

GARRETT CHAN

MARKOV STATE MODEL
CONSTRUCTION THROUGH
KEPLER WORKFLOWS

NATIONAL TAIWAN UNIVERSITY
TAIPEI

Wednesday, July 23, 2014

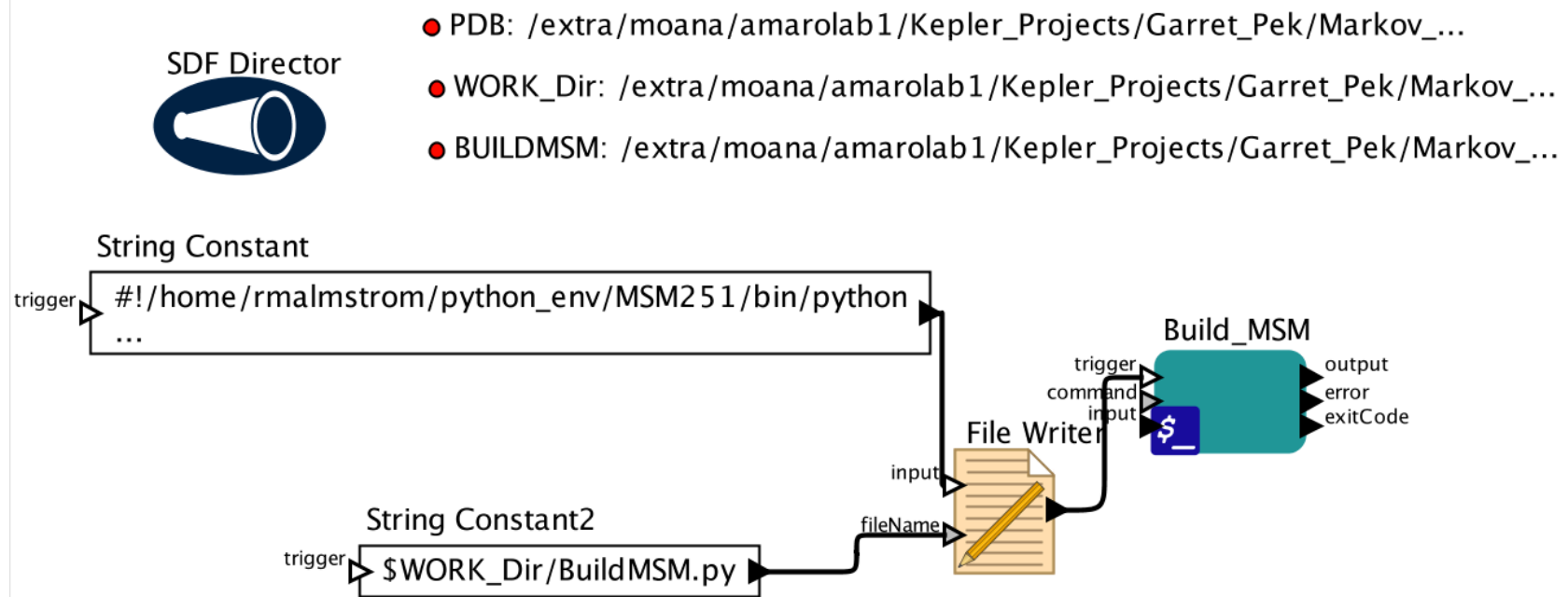
Progress Made This Week



- Tested the BuildMSM.kar workflow with the current system
- Retested past workflows to ensure compatibility with the BuildMSM.kar workflow
- Reorganized past workflows to ensure that they can be used both in series for continuous MSM construction or separately for other applications

Progress Made This Week

□ Tested part of the workflow so far (BuildMSM.kar):



- This workflow takes the clustered microstates and uses MSMBuilder 2 to make the Markov state model.

Plans for Next Week



- Collaborate with Dr. Malmstrom to elucidate next steps needed to complete workflow
- Look into faster remote desktop system, since X11 is slow and makes using Kepler difficult even when using cipher
- Clean up unnecessary and duplicate workflows

Taiwan has some seriously beautiful sights

Hiking up Elephant Mountain in the heat was completely worth it for this view.



And the Red House Theater in Ximending is so cool to look at night! This picture really doesn't do it justice.

Wow, how will I ever leave this place?



Look at this mango shaved ice.



I had seafood noodle soup for *lunch*.

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