GARRETT CHAN

MARKOV STATE MODEL CONSTRUCTION THROUGH KEPLER WORKFLOWS

NATIONAL TAIWAN UNIVERSITY
TAIPEI

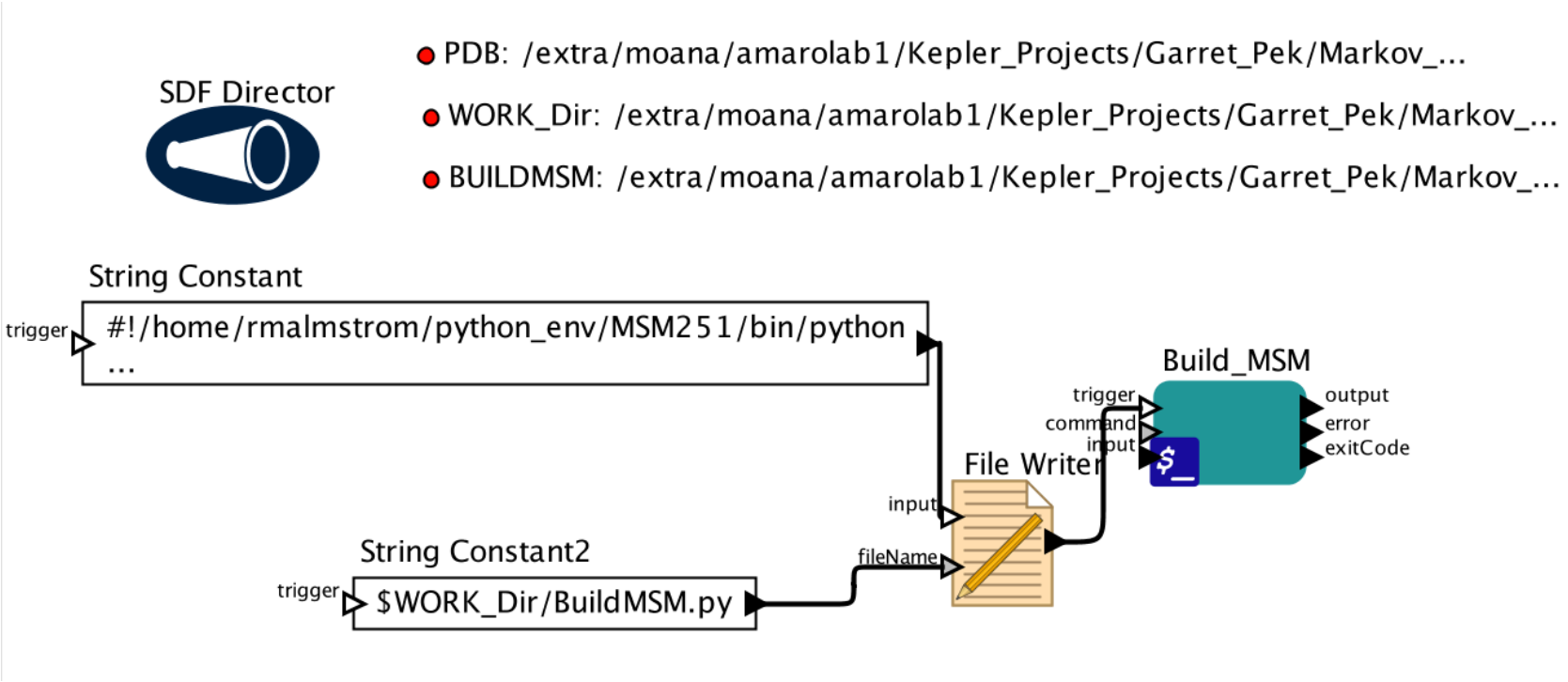
Wednesday, July 16, 2014

Progress Made This Week

- Decided not to build a Python module with NetworkX to display graph and began reworking existing visualization scripts to accommodate multiple systems
- Found the best way to try different parameters to get the implied timescale plots
- Retested the Cluster.kar workflow to make sure it was working correctly

Progress Made This Week

- 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

- Test the BuildMSM.kar workflow with the current system
- Retest past workflows to ensure compatibility with the BuildMSM.kar workflow
- Reorganize past workflows to ensure that they can be used both in conjunction with each other to build an MSM and separately for other potential uses

This week I went to…

A small and ornate temple that I found by chance.

A large and ornate temple to the arts, the National Palace Museum.

And I ate this really colorful bowl of *dou hua*

Dou hua

A Big *xièxie* To:

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