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

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Department of Computer Science  
SOUTHERN UNIVERSITY AND A&M COLLEGE  
9:00 AM

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Examination of the Hoxa1 Cell Signaling Pathway and Gene Regulatory Network in Mouse ES cells

D R .  E D U A R D O  M A R T I N E Z - C E B A L L O S  
Department of Biology  
SOUTHERN UNIVERSITY AND A&M COLLEGE  
9:45 AM

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

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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.
Examination of the Hoxa1 Cell Signaling Pathway and Gene Regulatory Network in Mouse ES cells

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The homeobox (Hox) family of transcription factors comprises important regulators of embryonic patterning and organogenesis. In mammals, the Hox genes are located in four separate chromosome clusters, and can be activated sequentially by retinoic acid (RA) in a manner that resembles their positions in the clusters, e.g. 3’ genes are activated by RA before 5’ genes. In vertebrate embryos, alterations of the normal pattern of Hox gene expression result in homeotic transformations and malformations. In mice, Hoxa1 has been shown to be required for proper patterning of the early hindbrain and the associated neural crest. Similarly, we have previously reported that Hoxa1 is required for the neuronal differentiation of mouse Embryonic Stem (ES) cells in vitro. However, little is known about the molecular mechanism by which this transcription factor directs either embryonic brain patterning or the differentiation in culture of ES cells along a neuroectodermal lineage. In this regard, our preliminary ChIP-on-chip data suggest that Hoxa1 may regulate ES neuronal differentiation by activating Ca$^{2+}$-mediated signaling events in Wild type mouse ES cells. Furthermore, treatment of Hoxa1 -/- ES cells with thapsigargin, an intracellular Ca$^{2+}$-pump inhibitor, correlated with increased levels of the neuronal marker beta-Tubulin III. Thus, these results suggest that Hoxa1 initiates neuronal induction by increasing intracellular Ca$^{2+}$ levels in RA-treated mouse ES cells. As an attempt to uncover additional signaling events occurring downstream of Hoxa1, we also sought to identify the Hoxa1 Gene Regulatory Network (GNR) from gene expression data. Here, we present our initial studies using a noise and redundancy reduction technique called NARROMI to infer the Hoxa1 GNR from time course RNA-sequencing data. All together, our studies provide an insight into the mechanism of Hoxa1 action in differentiating mouse ES cells.