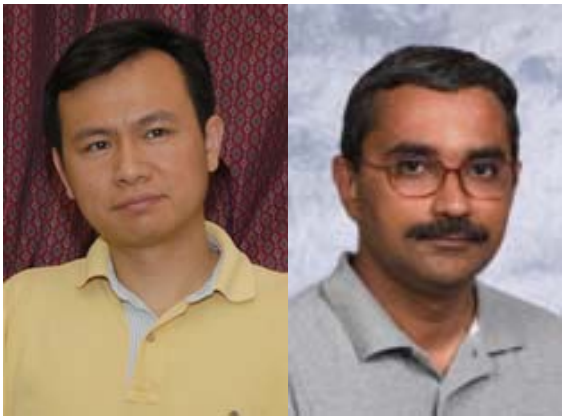
USF UNIVERSITY OF SOUTH FLORIDA
COLLEGE OF ENGINEERING

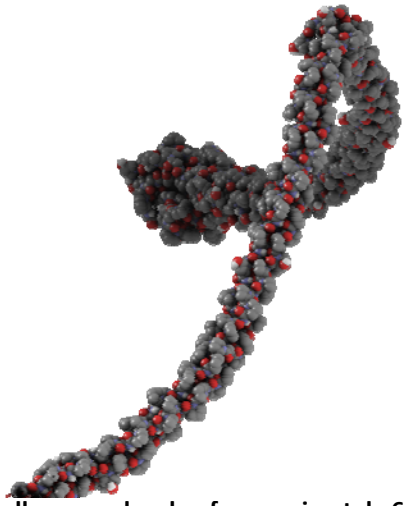
Computer Science & Engineering Professor Awarded
NIH Grant for Interdisciplinary Molecular Simulation Research



Yicheng **Sagar Pandit**

Tampa, Fla. (May 5, 2010) – Dr. Yicheng Tu, Assistant Professor of Computer Science and Engineering and principle investigator (PI), and Dr. Sagar Pandit, Assistant Professor of Physics and co-PI, have been awarded a five-year R01 grant from the National Institutes of Health (NIH), totaling $875,262 for "Database-centric Data Analysis of Molecular Simulations."

This is a collaborative project between Tu's group in CSE and Dr. Pandit's group from USF Department of Physics and Dr. Xingquan (Hill) Zhu from the Department of Computer Science and Engineering at Florida Atlantic University. The project addresses key data management challenges in performing molecular simulations, which is a major computational tool in studying the physical and chemical features of biological systems, for example, the mechanical properties the biomolecule collagen.



A model collagen molecule of approximately 63 nanometers in length.

A wide variety of body tissues like skin, bone, tendon, ligament, and cornea exhibit an enormous range of mechanical properties that result from the presence of collagen. Studying the processes underlying the structural and behavioral diversity of these properties using molecular simulations typically involves a great deal of user interaction with the molecular simulations. In this new scheme, the algorithm will dynamically make decisions regarding how to continue the simulations.

Such decisions are based on efficient evaluation of the current status of the simulation system. Existing methods to compute some of the critical system parameters such as multi-body correlation functions require an extremely long time (e.g., tens of days), making it infeasible to make simulation decisions on-the-fly. As a result, the simulations are often designed to run along multiple directions and the wrong directions are detected only after the whole simulation is done.

A major focus of this project is to design efficient data retrieval and query processing algorithms derived from modern database technology. In their initial design, the aforementioned system parameters can be computed in just a few minutes' time. Furthermore, simulation data from any research group's simulations can be made accessible to other groups by means of a distributed database, allowing for greater and more-timely accessibility to scientifically, peer-reviewed results.

The University of South Florida is one of the nation's top 63 public research universities and one of only 25 public research universities nationwide with very high research activity that is designated as community engaged by the Carnegie Foundation for the Advancement of Teaching. USF was awarded $380.4 million in research contracts and grants in FY 2008/2009. The university offers 232 degree programs at the undergraduate, graduate, specialist and doctoral levels, including the doctor of medicine. The USF System has a $1.8 billion annual budget, an annual economic impact of $3.2 billion, and serves more than 47,000 students on institutions/campuses in Tampa, St. Petersburg, Sarasota-Manatee and Lakeland. USF is a member of the Big East Athletic Conference.

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