LBRN Work-in-Progress

INBRE Seminar series

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Tuesday September 3, 2013

9:30 - 10:15AM

Simulating Protein-Substrate Interactions in 8R-lipoxygenase and Developing MPI-enabled MapReduce Framework for Molecular Dynamics Simulation

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DR. SHUJU BAI

Department of Computer Science

SOUTHERN UNIVERSITY AND A&M COLLEGE

9:30 AM

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Simulating Protein-Substrate Interactions in 8R-lipoxygenase and Developing MPI-enabled MapReduce Framework for Molecular Dynamics Simulation

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Dr. Shuju Bai

Associate Professor, Department of Computer Science

Southern University and A&M College

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Mentors:

Marcia Newcomer PhD

George C. Kent Professor, Department of Biological Sciences

LSU

Seung Jong Park PhD

Associate Professor, Division of Computer Science and Engineering

LSU

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Our research has two specific aims. 1) Model protein-substrate interactions in 8R-lipoxygenase; 2) Apply new computational technology into molecular dynamics applications to enhance the performance. We have finished molecular dynamics simulation of arachidonic acid:8R-lipoxygenase complex to confirm/verify the model we developed using ICM. The results suggest a model which could possibly explain the interactions between 8R-LOX and arachidonic acid. We are in the process of simulating the interactions of 5-LOX and arachidonic acid. Meanwhile, we incorporated MPI into MapReduce framework based on Hadoop. The MPI module we added enables Hadoop to monitor and manage the resources of Hadoop cluster so that computations incurred in MapReduce tasks can be performed in a parallel manner. We have carried out molecular dynamics simulations on the MPI-enabled MapReduce framework. Results showed that our implementation improves performance of Hadoop by effectively assigning tasks to task trackers and reducing the execution time of molecular dynamics applications.