Imperial College London
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MSc in Applied Computational Science and Engineering

Independent Research Project
Final Report

Conservative Interpolation Between Unstructured Meshes that Preserves Heterogeneity and Structure for Modeling Three-Dimensional Bone

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June 2022

1 Introduction

Discretizing complex 3D geometries into unstructured meshes is a challenging but vital process in computational science. This numerical discretization allows for solving systems of equations that model real-life processes such as weather changes, fractures, fluid dynamics, and propagation of fractures in bones. Just like every computational problem, solving a large system of equations requires attention to memory consumption, accuracy, and speed. Representing processes that vary each fraction of the second necessitates finding non-traditional ways of solving systems involving large unstructured meshes. Conservative interpolation is a popular approach to accomplish that. This class of methods ensures that the global integrals of the system are conserved, therefore preserving conservation properties under discretization. Farell et al. proposed a conservative interpolation method that uses an auxiliary mesh, called a supermesh, to map between two grids [1].

The purpose of this project is to ultimately be able to interpolate between 3D unstructured meshes that represent a section of a bone that has undergone a fracture. When a bone is subjected to a hit (or anything else that might cause it to break), a fracture will gradually grow with time, which evidently changes the mesh that represents this bone. In examining this propagation, we would be working on a very small scale [2]. Consequently, we end up having very large unstructured meshes stored in memory. Given that a small time step is taken in the simulation process to reduce the discretization error, this ends up being a costly task in terms of execution time [3]. In order to mitigate this issue, we can instead use conservative interpolation using a supermesh [1]. In this method, we begin by constructing a supermesh of both grids representing the current timestep and the next one. There is no out-of-the-box C++ supermesh generator that can do this, and this project focuses on developing such an algorithm.

1.1 Previous Attempts at Creating/Using a 3D Supermesh

Rinaldi et al. presented a flux-conserving method for non-conformal mesh block interfaces [4]. The method can be used for the finite-volume discretization of any system of conservation laws and uses an auxiliary 3D supermesh. This method does not involve any interpolation, and, by construction, guarantees conservation. It works by replacing the parent meshes in the flux balance calculation with the supermesh. In this method, the 3D elements may have either quadrilateral or triangular faces. The supermesh is constructed by intersecting all of the elements of mesh A and B together. For each pair, the vertices of E_A contained in E_B are found and vice-versa. Then the edges are intersected, and any duplicate points are removed. Lastly, if the resulting number of elements is greater than 2, new supermesh elements are defined.

Oner et al. present another example of using a supermesh [5]. In order to obtain highly accurate numerical results for viscoelastic flow problems, a parallel adaptive mesh refinement strategy is incorporated into the side-centered finite volume method. This approach for solving viscoelastic problems uses conservative interpolation and employs supermeshes as intermediaries to facilitate the interpolation. To do so, the parent geometries are split into hexahedral volumes, to be later split into triangular shapes in the refinement and supermesh. The Delaunay triangulation method is not used here, as it has proved complex for 3D geometries. Instead, element-by-element intersection calculations are done. A template-based side-centered refinement algorithm is proposed. The mesh elements are looped over, and a check is done for whether the parent element requires coarsening. If so, all children get set as inactive. Then for all the elements needing refinement, based on the number of nodes and level of refinement, a template is selected, and the element is refined; this is repeated until there are no more unrefined elements.

Menon et al. describe a method for conservatively remapping fields from one mesh to another for finite-volume computations [6]. The proposed method is also second-order accurate. The base and target meshes are not assumed similar, making this approach general at the high cost of calculating many intersections.

Evidently, supermeshing has been used for solving many computational problems. Conservative interpolation using a supermesh is a promising candidate for simulating bone fractures since most fractures are modeled at a microscopic level. The trabecular (porous honeycomb-like core) and cortical (stiff external shell) structures necessitate representing a complex geometry when modeling the fractures [7]. At a microscopic level, this simulation becomes highly costly in terms of both memory and time.

1.2 Theoretical Background for Conservative Interpolation Using a Supermesh

There exists a robust theoretical background for the supermeshing technique, and how it can speed up mesh adaptivity and increase its accuracy [1]. However, the detailed process of supermeshing is explained only for the 2D case. It certainly extends to the 3D case, with some additions and modifications.

A supermesh $\mathcal{T}_c$ of parent meshes $\mathcal{T}_A$ and $\mathcal{T}_B$ is defined as any mesh that fulfills the following 2 conditions:

(1) Any node $\mathcal{N}$ present in the parent mesh must exist in the supermesh. (i)
(2) The intersection of an element of $\mathcal{T}_c$ with any element of either of the 2 parent meshes must either be the empty set or the whole element $\mathcal{K}_c$. (ii)

Assuming such mesh is generated, in order to go forth with conservative interpolation, it is also essential to have mappings that can take any element in the supermesh and find its parent elements in the base and target meshes. Thus, the complete algorithm consists of three major steps. We start off by creating a supermesh $\mathcal{T}_c$ as well as the mappings $\mathcal{X}_{CA}$ and $\mathcal{X}_{BC}$. Then, for each element in $\mathcal{T}_B$, we find its integral value as the sum of that of its children in $\mathcal{T}_c$. Finally, after finding the elemental integrals, the nodal values are computed by means of a Galerkin Projection.

We are considering mesh $\mathcal{T}_A$ to be the base mesh and $\mathcal{T}_B$ to be the target mesh; the goal is to interpolate the values from $\mathcal{T}_A$ onto $\mathcal{T}_B$. Given a function $q(x)$, the integral of which is to be conserved in the discretized process of interpolation, the sum of the elemental integrals over $\mathcal{T}_A$ must be equal to that over $\mathcal{T}_B$, under a projection π_B.

$$\sum_{K_A \in \mathcal{T}_A} \int_{K_A} q(\boldsymbol{x})\, dV = \sum_{K_B \in \mathcal{T}_B} \int_{K_B} \Pi_B[q](\boldsymbol{x})\, dV$$

Since each element in $\mathcal{T}_B$ can be expressed as the union of its children in $\mathcal{T}_C$, we can therefore replace each elemental integral of $\mathcal{T}_B$ with the sum of the integrals of its children in $\mathcal{T}_C$, with π_C being the projection operator applied to the supermesh. Since no two child elements in $\mathcal{T}_C$ intersect, the problem boils down to interpolating from $\mathcal{T}_A$ to $\mathcal{T}_C$.

$$\sum_{K_A \in \mathcal{T}_A} \int_{K_A} q(\boldsymbol{x})\, dV = \sum_{K_C \in \mathcal{T}_C} \int_{K_C} \Pi_C[q](\boldsymbol{x})\, dV$$

Thus, for this process to be conservative, all that is left to do is find an operator that preserves the integral over the meshes from mesh A to mesh C. One such operator is defined as the fraction of the integral of the child element in C over that of its parent in A. Assuming the

function $q(x)$ is constant over a single element, the nodal values across $\mathcal{T}_B$ can then be recovered, and for each node, the value would be the integral across the element divided by the element's volume. Afterward, a Galerkin projection can be applied to obtain piecewise linear basis functions from constant elemental values.

2 Methodology

2.1 Process of Creating a Valid Supermesh

When working in 2D, given two meshes $\mathcal{T}_A$ and $\mathcal{T}_B$, for their supermesh $\mathcal{T}_C$ to be valid, all the nodes and edges of the parent meshes must be present in $\mathcal{T}_C$. This is proven in lemma 6 by Farell et al [1]. This lemma leads to the following algorithm.

The general steps for constructing the supermesh in 2D are as follows:

(1) Obtain the union $\mathcal{N}$ of all the nodes of $\mathcal{T}_A$ and $\mathcal{T}_B$
(2) Obtain the union $\mathcal{D}$ of all the faces of $\mathcal{T}_A$ and $\mathcal{T}_B$
(3) $\mathcal{N}$ and $\mathcal{D}$ form an imperfect piece-wise linear complex
(4) $\mathcal{N}$ and $\mathcal{D}$ are given to the Delaunay Triangulation method of the Triangle Library, and a triangulated supermesh is obtained

An underlying step in this algorithm is creating the parenthood mappings for the resulting supermesh's elements. Since each edge can be shared by a maximum of 2 elements, the edges are annotated with an encoding of two integers representing the parent elements in the original meshes. This encoding is a bijection from which the associated input elements are easily recoverable [8].

When working in 3D, there are slight modifications to be done. From lemma 6 mentioned above, one can infer that in 3D, a valid supermesh must have all the nodes of the parents, and all the faces, not only edges. This is easily achievable for any 2 arbitrary 3D meshes, by simply finding the union of their nodes and the union of their triangular faces. However, the Triangle library used by Farell et al. only works for 2D geometries. In this work, TetGen is used to generate tetrahedralized parent meshes in 3D. Nevertheless, it does not offer the option of tetrahedralizing a certain geometry, whilst keeping certain faces. Therefore, a supermeshing algorithm is constructed from scratch.

2.2 Method of Intersecting Tetrahedra

2.2.a Motivation for Algorithm

A common technique for tetrahedralizing a domain is the Delaunay Method. The method takes a set of points $\mathcal{S}$ in space and returns a list of tetrahedra such that each simplex (edge, triangle, or tetrahedron) follows this rule: all its vertices can be connected by a circumsphere that includes no other vertex [9]. As a result, this algorithm produces mostly "round" tetrahedra, and not so many "thin" ones [10]. The C++ library TetGen has an interface for using this algorithm. One can simply provide the vertices that form the exterior of the domain, or the Piecewise Linear Complex, and TetGen then decomposes this domain into Delaunay tetrahedra. One can also provide all the nodes (interior and exterior) of a mesh and get a tetrahedralization. TetGen also provides options for refining an existing mesh. One downside, however, is that TetGen does not allow us to fix certain faces of the domain.

One approach to producing a supermesh using TetGen would be to get the union of all nodes of both parent meshes and pass them on to TetGen's tetrahedralize() function. This approach of

course does not work because, as mentioned earlier, the presence of all the faces of the parents in the supermesh is essential for its validity.

The method discussed in this project involves getting two parent meshes that have already been tetrahedralized by TetGen, and then manually finding the tetrahedralization of their union. The resulting children tetrahedra at each intersection are repeatedly intersected with other parts of the domain, until there are no more intersections.

2.2.a Description of Algorithm

Despite being developed with input meshes being a result of TetGen's tetrahedralization method, the intersecting tetrahedra algorithm makes no assumptions about the input meshes in terms of the shapes of the domain. It does not require the input to be a Delaunay Tetrahedralization specifically and has no constraints on the number of elements of each parent mesh.

The algorithm works in a recursive manner and makes use of three meshes (or lists of tetrahedra), the first two lists representing the elements of $\mathcal{T}_A$ and $\mathcal{T}_B$, and the third one being an auxiliary list of tetrahedra that starts out empty, and gets progressively filled with elements as the algorithm progresses. The nodes of both parents as well as their elements (which are essentially groups of 4 nodes representing each original tetrahedra in the parent mesh) are first received. Then for each element of mesh $\mathcal{T}_A$, two major steps are done. Firstly, the element $\mathcal{K}_i$ of $\mathcal{T}_A$ is intersected with the auxiliary mesh, and child tetrahedra are obtained. The child tetrahedra are then intersected with the elements of $\mathcal{T}_B$.

2.2.b Pseudocode of Supermesh Algorithm and Notes

Algorithm 1 Intersecting Tetrahedra Algorithm for Generating a Supermesh

```
function supermesh(A, B):
    C = [ ] empty vector of tetrahedra
    marker = array of bools of size sizeof(B)
    for i in range(sizeof(A))
        AC , AB = [ ]  empty vectors of int
        temp = [ ] empty array of tetrahedra
        t , c = 0
        if (AC ! empty)
            for j in range(sizeof(C))
                if A(i) intersects C(j)                 *
                    temp.push(C(j))
        for j in range(sizeof(B))
            if (!marker[j])
                if A(i) intersects B(j)                 *
                    AB.push(j)
        while true
            if (temp[t] intersects C[AC[c]])            *
                X = get_intersection (temp(t),C[AC[c]] )
                if sizeof(X) == 1, go to else
                temp.remove(t)
                temp.push(X)
            else
                c++
                if ( c == sizeof ( AC ) )
                    c = 0;  t++
                    if ( t == sizeof ( temp ) )
                         break
        temp1 = [ ] empty vector of tetrahedra
        for j in range ( sizeof ( temp ) )
            if (one of temp(j)'s parents is unintialized)
                    temp.remove(temp(j))
                    temp1.push(temp(j))
        t , c = 0
        if ( AB ! empty )
            while true
                if ( temp1(t) intersects B(AB[c]) )     *
                    X = intersection temp1(t) and B(AB[c])
                    if sizeof(X) == 1, go to else
                    temp1.remove(t)
                    temp.push(X)
                else
                    c ++
                    if ( c == sizeof(AB))
                        c = 0
                        t++
                        if ( t == sizeof (temp1))
                            break
        for j in AB
           marker[j] = 1
        C.remove(all elements pointed at by AC and AB)
        C.push(temp, temp1)
```

In Algorithm 1, the two parent meshes A and B are taken as input, and an empty auxiliary mesh C is initialized. No assumptions are made about the order of the elements of the parent meshes, their orientation, or the order their nodes are stored in. The only assumptions made are that no two elements of A or two elements of B intersect, and that no elements in A or B are degenerate tetrahedra (have 4 coplanar points, or 3 or more collinear points).

The algorithm can be split into 4 blocks: initialize (block I), intersect with C (block II), intersect with B (block III), and update C (block IV). All four of these blocks are repeated for each element of mesh A.

Block I determines which elements of C and B does element i of A intersect. The ranks of these elements are saved in two separate arrays. An empty temporary vector of elements is initialized (temp can be thought of as a queue linked list, but for ease of implementation, an STL vector can be used).

Block II loops over each element of temp and checks if it intersects the predetermined elements of C. Each time an intersection occurs, the intersection function returns one or more tetrahedra, each with either two parents assigned, or only one, the one parent being $\mathcal{K}_{\mathrm{i}}$ of A. Then, the intersecting element is removed from temp and the resulting child elements are added to temp. The process keeps repeating until all of temp is checked for intersection with the predetermined elements of C.

Block III is similar to block 2. It takes the children elements that resulted from intersecting $\mathcal{K}_{\mathrm{i}}$ of A with C, such that these elements have been assigned only one parent. Then, the intersection of these child elements with the predetermined elements of B is done in the same way as before.

Block IV updates the elements of the supermesh, and marks the intersected elements of B to signify they are now part of the supermesh; no need to check them as part of mesh B.

2.2.b Subroutines of Supermesh Algorithm

In the supermeshing process, there are two essential functions that do most of the work. The first function is the boolean intersection function. This function takes 2 tetrahedra, and checks whether they intersect. This function is used in the lines marked with (*) and is called repeatedly for many elements each iteration. The way to check if two tetrahedra intersect is to essentially check if each edge of B intersects any face of A and vice versa. Checking whether an edge intersects a face repeatedly is an expensive process. A faster way is proposed by Ganovelli et al. [11]; this method makes use of the separating axis theorem but avoids some computations that are usually done while performing the separating axis test.

The separating axis theorem is used to detect overlap of convex polytypes. It states that if the convex polyhedral are separable, then there exists an axis on which their projections do not overlap. This axis is either orthogonal to a face of one of the two convex bodies, or to an edge for each of the two. [11] These two rules are theoretically certainly a step up from having to do edge-face intersections, however, computationally, determining if a separating axis orthogonal to a face or orthogonal to a pair of edges exists is costly. The algorithm proposed by Ganovelli et al. is referred to as GPR; its key advantage is that it does not explicitly test pairs of edges to find a separating axis. The algorithm instead checks if each of a pair of two faces of tetrahedra is a separating plane, saves some results, then in no separating axis is found, the results are used to determine if the edge shared by these two faces is separating.

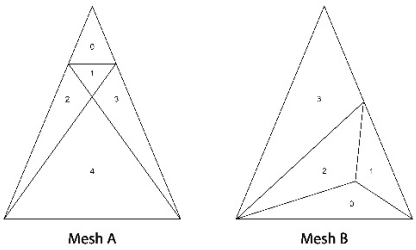
The second important function is one which takes 2 tetrahedra as input, finds their intersection points, and based on the finite number of ways 2 tetrahedra can intersect, returns a list of

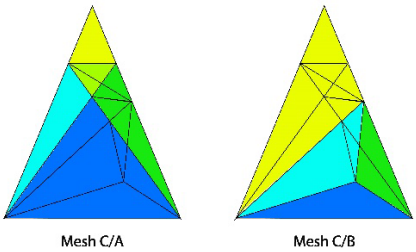
children tetrahedra. This was inspired by the work of McCoid et al. [ ] in which they prove that only 0, 3, or 4 intersections may exist between all of the edges of a tetrahedron X and a plane of another tetrahedron Y. With some additional constraints, this can lead to a general breakdown of how any two tetrahedra can intersect. But before getting into that, one must obtain the intersection points of the two tetrahedra. To do that, a get_intersection_points() function is used. This function is simple, but includes a lot of computational geometry subroutines: for each pair edge(A)-triangle(B) and edge(B)-triangle(A), we find the intersection point and add it to a vector of points to be returned.

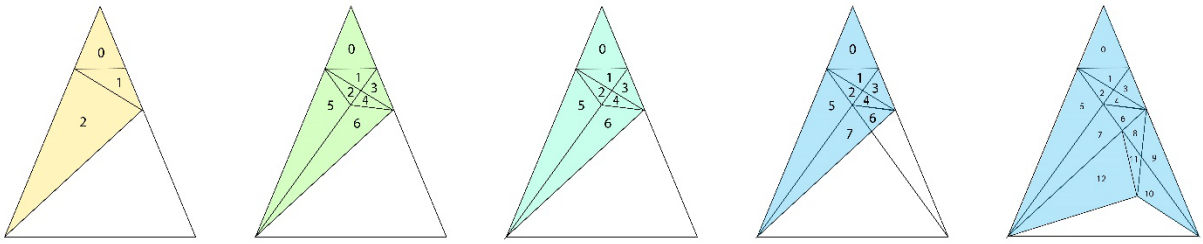
Below is a diagram showing the flow of execution of get_intersection_points():

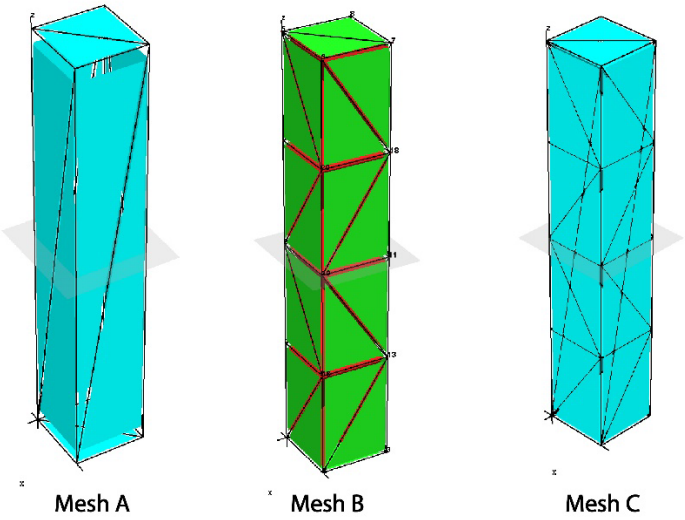
2.3 Library Code Breakdown

2.4 Results









3 Conclusion and Discussion

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