# Low-dimensional Representations for Learning Fast Molecular Dynamics Simulations

Miles Crosskey
Duke University

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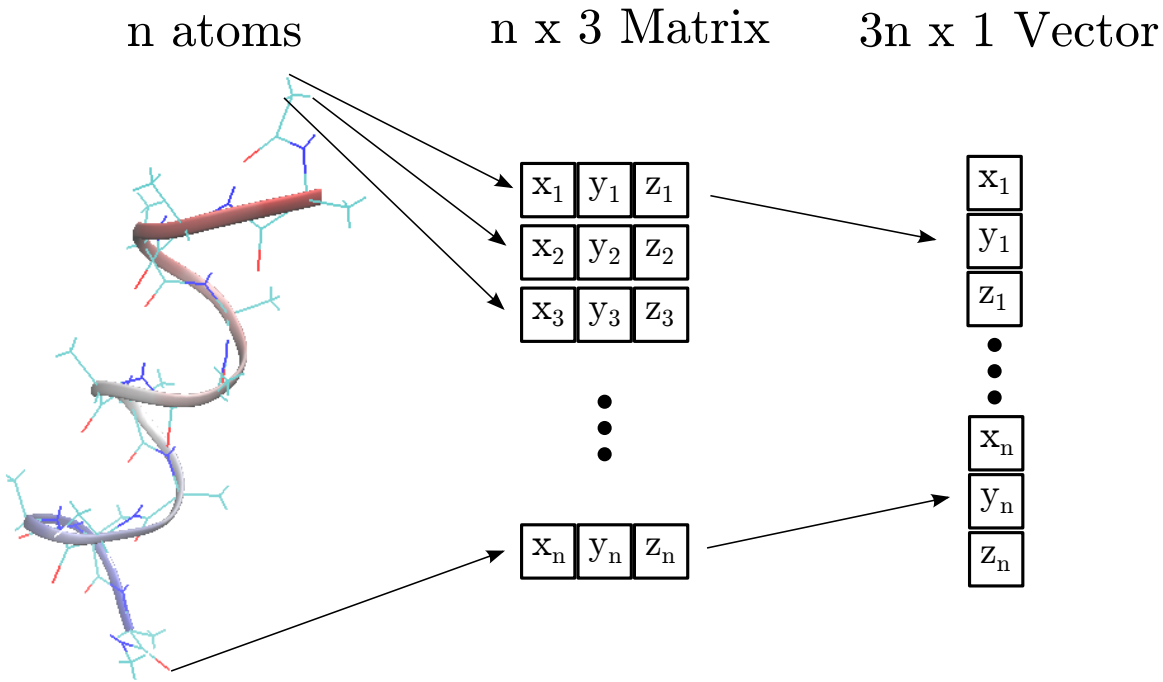
Joint work with Mauro Maggioni and Eric Monson

# Video: Molecular Dynamics

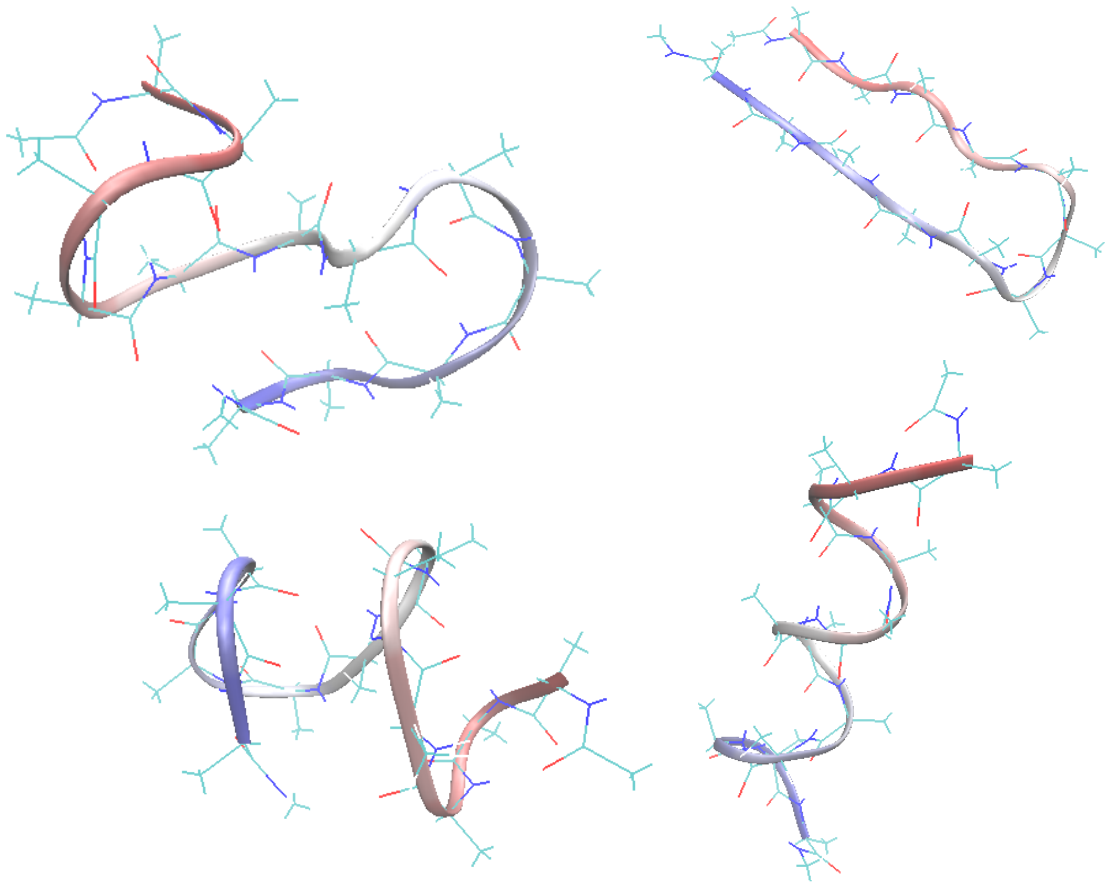
# Configuration storage

- view in 3-d
- write coordinates
- write as vector
- many constraints between entries



# Simulation Difficulties

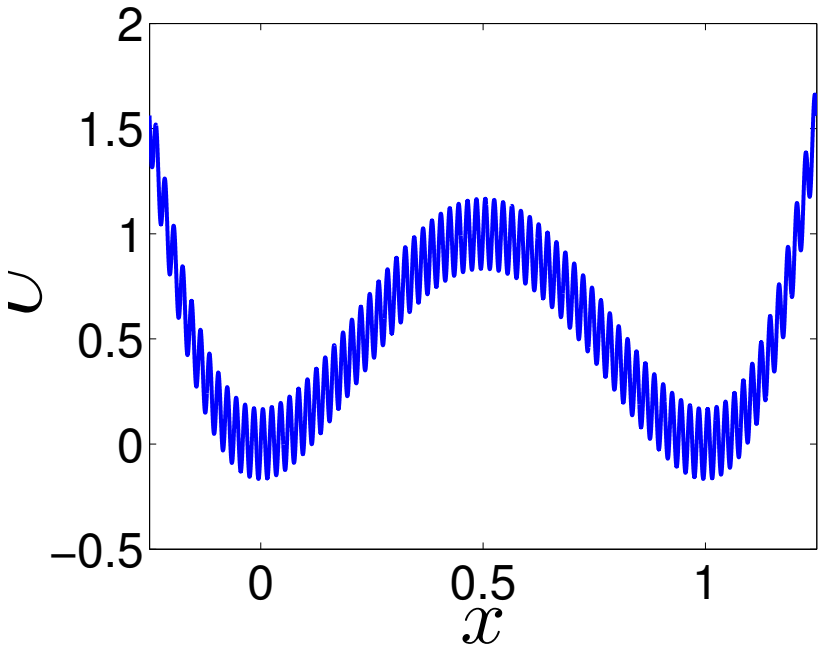
- High dimensional
- Expensive force computations
- Small time steps
- Transitions between configurations is slow



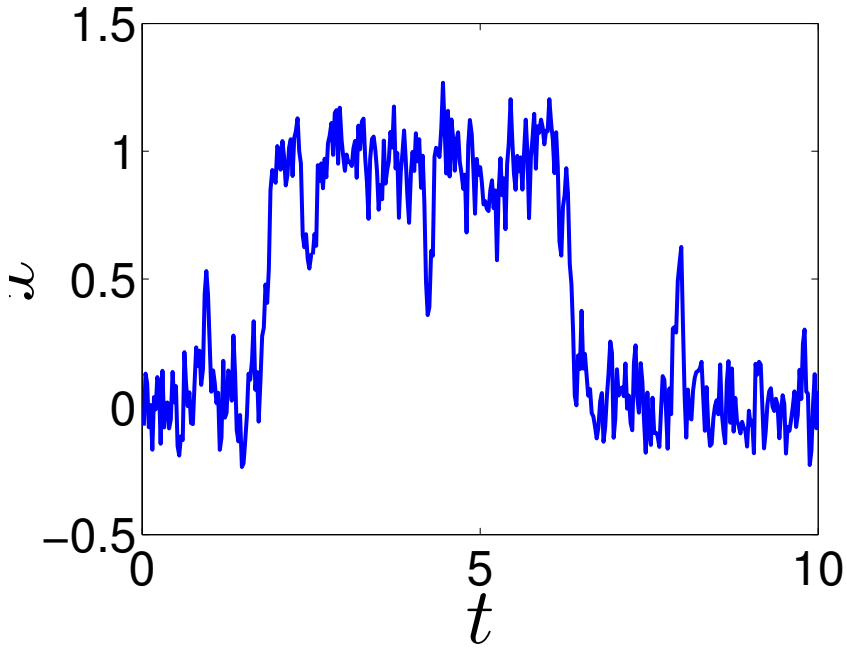
# 1d Example

Brownian motion in potential well

Potential Well



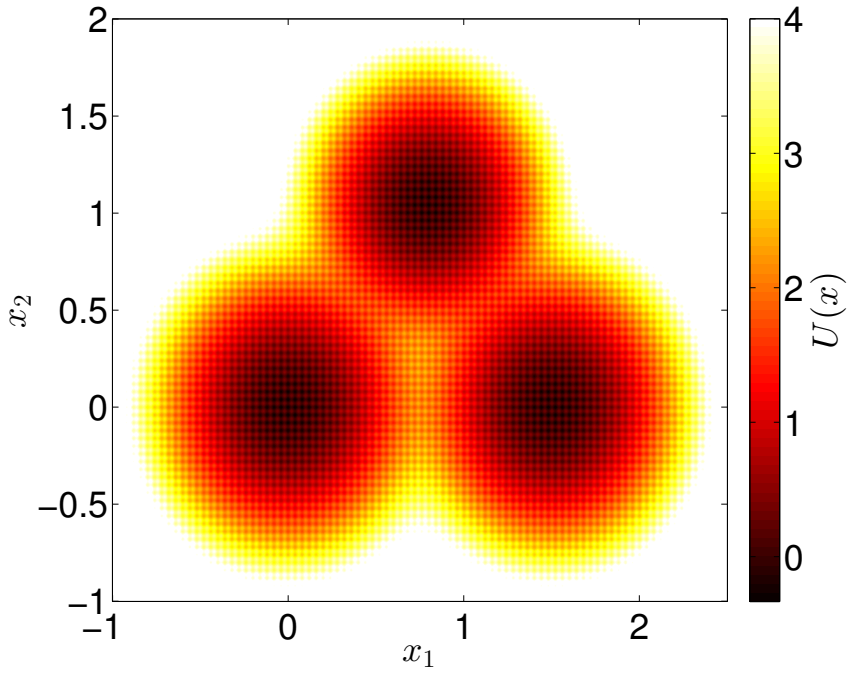

Sample Trajectory



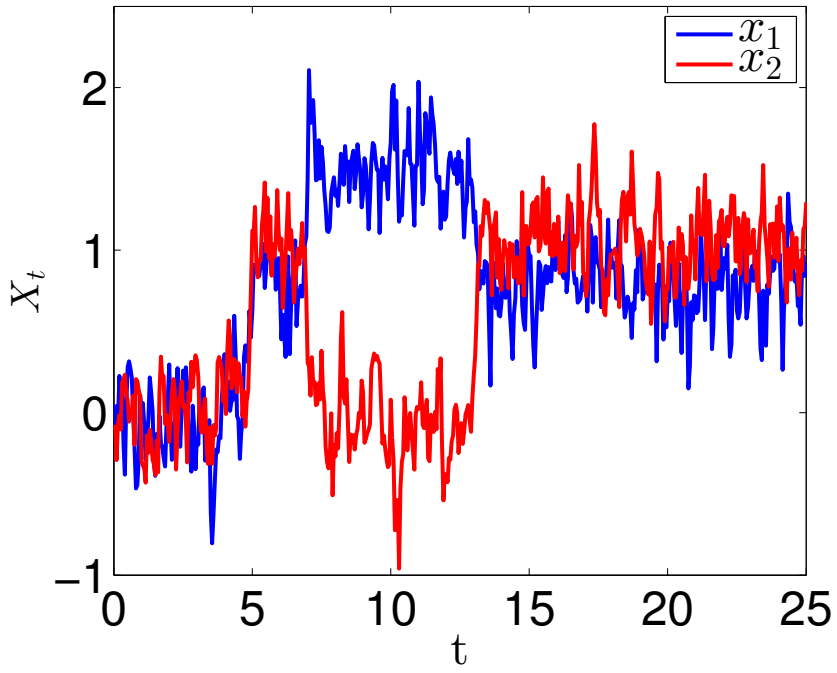
# 2d Example

Brownian motion in 2-d potential well

## Potential Well




## Sample Trajectory



# High Dimensional Example

Map 2-d vectors to images using the following procedure:

- Start with 2d vector $x$
- Map each pixel in 100 x 125 image to grid location
- Turn on pixel if grid point within $1/2$ of $x$

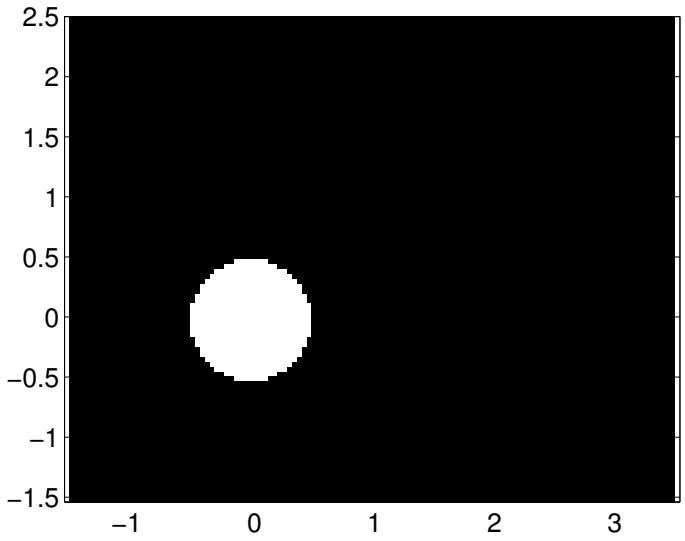
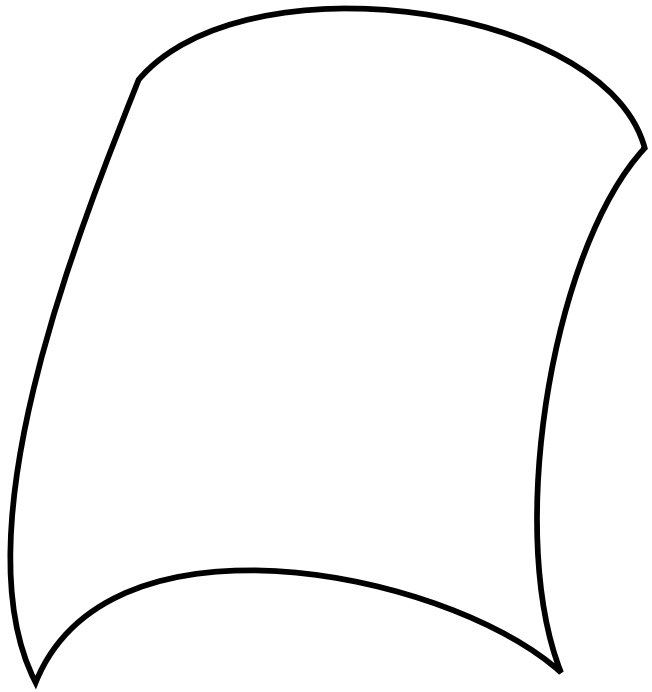



Figure : Image returned from [0,0]

# Video: Sample Trajectory

# Learning the Simulator

- Divide configuration space
- Fit planes to pieces
- Connect neighboring planes
- Learn simulators on planes



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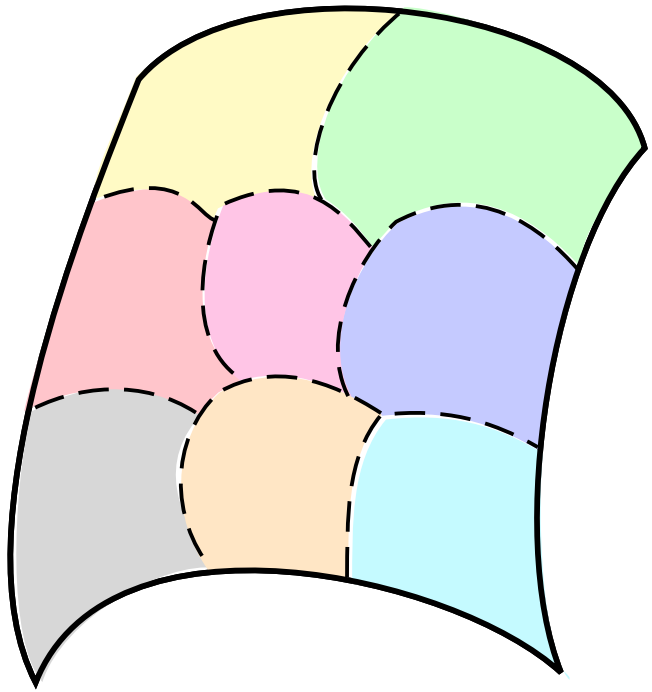

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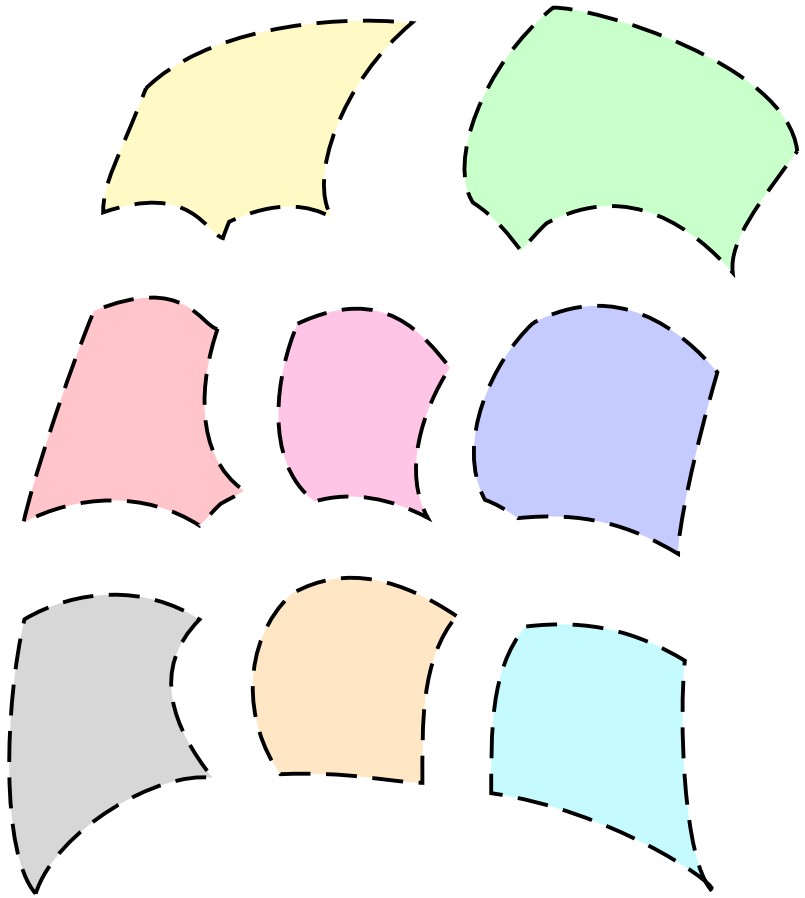

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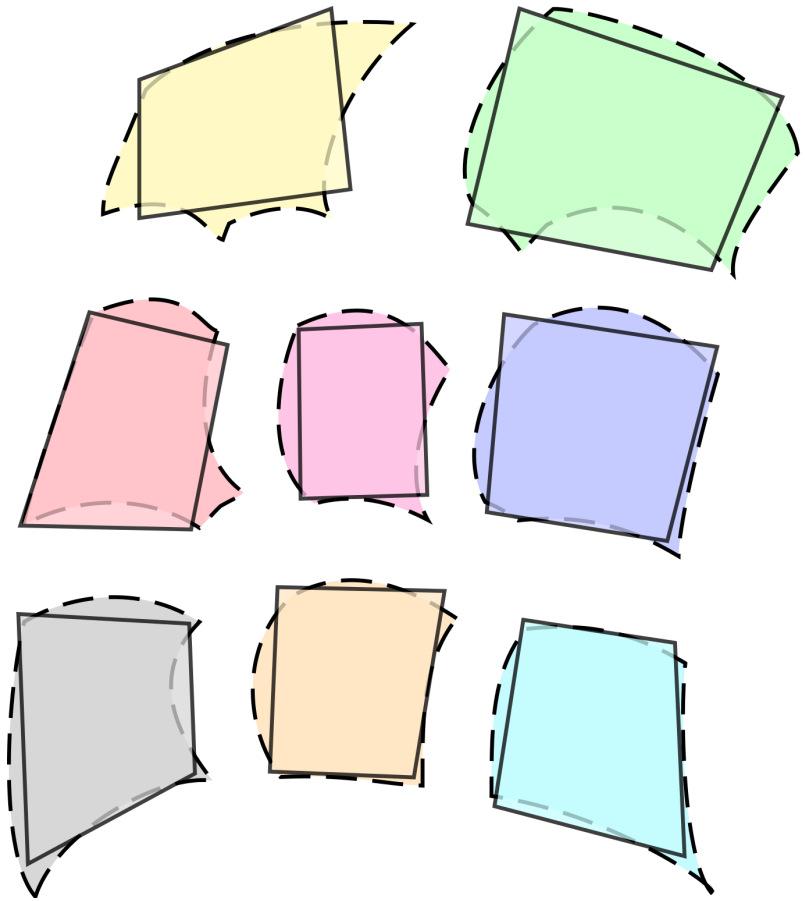

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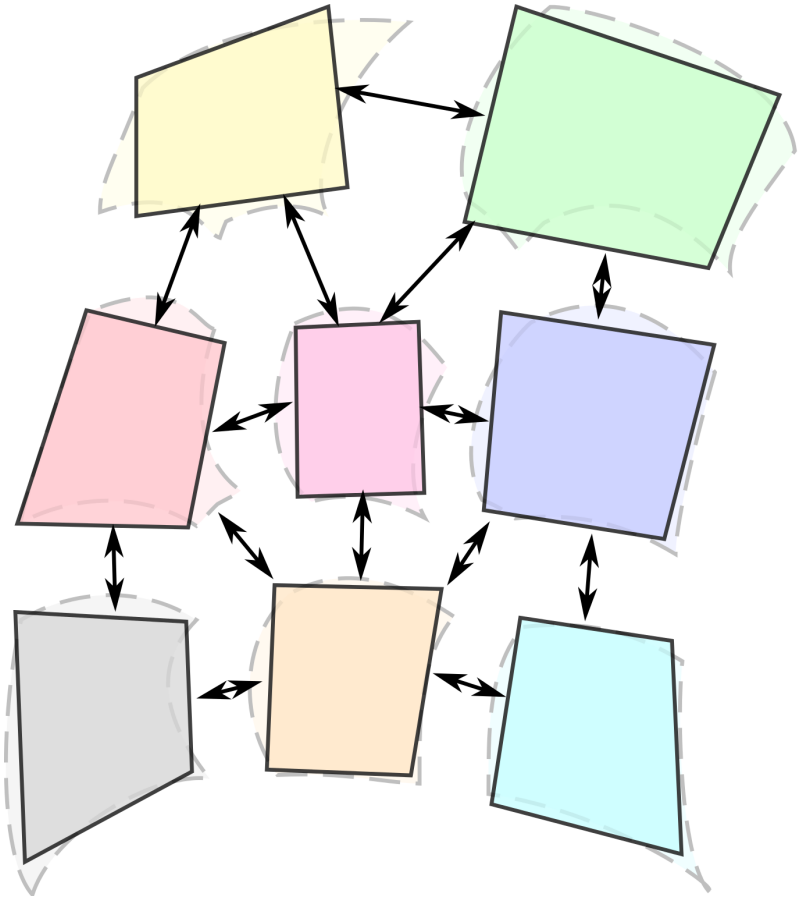

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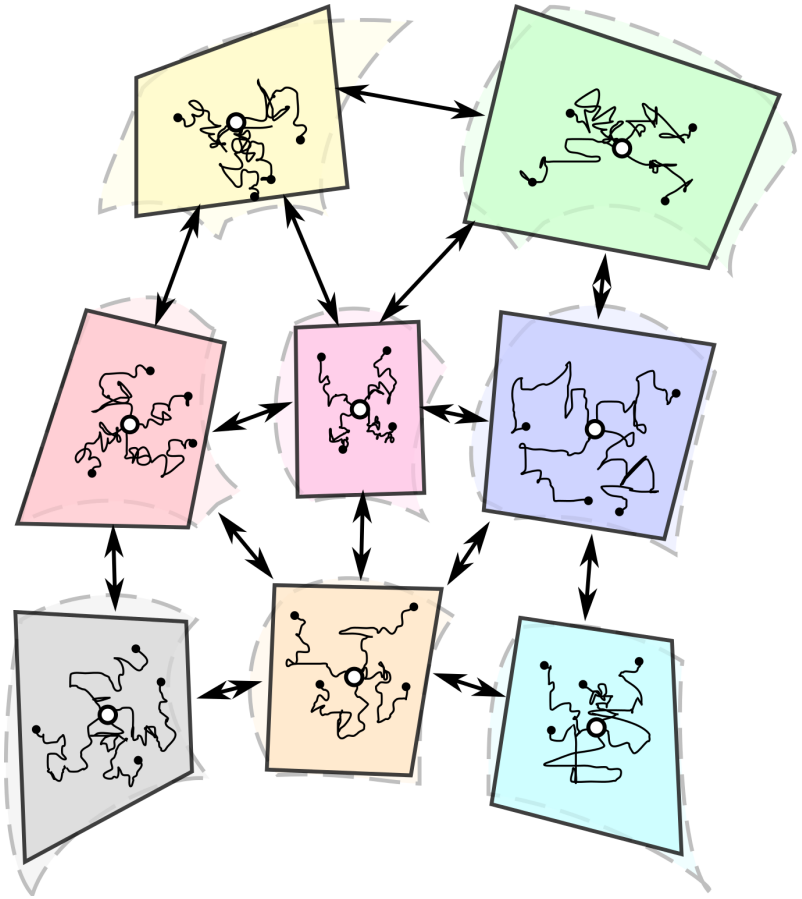
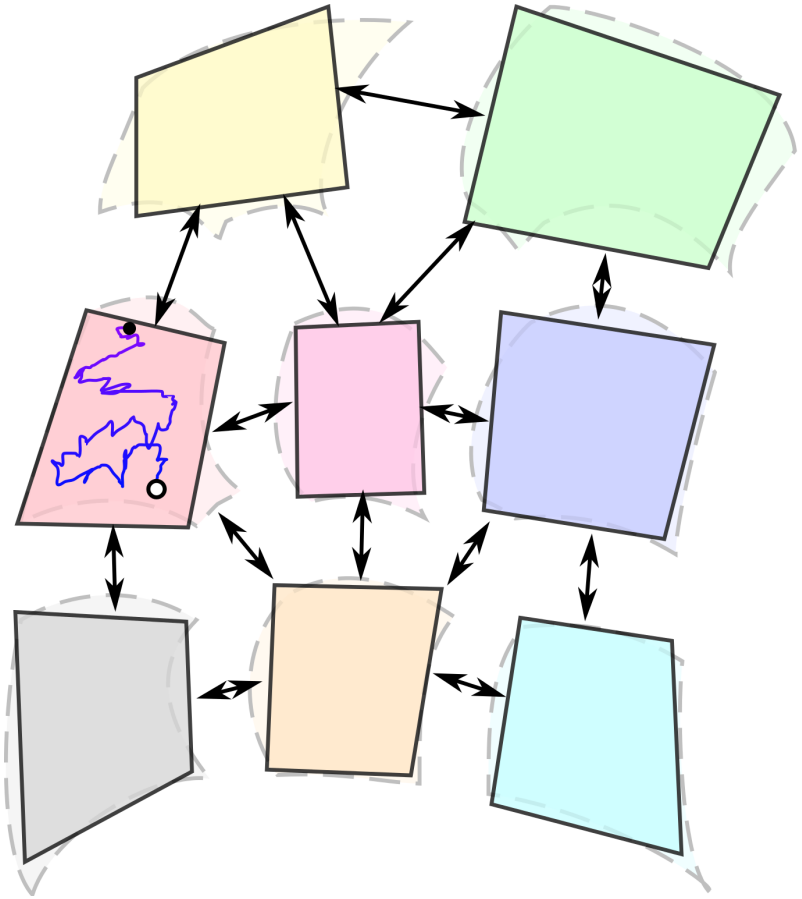


# Running the New Simulator

- Simulate on plane
- Switch to neighboring plane
- Take larger timesteps
- Simulate in fewer dimensions



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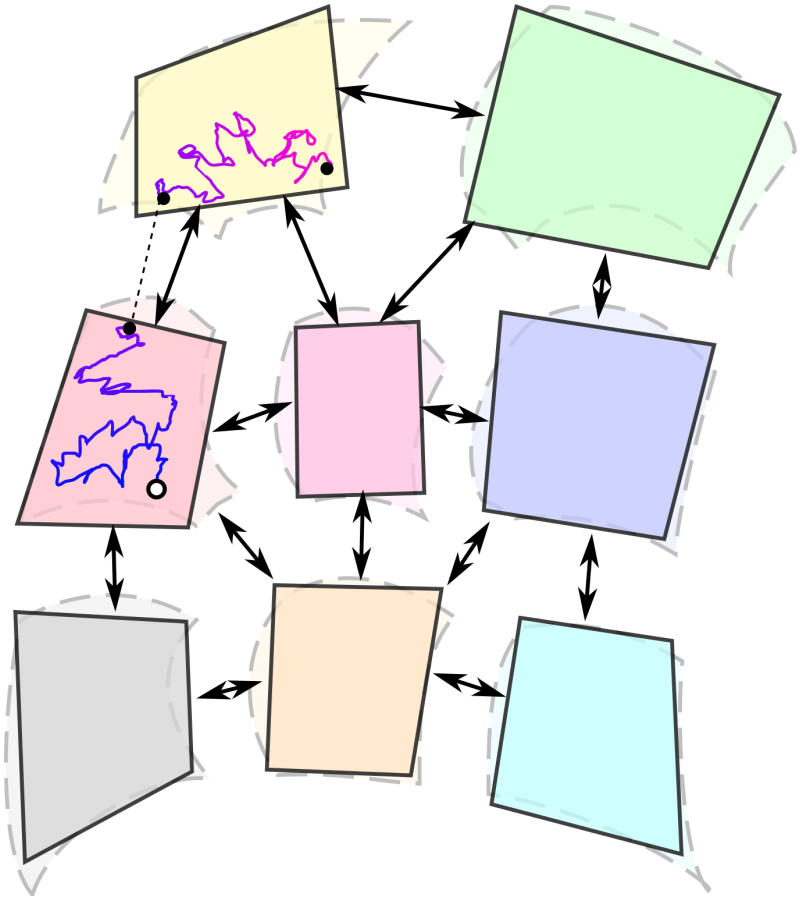

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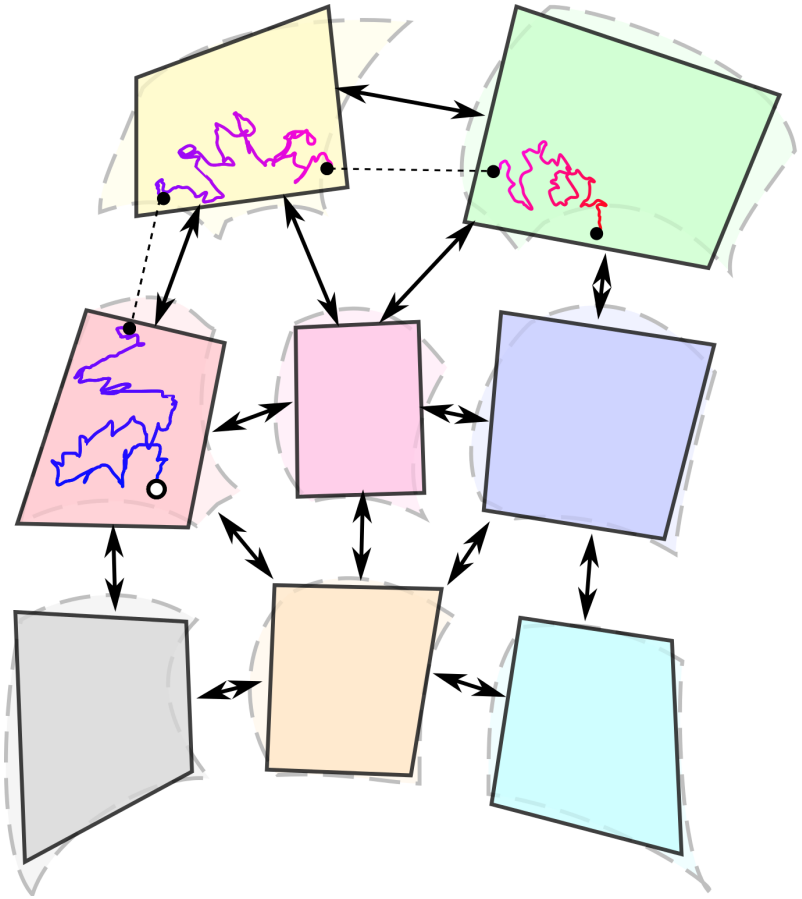

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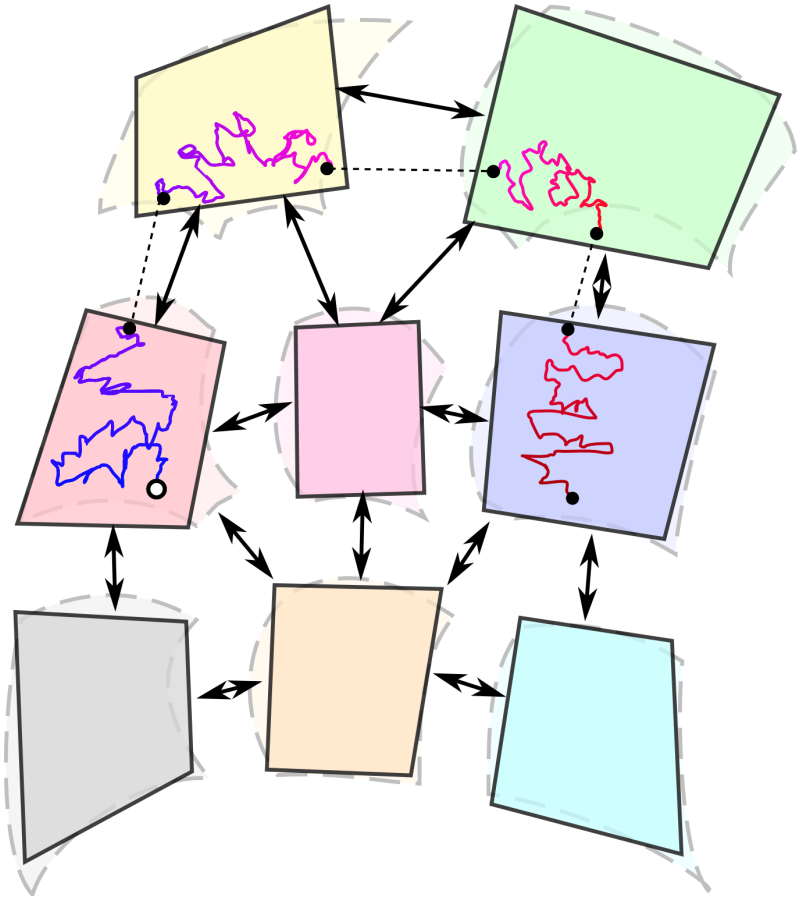
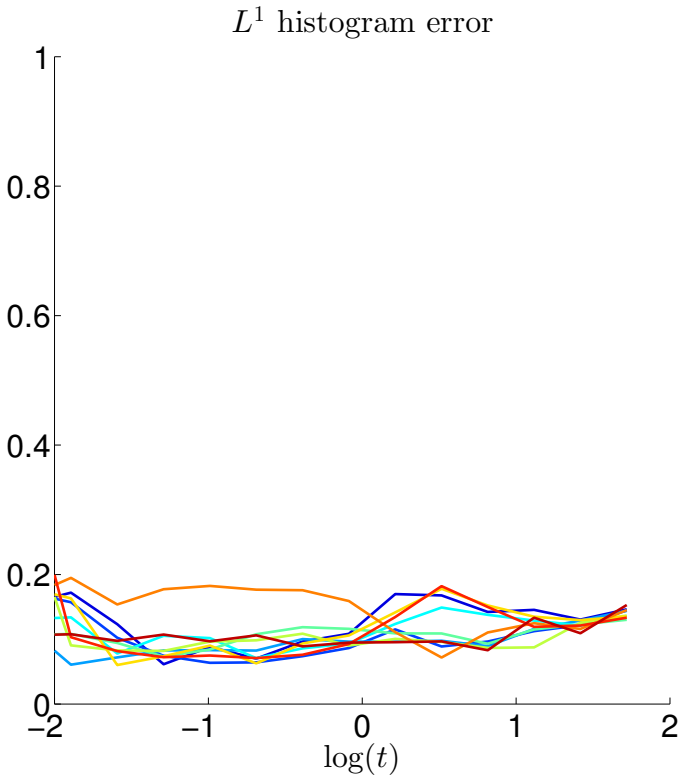


# Comparing Simulators

- Pick starting location
- Run many long paths
- Bin paths by pieces
- Compare histograms

## High Dimensional Example



# Results and Future Work

Results:

- Error bound proof
- Challenging toy examples

Future Work:

- Molecular Dynamics
- Weather Data