

GARRETT CHAN

MARKOV STATE MODEL
CONSTRUCTION THROUGH
KEPLER WORKFLOWS

NATIONAL TAIWAN UNIVERSITY
TAIPEI

Tuesday, August 26, 2014

Progress Made This Week



- ❑ Finalize the structure of the BuildMSM.kar workflow to bring it in line with the structure of the other workflows
- ❑ Finished working through inconsistencies in the BuildMSM.kar workflow
 - ❑ Workflow did not allow for several systems to run at the same time
 - ❑ Redo the second half of the workflow and resolve several errors
- ❑ Modified several actor lines to improve user accessibility
 - ❑ Custom parameters can be entered without going into the workflow

Progress Made This Week



- Began to rewrite visualization scripts to make visualization workflow for MSMs
 - ▣ Due to time limitations, this was not completed, but will be picked up at a later date

Final Conclusions



- Objective: To create a Kepler workflow that would facilitate the reproducible and time-efficient construction of Markov state models (MSMs)
- Workflow stages: trajectory preparation, clustering, implied timescale construction, MSM construction through MSMBuilder
- Using previous Molecular Dynamics simulation data on protein kinase A, an MSM was built using the Kepler workflow

Final Conclusions



- Workflow components kept separate to allow for flexible use of individual components if desired
- Parameters are user-accessible to allow for customizability of workflow, capable of accepting many different systems
- Visualization of MSM still under construction, but will allow for human analysis of MSMs once completed

Hiking in Wulai



Hiking in the mountains near Wulai was the perfect weekend escape from Taipei, and it provided for a wonderful opportunity to reflect on my experiences traveling through Taiwan.

Hiking in Wulai

The scenery was gorgeous, and it felt like I was going back in time to an untouched part of Taiwan.



The contrast between the urban grind of Taipei and the idyllic serenity of the mountains was amazing.



A Big *xièxie* To:



- The Ledell Family for their generous scholarship
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- Professor Rommie Amaro and Dr. Robert Malmstrom
- *Zaijian Taiwan!*