

## **Ongoing Research Support – Jeremy C. Smith.**

### 1) DOE - OBER

*Title:* Program Announcement LAB 07-12 New Analytical and Imaging Technologies for Lignocellulosic Material Degradation, and for Multiplexed Screening for Plant Phenotypes “Dynamic Visualization of Lignocellulose Degradation by Integration of Neutron Scattering Imaging and Computer Simulation”

*Funding period:* 10/1-07-10/1-10

*Amount:* \$2.1M

*Effort:* 1.2 months per year

*Role:* Co-PI.

*Abstract:* To combine neutron scattering and computer simulation for multiple length scale, real-time imaging of biomass during pretreatment and enzymatic hydrolysis. The combined capabilities of the Spallation Neutron Source, the High Flux Isotope Reactor, and the National Center for Computational Sciences at Oak Ridge National Laboratory will provide new information on lignocellulosic degradation.

### 2) DOE – OBER

*Title:* Bioenergy Science Center

*Funding Period:* 2007-2012

*Amount:* \$125M

*Effort:* 1.2 months per year

*Role:* Co-PI and Task Leader.

*Abstract:* Our task in this center is to perform computer simulations of enzymes involved in cellulose deconstruction, including cellulosome component modeling and quantum mechanical/molecular mechanical investigations of cellulase action.

### 3) NSF - IGERT

*Title:* SCALE-IT (Scalable Computing and Leading Edge Innovative Technologies) for Biology.

*Funding Period:* 10/09-10/14

*Amount:* \$3M (some of which could in principle fund research in our laboratory)

*Effort:* 0.5 months per year.

*Role:* Co-PI

*Abstract:* A team of biologists and computational scientists at the University of Tennessee in partnership with colleagues at Oak Ridge National Laboratory, is directing a five-year Integrated Graduate Education and Research Training (IGERT) Program. Our goal is to recruit and train future biologists in a new way of approaching biology— a seamless combination of computing expertise and research using emerging tools that can attack the most challenging problems in biology spanning sub-cellular to organismal scales.

#### 4) DOE – EpsCOR Implementation Award

*Title:* DE-FG02-08ER46528 Neutron Scattering Research Network for EPSCoR States.

*Funding Period:* 10/1/09-10/1/12

*Amount* \$1.97M plus 50% U. Tenn. matching, some of which could in principle fund research in our laboratory.

*Effort:* 0.5 months per year

*Role:* Co-PI

*Abstract:* With the completion of the Spallation Neutron Source (SNS) and upgrading of the High-Flux Isotope Reactor (HFIR) at the Oak Ridge National Laboratory (ORNL) the state of Tennessee is poised to lead the world in the capability of neutron scattering research. This proposal aims at directing the great impact of these facilities to the EPSCoR states and Tennessee in particular, by creating a research collaboration network around these facilities, and making the access to the facilities much easier for the researchers in the EPSCoR states. The plan consists of five parts: (1) Seeding research collaboration among the core participants and with the ORNL researchers, (2) Purchasing equipment widely used by the participants, (3) Supporting travels by the graduate students and participating researchers to the neutron facilities at the ORNL, (4) Partially supporting sabbatical leaves by the participating researchers, and (5) Holding workshops and schools on the application of neutron scattering for biological, life and physical sciences and engineering.

#### 5) NSF 07-597 EF - BIO CENTERS:

*Title:* Nimbios – Center for Synthesis of Mathematics and Biology

*Funding Period:* 10/1/09-10/1-12

*Amount:* \$15,907,538.

*Effort:* 1.2 months/year

*Role:* Co-PI.

*Abstract:* A major goal of mathematical models and analysis in biology is to provide insight into the complexities arising from the non-linearity and hierarchical nature of biological systems. The Center fosters the maturation of cross-disciplinary approaches in mathematical biology and fosters the development of a cadre of researchers who are capable of conceiving and engaging in creative and collaborative connections across disciplines to address fundamental and applied biological questions. The Center : 1) addresses key biological questions by facilitating the assembly and productive collaboration of interdisciplinary teams; and 2) fosters development of the critical and essential human capacity to deal with the complexities of the multi-scale systems that characterize modern biology.

#### 6) DOE - OBER Science Focus Area

*Title:* Biogeochemical and Molecular Mechanisms Controlling Contaminant Transformation in the Environment

*Funding Period* . 10/09-10/14

*Amount* \$3M/year

*Effort:* 1.2 months/year

*Role:* Co-PI and Task leader.

*Abstract:* The ORNL Science Focus Area (SFA) Program responds to Environmental Remediation Science Program (ERSD) needs by addressing the scientific issues that limit contaminant remediation at the Oak Ridge Reservation (ORR). Over the initial 5-10 year period, ORNL's SFA will address significant knowledge gaps regarding biogeochemical transformations that determine uranium (U) subsurface mobility and mercury (Hg) toxicity. This program integrates geochemical, microbiological, molecular, and modeling-simulation sciences to understand contaminant behavior in the field.

## 7) NIH - PEER

*Title:* Program for Excellence and Equity in Research

*Funding Period:* 01/01/09-01/01-14

*Amount:* \$3.9M.

*Effort:* 1.2 months/year

*Role:* Senior Personnel.

*Abstract:* The University of Tennessee Knoxville's (UTK) Program for Excellence and Equity in Research (PEER), an Initiative for Maximizing Student Diversity (IMSD) program in the MORE Division, through UTK's partnership with Oak Ridge National Laboratory (ORNL) and the partnership's UTK/ORNL Graduate School for Genome Science and Technology (GST), proffers underrepresented minority (URM) Scholars the opportunity to train in an unprecedented atmosphere of scientific excellence, engage in team-science fostered through the UTK-ORNL partnership, gain crucial 21st century professional skills, and be mentored by world class scientists, all within a supportive community created by and for the Scholars. PEER's goal is to leverage these attributes to create a "program of excellence" that will produce from PEER, the GST, and across the university, an increased number of accomplished, competitive and determined URM Ph.D.s who attain careers in biomedical research characterized by significant contributions to their fields, and thus contribute to our nation's health and well being.

## 8) DOE - ASCR

*Title:* LAB 08-19 Software Development Tools for Improved Ease-of-Use of Petascale Systems

ERKPE92 Scalable Development Environment for Petascale Computing

*Funding Period:* 09/09-09/12

*Amount:* \$2.1M

*Effort:* 1.2 months/year

*Role:* Co-PI

*Abstract:* Our goal is to reduce or eliminate at least some of the factors that hinder productive development of petascale scientific codes. Our starting point will be the development environment that plays a crucial role in the application development lifecycle. Long experience by the software engineering community has demonstrated that the use of integrated development environments is a key mechanism for improving productivity, so our intention is to use the open source Eclipse platform as the basis for the project.

9) DOE – Laboratory Directed Research and Development Fund

*Title:* Neutron Sciences 002-0507: Neutron scattering methodologies for the study of protein dynamics

*Funding Period:* 10/1/07-10/1/10

*Amount:* \$600K

*Effort:* 1.2 months per year

*Role:* PI

*Abstract:* To develop neutron scattering techniques for the analysis of protein dynamics. Calculations are being performed of spin-echo intensities from protein motions.

10) DOE – Laboratory Directed Research and Development Fund: Systems Biology 003-00044

*Title:* Computational Methods for Molecular Biophysics.

*Funding Period:* 10/1/06-10/1/09

*Amount:* \$1.067M

*Effort:* 1.2 months per year

*Role:* PI

*Abstract:* To develop computational methodologies in molecular biophysics.

11)DOE- OBER/ASCR

*Title:* ERKJE84 Multiscale Mathematics for the Simulation of Complex Biological Systems

*Funding Period:* 09/09-09/12

*Amount:* \$1060M.

*Effort:* 1.2 months/year

*Role:* PI

*Abstract:* Multiscale methods will be developed for biomolecular simulation and applied to critical problems in cellulosic ethanol production. Multiscale concepts will be used to parallelize molecular dynamics (MD) code for petascale capability supercomputing and to perform coarse graining. The coarse graining will involve development of the Realistic Extension Algorithm via Covariance Hessian (REACH) methodology, which maps results obtained from atomistic MD simulations onto models for larger-scale, coarse-grained MD. REACH will be extended to form PETA-REACH, a highly-parallelized algorithm based on a multiscale mathematical framework. The method will incorporate implicit solvation and develop the current coarse-grained REACH potential.