## CSol – Team Progress Report: Investigating Metabolic Phenomena Using Information Theory

Team Members: Frank DeVilbiss<sup>1</sup>, Maxim Raginsky<sup>2</sup>, Shakti Gupta<sup>3</sup>, Mano Maurya<sup>3</sup>, Shankar Subramaniam<sup>3</sup>, Mohan Gopaladesikan<sup>4</sup> Pablo Robles-Granda<sup>5</sup> and Doraiswami Ramkrishna<sup>1</sup>,

(1)School of Chemical Engineering, Purdue University, West Lafayette, IN,

(2)Department of Electrical and Computer Engineering, University of Illinois at Urbana-Champaign, Urbana, IL

(3) Department of Bioengineering, University of California San Diego, La Jolla, CA

(4) Department of Statistics, Purdue University, West Lafayette, IN

(5) Department of Computer Science, Purdue University, West Lafayette, IN

This year has been a successful year in terms of collaboration. With the aid of Prof. Subramaniam's group in UCSD, we have fruitfully modeled the metabolic behavior of macrophage cells responding to an inflammatory stimulus, Kdo<sub>2</sub>\_Lipid-A using an approach that approximates the control of metabolic reactions. From dynamic metabolite data, we have been able to predict gene expression data qualitatively using the control variables in the metabolic model. This is shown below

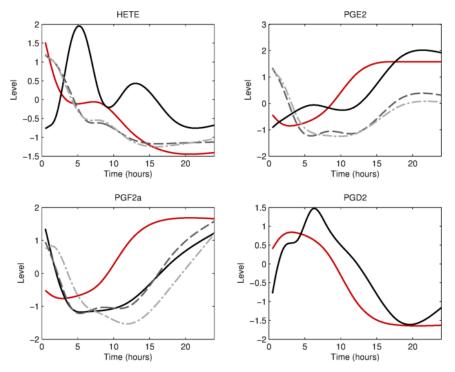


Figure 1 – Cybernetic variables modeling the control of different metabolic reactions are in red. Gene expression data for various genes is in black and grey. Note that the model is able to capture the qualitative effects of gene expression. For example in the pathway from Arachidonic Acid to 11-HETE (Upper Left), one can see how the gene expression profiles and cybernetic profile both start going downward, pause around 8 hours, and then continue their downward trend. Accounting for possible time delays, gene *Alox12b* also shows this trend.

The above result is an exciting validation of our modeling framework because it indicates that the cybernetic model of regulation matches data for the cell's mechanism of regulation.

Moreover, it shows that one can take biological information from one level of the system and infer the changes in data on another level.

## **Meetings This Year**

Frank DeVilbiss, Mano Maurya, Shakti Gupta, Prof. Subramaniam and Prof. Ramkrishna (Teleconference): 08/30/2013

Frank DeVilbiss, Mano Maurya, and Shakti Gupta (Skype): 10/01/2013

Frank DeVilbiss, Mano Maurya, and Prof. Ramkrishna (In Person at AIChE Conference): 11/06/2013

Frank DeVilbiss, Mohan Gopaladesikan, and Pablo Robles-Granda (In Person): 12/02/2014

Frank DeVilbiss, Mano Maurya, and Shakti Gupta (Skype): 04/18/2014

Frank DeVilbiss and Mohan Gopaladesikan (In Person): 05/12/2014

Frank DeVilbiss, Mano Maurya, and Shakti Gupta (In Person during CSol Summer School): 08/04/2014-08/07/2014

Frank DeVilbiss, Mano Maurya, and Shakti Gupta (Skype): 08/15/2014

Frank DeVilbiss, Mano Maurya, and Shakti Gupta (Skype): 09/02/2014

Note that aside from these meetings much communication also took place via email.a

## **Presentations This Year**

DeVilbiss, F. T., Raginsky, M., & Ramkrishna D. (2014, November). "Addressing the Need for a Model Selection Framework in Systems Biology Using Information Theory." Presented at American Institute of Chemical Engineers 2014, Atlanta, GA.

DeVilbiss, F. T., Jayachandran D., Maurya, MR, Gupta, S., Subramaniam, S. & Ramkrishna D. (2014, November). "Addressing the Need for a Model Selection Framework in Systems Biology Using Information Theory." Presented at American Institute of Chemical Engineers 2014, Atlanta, GA.