GARRETT CHAN

MARKOV STATE MODEL CONSTRUCTION THROUGH KEPLER WORKFLOWS

NATIONAL TAIWAN UNIVERSITY
TAIPEI

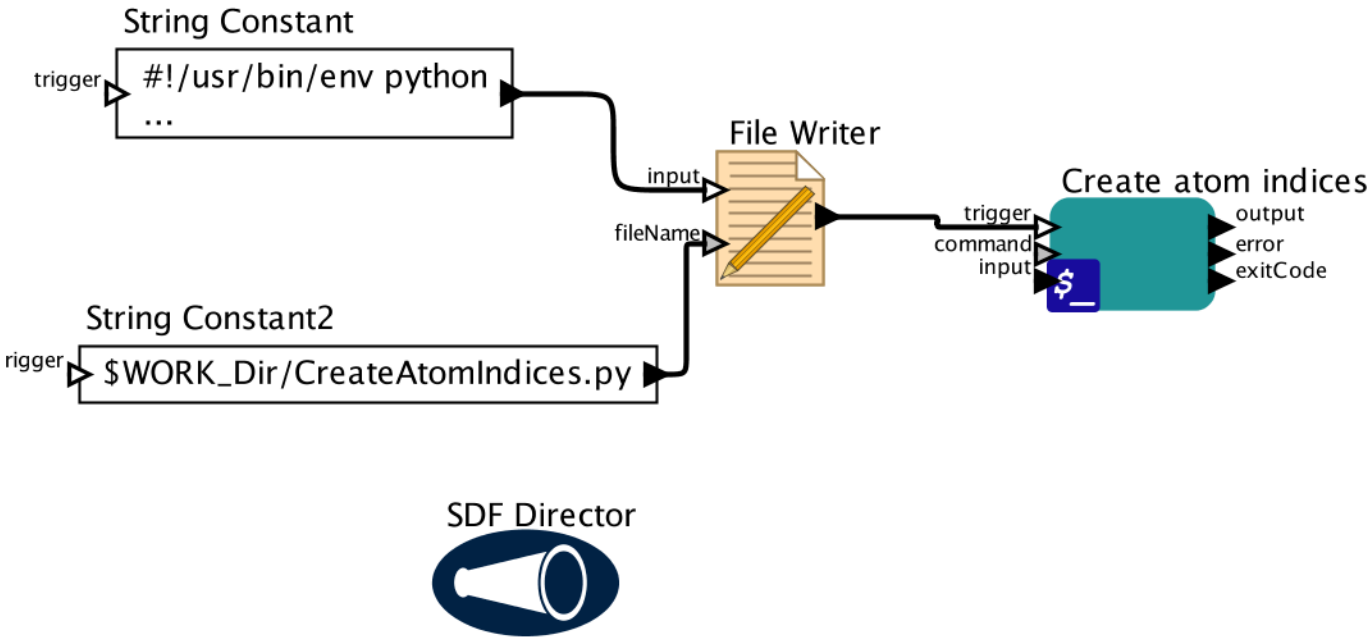
Wednesday, July 9, 2014

Progress Made This Week

- Ran buildMSM.py on all systems and created the tProb.mtx probability matrix for each system
- Began finding actors for the workflow for buildMSM.py
  - Decided to use actors similar to those I used in a previous workflow
- Read through for MSM visualization scripts
  - Asked for help about which one to use

Progress Made This Week

- Part of the workflow so far (createatomindices.kar):



- This workflow makes a list of the backbone atoms in the system of interest.

Plans for Next Week

- Build a Python module with NetworkX to display graph
- Decide on the best way to try different parameters to get the implied timescale plots
  - Will work on understanding the implied timescales and how to best approach incorporating them into the workflow

When I Wasn't in the Lab, I…

Saw Taipei from really high up.

Got melon and shrimp *xiaolongbao* from Din Tai Fung with Ashley.

Tried dragon fruit for the first time. It's mild and has seeds like a kiwi's.

And, of course…

I ate beef noodle soup!

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