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An integrated computational framework for modeling materials with complex and evolving microstructures

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The project focused on developing an automated computational framework for modeling materials with complex microstructures. Main achievements include: (i) Establishing a parallel, non-iterative mesh generation algorithm named CISAMR for meshing high complex domain geometries with super-linear speed-up in parallel enabling the construction of massive meshes with tens of millions of degrees of freedom; (ii) Developing a microstructure reconstruction algorithm consisting of virtual packing and optimization phases, for synthesizing realistic micro-structural models of various materials including fibrous composites, particulate composite, and entangled non-woven fibrous materials; (iii) Implementing the meshing and virtual reconstruction algorithms for modeling several real-world problems, including asteroidal rocks, fiber reinforced composites, and structural adhesives.

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## **An integrated computational framework for modeling materials with complex and evolving microstructures**

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## 1. Objectives

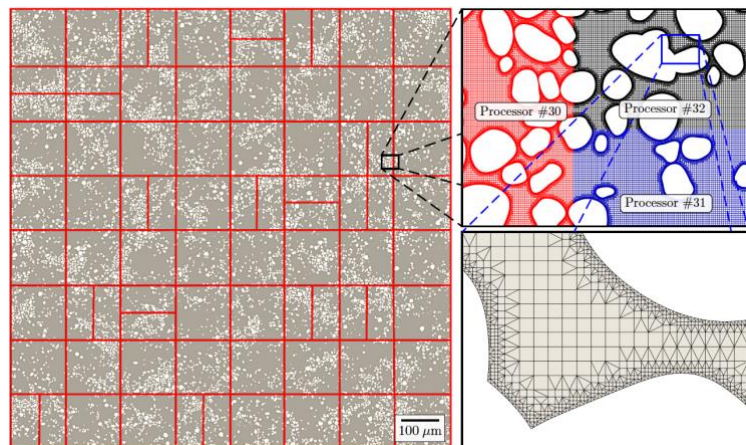
The primary objective of this research project is the creation of a cutting-edge computational framework for the automated modeling of novel materials involving complex and evolving microstructures. Hence, an integrated framework is proposed that combines three key components: (i) A novel algorithm for converting morphological and statistical features from imaging data into a realistic synthetic virtual microstructure; (ii) A novel non-iterative mesh generation approach which transforms a structured background grid into a high-quality conforming finite element mesh; and (iii) A non-isoparametric NURBS-enhanced mapping for a novel finite element (FE) formulation which eliminates geometric discretization errors without the computational overhead of introducing additional degrees of freedom (DOFs). Various algorithmic and data-structural aspects are carefully considered for designing this integrated framework, which aims to facilitate faster development of novel engineering materials by significantly reducing the labor and computational costs and by providing improved accuracy by the elimination of discretization errors. The proposed methodology also allows for parallelization, which can facilitate rapid solution of problems such as *Uncertainty Quantification (UQ)* [1,2] and *Integrated Computational Materials Engineering (ICME)* [3,4].

## 2. Research

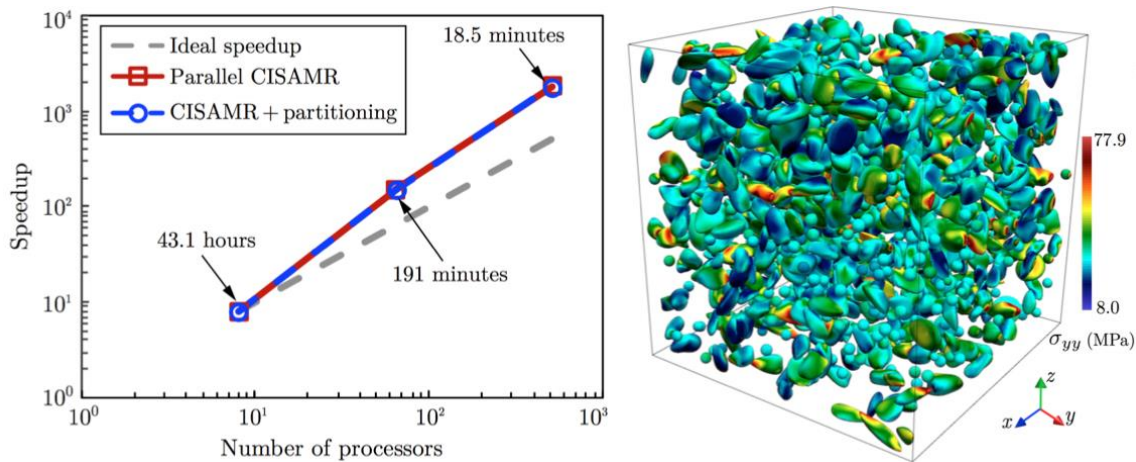
The first phase of the project was dedicated to the development and integration of two components, namely the *microstructure characterization* and the *conforming finite element (FE) mesh generation*. The second phase, executed in the past year, was dedicated to the development of a *parallel computational framework* [5] for conforming mesh generation. Specific algorithmic considerations were made to enhance the automated framework developed in phase one, improving both its computational efficiency and fidelity for handling large-scale complex problems, including those with high interest engineering materials such as carbon-fiber reinforced polymers (CFRPCs) [6], and cross-linked fiberglass packs [8].

### 2.1. Parallel CISAMR

The Conforming to Interface Structured Adaptive Mesh Refinement (CISAMR) introduced in first phase, was implemented in a parallel computational framework, with maximal code reuse from its sequential counterpart [5]. Here, the domain partitioning is tightly integrated with the microstructure reconstruction framework to ensure an optimal arrangement of partitions based on shapes/sizes of particles. This relatively inexpensive pre-processing phase is specifically designed for modeling heterogeneous material microstructures. For decomposing the domain, a set of hierarchical bounding box representations of inclusion morphologies, together with the number of refinement levels along each interface, are utilized to



**Figure 1:** RVE of a corroded steel sheet, together with the arrangement of 80 partitions used by parallel CISAMR to generate a conforming mesh. Portions of the resulting conforming mesh (generated using 40 partitions) are depicted in insets of the figure [5]



**Figure 2:** Stress patterns observed in particulate composite simulated using conforming mesh generated with parallel CISAMR, along with plots showing the scaling of mesh generation with increase in # of processors [5].

determine the computational load measure in each sub-region, and a multi-objective optimization problem is then solved to balance the computational load across the processors. **Figure 1** shows the conforming mesh generated for the portion of a corroded metal sheet using the parallel CISAMR with an optimized load distribution for 80 processors.

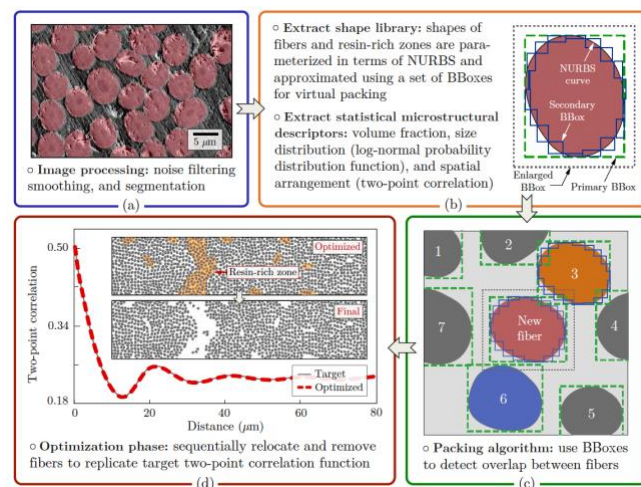
The distinct phases of the CISAMR algorithm are then executed independently inside the sub-meshes with minimal communication between the processors, while also retaining the highly desirable non-iterative aspect. The scalability tests performed on massive example problems showed linear (ideal), and at times, super-linear (fantastic) speedups, highlighting the suitability of the parallel CISAMR algorithm for generating massive conforming meshes. **Figure 2** illustrates the results of a scalability test performed on a 3D particulate composite microstructure, which shows the super-linear scalability of the CISAMR mesh generator, as well as the resulting stress fields from a high-fidelity micro-mechanical simulation performed in parallel using the same partitions.

### 3. Applications

In this section we describe some of the specific large-scale problems analyzed using the upgraded automated computational framework.

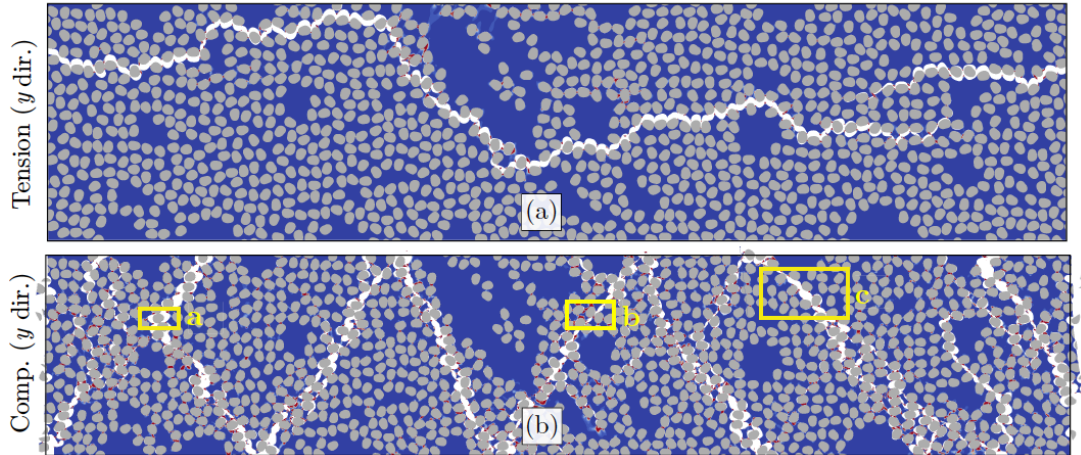
#### 3.1 Carbon-fiber reinforced Polymers (CFRPCs)

A numerical study was performed to measure the impact of size and spatial arrangement of resin-rich zones on the failure response of a carbon fiber reinforced polymer (CFRP), when subjected to loads applied transverse to the fibers direction [6]. The strategy involved the virtual reconstruction of large Statistical Volume Elements (SVEs) of CFRP based on imaging data, with varying size and spatial distribution of resin-rich zones. The process utilized the virtual microstructure reconstruction framework developed during phase one of the project and is visually depicted in **Figure 3**. The CISAMR meshing algorithm was then employed in parallel to generate high-quality, adaptively refined conforming meshes



**Figure 3:** Different steps of the algorithm used for the image-based virtual reconstruction of CFRP SVEs with resin-rich zones [6].

composed of millions of elements for each SVE. The FE approximations of failure response of SVEs were carried out using continuum ductile and cohesive-contact damage models for the epoxy matrix and fiber-matrix interfaces, respectively. **Figure 4** shows the damage response for the SVE at the failure point under transverse tensile and compressive loading. The study illustrated the suitability of the automated framework for analyzing the performance of engineering materials in the presence of microstructural

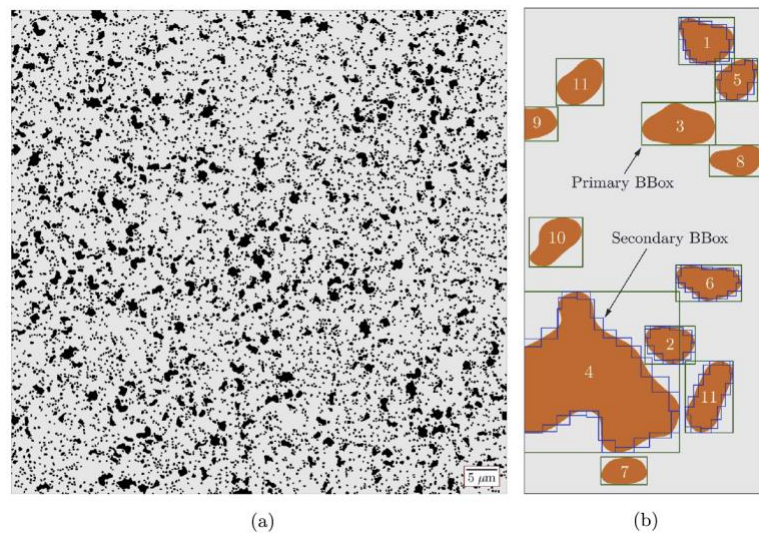


**Figure 4:** Damage patterns at the failure point in SVE subject to tension/compression in the y-direction [6].

defects, in this case being resin-rich zones formed as a result of the manufacturing process.

### 3.2 Homogenization-based fracture analysis

ZrB<sub>2</sub>-SiC is a two-phase particulate composite often used as a thermal coating, exhibiting sample-to-sample variations in elastic and fracture properties. This behavior is a result of micro-scale inhomogeneity, and hence the statistical volume elements (SVEs) are employed to homogenize the elastic and fracture properties [7]. The NURBS-based packing and optimization approach introduced in this project facilitated the automated generation of thousands of representative volume elements (RVEs) for the mesoscale analysis. **Figure 5** shows the hierarchical NURBS bounding boxes introduced for the innovative packing algorithm as well as a sample generated representative volume element (RVE). High quality 2D finite element models were efficiently generated using the CISAMR algorithm.



**Figure 5:** (a) Virtually reconstructed ZrB<sub>2</sub>-SiC RVE with 20% volume fraction; (b) packing based micro-structure reconstruction, used for the automated generation of SVEs [7].

The SVEs were analyzed under mixed, traction, and minimal kinematic boundary conditions to yield their angle-dependent tensile and shear fracture strengths and elastic stiffness. The results of this study showed a strong correlation between SVE size and particle spatial distribution on the homogenized fracture strengths, whereas elastic properties were found to be primarily dependent on the volume fraction.

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### 3.3 Cross-linked fiberglass packs

In this numerical study, fiberglass insulation packs with cross-linked fibers were analyzed under compressive loads. We made key algorithmic enhancements to the NURBS-based reconstruction algorithm to accurately synthesize realistic SVEs of this nonwoven entangled material. The virtual microstructures were generated using probability distribution functions associated with the diameter/length and spatial orientation of fibers, as well as the presence of fiber bundles and cross-linking binder phases. A reduced-order FE model was also proposed for cost-effective high-fidelity modeling of the mechanical behavior of fiberglass SVEs. This model utilized 1D beam and connector elements to discretize glass fiber and binder particles, respectively. The accuracy of this model was verified by comparing its results with high-fidelity 3D FE simulations. This study also investigated the use of appropriate boundary conditions for modeling SVEs under compression so as to replicate the power-law force-deflection response observed in experimental tests. The resulting model was then utilized to investigate the effects of the polymer binder and fiber bundles on the compressive stiffness of the fiberglass pack, which showed that the presence of fiber cross-linking and fiber bundles in the microstructure could increase the effective compressive stiffness of the fiberglass pack.

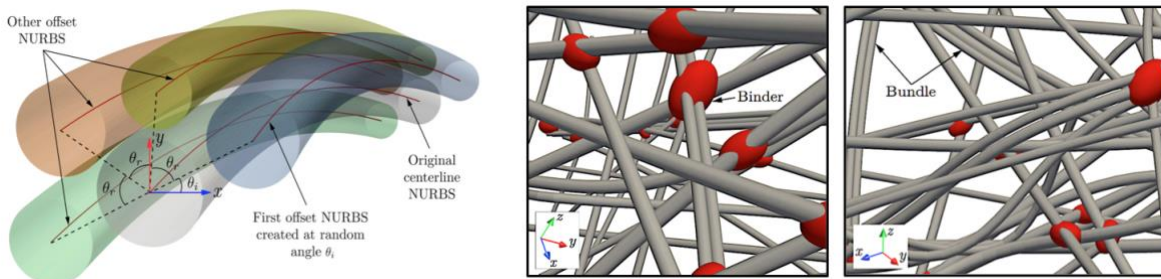


Figure 6: Generating fiberglass pack bundles and binder particles using NURBS [8].

### 3.4 Thermo-mechanical analysis of stony meteorites

In this application problem, the Micro-CT images of L6 ordinary chondrite (asteroidal rock) microstructure were converted into realistic microstructural models of the samples [9]. These NURBS based virtual microstructures were transformed into FE models using the CISAMR meshing algorithm for subsequent thermo-mechanical analysis. The micromechanical FE simulations showed the concentration of stress at matrix-particle interfacial regions with higher curvatures under mechanical loading, which can result in the nucleation and eventually propagation of cracks in such regions. However, thermal cycling causes a more uniform distribution of stress along the particle interfaces, resulting in their debonding from the surrounding matrix. Both observations were verified by experimental data obtained from an in-situ X-ray micro-computed tomography (micro-CT) setup capable of applying thermal and mechanical loads. The results of this study illustrate the high degree of accuracy that can be obtained using the cutting-edge numerical framework developed in this project.

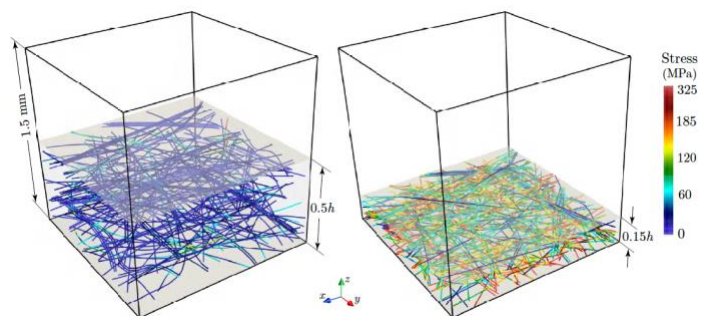
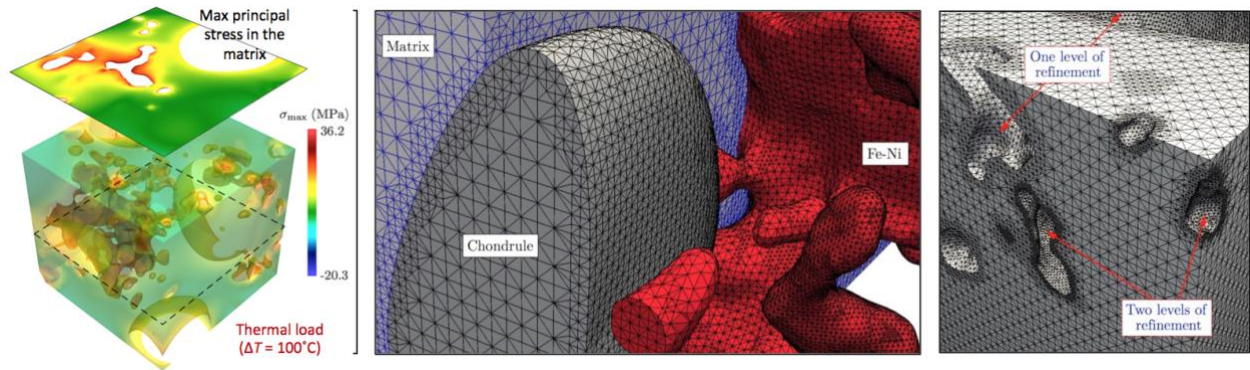


Figure 7: Reduced-order FE approximations of deformed shapes and stress fields in fiberglass SVEs when compressed to 50% and 15% of original height [8]



**Figure 8:** Synthesis of realistic 3D CFRPC microstructures: (a) BBox based packing; (b) Relocation based optimization; (c) Introducing misalignment and 3D extrusion [9].

## 7. Acknowledge/Disclaimer

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