Gamma}_c} - \langle \llbracket \boldsymbol{\phi} \rrbracket_{1-\lambda}, \llbracket \boldsymbol{\sigma}(\boldsymbol{\varepsilon}) \rrbracket \tilde{\mathbf{n}} \rangle_{\tilde{\Gamma}_c} - \langle \llbracket \boldsymbol{\phi} \rrbracket, \llbracket \boldsymbol{\sigma}(\boldsymbol{\varepsilon}) \rrbracket_\lambda \tilde{\mathbf{n}} \rangle_{\tilde{\Gamma}_c} + (\boldsymbol{\psi}, \boldsymbol{\varepsilon} - \nabla^s \mathbf{u})_{\Omega \setminus \tilde{\Gamma}_c} + \langle \boldsymbol{\phi}, \boldsymbol{\sigma}(\boldsymbol{\varepsilon}) \mathbf{n} - \mathbf{t}_N \rangle_{\Gamma_N} \\
& + \langle \llbracket \boldsymbol{\phi} \rrbracket, (\tilde{\mathbf{n}} \cdot \mathbf{n}) \mathbf{t}_{coh}(\mathbf{w}(\mathbf{u} + \nabla \mathbf{u} \mathbf{d})) \rangle_{\tilde{\Gamma}_c} + \langle \llbracket \boldsymbol{\phi} \rrbracket, \llbracket \boldsymbol{\sigma}(\boldsymbol{\varepsilon}) \rrbracket_\lambda \tilde{\mathbf{n}} - \llbracket \boldsymbol{\sigma}(\boldsymbol{\varepsilon}) + \nabla \boldsymbol{\sigma}(\boldsymbol{\varepsilon}) \mathbf{d} \rrbracket_\lambda (\tilde{\mathbf{n}} \cdot \mathbf{n}) \mathbf{n} \rangle_{\tilde{\Gamma}_c} \\
& + \langle \llbracket \boldsymbol{\phi} \rrbracket_{1-\lambda}, \llbracket \boldsymbol{\sigma}(\boldsymbol{\varepsilon}) \rrbracket \tilde{\mathbf{n}} - (\tilde{\mathbf{n}} \cdot \mathbf{n}) \llbracket \boldsymbol{\sigma}(\boldsymbol{\varepsilon}) + \nabla \boldsymbol{\sigma}(\boldsymbol{\varepsilon}) \mathbf{d} \rrbracket \mathbf{n} \rangle_{\tilde{\Gamma}_c} = 0 , \tag{66}
\end{aligned}$$

which, after simplifying some boundary terms, yields

$$\begin{aligned}
& (\boldsymbol{\phi}, -\nabla \cdot \boldsymbol{\sigma}(\boldsymbol{\varepsilon}) - \mathbf{b})_{\Omega \setminus \tilde{\Gamma}_c} + (\boldsymbol{\psi}, \boldsymbol{\varepsilon} - \nabla^s \mathbf{u})_{\Omega \setminus \tilde{\Gamma}_c} + \langle \boldsymbol{\phi}, \boldsymbol{\sigma}(\boldsymbol{\varepsilon}) \mathbf{n} - \mathbf{t}_N \rangle_{\Gamma_N} \\
& - \langle \llbracket \boldsymbol{\phi} \rrbracket, (\tilde{\mathbf{n}} \cdot \mathbf{n}) (\llbracket \boldsymbol{\sigma}(\boldsymbol{\varepsilon}) + \nabla \boldsymbol{\sigma}(\boldsymbol{\varepsilon}) \mathbf{d} \rrbracket_\lambda \mathbf{n} - \mathbf{t}_{coh}(\mathbf{w}(\mathbf{u} + \nabla \mathbf{u} \mathbf{d}))) \rangle_{\tilde{\Gamma}_c} \\
& - \langle \llbracket \boldsymbol{\phi} \rrbracket_{1-\lambda}, (\tilde{\mathbf{n}} \cdot \mathbf{n}) \llbracket \boldsymbol{\sigma}(\boldsymbol{\varepsilon}) + \nabla \boldsymbol{\sigma}(\boldsymbol{\varepsilon}) \mathbf{d} \rrbracket \mathbf{n} \rangle_{\tilde{\Gamma}_c} = 0 , \tag{67}
\end{aligned}$$

and corresponds to

$$-\nabla \cdot \boldsymbol{\sigma} - \mathbf{b} = \mathbf{0} , \quad \text{in } \Omega \setminus \tilde{\Gamma}_c , \tag{68a}$$

$$\boldsymbol{\varepsilon} - \nabla^s \mathbf{u} = \mathbf{0} , \quad \text{in } \Omega \setminus \tilde{\Gamma}_c , \tag{68b}$$

$$\boldsymbol{\sigma} \mathbf{n} - \mathbf{t}_N = \mathbf{0} , \quad \text{on } \Gamma_N , \tag{68c}$$

$$(\tilde{\mathbf{n}} \cdot \mathbf{n}) (\llbracket \mathbf{S}(\boldsymbol{\sigma}(\boldsymbol{\varepsilon})) \rrbracket_\lambda \mathbf{n} - \mathbf{t}_{coh}(\mathbf{w}(\mathbf{S}(\mathbf{u})))) = \mathbf{0} , \quad \text{on } \tilde{\Gamma}_c , \tag{68d}$$

$$(\tilde{\mathbf{n}} \cdot \mathbf{n}) \llbracket \mathbf{S}(\boldsymbol{\sigma}(\boldsymbol{\varepsilon})) \rrbracket \mathbf{n} = \mathbf{0} , \quad \text{on } \tilde{\Gamma}_c , \tag{68e}$$

where the first three equalities are the enforcement of the balance of forces, the definition of the strain, and the traction boundary conditions, while the last two conditions are associated with the crack interface. In particular, (68d) enforces the cohesive law - approximated by the Taylor expansion and (68e) enforces the continuity of the normal component of the stress - again with the Taylor approximation - along all of  $\tilde{\Gamma}_c$ .

**Remark 11** (Role of  $(\tilde{\mathbf{n}} \cdot \mathbf{n})$  in (68)). *The residuals (68d)–(68e) are multiplied by the weight  $(\tilde{\mathbf{n}} \cdot \mathbf{n})$ , which represents the projection of the curve/surface measure of the edges/faces in  $\tilde{\Gamma}_c$  onto  $\Gamma_c$ , in the two/three-dimensional case, respectively. This area correction term is essential for the correct computation of the work associated with the crack cohesive forces, and to avoid severe mesh dependencies in numerical computations. This is to say that the virtual work statement associated with (68d)–(68e) is automatically self-correcting for the effective true crack surface area. Instead, when node release techniques over the edges/faces of the grid are combined with cohesive zone models, the discrete crack area and associated virtual work statement are grossly*

inaccurate and induce severe mesh dependencies. We will return to this point when discussing, later on, the numerical results.

### 6.7. A stabilized Shifted Fracture Method

If equal-order piecewise linear interpolation is used for both variables  $\mathbf{u}$  and  $\boldsymbol{\varepsilon}$ , the overall finite element formulation is not numerically stable. It is however possible to stabilize the formulation (65a) by adding appropriate variational multiscale stabilization terms proposed in [28, 64, 80]. In these works, sub-grid components of the solution expressed by means of the residual of the discrete equations were used to enhance numerical stability. In the present project, the following modified form of the mixed system (65a) is used:

$$\begin{aligned} \mathcal{B}_{\text{SFM}}^{[\Omega \setminus \tilde{\Gamma}_c]}([\mathbf{u}, \boldsymbol{\varepsilon}]; [\boldsymbol{\phi}, \psi]) - \mathcal{L}_{\text{SFM}}^{[\Omega \setminus \tilde{\Gamma}_c]}([\boldsymbol{\phi}, \psi]) + (\nabla \cdot \boldsymbol{\sigma}(\psi), \tau_u h^2 / 2\mu (\nabla \cdot \boldsymbol{\sigma}(\boldsymbol{\varepsilon}) + \mathbf{b}))_{\Omega \setminus \tilde{\Gamma}_c} \\ - (\psi - \nabla^s \boldsymbol{\phi}, 2\mu \tau_\varepsilon (\boldsymbol{\varepsilon} - \nabla^s \mathbf{u}))_{\Omega \setminus \tilde{\Gamma}_c} = \langle \boldsymbol{\phi}, \mathbf{t}_N \rangle_{\Gamma_N}, \end{aligned} \quad (69)$$

where the parameters  $\tau_\varepsilon = 0.5$  and  $\tau_u = 10$  are chosen for all computations shown in Section 7. The choice of  $\tau_\varepsilon$  and  $\tau_u$  was already explored in [64, 80] for the Darcy flow operator, with an analysis of stability and convergence. The same choice of stabilization was made when adopting the Shifted Boundary Method for immersed solid mechanics computations [11], and was mathematically proved stable and accurate.

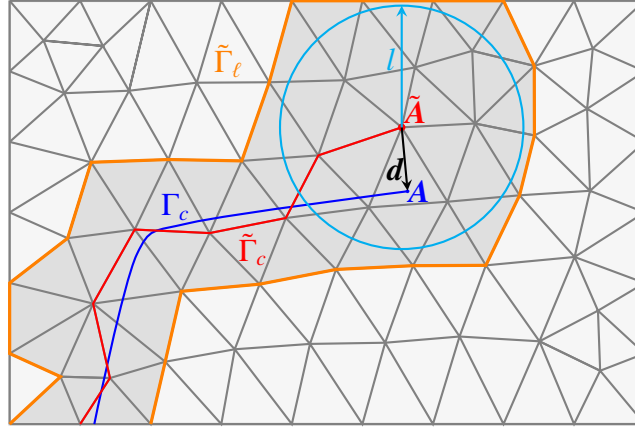


Figure 15: The true crack  $\Gamma_c$  (blue), the surrogate crack  $\tilde{\Gamma}_c$  (red), and the boundary  $\tilde{\Gamma}_L$  (orange) of the layer of elements.

### 6.8. An efficient numerical implementation: the shifted fracture layer

The SFM described so far relies on a mixed displacements/strains formulation, which could be undesirable, due to the increase in degrees of freedom and thus the associated computational cost. At the same time, a primal formulation with piecewise-linear interpolation of  $\mathbf{u}$  would lead to a first-order accurate method, because the cohesive traction conditions are akin to Robin conditions and the SFM would then require second-order derivatives of the displacement field. In fact, replacing  $\boldsymbol{\varepsilon} = \nabla^s \mathbf{u}$  in the stress definition leads to  $\nabla(\boldsymbol{\sigma}(\nabla^s \mathbf{u})) = \mathbf{0}$ , in the case of piecewise linear interpolation.

This section introduces a strategy that significantly reduces the computational burden of solving the mixed system without reducing the accuracy of the displacement solution  $\mathbf{u}$ . This approach was proposed by Atallah *et al.* [11] and successfully tested for Dirichlet and Neumann conditions in linear elasticity.

Recalling the definitions of  $\tilde{\Gamma}_c$  in Section 6.3, we define  $\tilde{\Omega}_\ell$  as the set of elements  $T \in \mathcal{T}_h$  with at least one node on  $\tilde{\Gamma}_c \cup B(\tilde{\mathbf{A}}, l)$  (here  $B(\tilde{\mathbf{A}}, l)$  is the ball of center  $\tilde{\mathbf{A}}$  and radius  $l$ ), that is,

$$\tilde{\Omega}_\ell = \{\cup_{T \in \mathcal{T}_h} T : T \cap (\tilde{\Gamma}_c \cup B(\tilde{\mathbf{A}}, l)) \neq \emptyset\} . \quad (70)$$

The set  $\tilde{\Omega}_\ell$  can be described as the set of elements that are neighboring the surrogate crack surface, augmented by a cluster of elements around the tip of the surrogate crack, as shown in Figure 15. The radius  $l$  of the ball  $B(\tilde{\mathbf{A}}, l)$  is chosen to scale like the mesh size  $h$ , and typically  $l \in [2h, 3h]$ . Observe that the boundary of  $\tilde{\Omega}_\ell$  may include a portion of the boundaries  $\Gamma_D$  and  $\Gamma_N$ . Consider now the variational formulation:

$$\text{Find } [\mathbf{u}, \boldsymbol{\varepsilon}] \in V_{u,h}(\Omega) \times V_{\varepsilon,h}(\tilde{\Omega}_\ell) \text{ such that, } \forall [\boldsymbol{\phi}, \boldsymbol{\psi}] \in V_{u,h}(\Omega) \times V_{\varepsilon,h}(\tilde{\Omega}_\ell) ,$$

$$\mathcal{B}_{\text{SFM}}([\mathbf{u}, \boldsymbol{\varepsilon}]; [\boldsymbol{\phi}, \boldsymbol{\psi}]) = \mathcal{L}_{\text{SFM}}([\boldsymbol{\phi}, \boldsymbol{\psi}]) , \quad (71a)$$

where

$$\mathcal{B}_{\text{SFM}}([\mathbf{u}, \boldsymbol{\varepsilon}]; [\boldsymbol{\phi}, \boldsymbol{\psi}]) = (\mathbf{C} \nabla^s \mathbf{u}, \nabla^s \boldsymbol{\phi})_{\Omega \setminus \tilde{\Omega}_\ell} + \mathcal{B}_{\text{SFM}}^{[\tilde{\Omega}_\ell \setminus \tilde{\Gamma}_c]}([\mathbf{u}, \boldsymbol{\varepsilon}]; [\boldsymbol{\phi}, \boldsymbol{\psi}]) , \quad (71b)$$

$$\mathcal{L}_{\text{SFM}}([\boldsymbol{\phi}, \boldsymbol{\psi}]) = (\boldsymbol{\phi}, \mathbf{b})_{\Omega \setminus \tilde{\Omega}_\ell} + \langle \boldsymbol{\phi}, \mathbf{t}_N \rangle_{\Gamma_N} + \mathcal{L}_{\text{SFM}}^{[\tilde{\Omega}_\ell \setminus \tilde{\Gamma}_c]}([\boldsymbol{\phi}, \boldsymbol{\psi}]) . \quad (71c)$$

This variational formulation is a combination of a standard primal formulation for the displacement unknown  $\mathbf{u}$ , and the mixed formulation (65) described in Section 6.5, but this time restricted to the domain  $\tilde{\Omega}_\ell \setminus \tilde{\Gamma}_c$ . Using integration by parts, it is possible to recover the following Euler-Lagrange equations. Here we focus on their restriction to  $\Omega \setminus \tilde{\Omega}_\ell$  and its boundaries:

$$-\nabla \cdot \boldsymbol{\sigma}(\nabla^s \mathbf{u}) = \mathbf{b} , \quad \text{in } \Omega \setminus \tilde{\Omega}_\ell , \quad (72a)$$

$$\boldsymbol{\sigma}(\nabla^s \mathbf{u}^+) \mathbf{n}^+ + \boldsymbol{\sigma}(\boldsymbol{\varepsilon})^- \mathbf{n}^- = \mathbf{0} , \quad \text{on } \tilde{\Gamma}_\ell , \quad (72b)$$

$$(\mathbf{C} \nabla^s \mathbf{u}) \mathbf{n} = \mathbf{t}_N , \quad \text{on } \Gamma_N \cap \partial(\Omega \setminus \tilde{\Omega}_\ell) , \quad (72c)$$

where the "+" and "-" signs refer to the primal ( $\Omega \setminus \tilde{\Omega}_\ell$ ) and mixed ( $\tilde{\Omega}_\ell$ ) sides of the domain, respectively. Equation (72b) enforces continuity of the normal component of the stress across the interface  $\tilde{\Gamma}_\ell$ . Note that the discrete displacement  $\mathbf{u}$  is by definition continuous over all of  $\Omega \setminus \tilde{\Gamma}_c$ .

**Remark 12.** *The formulation (71) requires to solve the irreducible primal formulation over the major portion of the domain,  $\Omega \setminus \tilde{\Omega}_\ell$ , and to restrict the mixed variational formulation only on a small layer of elements  $\tilde{\Omega}_\ell$  near the surrogate fracture  $\tilde{\Gamma}_c$ . In this context, the mixed formulation (65) described in Section 6.5 can be interpreted as a gradient reconstruction technique, built to ensure optimal error convergence for the SFM.*

**Remark 13.** *In the case in which multiple cracks are present with multiple (possibly overlapping) regions  $\Omega \setminus \tilde{\Omega}_\ell^i$ , the proposed efficient implementation would still be applicable and effective, since*

it would amount to use the mixed formulation on the union  $\cup_i (\Omega \setminus \tilde{\Omega}_\ell^i)$ , and the primal formulation elsewhere.

## 7. Numerical Results

A number of computational tests in two and three dimensions are presented, with comparison with classical benchmark tests in the field.

### 7.1. Two-dimensional tests

We consider here three classical examples that have been widely studied in the literature, both experimentally and numerically: the three-point bending specimen test [33, 84, 116], the L-shape panel test [53, 138, 142] and the four-point bending specimen test [34, 84, 116]. The first produces a straight crack path, while the other two produce curved crack paths. The tests are ordered so as to respect the increasing complexity of the nonlinear snap-back response in the case of brittle materials. The plane strain assumption is adopted for all two-dimensional numerical simulations.

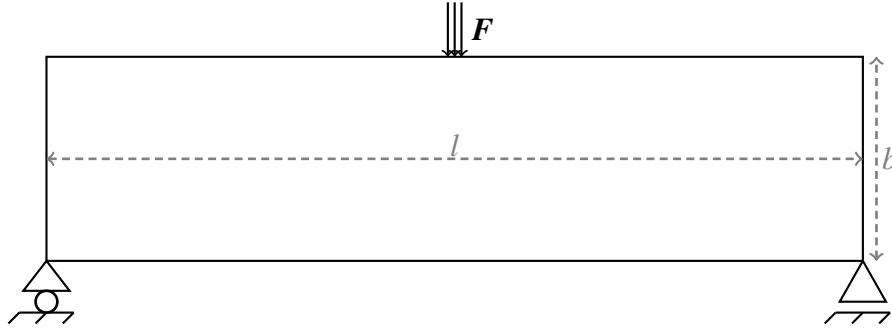


Figure 16: Geometry and setup of the three-point bending specimen.

#### 7.1.1. Three-point bending specimen

The geometry of the three-point bending specimen is shown in Figure 16 and is constituted of a rectangular beam of height  $b = 0.15$  m, length  $l = 4b$ , and thickness  $s = b$ . The material properties are:  $E = 36.5$  GPa,  $\nu = 0.1$ ,  $t_{cr} = 3.19$  MPa, where  $E$  is Young's modulus,  $\nu$  is Poisson's ratio and  $t_{cr}$  is the normal critical stress. The load  $F$  is distributed over a strip of length 0.01 m, symmetric with respect to the midpoint of the beam. The beam is simply supported at both ends and the horizontal displacement is prevented by the right support, as shown in Figure 16. The performance of the SFM is assessed for values of the fracture energy  $G_F = 5$  N/m,  $G_F = 50$  N/m and  $G_F = 200$  N/m, which span from brittle to ductile fracture behavior.

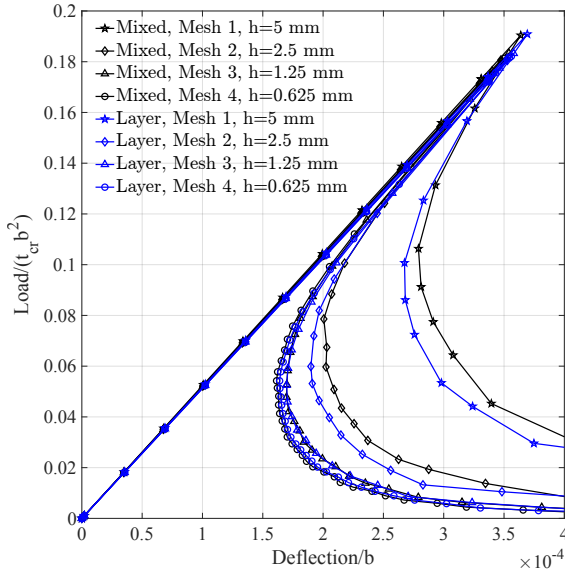
Four computational grids (denoted Mesh 1, 2, 3 and 4) are used in the calculations, whose details are presented in Table 2. Meshes 1, 2, 3, and 4 have an average mesh size  $h = 5$  mm,  $h = 2.5$  mm,  $h = 1.25$  mm and  $h = 0.625$  mm. Meshes 2, 3, and 4 are obtained by nested refinement of Mesh 1, and the sizes of the grids refer to a neighborhood of the crack path, since they are slightly coarsened away from it.

As the load  $F$  increases, the bottom of the mid section is the location where the principal stress first reaches the normal critical stress  $t_{cr}$ , and a crack develops upward. Because of the symmetry of the problem, the crack path is vertical.

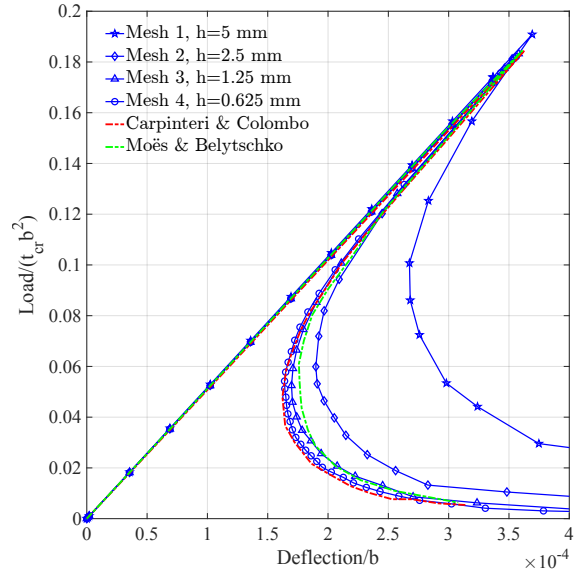
| Meshes | Number of elements | Number of nodes | Average element size around crack path |
|--------|--------------------|-----------------|----------------------------------------|
| Mesh 1 | 1,565              | 851             | 5 mm                                   |
| Mesh 2 | 3,477              | 1,828           | 2.5 mm                                 |
| Mesh 3 | 10,513             | 5,385           | 1.25 mm                                |
| Mesh 4 | 19,318             | 9,774           | 0.625 mm                               |

Table 2: Mesh properties for the three-point bending specimen.

Figure 17a shows the non-dimensional load-deflection curves for both the fully mixed formulation described in Section 6 and the fracture layer approach described in Section 6.8. The fracture energy is  $G_F = 5$  N/m and induces a sharp snap-back response. For both formulations, the load-deflection curves converge to the same limit after four levels of mesh refinement. Since the fracture layer approach gives very similar results to the mixed variational formulation, we will only show results for the former from now on. Figure 17b shows that the SFM solution converges to values in very good agreement with both the work of Carpinteri and Colombo [33], which used adaptive mesh refinement in combination with a node release technique, and of Moës and Belytschko [84], which used the XFEM. Figure 18 shows the true/surrogate crack paths and the subdomains  $\tilde{\Omega}_\ell$



(a) Comparison between the fully mixed formulation (65) and fracture layer variational formulation (71).



(b) Comparison of the fracture layer SFM formulation against references.

Figure 17: SFM computations of the three-point bending test: Non-dimensional load-deflection curves for brittle response ( $G_F = 5$  N/m).

and  $\Omega \setminus \tilde{\Omega}_\ell$  for the fracture layer implementation of the SFM. We consider here different loading stages for Mesh 1 and again  $G_F = 5$  N/m. Note that, for the SFM, the true crack path is computed from the surrogate crack path using the distance vector  $\mathbf{d}$  and the maximal principal tensile stress criterion.

**Remark 14.** *The SFM estimate of the true crack path is very accurate, considering that the computational grid is unstructured and without symmetries. We believe this is due to the combination of the use of a cohesive zone model, which prevents gradients to grow unbounded as the grid is refined, and the approximation properties of the Taylor expansion, which remain valid under these conditions.*

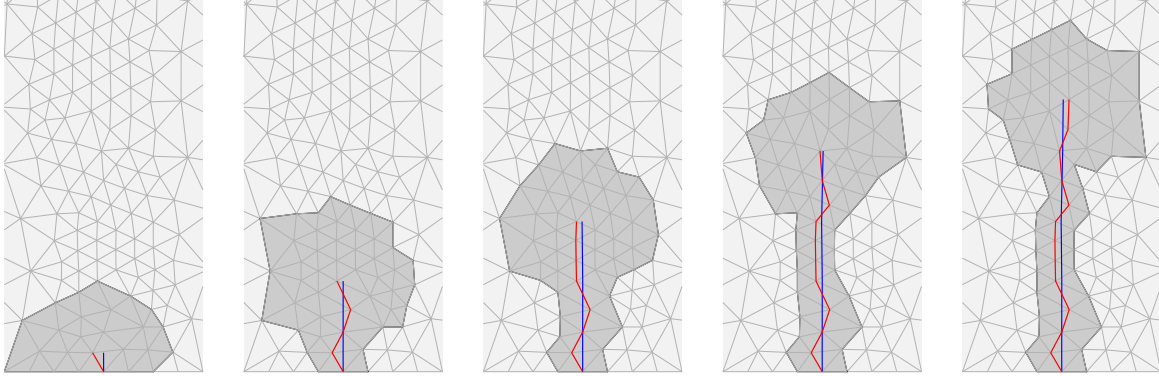


Figure 18: SFM computations of the three-point bending test: Crack path and layer at different stages of the fracture propagation. Simulations are performed for a brittle material ( $G_F = 5$  N/m) and Mesh 1. The estimated true crack path is plotted in blue and the shifted (surrogate) crack path is plotted in red for different loading stages. The estimated true crack path is obtained by shifting the edges of the surrogate crack path by the distance vector  $\mathbf{d}$ . The dark gray area represents  $\tilde{\Omega}_\ell$ , the layer where the mixed SFM formulation is applied. A standard displacement-based primal formulation is applied elsewhere.

It is worthwhile at this point to compare the SFM with the node-release technique (NRT), which in practice corresponds to the case of a primal (displacement-based) variational formulation of the SFM with the distance vector enforced to be  $\mathbf{d} = \mathbf{0}$ . Figure 19 shows a comparison of the numerical results obtained with the SFM and the NRT (the latter is clearly mesh dependent), for a fracture energy  $G_F = 5$  N/m. For the NRT, the approximate crack path follows the edges of the grid, and the cohesive interface conditions are imposed on the approximate crack (depicted in green in the two plots on the left of Figure 19). As already mentioned, in the case of the SFM, the crack path is estimated from the surrogate crack path using the distance  $\mathbf{d}$ , and this results in a considerably more accurate result (marked in blue). For comparison, the black dashed line indicates the exact fracture path.

This difference in approximation has also very important consequences in the profiles of the non-dimensional load-deflection curves, shown in the right panel of Figure 19. The NRT produces large oscillations in the load-deflection curves and a large overshoot for the peak load, because the direction of propagation of the crack is highly influenced by the orientation of the candidate edges. The edges in the crack path obtained with the NRT can easily form angles between  $30^\circ$  and  $90^\circ$  with respect to the true crack direction. As a result, whether the crack propagation direction is chosen by way of stress intensity factors or maximum (averaged) principal stresses, a much larger load is required to reach the critical value  $t_{cr}$  on those edges. In this way, both overshoot and oscillations can be observed in the load-deflection curves. Instead, for the SFM, the crack direction is not tied

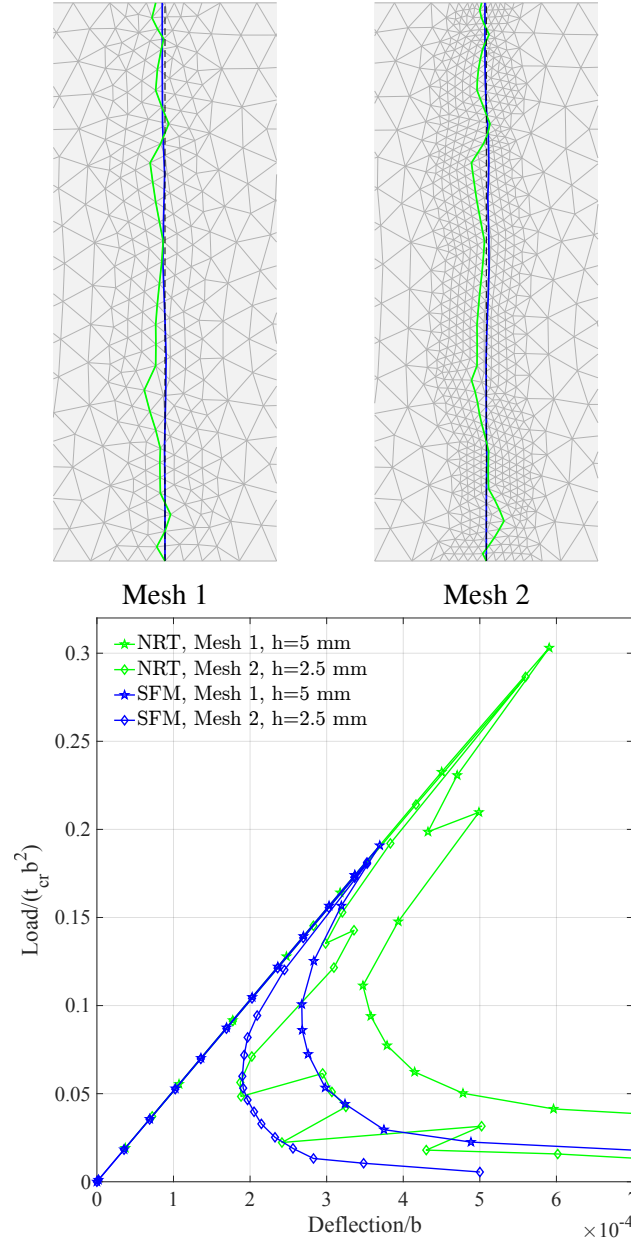


Figure 19: Three-point bending specimen with fracture energy  $G_F = 5 \text{ N/m}$ . On the left, the crack path for the NRT (green) and the SFM (blue) with fracture energy  $G_F = 5 \text{ N/m}$  on different meshes. The black dashed line shows the exact vertical crack path. On the right, the non-dimensional load-deflection curves for the NRT (green curves) and the SFM (blue curves).

to the edges' orientation, and, as a consequence, we obtain very smooth load-deflection curves without overshoots or oscillations. Note also that the SFM produces a very good approximation to the overall fracture surface area, because of the area correction factor  $\mathbf{n} \cdot \tilde{\mathbf{n}}$  discussed in Remark 11 of Section 6.6.

The three-point bending specimen test can also be used to evaluate the accuracy of the SFM and NRT in estimating the position of the crack path at various resolutions. A measure of the error

in location of the surrogate crack and the exact crack path is the shaded area shown on the left of Figure 20. An analogous definition would hold for the error between the estimated true crack path location and the exact crack path location. A definition that encompasses all these measures of error is

$$e_p = \int_{\Gamma_p} |x_e - x_p| |\mathbf{n}_p \cdot \mathbf{n}_e| d\Gamma_p \quad (73)$$

where  $\Gamma_p$  is a computed crack path, and  $x_e$  and  $x_p$  are the  $x$ -components of points  $\mathbf{x}_e$  and  $\mathbf{x}_p$  on the exact and computed crack paths  $\Gamma_{c,e}$  and  $\Gamma_p$ , respectively. In the specific case of the SFM, (73) can be evaluated with  $\Gamma_p = \tilde{\Gamma}_c$ , for the surrogate crack path, or  $\Gamma_p = \Gamma_c$ , for the estimated true crack path. In the case of the NRT, instead, (73) can only be evaluated on  $\Gamma_p = \tilde{\Gamma}_{c;\text{NRT}}$ , that is a fracture path composed of full edges of the grid. Note that, in general,  $\tilde{\Gamma}_{c;\text{NRT}} \neq \tilde{\Gamma}_c$ , because of the known mesh dependencies in the selection of the fracture path in the NRT. See the left panel of Figure 20 for a visual depiction of the error  $e_p$ , represented as the shaded area between the surrogate and exact crack paths. Note also that in the case of the three-point bending specimen, the exact crack path is vertical and  $\mathbf{n}_e = (1, 0)$ .

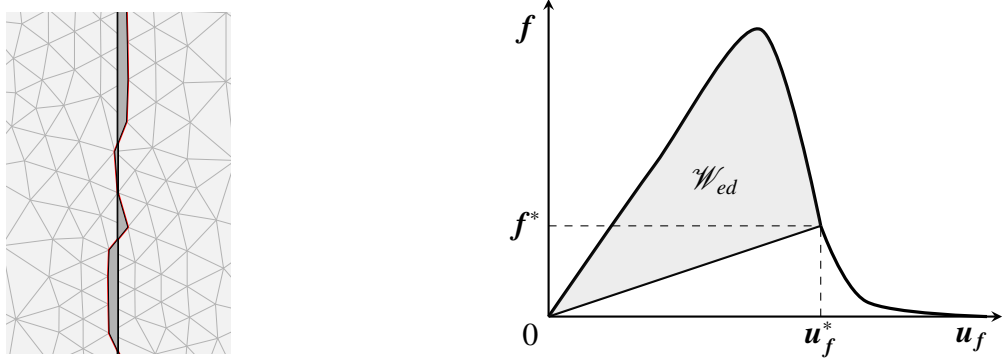


Figure 20: On the left, the crack position error, depicted as the dark gray area between the surrogate crack path (red) and the exact path (black). On the right, the work of external load in a load-displacement plot.

Another measure of the accuracy of the proposed approach is the error between the total dissipated fracture energy and the total work of external loads. The work of an external load  $\mathbf{f}$  that produces a cumulative displacement  $\mathbf{u}_f$  at its point of application can be abstractly defined as

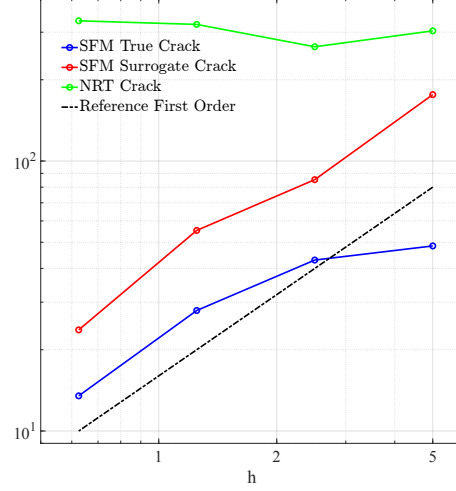
$$\mathcal{W}_{ex} = \int_0^{\mathbf{u}_f} \mathbf{f} \cdot d\mathbf{u} , \quad (74)$$

where the case of a distributed load can be handled with slight modifications. In the case of the three-point bending specimen the load is applied vertically but it is distributed over a small area, over which the work has to be integrated. Part of  $\mathcal{W}_{ex}$  is dissipated by the crack and the other is stored as elastic energy in the domain. The dissipated energy by the crack can be computed as  $\mathcal{W}_{ed} = \int_0^{\mathbf{u}_f^*} \mathbf{f} \cdot d\mathbf{u} - \frac{1}{2} \mathbf{u}_f^* \cdot \mathbf{f}^*$ . Once the crack has completely separated the structural specimen, all the external work would be dissipated by the crack, that is  $\mathcal{W}_{ed} = \mathcal{W}_{ex}$ . As shown in Figure 20,  $\mathcal{W}_{ed}$  is graphically depicted as the shaded area. The energy dissipated by the crack can be calculated as the integral of the fracture energy over the surface of the crack. As shown in Figure 13, for a

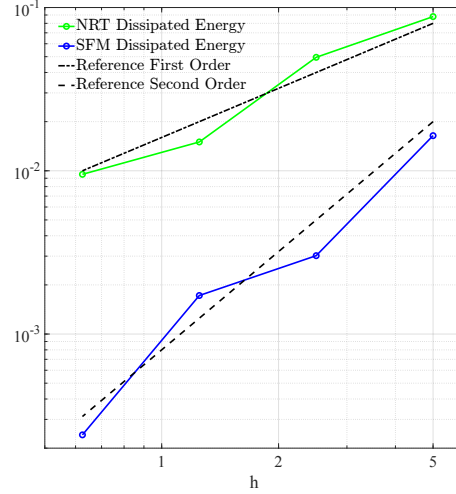
cohesive zone model, the dissipated energy by the crack is

$$\mathcal{W}_{cd} = \int_{\Gamma_c} \left( \int_0^{w^*} t dw - \frac{1}{2} t^* w^* \right) d\Gamma_c . \quad (75)$$

Similarly, when the crack is fully developed,  $\mathcal{W}_{cd} = \int_{\Gamma_c} \left( \int_0^w t dw \right) d\Gamma_c \approx \int_{\tilde{\Gamma}_c} G_F |\tilde{\mathbf{n}} \cdot \mathbf{n}| d\tilde{\Gamma}_c$ . Then we



(a) Crack position error  $e_p$ .



(b) Dissipated fracture energy error  $e_{\mathcal{W}}$ .

Figure 21: Three-point bending specimen: Convergence rate of the SFM and the NRT on crack position error  $e_p$  and the error in the fracture energy budget  $e_{\mathcal{W}}$ , for  $G_F = 5$  N/m.

can introduce

$$e_{\mathcal{W}} = |\mathcal{W}_{ed} - \mathcal{W}_{cd}| , \quad (76)$$

that is, the misfit between the fracture energy and the work of the external load(s).

Figure 21 shows the errors  $e_p$  and  $e_{\mathcal{W}}$  for the three-point bending specimen test, comparing the SFM and NRT. The left panel of the picture shows that the crack position error  $e_p$  *does not converge* for the NRT, while it converges with first-order accuracy for the SFM. The right panel of

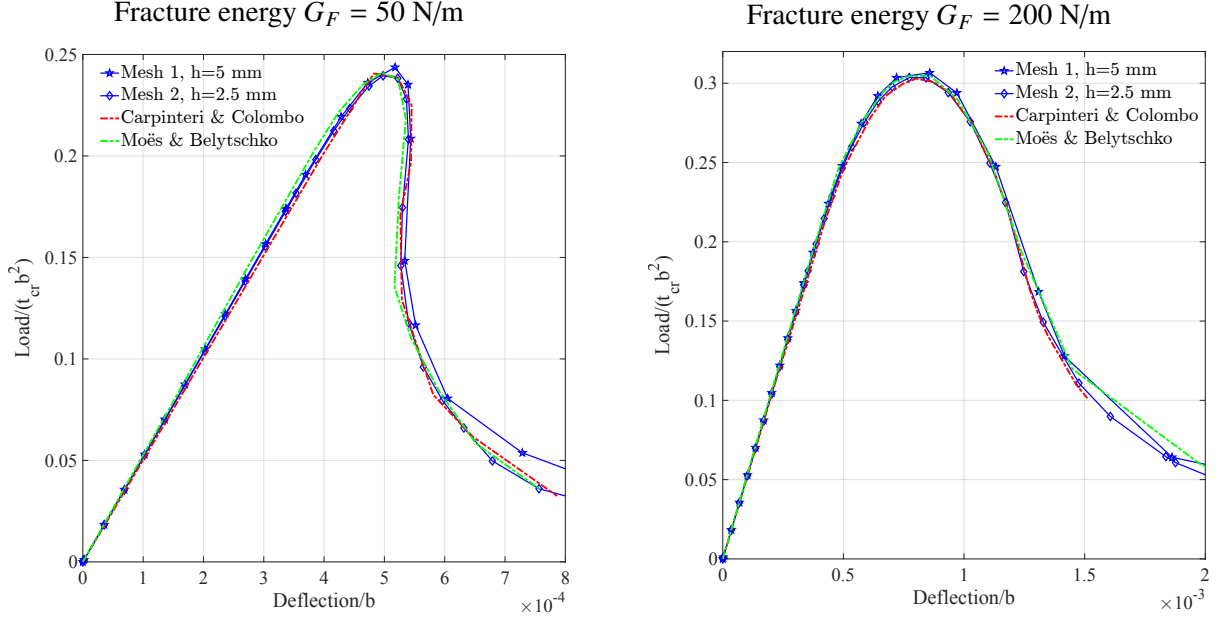


Figure 22: Non-dimensional load-deflection curves for the three-point bending test with fracture energy  $G_F = 50$  N/m and  $G_F = 200$  N/m.

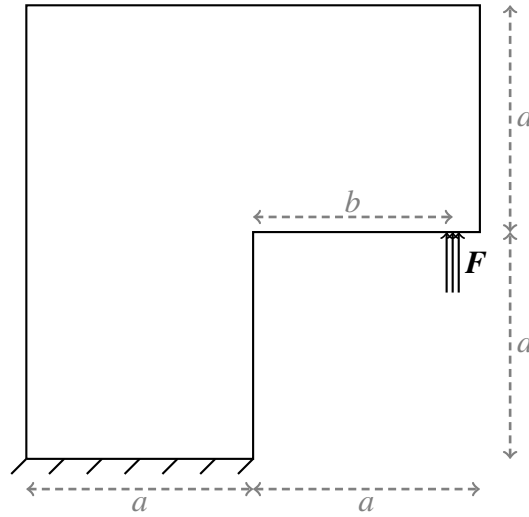
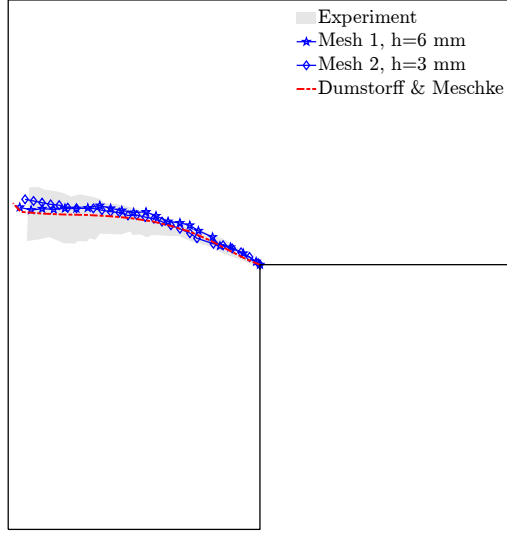


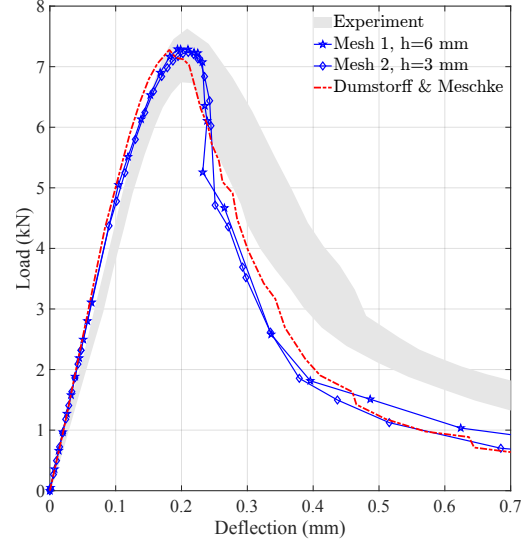
Figure 23: Geometry and setup of the L-shape panel.

the picture shows that while the NRT has a first-order converging  $e_{\mathcal{W}}$ , the SFM provides a quadratic convergence for the same quantity.

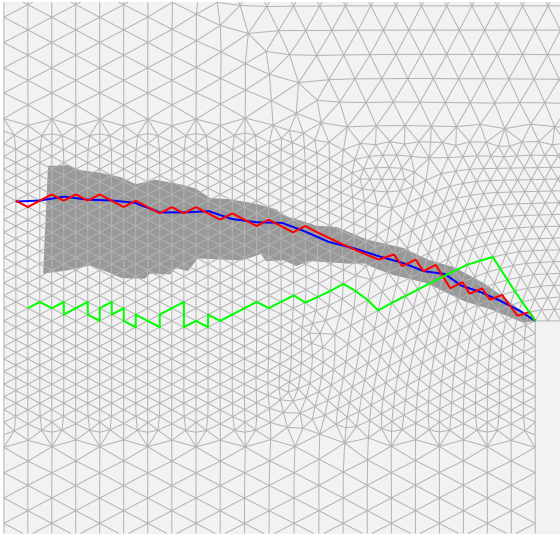
For completeness, we show in Figure 22 the results from three-point bending specimen simulations with the SFM and higher levels of fracture energy, which induce more ductile behavior. In particular, Figure 22 shows the non-dimensional load-deflection curves with fracture energy  $G_F = 50$  N/m and  $G_F = 200$  N/m. Also in this case the SFM solutions agree closely with the classic references [33, 84]. Similar fracture energetic considerations apply in this case.



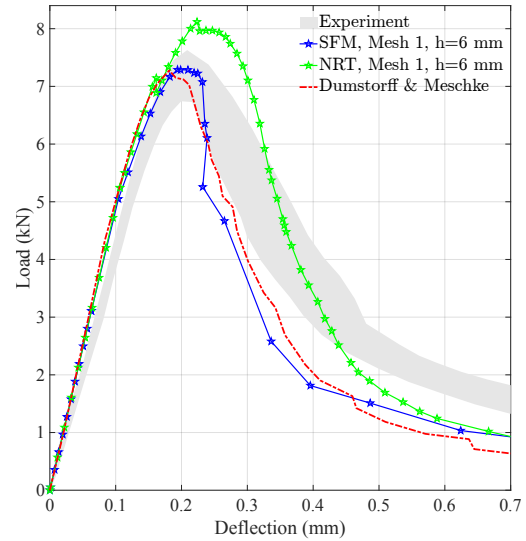
(a) SFM true crack path for the L-shape panel test with SIF.



(b) Load-deflection curve for the L-shape panel test with SIF.



(c) SFM true crack path (blue), surrogate crack path (red) and NRT crack path (green) for the L-shape panel test.



(d) SFM and NRT load-deflection curves for the L-shape panel test.

Figure 24: L-shape panel test [53, 142]. Crack path (left) and load-deflection plot (right).

### 7.1.2. L-shape panel

In this second numerical example, a mixed-mode crack is investigated in an L-shape panel [53, 138, 142]. The geometry, loading and boundary conditions are shown in Figure 23, where  $a = 0.25$  m,  $b = 0.22$  m and the thickness  $t = 0.1$  m. The material properties are Young's modulus  $E = 20$  GPa, Poisson's ratio  $\nu = 0.18$ , fracture energy  $G_F = 100$  N/m, normal critical stress  $t_{cr} = 2.2$  MPa and shear effect parameter  $\beta = 1.5$ . The load  $F$  is distributed over a strip of length 0.01 m centered at the location indicated in Figure 23. As mentioned by references [53, 138], the maximal tensile principal stress criterion does not produce a correct crack path for this mixed-

mode I-shape panel test. In fact, for this approach, shear effects are not fully accounted for around the crack tip, leading to a less accurate direction of propagation of the crack. Therefore, the Stress Intensity Factors (SIF) are used here to select the crack propagation direction. Figure 24a shows the comparison of the SFM true crack path against Dumstorff and Meschke's [53] numerical result and Winkler's [142] experimental results. The SFM solution agrees well with the reference numerical result of Dumstorff and Meschke [53] and lies within the experimental uncertainty bracket of the experiments of Winkler [142]. In Figure 24b, the load-deflection curves of SFM also match the reference numerical and experimental results. Figure 24c shows a comparison of the crack paths obtained from SFM and NRT for Mesh 1. The NRT crack path does not match the experimental results. Figure 24d compares the load-deflection curves for SFM and NRT. The NRT produces a higher peak load compared with the SFM and the reference computational and experimental results. Note that the SFM estimate of the curved true crack path is fairly accurate. The cohesive zone model prevents the stress gradients to become unbounded and this in turns guarantees the validity of the Taylor expansion approach.

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