#### GARRETT CHAN

MARKOV STATE MODEL
CONSTRUCTION THROUGH
KEPLER WORKFLOWS

NATIONAL TAIWAN UNIVERSITY TAIPEI

## 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

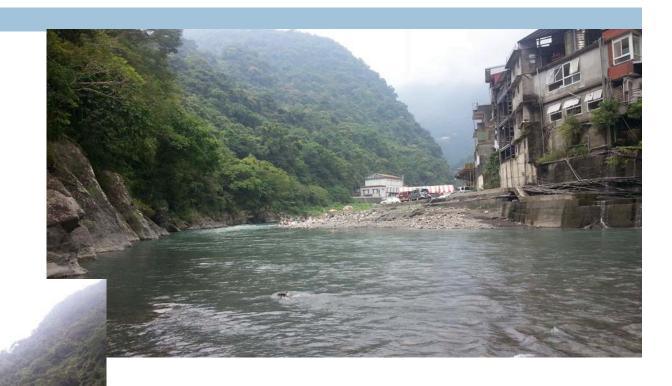
- Workflow components kept separate to allow for flexible use of individual components if desired
- Parameters are user-accessible to allow for customizability of workflow, capable of accepting many different systems
- Visualization of MSM still under construction, but will allow for human analysis of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

# Hiking in Wulai



# Hiking in 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
- Dr. Gabriele Wienhausen, Teri Simas, and everyone at PRIME who made this program possible
- Professor Jung-Hsin Lin and everyone in his lab for being wonderful hosts
- Professor Rommie Amaro and Dr. Robert Malmstrom
- □ Zaijian Taiwan!