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A formulation to exactly integrate multiple discontinuities in 2D/3D finite elements by means of equivalent polynomials in XFEM analysis

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Declaration

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Numerical integration of discontinuous functions is a longstanding problem explored by numerous authors over time. This topic acquired even greater attention in fracture mechanics, particularly in the eXtended finite element method (XFEM) context, in which the exact integration of discontinuous functions is essential in order to obtain precise and accurate results. In this scope, equivalent polynomials stand as an efficient method to address the problem harnessing traditional Gauss quadrature rule to exactly integrate polynomials times step function. Specific situations, however, require polynomials times multiple step functions to be integrated (i.e., problems involving crack branching, kinking, and junctions within a single finite element).

This Thesis focuses on the development of a method to exactly integrate polynomials times multiple step functions over various 2D and 3D domain shapes using standard Gauss quadrature, without splitting the integration domain. Traditional integration methods adopted in the XFEM framework may struggle to handle step functions, resulting in inaccurate numerical solutions or requiring multiple domain subdivisions. To address this issue, the research explores the mathematical foundations of equivalent polynomials for the integration of polynomials times step function in the context of XFEM analysis. The concept is then extended to the case of multiple step functions within the integration domain in order to deliver a formulation to smooth the overall integration process.

As a first step towards the integration of an arbitrary number of discontinuities, a closed form solution for the exact numerical integration of polynomials times double step function over quadrilateral domains is proposed. A software implementation of the proposed formulation, the Fortran library *double discontinuity equivalent polynomials* (*DD_EQP*), is also presented, delivering a practical application of the method and demonstrating its ease of implementation, precision and effectiveness. The *DD_EQP* is used to validate the proposed solution by means of numerical testing, providing exact results. The presented formulation is then extended to triangular, tetrahedral and hexahedral domains, demonstrating its effectiveness and the accuracy

for each analysed element shape. Additionally, by means of isoparametric mapping, the solution can be employed on 2D and 3D elements however defined in a global coordinate system, bringing them back to a regular parent element geometry. The effect on the results accuracy in the case of distorted elements is also discussed and mitigation strategies are explored. The extension of the proposed method to an arbitrary number of discontinuities is then addressed and a closed form solution for standard bi-dimensional quadrilateral domains is presented. The results demonstrate that the presented formulation offers an accurate and robust method for the exact integration of polynomials times multiple step functions, which is crucial for the stiffness matrix evaluation of enriched elements in XFEM simulations. The proposed technique provides a mathematical framework which can be also used as a reliable numerical tool to integrate polynomials over complex geometries and non-trivial domain shapes by way of standard Gauss quadrature.

In conclusion, the proposed method provides new pathways for exactly numerically integrate polynomials times multiple step functions, which is essential in simulations of complex physical phenomena in engineering and scientific applications. Moreover, the proposed formulation, as well as the *DD_EQP* library, have a wide application range, not limited to XFEM and fracture mechanics, but also including computational mechanics, mathematical computing of complex geometric regions, and computer graphics.