YEAR 2:

**Major activities**

Developments during year two focused on three aspects of this project including:

* Examination and initial implementation of tools for parallel exchange of data between scales in the execution of parallel multiscale simulations.
* Execution of multiscale biomaterial investigations using an extended microscale RVE.
* Implementation of massively parallel unstructured mesh methods for adaptive simulations.

A key requirement of parallel multiscale simulations is supporting the transfer of fields between single scale analysis components on a massively parallel computer. To date efforts on the development of methods to exchange information between scales have relied on ad-hoc methods specific to the scale transfer being carried out. Since the development of effective parallel algorithms to execute such processes is quite complex and time consuming, it is highly desirable to have a generalized means to transfer the data between the single scale components in parallel that is independent of the specific scale linking transformations executed. Building on methods of generic programming, a method of defining and controlling process sets for parallel data transfer has been defined and is being implemented.

A key complication addresses in the development of the current multiscale process set methods is their execution and control on massively parallel computers. At the highest level adaptive control of must follow a single program single data mechanism. However, the actual execution of the transfers must at a minimum employ a single program (of overall control) multiple data mechanism. The mechanism developed for doing this supports process sets in which the data is transferred between single scale simulation components that are operating in parallel using their own distribution of operations and data across processing cores. The completion of this model into a multiscale simulation code and its extension to methods with increased scalability is underway. In particular, these methods are also now being integrated into two-scale adaptive simulation code for fibrous materials.

As part of the development of that multiscale fibrous material simulation code, efforts have also been carried out to generalize the microscale RVE to extend the pre existing fiber only representation to include support a fiber plus matrix representation. The development and use of the fiber plus matrix RVE first had to address the development of correct non-manifold geometric models and the automatic generation of the meshes in the RVE’s. With that task carried out, studies were preformed that clearly showed that for specific materials the inclusion of the matrix in the RVE is critical to the accurate prediction of local solution parameters of importance for the prediction of tissue damage [1,2]. The key challenge in the application of this RVE in the execution of multiscale tissue analyses is the high level of computational effort required for each RVE, which is now a substantial finite element model. Multiscale analyses of this type will only be feasible on massively parallel computers where even the individual RVE analyses step are executed in parallel over multiple cores. Efforts to support such multiple level parallelism have been initiated and will be a focus in the coming year.

**Specific Objectives**

The specific objectives of this project are to:

* Define abstractions and methods that bridge physics and mathematics formalisms to the models and computational methods needed for component-based adaptive multimodel analysis. This infrastructure must maintain a clear understanding of all the relations and transformations executed and relate them to a multiscale design specification. Such capabilities are essential to tracking design sensitivities and uncertainties within a multiscale design process.
* Implement interoperable components that support the relations and transformations associated with the domain, model and field interactions of the abstracted simulation components.
* Define and implement a methodology to supports the full range of adaptive model, scale linking and discretization control techniques needed for multiscale simulations.
* Develop multilevel dynamic load balancing techniques to support the scalable execution of adaptive multiscale simulations on massively parallel computers.
* Develop multiscale simulation applications that demonstrate the effectiveness of the tools and technologies developed.

RESULTS and achievements

The partial results and achievements to date are indicated in the activities. As a project focused on the development of an overall software infrastructure, there is the need to address a large number of base technical issues and methods before useful results can be obtained.