Gecko

Design for IGA-type discretization workflows

Gecko Technical Report 1

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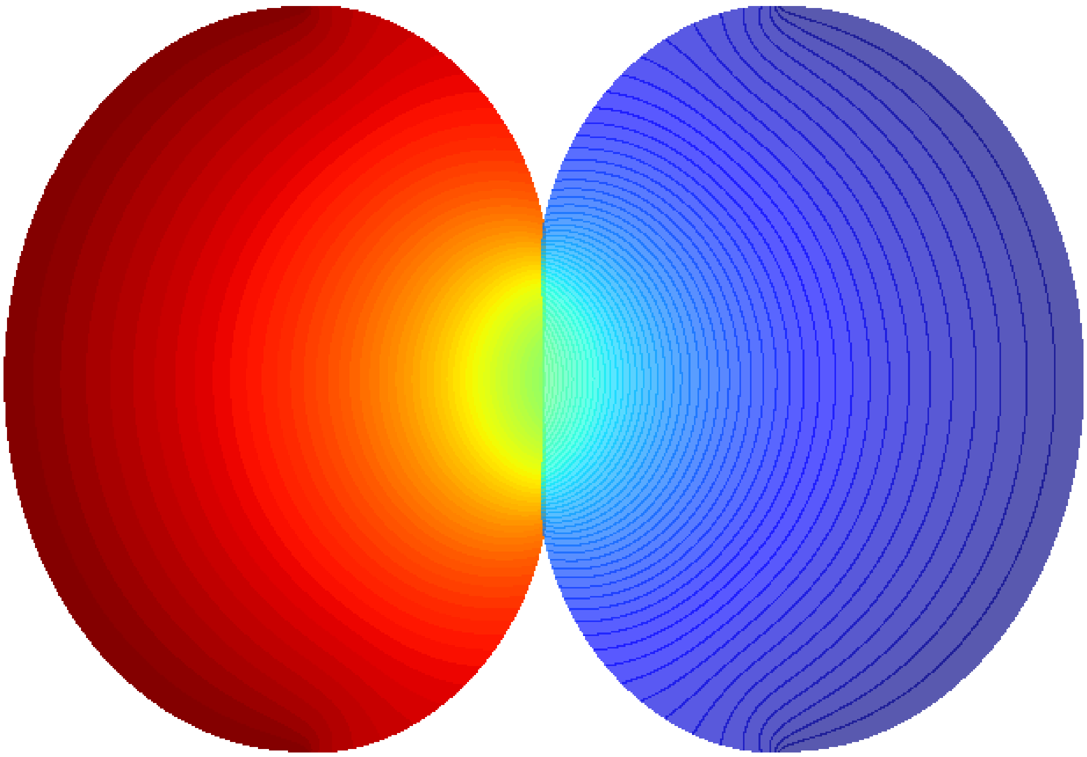

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Executive summary

This document presents the integration of the Shifted Boundary Method (SBM) into the framework of Isogeometric Analysis (IGA), creating a robust and efficient approach for solving structural and contact mechanics problems. The synergy between SBM and IGA addresses longstanding challenges in computational mechanics, particularly those related to handling complex geometries and accurately simulating contact interactions.

The Shifted Boundary Method enhances the flexibility of computational frameworks by shifting boundary conditions to surrogate boundaries, avoiding the need for watertight meshes and simplifying preprocessing. When combined with IGA, which uses smooth spline-based basis functions like B-splines and NURBS, this approach ensures high continuity and exact geometric representation. These features make the framework particularly effective for intricate geometries and scenarios where precision is critical, such as contact mechanics.

In the context of contact mechanics, a novel penalty-free Nitsche formulation has been developed. This method simplifies the enforcement of contact constraints, eliminating the need for additional variables like Lagrange multipliers or penalty parameters, while maintaining accuracy and numerical stability. The approach has been validated through classical benchmarks such as the Hertz contact problem and patch test, demonstrating its ability to handle large deformations and complex contact conditions with precision. Key achievements include:

1. Successful integration of SBM and IGA for complex geometries, preserving high accuracy and reducing computational overhead.
2. Development of a penalty-free Nitsche formulation for contact mechanics, simplifying implementation and ensuring robust constraint enforcement.
3. Validation of the framework through benchmark problems, highlighting its accuracy, stability, and efficiency compared to traditional FEM.

Looking forward, this framework is well-positioned to extend to immersed contact mechanics, enabling the simulation of even more complex systems. The flexibility of SBM combined with the precision of IGA opens new possibilities for tackling challenging multi-scale and large-deformation problems in various engineering fields.

In conclusion, the integration of SBM and IGA represents a transformative step in computational mechanics, delivering a powerful tool that combines theoretical innovation with practical applicability to meet the demands of modern engineering challenges.

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List of abbreviations

ALM	*Augmented Langrangian Multiplier method*
FEM	*Finite Element Method*
IGA	*IsoGeometric Analysis*
LM	*Lagrangian Multiplier method*
SBM	*Shifted Boundary Method*

Introduction

Isogeometric Analysis (IGA) has revolutionized computational mechanics by bridging the gap between Computer-Aided Design (CAD) and numerical simulations, enabling exact geometric representation and high continuity across element interfaces. This integration is particularly advantageous for applications such as contact mechanics, where precision in stress distribution and deformation modeling is critical. IGA employs smooth basis functions like B-splines and Non-Uniform Rational B-Splines (NURBS), ensuring geometric fidelity and reducing the degrees of freedom required for accurate simulations compared to traditional Finite Element Methods (FEM).

Despite these advantages, traditional boundary-fitted IGA implementations face significant challenges when applied to complex geometries. The need for watertight models and the computational cost of handling trimmed or discontinuous surfaces can hinder efficiency. To address these challenges, the Shifted Boundary Method (SBM) has emerged as a complementary technique. By shifting boundary conditions to surrogate boundaries and modifying them using Taylor expansions, SBM avoids issues like small cut cells and simplifies preprocessing. Its integration into the IGA framework enhances flexibility in handling intricate geometries and boundary conditions, particularly for immersed scenarios.

This document presents the integration of SBM within IGA, with a particular focus on its application to contact mechanics. The combination of SBM and IGA addresses challenges related to boundary imposition and geometric complexity, while also advancing contact mechanics formulations through a penalty-free Nitsche approach. Benchmarks such as the patch test, Hertz contact problem, and punch test validate the robustness, efficiency, and accuracy of these methods. By balancing SBM's versatility in geometry handling with IGA's precision and computational advantages, this work highlights a comprehensive framework for tackling complex structural and contact mechanics problems.

1. The Shifted Boundary Method in IGA

Isogeometric Analysis (IGA) has emerged as a transformative approach in computational mechanics, bridging the longstanding gap between Computer-Aided Design (CAD) and Computer-Aided Engineering (CAE). Initially proposed by Hughes et al. [1, 2, 3, 4, 5], IGA delivers precise geometric representations and high levels of continuity at element interfaces [6], making it especially effective for accurately modeling intricate geometries [7, 8, 9]. The foundation of IGA lies in employing B-Splines and NURBS basis functions, which provide smooth transitions and enable localized refinements, ultimately enhancing the reliability and precision of simulations [10, 11].

Despite its strengths, traditional boundary-fitted implementations of IGA encounter notable hurdles with complex geometries. These include the need for watertight models and the computational overhead of managing trimmed or discontinuous surfaces [12, 13]. To address these challenges, immersed boundary techniques, such as the Finite Cell Method (FCM) [14, 15] and Isogeometric Boundary Representation Analysis (IBRA) [16, 17, 18, 19, 20], have been introduced. These methods bypass the need for strict boundary conformity by working with non-boundary-fitted meshes. However, a persistent issue in these approaches is the handling of small cut cells [21, 22], which can degrade computational performance and complicate solver convergence.

The Shifted Boundary Method (SBM) [23,24], originally developed in the context of the Finite Element Method (FEM), provides an innovative approach to overcoming challenges associated with traditional boundary-fitted methods. By shifting boundary conditions to a surrogate boundary and leveraging Taylor expansions for accurate boundary value modifications, SBM effectively eliminates the issues caused by small cut-cells. This simplification not only maintains optimal accuracy but also reduces the complexity of mesh generation and refinement. Applications of SBM in FEM have already demonstrated its efficacy in elasticity and incompressible fluid dynamics [25,26,27,28].

1.1 A brief comparison: IGA and FEM

A key step in advancing the use of IGA was the implementation of a general body-fitted problem, where a flexible, nonlinear mapping between the parameter and physical spaces was developed. This mapping leverages IGA's inherent capability to describe CAD geometries perfectly, ensuring precise simulation of even the most complex domains.

- **Advantages of IGA over FEM in Body-Fitted Scenarios**

Comparative studies between IGA and FEM have revealed several advantages of IGA in body-fitted scenarios:

1. **Reduced Degrees of Freedom (DOFs)**:
   IGA requires fewer DOFs to achieve the same error level compared to FEM. This is due to the higher-order continuity of NURBS, which reduces the number of elements and control points needed for accurate approximations.
2. **Exact Geometry Representation**:
   Unlike FEM, where mesh generation can introduce geometric inaccuracies, IGA ensures that the computational domain is an exact replica of the CAD model (Figure 1). This exactness is particularly beneficial for problems where geometric fidelity is critical, such as those involving contact mechanics.

3. **Simplified Refinement**:
   Refinement in IGA can be achieved without altering the underlying geometry, making it more straightforward to adapt the computational model to different levels of precision.
4. **Higher Convergence Velocity**:
   Both FEM and IGA exhibit similar convergence orders when using the same polynomial degree. However, IGA's ability to easily increase the order of basis functions without remeshing provides a significant edge. Higher-order basis functions lead to enhanced convergence rates, enabling IGA to achieve desired accuracy more efficiently and lower numbers of degrees of freedom (Figure 2).

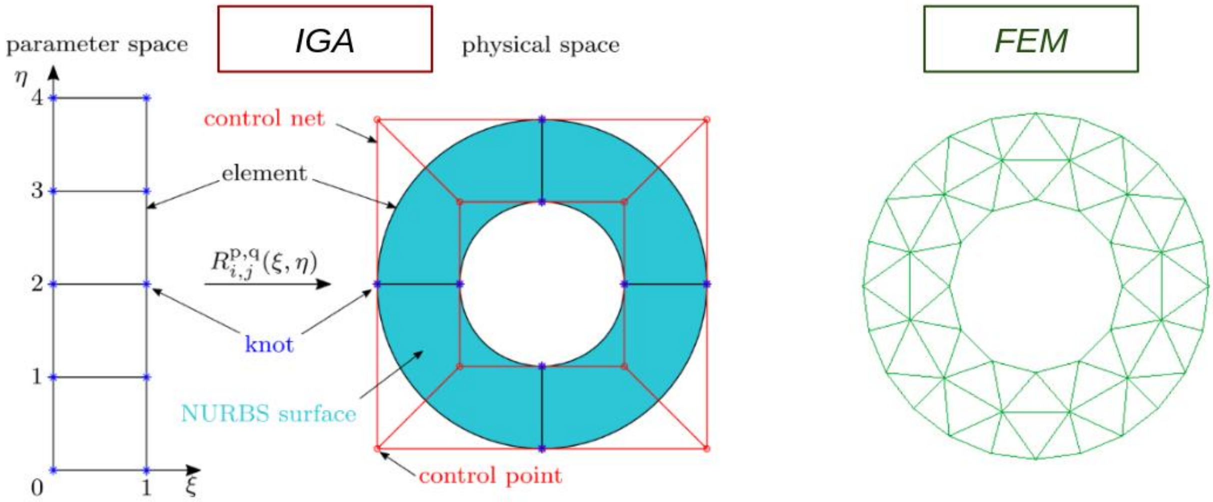


***Figure 1**. Comparison of IGA and FEM discretizations.*

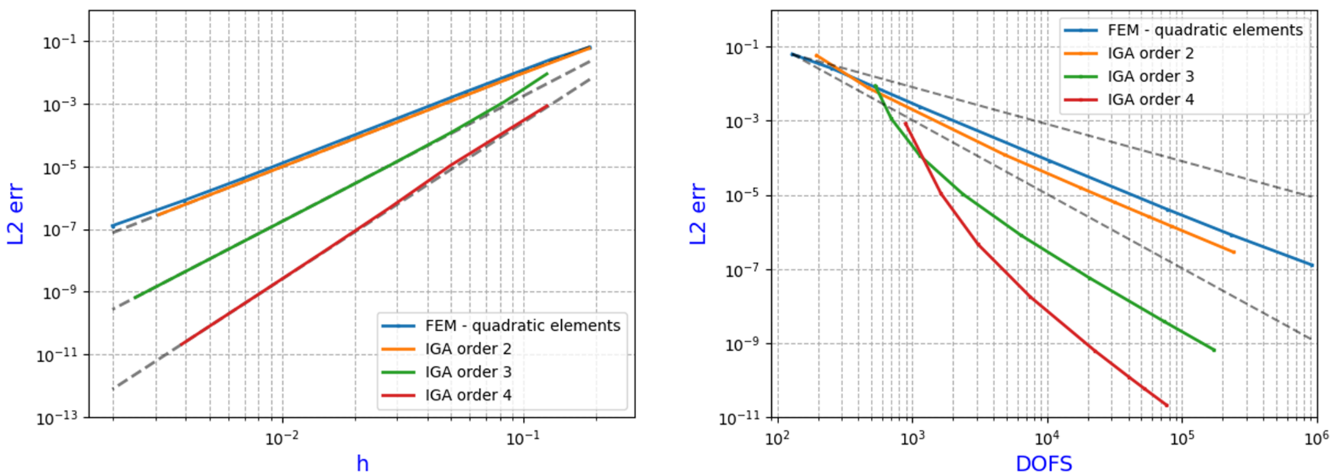


***Figure 2**. Comparison of IGA and FEM convergence and DOFs utilization.*

1.2 The Shifted Boundary Method

The Shifted Boundary Method (SBM) offers a flexible framework to address challenges in numerical integration over complex domains, including contact mechanics. As outlined in [29], SBM shifts the imposition of boundary conditions from the true boundary Γ to a surrogate boundary Γ_h , composed of edges of a computational grid.

Boundary conditions are modified using Taylor expansions, ensuring optimal convergence rates. This approach avoids challenges associated with small cut cells and simplifies numerical integration, making it particularly suited for embedded methods and large deformation problems.

In this context, the SBM complements Isogeometric Analysis (IGA) by leveraging exact geometry descriptions and avoiding trimmed knot spans. This synergy improves the representation of physical geometries and enhances computational efficiency.

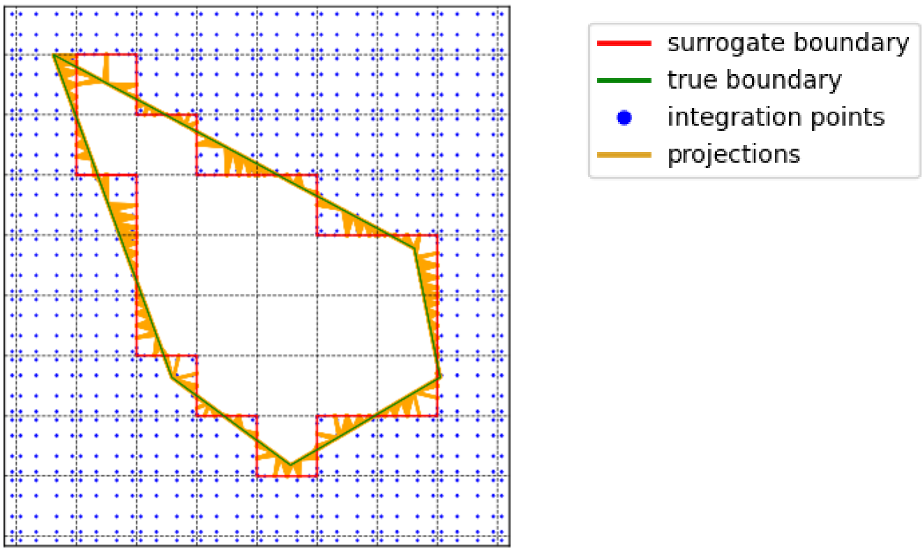
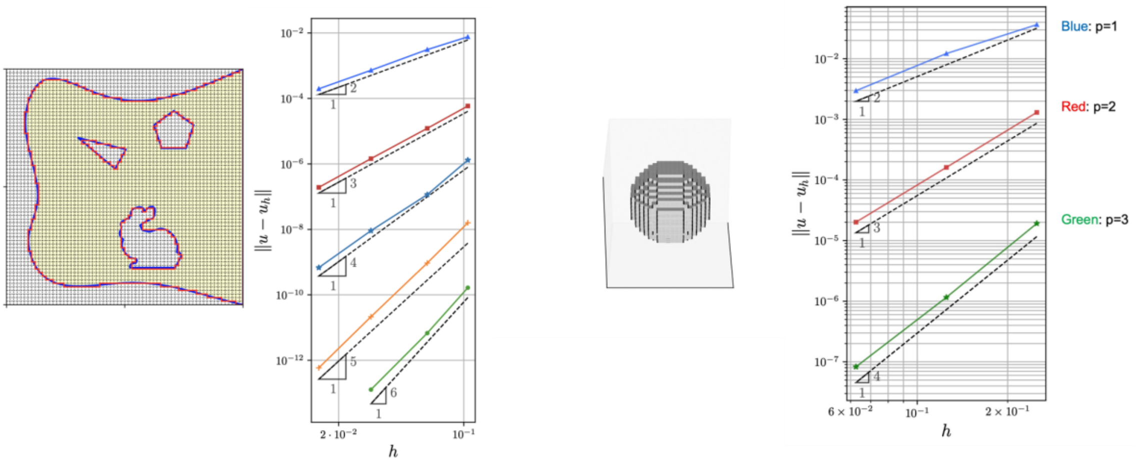


Figure 3: *SBM main characteristics.*

The SBM for IGA has been implemented inside the Kratos Multiphysics framework (KratosMultiphycsGithub) to handle 2D fluid and structural mechanics problems with complex geometries.

The SBM implementation preserves the optimal convergence of body-fitted cases under Dirichlet boundary conditions, though it experiences a one-order reduction in convergence for Neumann (load) conditions. This functionality has also been extended to 3D problems, broadening its applicability (Figure).



■ ***Figure 4.*** *IGA+SBM for 2D/3D problems.*

Finally, Figure 5 shows a convergence comparison between standard IGA and IGA with SBM for the case of circular geometry. No big loss is evident for the use of the SBM against the exact geometry of the body-fitted scenario.

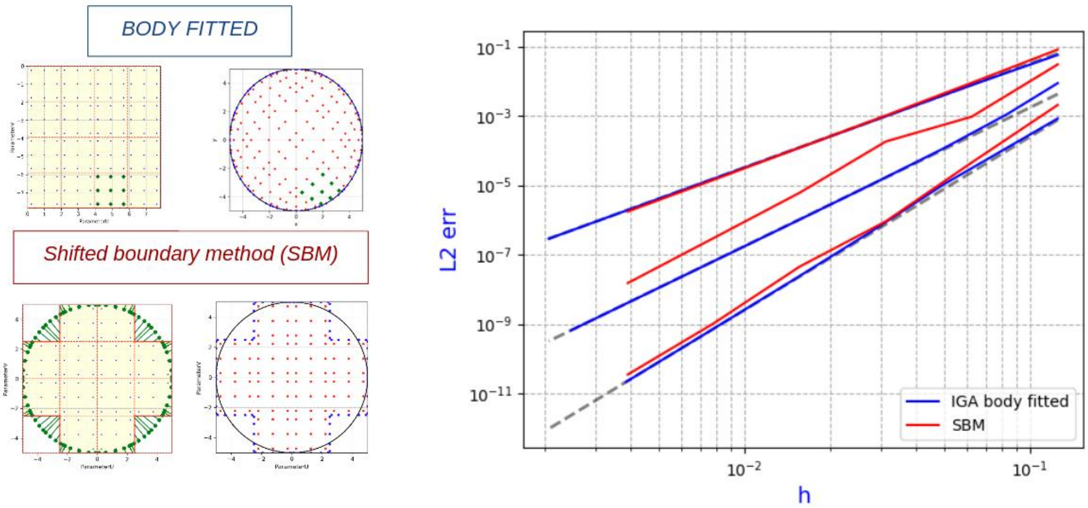


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Figure 5. *Comparison of IGA body-fiitted and IGA + SBM convergence for a circle.*

2. Towards a “penalty-free” Contact mechanics

Contact mechanics investigates the interaction of surfaces under load, with emphasis on stress distribution, deformation, and phenomena such as friction and adhesion. This field is essential in various engineering applications, including mechanical systems, aerospace structures, and biomechanics, where precision is paramount for safety and performance.

The theoretical foundations of contact mechanics were laid by Hertz [30], who developed analytical solutions for elastic contact between simple geometries. With the advent of computational methods, the field expanded significantly, particularly through the Finite Element Method (FEM). FEM allowed researchers to tackle more complex geometries and material behaviors, extending contact analysis to elastic-plastic transitions [31,32]. Additionally, multiscale models emerged, enabling the integration of microstructural interactions into macroscopic contact problems [33].

Contact Detection and Constraints in FEM

Key challenges in FEM for contact mechanics include accurate contact detection and robust constraint enforcement. Standard techniques such as Lagrange multipliers and penalty methods have been extensively employed. The augmented Lagrangian method offers a compromise by combining the advantages of both approaches, providing better accuracy and stability at the cost of computational effort [34]. Advances in frictional and adhesive models, such as those developed by Kogut and Etsion [35], further enriched the analysis of contact behavior in applications like gear systems and material forming processes.

Despite its strengths, FEM encounters limitations when dealing with complex geometries. Generating watertight meshes and ensuring continuity across complex surfaces are time-consuming processes. These challenges prompted the development of alternative techniques, including Isogeometric Analysis (IGA).

Isogeometric Analysis and Contact Mechanics

Isogeometric Analysis (IGA), introduced by Hughes et al. [1], bridges the gap between Computer-Aided Design (CAD) and Finite Element Analysis (FEA), enabling a direct integration of exact CAD geometries into computational workflows. Unlike traditional FEA, which approximates geometries with faceted meshes, IGA employs smooth spline-based basis functions, such as B-splines and Non-Uniform Rational B-Splines (NURBS), to achieve precise geometric representation and high continuity across elements [36]. These features make IGA particularly advantageous in simulating complex contact mechanics problems, which are inherently nonlinear and exhibit non-smooth interactions.

In the early applications of IGA to contact mechanics, Temizer et al. [38] and De Lorenzis et al. [38] highlighted its potential for handling complex scenarios, including large deformations and frictional behavior. IGA’s ability to eliminate geometric discontinuities reduces non-physical oscillations in contact interactions, a common issue in traditional FEA. The inherent smoothness and continuity of NURBS basis functions enable IGA to tackle the challenging mathematical formulations of contact mechanics effectively.

To enforce contact constraints, IGA leverages several methods such as penalty methods, Lagrange multipliers [34], and augmented Lagrange methods [39]. Discretization strategies tailored to IGA, including the Mortar approach [40], Gauss Point-to-Segment (GPTS) methods

[41], and Segment-to-Segment (STS) methods [42], have been instrumental in enhancing the robustness and accuracy of contact simulations.

Recent advancements, including adaptive refinement techniques using hierarchical NURBS and T-splines [43, 44], address challenges such as the small cut-cell problem and high computational costs associated with high-order continuity.

The SBM has demonstrated success in solving elasticity and incompressible fluid dynamics problems, showing promise for extending IGA to more challenging applications, including immersed contact mechanics [45,46]. Its ability to handle complex 2D and 3D geometries with optimal convergence under Dirichlet boundary conditions highlights its potential as a game-changing approach in computational contact mechanics.

2.1 Governing equations and variational formulation

Contact mechanics deals with the study of stresses and deformations arising at the interface between contacting bodies. In computational mechanics, the weak form of the governing equations is often employed to facilitate numerical implementation.

The formulation of contact mechanics begins with the total elastic potential energy of the system, expressed as:

$$W = \int_{\Omega} \Psi d\Omega + \int_{\Gamma_C} \lambda g_n ds$$

where Ψ is the strain energy density, Γ_C denotes the contact interface, λ is the Lagrange multiplier associated with the contact stress, and g_n is the gap function, which measures the normal separation between contact surfaces.

By introducing the variation of the potential energy, the weak form of the contact problem becomes:

$$\delta W = \int_{\Omega} \sigma : \delta\epsilon d\Omega + \int_{\Gamma_C} (\lambda \delta g_n + g_n \delta\lambda) ds = 0,$$

where σ is the Cauchy stress tensor, and ϵ is the strain tensor. The term $\lambda \delta g_n$ enforces the contact condition through the Lagrange multiplier, while gn $g_n \, \delta\lambda$ imposes the constraint on the gap.

The challenge lies in enforcing the contact constraints, $g_n \leq 0$ and $\lambda \geq 0$, which together satisfy the complementarity condition $\lambda g_n = 0$.

2.1.1 Approaches to Enforcing Contact Constraints

Several methods have been developed to enforce contact constraints, each with its own advantages and limitations. Two of the most widely used are the Lagrange multiplier method and the penalty method, both of which are foundational to modern contact mechanics algorithms.

Lagrange Multiplier Method

The Lagrange multiplier method introduces an additional field, λ\\lambdaλ, to explicitly enforce the contact constraints. The augmented variational form becomes:

$$\int_{\Gamma_C} \lambda g_n \, ds,$$

where λ acts as a contact force. This approach ensures exact constraint satisfaction but increases the number of unknowns in the system. The method is robust but computationally expensive due to the saddle-point nature of the resulting system. Furthermore, poor conditioning of the system matrix can complicate numerical solution strategies.

Penalty Method

The penalty method simplifies the implementation by replacing the constraint with a penalty term in the variational form:

$$\int_{\Gamma_C} \frac{\epsilon}{2} {g_n}^2 ds,$$

where $\epsilon > 0$ is the penalty parameter. Larger values of ϵ enforce the constraints more strictly but can lead to numerical instability, while smaller values introduce constraint violations. Striking the right balance requires careful calibration, which can be problem-specific and nontrivial.

Nitsche's "penalty free" Method

Nitsche's method combines the strengths of both approaches by weakly enforcing contact constraints without introducing a Lagrange multiplier or requiring explicit penalty parameters. This formulation introduces stabilization terms that ensure numerical consistency and stability. The main idea is to substitute the lagrangian multiplier, λ, which physically represents the normal stress at the contact boundary, exactly with the stress at the contact, $\bar{\sigma}$, that it's directly computed from the displacements of the bodies involved in the contact and does not require additional degrees of freedom in the system. We can choose

$\bar{\sigma} = \gamma\sigma^+ + (1-\gamma)\,\sigma^-$, with $\gamma \in [0,1]$

to set the contact stress closer to the master or slave contact stresses. In this way the perturbation to the potential results as

$$\int_{\Gamma_C} \bar{\sigma} g_n \, ds.$$

2.1.2 Remarks on Computational Implementation

The implementation of these formulations is heavily dependent on the choice of discretization. In the context of this deliverable, IsoGeometric Analysis (IGA) and the Shifted Boundary Method (SBM) provide a robust framework for handling contact mechanics. IGA leverages NURBS basis functions for seamless integration with CAD geometries, eliminating geometric errors. SBM enhances flexibility in defining boundaries, addressing challenges in handling immersed geometries.

The penalty-free formulation adopted here simplifies implementation and avoids the challenges associated with Lagrange multipliers and penalty parameters, making it well-suited for complex industrial scenarios. As emphasized in Wriggers' *Computational Contact Mechanics* [34], the choice of method must balance accuracy, computational cost, and ease of implementation. The penalty-free Nitsche formulation represents a significant step forward in this balance.

2.2 Contact Algorithm and Benchmarks

2.2.1 Contact Algorithm

The contact algorithm developed in this work leverages a robust framework to handle volume-to-volume contact using the Nitsche penalty-free formulation in the IsoGeometric Analysis (IGA) framework. The methodology includes the following components:

1. Nearest Projection Search for Contact Pairs

The identification of contact pairs is performed using a nearest projection algorithm. For each integration point on the master surface (the mortar surface in this formulation), a projection is performed onto the slave surface. This ensures the identification of the closest corresponding points, forming potential contact pairs. The search accounts for the deformation of the bodies, allowing for dynamic updates to the contact pairs at each load step. This capability is particularly important for scenarios involving large deformations, where the contact interface evolves over time.

2. Activation and Deactivation Strategy

The contact algorithm employs a strategy for activating and deactivating contact pairs during the Newton-Raphson iterative process. At each iteration:

- The normal gap g_n and the contact stress λ are evaluated for each contact pair.
- **Activation**: Contact pairs are activated if $g_n \leq 0$, indicating penetration. The activation enforces the contact condition in subsequent iterations to resolve the penetration.
- **Deactivation**: If the contact stress λ>0, indicating traction (pulling apart), the contact pair is deactivated to prevent unphysical behavior such as "gluing." The iterative process continues until no contact pairs are updated between successive iterations, ensuring a stable and consistent solution.

2.2.2 Benchmarks

To validate the implementation, two classical benchmark problems were analyzed:

1. Patch Test

The patch test evaluates the ability of the algorithm to maintain stress and displacement continuity across a contact interface between two squares with non-coincident meshes. The Nitsche penalty-free formulation demonstrated excellent accuracy, achieving stress and displacement continuity within numerical tolerances. This result confirms the robustness of the nearest projection search and the contact activation/deactivation strategy.

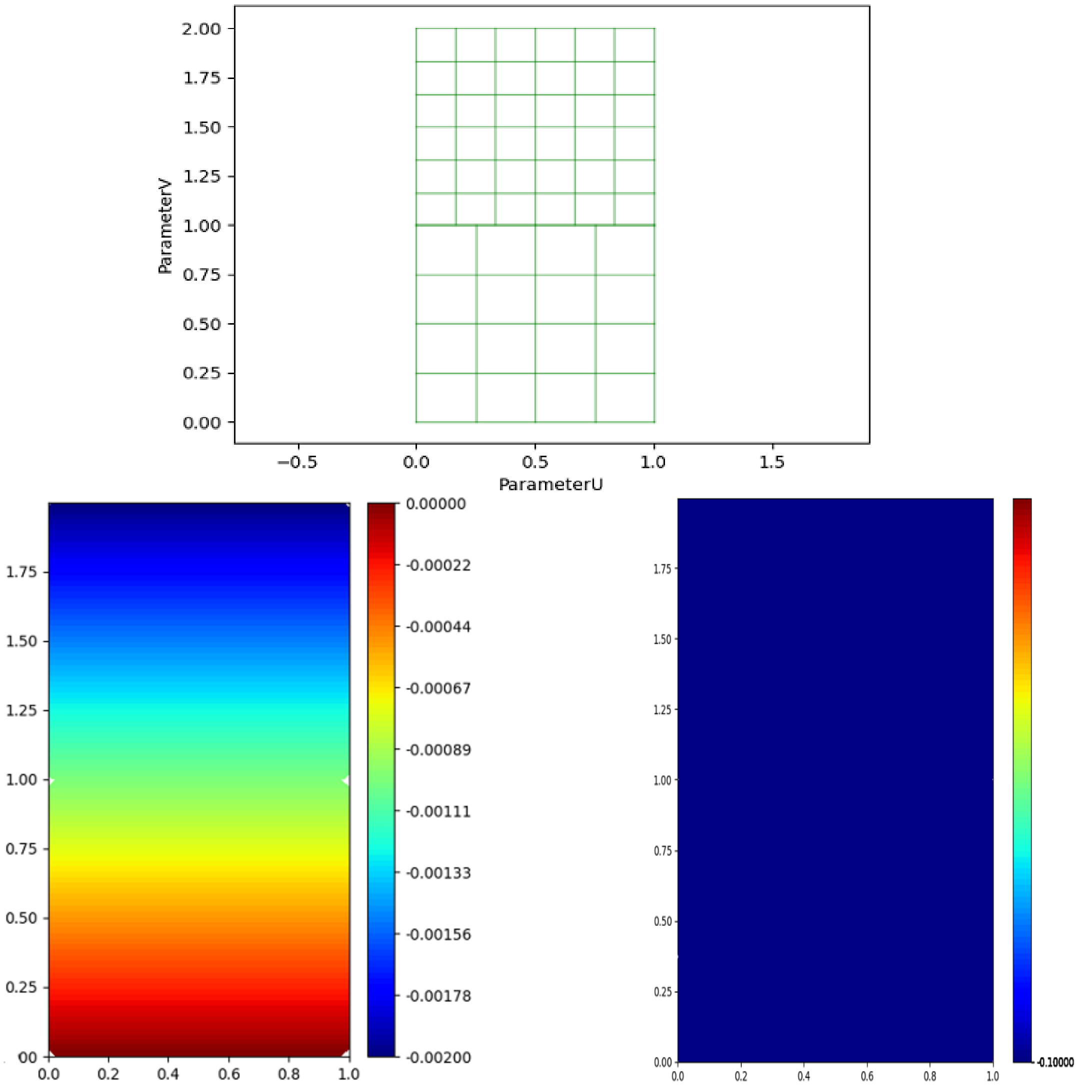

Figure 3: Patch test, Mesh (above), vertical-displacent (left) vertical stress (right).

2. Hertz Contact Problem

The Hertz contact problem involves the interaction of a cylinder (or circle in 2D) with a rigid wall, serving as a well-known analytical reference for contact mechanics. The implementation accurately reproduces the contact pressure distribution, confirming the capability of the algorithm to capture normal stresses and displacements. In this case:

- The pressure distribution follows the classical parabolic shape, consistent with the analytical solution.
- The vertical displacement along the contact interface matches the derived theoretical solution, further validating the accuracy of the contact formulation.

These benchmarks highlight the robustness and accuracy of the contact algorithm, demonstrating its applicability to a wide range of contact problems, from simple linear cases to more complex non-linear scenarios. The results also underscore the advantages of the penalty-free Nitsche formulation in maintaining stability and avoiding the pitfalls associated with traditional penalty-based methods.

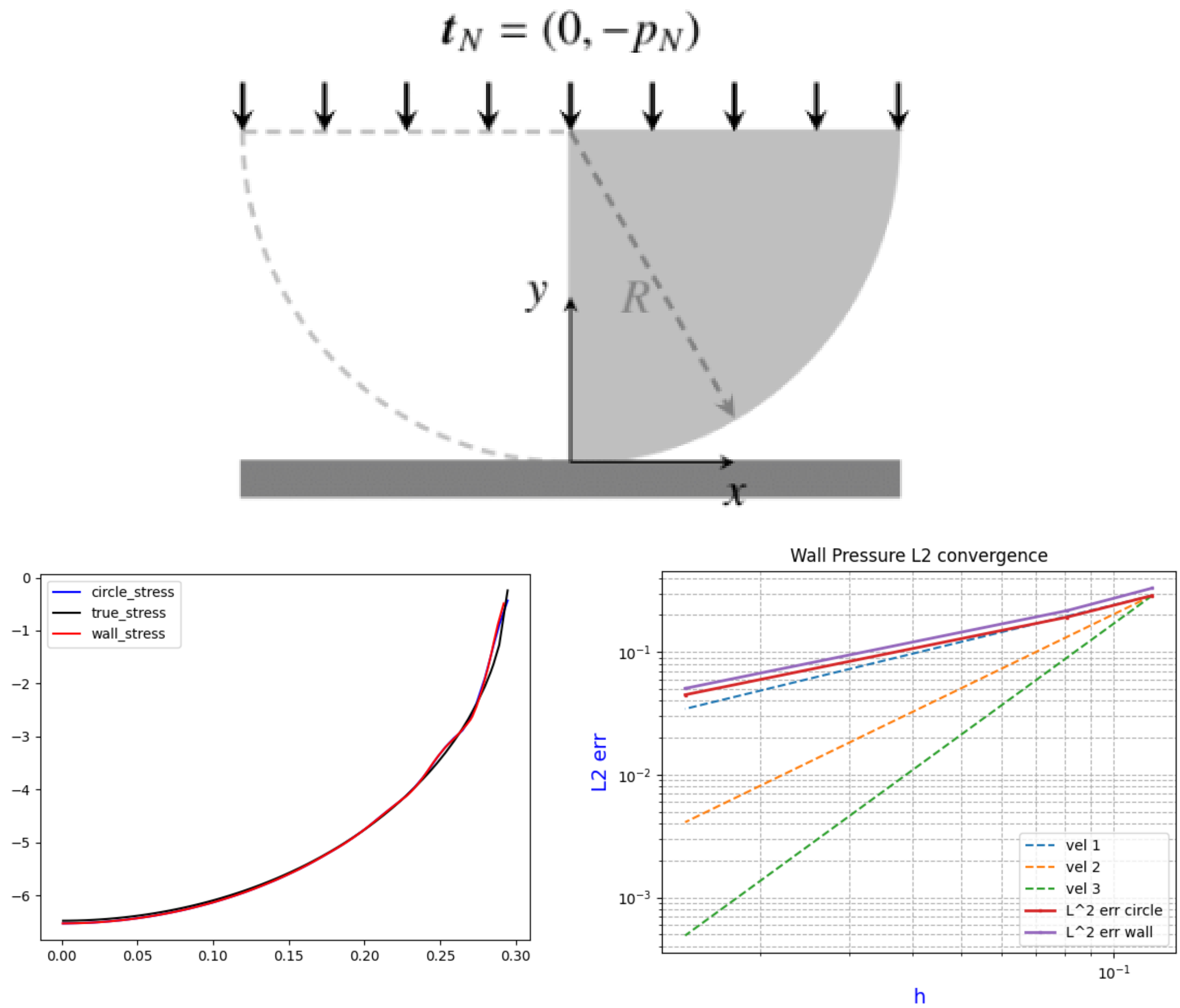

Figure 4: *Hertz Circle-Wall contact, stress comparison with the true solution on the contact boundary.*

3. Comparison with FEM

Finally a punch test has been checked against a well tested FEM contact solver with ALM. The penalty-free/IGA body fitted algorithm proves to converge fast the FEM accurate solution.

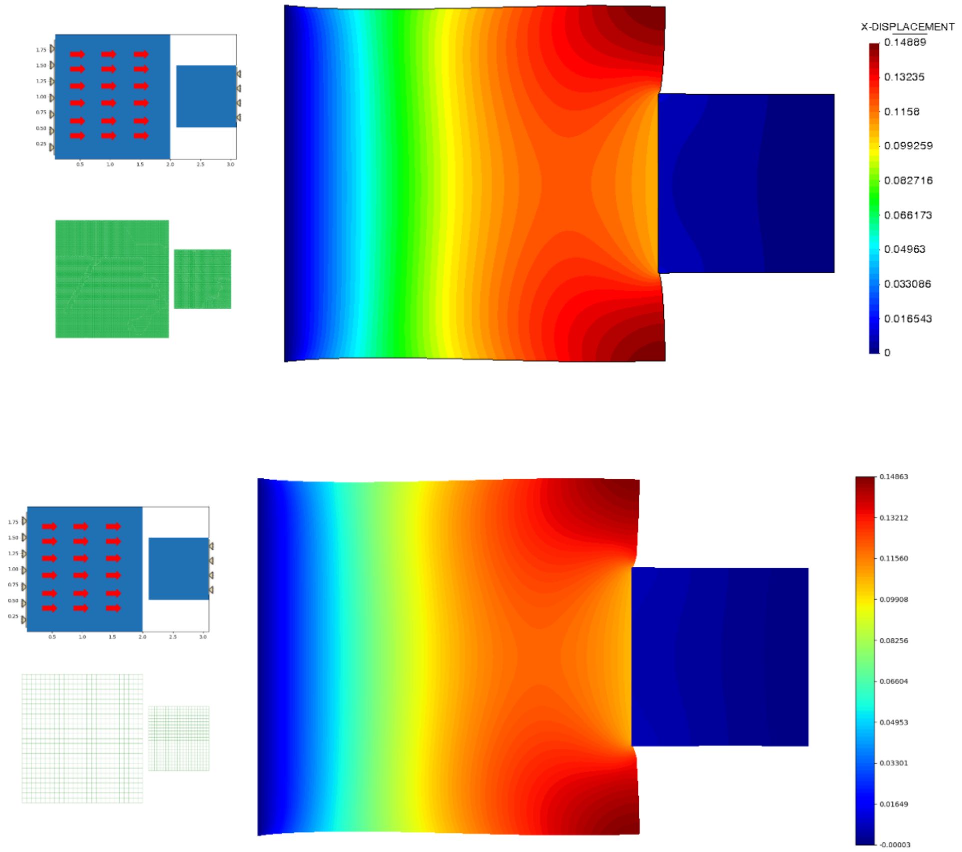

Figure 5:*Punch test horizontal displacements, FEM (above) vs. IGA(below)*

2.3 Road to Immersed Contact in Kratos

The next step in this research is to extend the current contact mechanics framework to handle immersed contact scenarios, leveraging the Shifted Boundary Method (SBM) within the IsoGeometric Analysis (IGA) framework. The SBM offers a flexible and robust technique for solving problems involving complex geometries and immersed boundaries, making it an ideal candidate for immersed contact mechanics.

Current Capabilities

At present, the SBM has been successfully implemented in Kratos Multiphysics framework for solving 2D structural mechanics problems under the IGA framework. Both body-fitted and SBM approaches have been validated, demonstrating the following:

- **Optimal Convergence for Dirichlet Boundary Conditions**: The SBM preserves optimal convergence rates when only Dirichlet boundary conditions are applied, matching the performance of body-fitted techniques.
- **Handling Neumann Boundary Conditions**: While the SBM loses one order of convergence for Neumann boundary conditions, it still provides accurate results with reduced pre-processing and increased flexibility in handling complex geometries.

- **Boundary Condition Imposition**: Both the standard Nitsche method and the penalty-free formulation perform reliably for imposing boundary conditions within the SBM framework.

3. CONCLUSIONS

The integration of the Shifted Boundary Method (SBM) into the Isogeometric Analysis (IGA) framework represents a significant advancement in computational mechanics. This synergy addresses challenges in complex geometry handling and contact mechanics, leveraging SBM's flexibility and IGA's precise geometric representation to achieve robust and efficient simulations.

The SBM simplifies the imposition of boundary conditions by shifting them to surrogate boundaries, reducing preprocessing complexity while preserving the accuracy of IGA. This approach proves particularly effective for intricate geometries, ensuring reliable results even for Neumann boundary conditions, though with a minor reduction in convergence order.

In contact mechanics, the penalty-free Nitsche formulation stands out for its ability to enforce constraints without requiring Lagrange multipliers or penalty parameters. This simplifies the computational framework while maintaining accuracy and stability, as demonstrated by benchmarks such as the Hertz contact problem and the patch test. IGA's inherent smoothness and exact geometry representation further enhance its ability to model contact interactions with precision and efficiency.

Looking ahead, the SBM-IGA framework offers significant potential for tackling immersed contact mechanics, enabling simulations of even greater complexity. This combination of theoretical innovation and practical efficiency provides a solid foundation for advancing computational mechanics to meet the demands of modern engineering challenges.

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