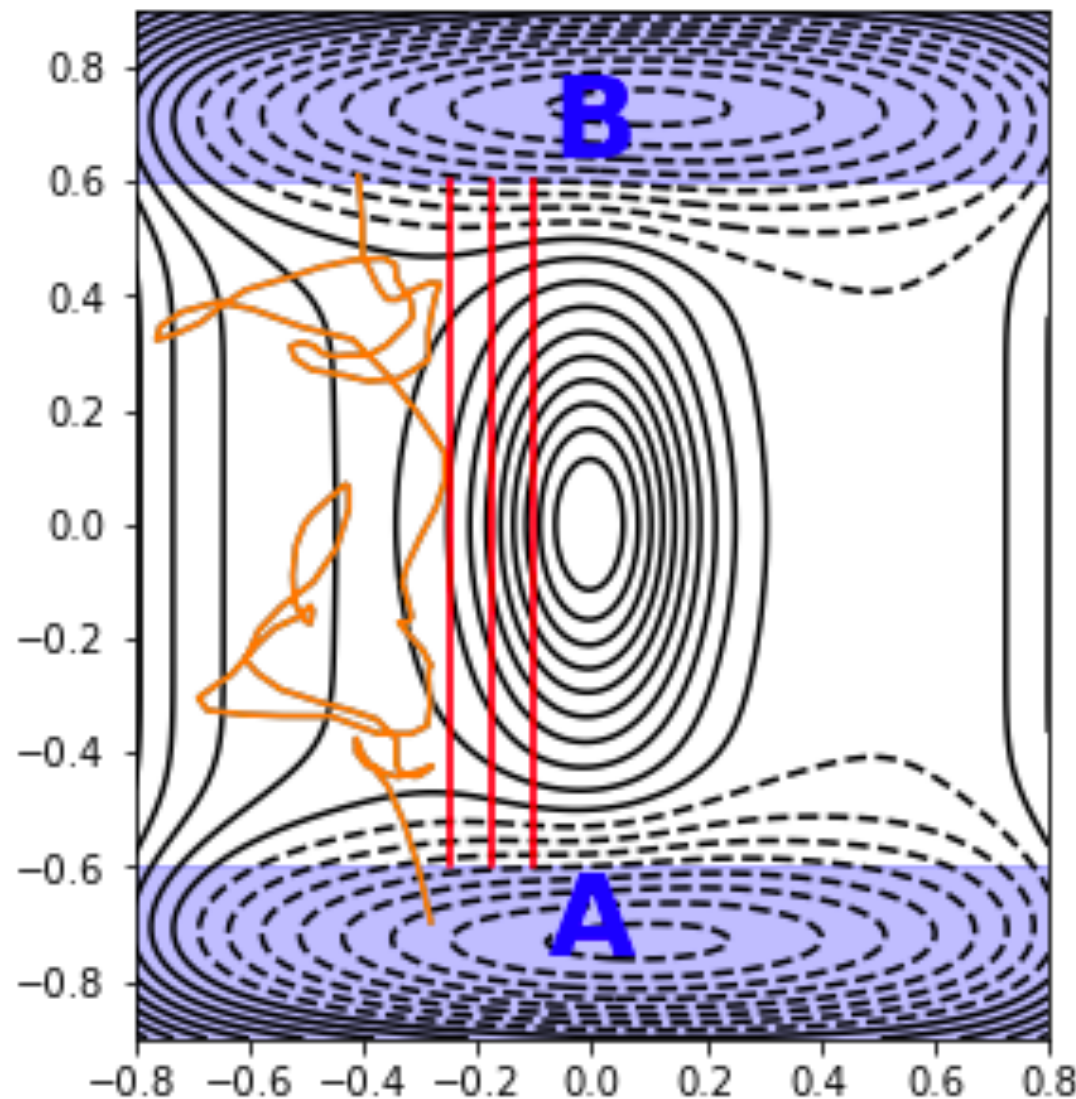


# Enhancing Switching



- Use TIS-like approach to “push” trajectories to the other channel
- Bias shooting point selection to switching region

# OpenPathSampling



<http://openpathsampling.org>

Twitter: @pathsampling

Development at: <http://github.com/openpathsampling/>

A Python library for path sampling simulations

## New features!

- Gromacs integration
- PLUMED integration
- Reactive Flux (Bennett-Chandler)
- Faster datafile format
- Spring Shooting\*
- Hooks for simulation customization\*

\* will be in next release (1.5)

***Now with a command  
line interface!***

## Coming soon:

- Parallel RETIS
- Simulation setup wizard