**Theoretical basis and practical applications of computational methods relevant to agricultural and food research problems.**

 The objective of this mini-course is learning, developing and using molecular modeling methodologies useful for research work. We will talk about theoretical concepts and techniques used in modern computer simulations, with a special emphasis on all-atom molecular dynamics simulation of protein and carbohydrate systems.

Topics include:

* Introduction to molecular modeling and applications
* Molecular dynamics simulations: strength and limitation
* Molecular Force fields: classical and polarizable
* Simulation Environment: Vacuum, implicit and explicit solvents
* Molecular dynamics analysis techniques
* Common modeling software
* Hands-on tutorials and exercises, introduction to Linux OS
* Discussions of applications of computational tools in research

Date: July 10-20, 2017

Additional presentations: September 2017

Instructors: Prof. Ganesan Narsimhan, Dr. Xiao Zhu

Bio of instructors:

Ganesan Narsimhan:

Dr. Narsimhan is a Professor of Agricultural and Biological Engineering at Purdue University, USA. Dr. Narsimhan’s main area of research is in Colloidal and Interfacial Phenomena with emphasis on the formation and stability of protein stabilized foams, emulsions and dispersions. Dr. Narsimhan has developed a methodology for identification of antimicrobial peptides from protein and has applied these methods to soy protein. He has elucidated the mechanism of pore formation in cell membranes by antimicrobial peptides using molecular dynamics (MD) simulation. He has also employed MD simulation to investigate the secondary and tertiary conformational changes of peptide adsorbed as well as tethered to silica surface. He is currently investigating interaction of cyclodextrin and curcurmin with cell membranes.

Xiao Zhu:

Dr. Zhu is a Senior Research Scientist at Purdue University with expertise in computational modeling and molecular simulations. He develops and applies computational tools to understand the structure-dynamics-function relationship in complex molecular and nanoscale systems. Currently, a few specific problems of interest include carbohydrate interactions guest molecules, *in silico* identification of antimicrobial peptide from natural proteins and design of inhibitors for fungal pathogens.