

GARRETT CHAN

MARKOV STATE MODEL
CONSTRUCTION THROUGH
KEPLER WORKFLOWS

NATIONAL TAIWAN UNIVERSITY
TAIPEI

Wednesday, July 30, 2014

Progress Made This Week



- Tried to find a faster remote desktop system, since X11 is slow and makes using Kepler difficult even when using cipher, but had to continue using cipher
- Worked Dr. Malmstrom to elaborate next steps needed to complete the final components of the workflow
- Tested viability of using visualization scripts with the current workflow

Progress Made This Week



- Re-tested the last part of the workflow (BuildMSM.kar)
 - ▣ Needed to know if visualization scripts would work with workflow
 - ▣ Looked into changing the final stage of the workflow into a system that would work with any general system

Plans for Next Week



- Finish organizing the back half of the workflow to meet the needs of building an MSM
- Combine and separate workflow components as needed
 - ▣ I will need more guidance on this, because I am unsure as to how the separate components can be used

Successes



❑ Roadblocks

- ❑ Working with systems at UCSD can be slow, because the connection with *MSMBuilder* and *Kepler* is difficult to run over a remote desktop system



Successes

- ❑ Fabricated the final components of the entire *MSM*-constructing workflow system
- ❑ Tested newly created workflow components and retested components that had been made earlier; found that the workflows ran correctly

Taiwan has some great museums



Left: Taipei 228 Memorial, commemorating the victims of the 228 Incident

Right: National Taiwan Museum, containing exhibits about the history of Taiwan



I ate a lot of desserts this past week

Taiwan is known for its tropical fruits, such as passion fruit as litchi, so naturally, I had to get both in a cake.



The buns are delicious and soft and filled with sweet taro paste

A Big *xièxie* To:



- The Ledell Family for their generous scholarship
- Professor Rommie Amaro and Professor Jung-Hsin Lin for being a gracious host
- Dr. Robert Malmstrom, for his guidance on MSM construction
- Teri Simas, Dr. Gabriele Wienhausen, and everyone at PRIME who made this program possible