Final Technical Report for contact number DE-FG02-08ER25862 (08/14/2011-08/14/2016; Total Award Period Covered: 08/15/2008-08/14/2016)

Tittle: Finite Dimensional Approximations for Continuum Multiscale Problems

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Abstract. The completed research project concerns the development of novel computational techniques for modeling nonlinear multiscale physical and biological phenomena. Specifically, it addresses the theoretical development and applications of the homogenization theory (coarse graining) approach to calculation of the effective properties of highly heterogenous biological and bio-inspired materials with many spatial scales and nonlinear behavior. This theory studies properties of strongly heterogeneous media in problems arising in materials science, geoscience, biology, etc. Modeling of such media raises fundamental mathematical questions, primarily in partial differential equations (PDEs) and calculus of variations, the subject of the PI's research. The focus of completed research was on mathematical models of biological and bio-inspired materials with the common theme of multiscale analysis and coarse grain computational techniques. Biological and bio-inspired materials offer the unique ability to create environmentally clean functional materials used for energy conversion and storage. These materials are intrinsically complex, with hierarchical organization occurring on many nested length and time scales. The potential to rationally design and tailor the properties of these materials for broad energy applications has been hampered by the lack of computational techniques, which are able to bridge from the molecular to the macroscopic scale. The project addressed the challenge of computational treatments of such complex materials by the development of a synergistic approach that combines innovative multiscale modeling/analysis techniques with high performance computing.

Keywords: bio-mimetic, multiscale modeling, coarse-graining, computational complexity, high performance computing.

Specific results obtained by the PI and his collaborators and supported by this award are in two areas:

Area 1. *Coarse-graining in stationary multiscale continuum problems.* In the work [1], the PI *et al.* proposed a new variational method for the numerical homogenization (coarse-graining) for linear PDEs with arbitrarily rough coefficients. This is called the

Rough Polyharmonic Splines (RPS) method and it is the most recent development of the approach from [2, 3]. The novelty of this approach is that it does not rely on the concepts of ergodicity or scale-separation of the coefficients, but relies instead on the compactness properties of the solution space used to construct a new localized, variational basis that is also meshless. This approach constructs "custom-made" multiscale finite elements for problems where the standard finite element methods do not provide the necessary accuracy due to the presence of many scales in the coefficients. Recently, an extension of the RPS method to nonlinear PDE problems has been developed by the PI and his collaborators in the course of this research [4].

Area 2. *Coarse-graining in dynamic problems for large systems of interacting particles.* In work [5], the PI *et al.* developed a novel computational approach for the time evolution of a system of a large number of interacting particles. The key features of such systems are the presence of (a) *strong interactions* and (b) *randomness* in the initial data due to the uncertainty of the locations of the particles. Current computationally efficient methods for a large system of interacting particles efficiently apply in a deterministic setting, but may be very costly in a random setting as one has to run it over many realizations. Thus, the novelty of the proposed approach is in addressing both challenges (a) and (b) simultaneously. The goal is to model collective behavior, and, in particular, the transition from an individual to a collective state, as well as the development of correlations, i.e., how initially independent particles become dependent with time due to interactions. A major theoretical step in this direction has been made in [5], where a closed system for one- and two-point probability distribution functions was obtained. The method has been validated through a large number of numerical experiments implemented using parallel computing (GPU).

In addition to the work in Areas 1 and 2, the PI and his collaborators applied the computational techniques developed in this research to active materials exemplified by bacterial suspensions. The results were published in papers [6–10] with the acknowledgment to the support of this award.

The papers [1, 5–10] resulted from this grant's support (renewal period 2011-2016). The work of the PSU graduate student Shawn D. Ryan (currently Assistant Professor in Cleveland State University) and post-doc Mykhailo Potomkin was supported by this award.

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