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 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
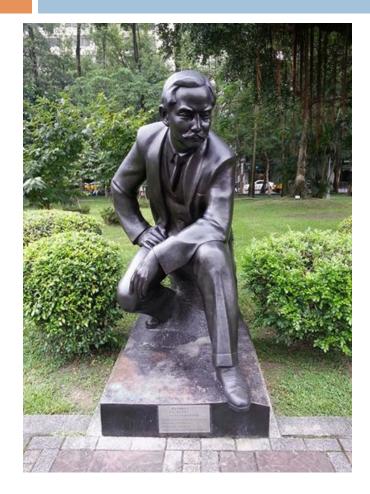
Progress Made This Week

- 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...

Sun Yat-sen: Chinese revolutionary, possible Calvin Klein model.

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

Went to Longshan Temple and enjoyed the incense.

A Big *xièxie* 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