GARRETT CHAN

MARKOV STATE MODEL CONSTRUCTION THROUGH KEPLER WORKFLOWS

NATIONAL TAIWAN UNIVERSITY TAIPEI

Wednesday, July 2, 2014
Proposed Research

- Markov state models (MSMs) can be used to represent the probabilities of conformational changes in a protein.
- Because MSM construction is a time-consuming process, a Kepler workflow can automate the process, improving reproducibility.
- This Kepler workflow, ideally, can be applied to MSM construction for a variety of systems.
Progress Made This Week

- Set up secure shell protocol to access the UCSD network and Kepler
- Continued researching the calculateprojectRMSD.py scripts needed for the BuildMSM stage of the workflow
- Realized that several different scripts exist to calculate the RMSD
Plans for Next Week

- Clarify which distance metric is best to use
- Decide on the best way to graphically represent the MSM data
- Begin integrating distance metric-calculating into Kepler workflow
When I Wasn’t in the Lab, I…

Visited the Sun Yat-sen Memorial Hall and learned about his storied life.

Went to Longshan Temple and enjoyed the incense.

Sun Yat-sen: Chinese revolutionary, possible Calvin Klein model.
A Big xièxiè To:

- The Ledell Family for their generous scholarship
- Professor Jung Hsin-Lin and Professor Rommie Amaro
- Gabriele Wienhausen, Teri Simas and everyone at PRIME who made this program possible