Thesis Proposal:
High Performance Simulation and Validation of Finite Element Method for Soft Tissues

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1 Introduction

With the development of the theory of non-linear finite elements and improvement of computation hardware, in recent years, using physics-based simulation for biomaterials became popular in biomechanics community in the examination of joint loading, tissue failures or for surgery prediction [1, 2, 3].

Soft tissues, including tendons, ligaments, blood vessels, skins or articular cartilages, and many others, serve important roles both biologically and mechanically. They bind, support, and protect the human body and structure. For instance, tendons connect bones and muscles to bones for stabilization or enabling motion. Ligaments connect bone groups to restrict relative movement. Blood vessels distend in response to pulse waves. Skin is the largest organ, it supports internal organs and serves as a protective barrier that helps regulating heat and fluid loss, and absorbs shock and radiation etc. Articular cartilages exist as a 1-5mm layer on top of the joint connective parts to distribute load and reduce contact stress and friction [4]. Soft tissues are fibre-reinforced complex materials. They mainly consist of a structural arrangement of collagen and elastin fibres that are embedded in the hydrated matrix of proteoglycans. Their stress-strain response has been experimentally measured and categorized as highly non-linear and viscoelastic [5, 6].

Due to the complexity of the material properties, the computational analysis and simulation of soft tissues are conducted using commercially available software [7, 8]. Those types of software tools are very robust in terms of supporting various constitutive models, but they are built on generic numerical linear algebra libraries that forego opportunities for problem-specific optimizations, and require complex steps for setting up boundary conditions which limits their use to trained engineers. The long time for setup and running simulation makes it a poor option for efficient clinical applications. As for the quality of discretization, those commercial software tools usually choose to use conforming tetrahedral or hexahedral mesh as their finite element discretization. These discretization schemes generally converge to the continuous solution under refinement, for simple instances of problems such as Isotropic Linear Elasticity, or the Poisson equation. However, they are prone to a number of artifacts in less trivial scenarios, which can prevent convergence to the expected result. Locking, for instance, is the behaviour of the linear tetrahedral element exhibiting an unnaturally higher stiffness due to the fact that the incompressibility of each element can impose much higher number of constraints than total degrees of freedom [9]. Similarly, for hexahedral mesh the artifact of locking instability will be present when there is an improper quadrature rule applied for element integration [10]. We can see in the quality of discretization that whether it will converge to the continuous solution and how fast it will converge is very much related to the constraints imposed by the constitutive model. In their effort to separate discretization and modeling of material response laws (constitutive laws), present FEM packages are often limited in addressing such challenges without adversely affecting performance and optimization.

The simulation of soft tissue has also been of great interest in the field of virtual surgery. Either for training or for surgery planing, using accurate simulation can both reduce cost and decrease error. But in contrast to tissue analysis, virtual surgery applications require the simulation running at an interactive rate. Early works [11, 12] use mass-spring system for simulation, and even though they can give fast simulation speed and benefits such as online cutting, a mass-spring system does not solve the underlining continuum equation correctly.

Earlier products by various researchers provide an indication of present capabilities, and lingering limitations. For example, Taylor et al. [13] proposed a GPU accelerated FEM simulator. Even though the system supports an anisotropic viscoelastic material model, the simulation was integrated explicitly for performance. GPU was also used for acceleration of the simulation by Lapeer et al. [14]. Three isotropic material models were considered along with mid point integration and the material parameters are fitted through experiments. The highest element count is 50,000 for this work. In work by Mitchell et al. [15] the authors have used a non-conforming regular hexahedron grid and matrix free solver for better performance, that supports complex boundary conditions such as collisions. But they only used single quadrature integration and limited to simple material models.

As for in the field of computer graphics, the use of physics based simulation to enhance animation has also attracted much attention and interest in the past decade [10, 16, 17]. Due to the fact visual appearance is the primary concern, those applications can often create visually convincing result by artists. However, they usually use very simple material models, lack validation, and trade fidelity with artistic control and performance. Most of the work in graphics in skinning, for instance [18], focuses only on the surface. Even though it handles collision and has some quasi-elastic behavior and runs in realtime, it only creates plausible surface deformation of the skin and does not generate any dynamic secondary motion. McAdams et al. [10], proposed an efficient and stable single quadrature FEM simulation on a non-conforming Cartesian grid. Though the system has been used for simulating character anatomically [19], the material is limited to co-rotated linear elasticity. Since the goal of the system is to create efficient and simple ways to generate contact collision and secondary motion in a believable fashion for animation, co-rotated linear elasticity is sufficient.

Among all the previous works, there is always the trade off between the performance and accuracy. For my thesis, using a combination of high-performance computing platforms, efficient data structure, high order finite element method, and accurate material model, I hope to aspire to engineer a solution for interactive high accuracy soft-tissue simulator.

2 Research questions

In my thesis the following questions will be examined and addressed:

- Are existing components of a computational simulation pipeline adequate for capturing the intricate behaviors of highly non-linear soft tissues? In particular, how do design choices in (a) constitutive modeling the mechanical response of tissue, (b) discretizing the governing equations, (c) representing state via data structures, and (d) solving the resulting discrete equations help or hinder this goal?
- If the previous investigation reveals deficiencies, how can those be treated without compromising features or performance?
- By improving the finite element modeling technique, how is the scope of application broadened?
- How do the design decisions in modeling and discretization affect performance and scalability in modern and emerging computational platforms?

I will pursue answers to these questions based on the following central hypothesis: *Experimental testing and validation on physical proxies can assert the adequacy or reveal deficiencies in methods for computational soft tissue modeling and simulation, and suggest enhancements across the modeling pipeline.*

3 Problems & Challenges

In this section, I will describe the problems I intend to investigate during the period of my Ph.D. study, what challenges they may impose, and finally the potential solutions to overcome them.

3.1 Constitutive model selection and validation

Problem overview

Biological soft tissues exhibit mechanical properties such as non-linearity, anisotropy [5], and viscoelasticity [6]. Many pieces of literature have proposed material models and parameters based on the experimental data. In general, there are two different approaches in picking or designing constitutive models: phenomenological and structurally based. Examples of *Phenomenological constitutive models* are seen in the work of Bischoff et al. [20], where the skin is modeled as an isotropic non-linear hyperelastic material using the material model proposed by Arruda et al. [21]. The parameters were fitted using an experimental result of a biaxial stretch test. Tepole et al. [2] and Delalleau et al. [22] used isotropic linear elasticity to estimate the parameter of the experimental result of an indentation test. Sun et al. [23]

proposed a generalized Fung-elastic constitutive model that is based on the polynomial expansions of the entries of the strain tensor. On the side of the *Structural-based constitutive modeling*, soft tissues are considered to be an isotropic incompressible water-based matrix reinforced by a network of fibres. Tepole et al. [2] modeled skin as a Mooney-Rivlin hyperelastic material with a decoupled non-linear fibre term contribute to energy to capture the anisotropy. Gasser et al. [24] extended the idea of decoupling the single directional fibrous structure energy from the underlining matrix energy by introducing a fibre distributing function. There is no universally agreed constitutive model for soft tissues. Therefore, to be able to support many constitutive models is important in my exploration of the pros and cons for each option, and validate their quality in predicting mechanical properties of soft tissues.

Challenges and possible solutions

There has been many attempts in proposing constitutive models for soft tissues. However, many of them are designed and tuned to a very specific load test, for instance, uniaxial stress test, bi-axial stress, indentation test, etc. Even though the simulation of a given constitutive model with tuned parameter has matched the experimental data, there is no guarantee such model will predict the soft tissue behaviour under an arbitrary load. But it is difficult to set up experiments for arbitrary loads for the following several reasons. First, to tune the parameters or validate the constitutive model, both strain and stress field need to be measured. Most of the strain measurement can only record the strain field on the surface, but a vigorous validation would require the volumetric strain field as well. As for the stress measurement, usually, they are measured by a force sensor attached to a probe that applies stress to the specimen. Those probes have a limited degree of freedom, and can't deform the specimen in arbitrary ways. Secondly, bio-tissues has a very limited period of viability, after several hours living bio-tissue will degenerate with a noticeable change of mechanical property. It is very difficult to perform several tests on the same specimen, and every specimen is unique due to the nature of the biological tissues. There is the possibility of using tissues from a cadaver. But those tissues are heavily processed and does not share the same mechanical properties as the living tissues in general.

Due to the constraints imposed by living tissues, for the scope of my study, I intend to use silicone rubber as a substitute. Such material has been used in surgical training and the field of special effect for many years. Even though silicone rubber has quite different mechanical properties than bio-tissues, it has a highly non-linear response [25] and highly reproducible behavior. Instead of constraining the test to be under simply loading conditions and captures only the force and displacements at the end of the samples I plan to impose boundary conditions that involve both displacement and rotations for thin 2D like samples and captures the displacement field across the whole sample. Then perform the comparison using results from simulations of different tuned constitutive models to the captured displacement field. In further tests, silicon substitutes can be enhanced with additional materials inserted in their volume, such as directional woven fibres, to emulate anisotropy or hard strain limits.

3.2 Homogenization based multigrid solver

Problem overview

Finite element simulations involve solving a large sparse linear system. There is a class of direct solvers such as Guass elimination, Cholesky decomposition etc. Those algorithms provide correct answer at the cost of high complexity of $O(n^2)$ or worse even for sparse problems, where n is the total number of unknowns. Such complexity limits the application of using direct solver on large problems. Another class of solvers, namely iterative solvers, converges to the solution with each iteration of cost $O(n)$. If terminated early, an iterative solver will still give an approximate answer. For solving large problems, iterative solvers with a fixed iteration count or residual tolerance are popular choices. In recent years, a class of iterative solvers called multigrid has become a popular choice due to fast convergence rate along with the global convergence behavior. It has demonstrated excellent performance for both fluid [26] and linear elasticity [27]. But in both cases, the materials are homogenous cross the domain.

Challenges and possible solutions

Bio-tissues are usually highly heterogeneous in terms of the material compositions. For instance, the skin consists of three distinct layers, and the outer most layer epidermis is approximately 1000 times stiffer than the inner layers. For those heterogeneous problems, standard algebraic multigrid can still be used [28], but the rate and behavior of convergence are much compromised.

The theory of homogenization seeks to solve a class of problems with highly varying materials, by replacing it with a single material. The classical case of homogenization is to replace two springs in parallel or series with one single spring. Of course, combining materials in two or three dimensions is much more complex than the one dimensional problem of composing springs. The theory of homogenization can provide a method to construct a multigrid hierarchy. But there are still missing pieces need to be solved, such as efficient smoother and transfer operators between levels of the hierarchy.

3.3 Discretization and data structure for efficient FEM simulation

Problem overview

Traditionally there are three different discretizations for FEM simulation: conforming mesh, non-conforming mesh, and meshless method. Conforming method means that the discretized solution space is a subset of the continuous solution space. Even though conforming method can give more accurate result around boundaries without any special treatment, constructing quality discrete conforming elements is both difficult and time-consuming in 3D. A poor quality mesh can cause the system to be close to singular and difficult to solve with limited floating point accuracy. Even with high quality mesh, given the connectivity between elements of a conforming mesh is non-trivial, the neighboring information needs to be stored and can incur significant overhead in computation.

Using non-conforming mesh, specifically surface embedding in a structured Cartesian grid, can be very efficient computationally, but regarding the boundary conditions, due to the fact that the discretized solution space is not a subset of the continuous solution space, there can be large errors along the boundaries. Belyschko et al. [29] proposed an extended finite element method (X-FEM) and captures the surface by sampling point around the boundary and using radial basis functions to reconstruct the boundary equations. Kumar et al.[30] used a levelset representation of the surface and step functions for the basis of the elements at the boundary. By doing so, captures the boundary condition exactly. Similarly, Zhu et al. [31] proposed a virtual node method for 2nd order accurate boundary condition capturing. But it was for linear elasticity. Another way to capture boundary conditions in a non-conforming simulation was proposed by Patterson et al. [32]. In this work, a Monte-Carlo sampling method was used to find the quadrature points for the integration of each boundary elements. To capture 2nd order accurate result, only 4 quadrature points were needed per element. But such method, even though highly efficient during the integration process, requires relatively expensive preprocessing time to find the quadrature points.

Another problem that rises with non-conforming mesh is embedding thin cuts in elements. Standard non-conforming mesh assumes continuity within an element, while thin cuts within element would break such assumption. To overcome this issue method such as non-manifold level set representation of implicit surface combining with cut cell [33] has been proposed.

Possible solutions

For the reason of efficiency, I will focus on simulation in non-conforming mesh based methods using a regular Cartesian background grid. Setaluri et al. [34] proposed a novel data structure that utilizes the virtual memory system for efficient storage of sparse and adaptive grid data. It will be the primary data structure for storage. The adaptivity provided by SPGrid can also enable capturing high resolution and more local details.

As stated in the overview, using non-conforming method will suffer from low accuracy along boundary and inability to capture thin cut features. To overcome those problems, I plan to use non-manifold level set proposed in [33] as the storage for the implicit surface, and extended finite element method can be used along the boundaries to resolve boundary conditions.

Challenges

As mentioned in the introduction, discretization, as an estimation of the continuous equation, in an ideal case will converge to the continuous form of the solution under refinement. But in reality, under many cases, they exhibit different asymptotic behaviours based on the constraints imposed. This discrepancy has been extensively studied for linear elasticity and other forms of PDE. But for nonlinear elasticity, there is very limited number of literature that studies the discretization artifacts for different constraints and there is very little understanding of the accuracy and convergence in this field. Many validations for the discretization are limited in single element test with prescribed affine transformation. Those tests can validate that the discretization equations are solved correctly, but are not sufficient in testing discretization artifact. In work by Zhu et al. [31], they have prescribed analytical deformations field to validate the 2nd order convergence rate of their discretization. But such technique only works for linear elasticity due to the uniqueness of the solution. For nonlinear elasticity, the solution may not be unique and a new verification technique is needed.

Biological soft tissues exhibit properties such as viscoelasticity, transversely isotropy, and highly non-linear strain-stress response [4]. Besides the challenge of finding suitable constitutive models that describe their mechanical behavior, there is the challenge of finding a proper efficient discretization and converges to the analytical expression of the constitutive model with refinement.

3.4 Dynamic topology change

Problem overview

Either for surgical incision or for tissue failure under excessive tearing force, dynamic topology change during simulation is important for handling interactions with soft tissues and capturing their behaviour. Mesh cutting has always been considered a hard problem. After cutting, both the shapes of the elements and topology of the mesh will change.

Many techniques have been developed for tetrahedral meshes. In work of Delingette et al. [35], the algorithm simply deletes the tetrahedral element that is been cut during simulation. Another work for cutting tetrahedral mesh was proposed by Sifakis et al. [36]. The authors proposed a robust cutting algorithm for tetrahedral meshes that with a high-resolution triangle surface meshes as the surface representation. Later Wang et al. [37] have proposed another algorithm, that uses virtual node algorithm that can efficiently cut a tetrahedral mesh with a triangle surface.

As for non-conforming FEM simulation with a hexahedron background grid, the elements of the background grid can not be cut into arbitrary shapes in comparison tetrahedral element simulation. But techniques, such as virtual node, discontinuous Galerkin method, and extended finite element can be used for dynamic cuttings of non-conforming FEM simulation. In work of Molino et al. [38], 6 nodes were embedded in each tetrahedral mesh which allows a maximum of three cuts per element. Though the technique is developed for tetrahedral element mesh, using embedded nodes, we can also split a hexahedron element in a similar fashion. Kaufmann et al. [39] used discontinuous Galerkin method to support cuttings for hexahedron elements. But new hexahedron elements were created during the cutting due to the new degrees of freedoms introduced by the discontinuity at the cut. XFEM has been used to model structure fracture and cutting in the field of mechanical engineering for a long time. But mostly they are been used for rigid body or linear elasticity materials that undergo small deformation. Jerabkova et al. [40] have proposed a fast and stable XFEM method for cutting nonlinear materials. But this work was only proposed for tetrahedral element meshes.

Challenges and Possible solutions

Even though most techniques for cutting are developed for tetrahedral mesh simulation, they theory can potentially work for non-conforming mesh simulation with a hexahedron background grid with some adjustment. The virtual node algorithm and XFEM algorithms have been combined with hexahedron mesh for other features in literature. For instance, a second-order virtual node FEM algorithm has been combined with a 2D background grid by Zhu et al. [31] for simulating nearly incompressible linear elasticity. In work of Dolbow et al. [41], XFEM is proposed to model discontinuity(crack) in a hexahedron mesh with linear elasticity.

Whether it is virtual node algorithm or XFEM, in comparison to standard FEM algorithm, besides the extra computation, requires extra storage in the elements that contain discontinuity. To support online cutting or tearing, such storage must be able to grow with the simulation progress. The virtual node algorithm, as presented by Molino et al. [38], has a maximum number of cuts supported per element. As for XFEM, it introduced a discontinuous shape function inside the element to model the cut. Standard 8 point Gauss quadrature rule works well for continuous shape function up to third order, but for a discontinuous shape function, a new integration method may need to be developed for accurate integration within an element.

3.5 Vectorization and optimization for stream optimized platforms

Problem overview

Finite element simulations can be algorithmically formulated as sparse matrix operations or stencil operations. Those operations for each node only require information from a small surrounding region as input to compute the compute the output. Especially for non-conforming FEM simulation with a uniform hexahedron background grid, the sparsity patterns and stencils for each element are identical. Such characteristic exposes the opportunity to use SIMD (single instruction multiple data) hardware to speed up the performance of simulation. In recent years, SIMD hardware such as GPU or xeon Phi, features over 10 times more floating point operations per second (FLOPS) than traditional CPUs and 5 times more memory bandwidth. They have been used for physics based simulation for performance improvement for decades now. McAdams et al. [10] have used SSE instructions on CPU for data level parallelism, and achieved 3-7 times speed up using GPU. Mitchell et al. [15] have used the **Intel Xeon Phi** hardware which features a 512-bit SIMD width for the FEM simulation.

Challenges and possible solutions

The first challenge a parallel algorithm faces is write-dependency. For FEM simulation, the computation usually involves reading nodal information and compute the contribution of each element and accumulate back to the nodes. But each node is shared by many elements. To prevent the situation of many threads computing different elements writing back to the same node, the final accumulation operation cannot be safely executed without a lock. But frequent locking can be extremely expensive and easily become the bottleneck of the computation. McAdams et al. [10] used a two pass algorithm to avoid such write dependency. First, a cell center stress value was computed in the first pass, then the nodal force was computed by taking the divergence of the adjacent cell stresses without the need of the accumulation operation. But this solution is very specific to the constitutive and single point integration scheme of their choice. Another potential solution for eliminating the accumulation operation is to do duplicated computation, instead of split elements to threads, we can split nodes to threads, and for each node, we compute the force contributing of all elements that contain this node. A limitation to this strategy is, even though the write dependency is eliminated, a significantly more amount of computation is needed, for each element is computed many times.

4 Work to date

A scalable Schur-complement fluids solver for heterogeneous compute platforms

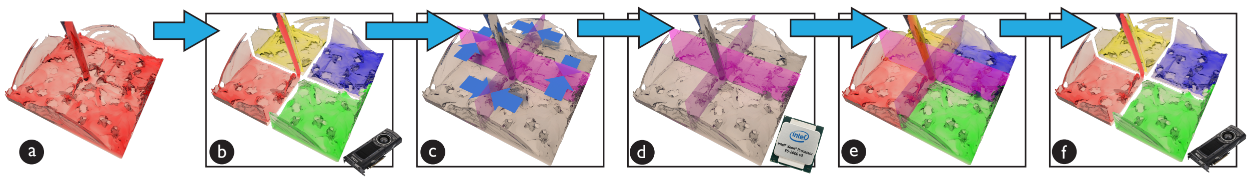

Figure 1: Illustration of the core concept of our method: (b) We split the computational grid into subdomains, and independently solve them on the GPU(s), using zero Dirichlet conditions on subdomain boundaries. (c) Fluxes of the subdomain solutions are computed and sent to the CPU. (d) A specially formulated system is solved on the interface, using the CPU. This produces the exact value of the interface variables. (e) Those values are sent to the subdomains, and set as Dirichlet conditions. (e) A final subdomain solve on the GPU yields the global solution.

In resent work [42], my co-authors and I developed a solution for solving large-scale finite-difference discretized Poisson problem in an efficient distributed fashion utilizing multiple stream optimized accelerators. The core contributing of the work is that we re-formulated the discrete Poisson problem into a collection of independent subdomain problems and a global interface problem that is the Schur-complement of the subdomains.

Each subdomain problem is solved based on the geometric multigrid algorithm proposed by McAdams et al. [26] given that finite difference 3D Poisson problem is a uniform 7 point stencil operation, we utilized the high bandwidth and high computational throughput of stream optimized accelerators and created highly efficient subdomain solvers.

As for the interface problem, in comparison to the subdomain problems, is highly irregular and, if written in explicit matrix form, a dense matrix operation while the subdomain problems are extremely sparse. To solve interface exactly would require super-linear complexity and it will easily be the bottle-neck of the solver. Instead of solving the interface exactly, we proposed an approximate solver for the interface using an adaptive approximation and multigrid V-cycle that executes in linear time with respect to the total number of degree of freedom on the interface. But as our solver by itself is only approximate, we used it as a preconditioner for the conjugate gradient method. As a whole, our iterative solver has linear complexity per iteration and the number of iteration required to reduces residual in an order of magnitude is independent of the solution resolution.

Power Diagrams and Sparse Paged Grids for High Resolution Adaptive Liquids

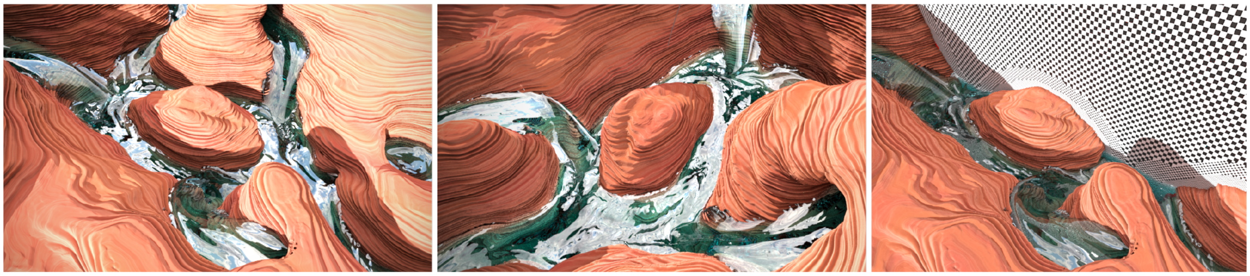

Figure 2: Close-up view of the simulation of a river flowing through a canyon. The adaptivity pattern, based on proximity to rigid boundaries, is shown along a vertical cross-section, on the right. A narrow band level set with resolution 2048^2 x 4096 is used for interface tracking.

My recent paper on adaptive fluids [43] presented a 2nd order adaptive scheme for liquid simulation. The key contribution of this work is that a 2nd order pressure solver that allows interface cross different grid of different resolution. Previous adaptive methods on a regular grid either require refine the surface of the liquid completely and change grid topology every time step [44] or only achieved 1st order accuracy along grid resolution changes [45]. To achieve 2nd order accuracy cross grid resolution, we combined the data structure of SPGrid [34] and power diagram [46] and developed a new fast marching and advection scheme.

Efficient Elasticity for Character Flesh Simulation on Octrees

This is the project I was working on during my internship with Disney Animation Studio in the summer of 2016. In this project, we extended the work [10] by McAdams et al. to use an adaptive grid for flesh simulation. In an animation production setting, the visual interests usually lie only on the surface. High resolution details underneath the surface are very costly to simulate and adds very little visual detail to the resulting character. We used a balanced linear octree as our main data structure, and developed parallel algorithms for the multigrid solver, collision detection, and varies time integration schemes.

5 Research Plan

In this section, the tentative schedule for the research projects and the problems they are to address will be presented. The intent is to finish my dissertation within 16 months.

5.1 Homogenization based multigrid solver

Details For this project, we intend to design a highly efficient multigrid solver for heterogenous linear elasticity using hexahedral elements on SPGrid with SIMD acceleration. Currently a plain CG solver has been implement, we are still working on the theoretical exploration of homogenization based multigrid solver. In this project, I will focus on applications with known heterogenous materials, such as topology optimization or 3D fabrication.

Estimated Completion Winter 2017

5.2 Constitutive models and discretization validation

Details For this project, I intend to validate for different constitutive models, how well are the qualities of the discretization, and how close is the simulation result in comparison to the physical experiment. The experiment will be conducted on physical proxies of soft-tissues such as silicon rubbers or other synthetic materials. The material will be processed into thin samples that can be considered as 2D. I will design the experiment to impose extended boundary conditions to the samples and capture the displacement field. The boundary condition will be changed slowly with time, so that the experiment can be considered quasi-static. Along side with the physical experiment validation, I will also validate the discretization quality for the constitutive models by applying a known deformation field and compare the analytical result with the simulation outcome.

Estimated Completion Spring - summer 2018

5.3 Online topology change

Details For this project, I plan to explore using XFEM to support online topology change with hexahedral element. Hexahedral elements in contrast to tetrahedral elements, which is also called linear elements, require more complex integration rules. With the discontinuity and singularity introduced by XFEM, new methods will be needed for minimizing storage and computation overhead with in cooperation with this new feature.

Estimated Completion Fall 2018

5.4 Dissertation Writing

Estimated Completion Winter 2018

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