Gecko
Design for IGA-type discretization workflows

Gecko Technical Report 1

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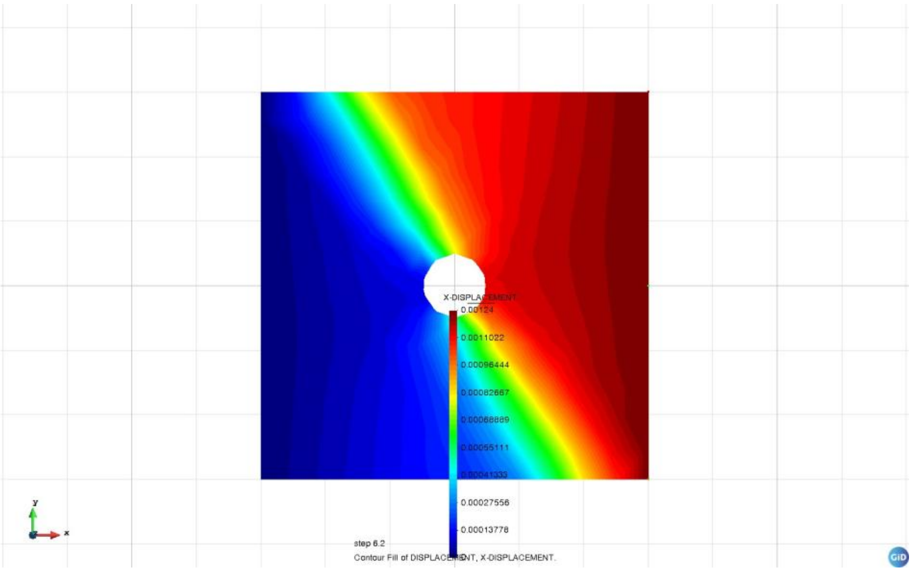


Funded by the European Union

This project has received funding from the European Union's Horizon Europe research and innovation programme under grant agreement No 101073106
Call: HORIZON-MSCA-2021-DN-01

Executive summary

This report summarizes the progress and ongoing research activities in the second year of a PhD project focused on advancing computational solid mechanics, with particular emphasis on damage mechanics and the application of Isogeometric Analysis (IGA). The work aims to build a comprehensive understanding of solid mechanics principles, improve numerical modeling capabilities, and develop computational tools for the simulation of material damage and failure.

Key developments in this phase of the project include:

1. **Strengthening Theoretical Foundations in Solid Mechanics**
   A thorough review of fundamental concepts in structural analysis and solid mechanics has been undertaken, primarily based on Oñate's *Structural Analysis with the Finite Element Method* [2]. This theoretical groundwork supports the understanding and implementation of computational methods for material behavior modeling.
2. **Numerical Modeling and Computational Implementation**
   Practical experience was gained through the implementation of finite element methods (FEM) for basic structural problems. This included solving 1D truss displacement problems and extending the models to include damage mechanics behavior using isotropic damage models based on the work of Oliver et al. [1]. Python and C++ programming languages were used to develop object-oriented codes that simulate stress-strain behavior during loading and unloading cycles.
3. **Advancing to 2D and 3D Damage Models**
   Progress has been made in formulating 2D isotropic damage models with the goal of extending this to 3D solid elements. This includes adapting linear elastic models and introducing nonlinear constitutive models relevant to damage mechanics. A key focus is on integrating regularization techniques to address mesh dependence caused by strain softening, specifically through the refinement of the characteristic length parameter.
4. **Integration with Kratos Multiphysics**
   Efforts have been directed toward understanding and adapting Kratos Multiphysics for damage mechanics applications. The definition of the characteristic length in FEM was reviewed, and a new formulation for IGA was proposed to ensure mesh independence by linking the characteristic length to the NURBS-based geometry representation.
5. **Ongoing and Future Work**
   Current work involves the implementation and validation of the proposed characteristic length formulation for IGA within Kratos Multiphysics. Future research will focus on extending damage models to 3D, validating numerical results, and comparing the performance of FEM and IGA in modeling damage and fracture mechanics.

This report reflects steady progress in building a strong theoretical and computational foundation necessary for addressing complex problems in solid mechanics. The current stage sets the groundwork for more advanced research in damage mechanics and computational modeling in the upcoming phases of the PhD project.

Introduction

In the evolving landscape of computational solid mechanics, the integration of design and analysis workflows remains a critical challenge, particularly in industries that handle complex geometries such as automotive and aerospace engineering. Traditional design processes rely heavily on Computer-Aided Design (CAD) for geometry modeling and the Finite Element Method (FEM) for numerical analysis. However, this separation introduces significant pre-processing efforts, primarily due to the need for meshing CAD geometries for FEM analysis.

Isogeometric Analysis (IGA) has emerged as a promising solution to bridge this gap by utilizing Non-Uniform Rational B-Splines (NURBS)—the foundational elements of CAD—directly in numerical simulations. This approach eliminates the meshing bottleneck and offers high continuity and precision in geometric representation. Yet, applying IGA to complex non-linear solid mechanics problems poses challenges, especially when integrating sophisticated material models like plasticity, damage, and hyperelasticity. These issues are compounded when handling trimmed or irregular geometries where conventional IGA struggles to maintain accuracy and consistency.

Immersed Boundary Representation Analysis (IBRA)-type discretizations present an innovative extension to IGA by facilitating the analysis of geometries with trims, holes, and other irregularities without the need for conforming meshes. This method allows for flexible and efficient modeling of complex 3D solids by embedding the geometry within a structured computational domain. The combined use of IGA and IBRA holds significant potential for improving the stability and accuracy of simulations involving non-linear material behaviors in industrial applications.

Current research focuses on enhancing these discretization methods to handle trimmed volumetric solids and complex material interactions, aiming to deliver reliable and industry-relevant computational tools. This integration promises to streamline the design-to-analysis pipeline, reduce computational costs, and increase the fidelity of simulations, marking a significant advancement in computational solid mechanics.

1. MATHEMATICAL FRAMEWORK IN SOLID MECHANICS

In computational solid mechanics, mathematical equations form the foundation for modeling the mechanical behavior of solid materials under external forces. These equations describe the relationship between external loads, material properties, and the response of the solid body, including stress, strain, displacement, and deformation. The mathematical framework for solving problems in solid mechanics is built on **balance laws**, **constitutive models**, and **boundary conditions**.

1.1 Governing Equations of Solid Mechanics

The primary governing equations in solid mechanics are derived from fundamental principles such as **Newton's laws of motion**, **conservation of mass**, and **conservation of energy**. For a solid body, the basic set of equations can be summarized as follows:

- **1.1.1 Equilibrium Equations**

The equilibrium equations represent the balance of forces acting on a material body. They ensure that the internal forces (stresses) balance the external loads applied to the body. The equilibrium equations in solid mechanics are given by:

$$\sigma_{ij,j} + b_i = 0 \text{ in } \Omega \quad (3.1)$$

where:

- σ_{ij} is the **stress tensor** (with components $\sigma_{xx}, \sigma_{yy}, \sigma_{zz}, \sigma_{xy}, \sigma_{yz}, \sigma_{zx}$)
- b_i represents the **body forces** (per unit volume, e.g., gravitational forces),
- Ω is the domain of the solid body, and
- The comma (,) denotes a derivative with respect to the spatial coordinates.

This equation ensures that the internal forces (the divergence of the stress tensor) balance the body forces at every point in the material.

- **1.1.2 Kinematic Equations**

The kinematic equations describe the relationship between the displacement of points in the solid body and the strain developed due to the deformation. The displacement vector uiu_iui gives the change in position of a point in the body:

$$u_i = u_i(x_1, x_2, x_3, t) \text{ where } i = 1,2,3 \quad (3.2)$$

The **strain tensor** ϵ_{ij} is related to the displacement field through the following equation:

$$\epsilon_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)$$

where:

- u_i is the displacement field (i.e., the movement of material points),
- ϵ_{ij} is the **strain tensor**, which characterizes the deformation of the material,
- x_i are the spatial coordinates.

1.1.3 Constitutive Models

The **constitutive relations** describe the material behavior and how stresses are related to strains. These models depend on the type of material (elastic, plastic, viscoelastic, etc.). For **linear elastic materials**, the relationship is given by Hooke's law:

$$\sigma_{ij} = C_{ijkl}\epsilon_{kl}$$

where:

- C_{ijkl} is the **elastic modulus tensor** that characterizes the material's resistance to deformation,
- ϵ_{kl} is the strain tensor.

For **isotropic linear elasticity**, this simplifies to:

$$\sigma_{ij} = \lambda\delta_{ij}\epsilon_{kk} + 2\mu\epsilon_{ij}$$

where:

- λ and μ are **Lamé's parameters** (related to material stiffness),
- ϵ_{kk} is the trace of the strain tensor (the volumetric strain),
- δ_{ij} is the **Kronecker delta**.

In the case of **nonlinear materials** (e.g., plasticity, damage), the constitutive equations will be more complex, incorporating material behavior under large strains, plastic deformation, or damage evolution.

1.2 Damage Mechanics

In **damage mechanics**, the material is considered to degrade over time or under loading, leading to a reduction in the material's stiffness and strength. The mathematical formulation of damage mechanics requires additional equations to model the material's response to damage, including **damage evolution** and **failure criteria**.

1.2.1 Damage Variable

Damage is often modeled using a **scalar damage variable** d that ranges from 0 (undamaged) to 1 (completely damaged). The damage variable affects the material's stiffness and strength. The **effective stress** is related to the damage variable as:

$$\sigma_{eff} = (1 - D)\sigma$$

where:

- σ_{eff} is the effective stress,
- σ is the nominal stress,
- D is the damage variable.

- **1.2.2 Damage Evolution**

The evolution of the damage variable can be described by various models, such as the **continuum damage mechanics (CDM)** approach. One commonly used formulation is based on **plasticity-damage coupling**, where the damage evolves as a function of the accumulated plastic strain or equivalent stress. The rate of change of the damage variable DDD is given by:

$$\dot{D} = f(\sigma_{eff}, \epsilon_{pl})$$

where:

- $\dot{D}$ is the rate of change of the damage variable,
- f is a damage evolution function,
- ϵ_{pl} is the **plastic strain**.

Various damage evolution laws, such as **strain-based** or **stress-based** laws, can be used depending on the material behavior and failure modes.

- **1.2.3 Failure Criteria**

To predict material failure, several failure criteria can be used in damage mechanics. One common criterion is the **maximum stress criterion**, where failure occurs when the stress reaches a critical value:

$$|\sigma| = \sigma_{fail}$$

where σ_{fail} is the **failure stress** of the material. In more advanced models, failure may depend on both **stress** and **strain** or other factors, such as **cycle loading** in fatigue.

2. COMPARISON OF IGA & FEM IN COMPUTATIONAL SOLID MECHANICS

In the field of computational solid mechanics, the prediction of mechanical behavior and damage evolution in materials is a critical challenge. Among the most widely used numerical techniques for solving solid mechanics problems, **Isogeometric Analysis (IGA)** and **Finite Element Method (FEM)** stand out due to their ability to model complex material behaviors, including damage, cracks, and deformations. This chapter provides an in-depth comparison of **IGA** and **FEM** in the context of computational solid mechanics, focusing on **damage mechanics** and the ability to simulate material failure and crack propagation.

2.1 Introduction to Isogeometric Analysis and Finite Element Method

Isogeometric Analysis (IGA), introduced by Hughes et al. (2005), integrates **Computer-Aided Design (CAD)** representations directly into the analysis process, enabling a seamless representation of geometry and the solution fields. The basis of IGA is the use of **Non-Uniform Rational B-Splines (NURBS)** or **B-splines** for both the geometry and the solution field (e.g., displacements, stress, etc.). This exact representation of geometry provides significant advantages over traditional finite element methods.

The **Finite Element Method (FEM)**, on the other hand, has been the standard numerical method for solving solid mechanics problems for decades. FEM discretizes the domain into small elements, where the problem is solved numerically using polynomial approximations. While FEM has proven to be highly versatile and effective in a wide range of problems, it typically involves approximations of the geometry, leading to potential errors, especially in complex structures.

Both methods are widely used in computational solid mechanics, including in the study of **damage mechanics**, where the goal is to predict the evolution of damage in materials under various loading conditions. However, their differences in geometry representation, element formulation, and crack modeling make them suitable for different types of damage problems.

2.2 Geometry Representation and Continuity

- **Isogeometric Analysis (IGA)**: A key feature of IGA is its **exact representation of geometry**. Using NURBS or B-splines, IGA can represent **curved** and **complex geometries** exactly without the approximation errors seen in FEM. This is particularly beneficial when modeling intricate geometries, such as those encountered in **damage mechanics** simulations involving cracks or material interfaces. IGA also provides **higher-order continuity** (C^1, C^2, etc.) in its shape functions, making it ideal for simulating smooth deformation and material behavior.

- **Finite Element Method (FEM)**: FEM approximates geometry using a **discretized mesh**, which can lead to errors when modeling complex geometries. The accuracy of the geometry representation in FEM depends on the mesh resolution and element type used. FEM typically employs **lower-order continuity** (C^0), meaning that while displacement continuity is maintained, higher-order derivatives such as stress and strain may exhibit discontinuities. This lower continuity can be a limitation when dealing with smooth material behavior but is suitable for handling discontinuous damage such as cracks.

- **Comparison**: While IGA provides a more accurate and continuous representation of the geometry, FEM is more flexible in handling different types of element formulations, which makes it more adaptable to problems involving localized damage and cracks.

2.3 Element Design and Mesh Sensitivity

- **Isogeometric Analysis (IGA)**: IGA uses **higher-order elements** that are capable of capturing complex material behavior with fewer degrees of freedom compared to FEM. The **higher-order basis functions** in IGA provide better accuracy for problems involving **smooth deformations** and **damage evolution**. In many cases, IGA requires **fewer elements** to achieve the same level of accuracy, especially for problems involving complex geometries.

- **Finite Element Method (FEM)**: FEM typically uses **lower-order elements** that require finer meshing and local refinements to achieve the desired level of accuracy. In problems involving **damage localization**, such as crack propagation, **fine mesh refinement** near the crack tip is often necessary. Mesh sensitivity is a common issue in FEM, especially when dealing with stress concentrators or sharp damage features.

- **Comparison**: While IGA generally requires fewer elements for high accuracy in smooth problems, FEM's flexible meshing and **adaptive refinement** capabilities make it better suited for problems involving **sharp damage features**, such as cracks, where localized refinement is needed.

2.4 Modeling Cracks and Damage Propagation

- **Isogeometric Analysis (IGA) and Crack Propagation**: A significant challenge in **damage mechanics** is simulating the propagation of **cracks**. IGA's smooth basis functions are not naturally suited for capturing the **discontinuities** introduced by cracks, as they lead to sharp changes in displacement and stress fields. The inherent **higher continuity** of IGA can create difficulties in modeling **crack initiation** and **propagation** in a realistic manner, especially in mode I fracture where stress singularities are present.

- **Approaches to Handle Cracks in IGA**: To address this challenge, several strategies have been developed:
  - **Phase-Field Models**: These models introduce a continuous representation of cracks, simulating crack growth as a **gradual transition** from intact to damaged material. Phase-field models are particularly well-suited to IGA, as they allow for the smooth evolution of damage without the need for sharp discontinuities (Miehe et al., 2010).
  - **Extended Finite Element Method (XFEM)**: XFEM can be combined with IGA to enrich the basis functions near the crack region, allowing for the representation of cracks without the need for remeshing (Belytschko et al., 2009).

- **Finite Element Method (FEM) and Crack Propagation**: FEM, due to its **lower continuity** nature, is better suited for simulating **cracks** and **discontinuous damage**. FEM can easily accommodate cracks using various methods:
  - **Extended Finite Element Method (XFEM)**: XFEM extends the FEM by enriching the displacement field near crack regions to capture **discontinuities** in displacement and stress without the need for remeshing (Moës et al., 1999).

● **Comparison**: While IGA faces challenges in directly simulating cracks due to its smoothness and higher continuity, techniques like **phase-field models**, and **XFEM** allow IGA to simulate cracks effectively. On the other hand, FEM is naturally suited to handle **discontinuous damage** and crack propagation due to its ability to introduce **sharp discontinuities** and perform **adaptive meshing**.

2.5 Computational Efficiency

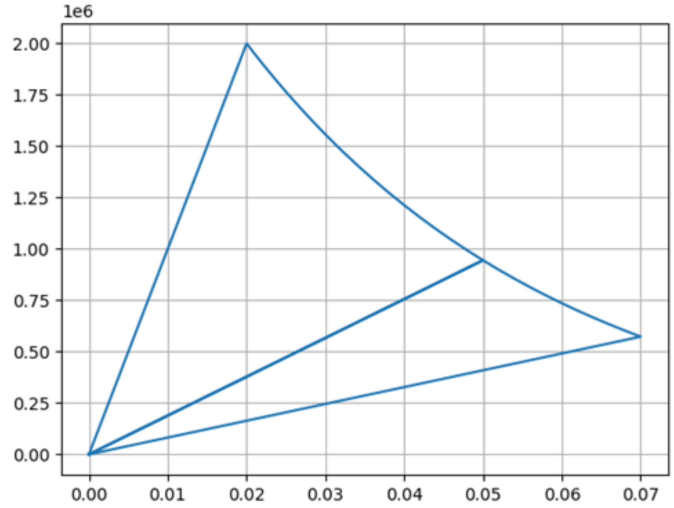
● **Isogeometric Analysis (IGA)**: IGA's exact representation of geometry and higher-order elements make it computationally efficient for problems with smooth damage evolution and complex geometries. The use of fewer elements can lead to significant computational savings. However, when applied to highly **nonlinear damage models**, the integration over higher-order elements can be computationally expensive (Hughes et al., 2005).

● **Finite Element Method (FEM)**: FEM is highly adaptable and can be computationally efficient, especially when **adaptive meshing** or **parallel processing** techniques are used. However, problems involving cracks or localized damage often require fine mesh refinements, increasing computational cost. **Remeshing** during crack propagation can add further overhead (Zienkiewicz et al., 2005).

● **Comparison**: IGA is more efficient for problems with smooth damage evolution and less complex crack behavior, while FEM is better suited for **large-scale problems** involving **crack propagation** and **local damage**.

3. ISOTROPIC DAMAGE MODELS

- **3.1 Isotropic Damage Models in One-Dimensional Systems**



■ *Figure 3.1. Stress-strain curve during both loading and unloading phases for the given material properties, with a Young's modulus (E) of 1.00E+08 Pa, yield stress of 2.00E+06 Pa, and fracture energy of 5.00E+04 J/m2*

A critical area of study in damage mechanics is the development of **isotropic damage models**, which describe the degradation of material properties due to loading and unloading cycles. A commonly used formulation for such models is that introduced by **Oliver et al.** (Oli+90), which characterizes the **stress-strain relationship** of materials undergoing damage.

In the 1D isotropic damage model, the material response is governed by the evolution of a damage variable, which reduces the effective stiffness of the material as damage accumulates. This model accounts for both loading and unloading behavior, and its implementation involves solving the system of equations that govern the damage evolution process. For instance, by considering a material with properties such as **Young's modulus (E)** of 1E+08 Pa, a **yield stress** of 2 MPa, and a **fracture energy** of 5E+04 J/m², the material's degradation can be studied by solving the stress-strain relations for different loading paths, as illustrated by the stress-strain curve (Figure 3.1).

3.2 Extension to Two-Dimensional Damage Models

Building on the 1D isotropic damage model, a natural progression is to extend the formulation to **two-dimensional** systems. In these models, the material exhibits strain-softening behavior, which requires careful attention to **regularization techniques** to prevent mesh dependence in simulations. The **characteristic length (l_c)** is a critical parameter in this context, as it determines the scale at which damage is regularized, ensuring that damage and fracture processes are not overly influenced by the numerical mesh.

In traditional FEM formulations, the characteristic length is computed based on the maximum distance from the centroid of an element to its nodes. For a triangular element, the characteristic length l_c is given by:

$$l_c = max(\| \mathbf{x}_c - \mathbf{x}_i \|), i = 1,2,3$$

where xc\mathbf{x}_c is the centroid and xi\mathbf{x}_i are the coordinates of the element's vertices. This approach is effective in FEM, where the mesh is discretized with nodes. However, this definition is not directly applicable to **Isogeometric Analysis (IGA)**, where elements are defined in terms of **NURBS** (Non-Uniform Rational B-Splines) basis functions rather than nodal points.

3.3 Characteristic Length in Isogeometric Analysis (IGA)

In IGA, the elements are not tied to a discrete mesh of nodes, but rather defined by the continuous nature of the NURBS basis functions. To maintain the role of the characteristic length in regularizing damage mechanics models within IGA, a new formulation is needed.

The characteristic length l_c in IGA is defined based on the **parametric spans** of the NURBS basis functions, rather than relying on the geometry's nodal discretization. For instance, for a quadrilateral element, the characteristic length can be expressed as:

$$l_c = max(\square \mathbf{x}(u_{i+1}, v_j) - \mathbf{x}(u_i, v_j) \square, \square \mathbf{x}(u_i, v_{j+1}) - \mathbf{x}(u_i, v_j) \square),$$

where $\mathbf{x}(u, v)$ is the mapping from the parametric space to the physical space, and uu and vv are the parameters defining the NURBS surface. This definition ensures that the characteristic length in IGA reflects the smooth, continuous nature of the geometry and maintains the regularization properties needed for accurate damage modeling.

3.4 Role of Regularization in Damage Mechanics

In damage mechanics, the **regularization** of strain-softening behavior is critical to obtaining stable and physically meaningful solutions. Without regularization, damage models can exhibit **mesh dependence**, where the results vary significantly with the mesh size, leading to unphysical crack patterns and non-converging solutions. The characteristic length l_c, whether defined in FEM or IGA, serves as a scale factor that regularizes the damage evolution, ensuring that the results are independent of the discretization used.

The regularization process is particularly important in the simulation of **fracture** and **material degradation**, where local damage must be captured without introducing numerical artifacts. By defining l_c in a way that is consistent with the underlying geometry, as in the case of the IGA-based definition, the approach mitigates mesh dependency and allows for more accurate simulations of complex material behavior.

4. CONCLUSIONS

The integration of advanced computational methods, such as **Isogeometric Analysis (IGA)** and **damage mechanics**, represents a significant step forward in the modeling of complex material behavior, particularly in the context of fracture and degradation. By extending traditional FEM formulations to IGA, a mesh-independent framework has been developed that improves the accuracy and efficiency of damage simulations.

Future work will focus on implementing these formulations within comprehensive computational frameworks, such as **KRATOS Multiphysics**, and conducting numerical experiments to validate the effectiveness of the IGA-based characteristic length in capturing the true material response to loading and damage. This work aims to provide more reliable and physically realistic models for the analysis of material failure, with potential applications in a wide range of engineering problems.

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