Molecular Dynamics Analysis Toolkit

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Molecular Dynamics Simulation

- Computer simulation of physical motions of atoms & molecules
- Applications in physics, chemistry, biology
- Several different programs developed by different groups
- Output to diverse text and binary formats
Cross-Platform Tools

- Several tools exist for reading and analyzing different formats
- Allows one analysis function to be written for multiple formats
- These leave data storage and organization up to the user
Molecular Dynamics Analysis Toolkit

- Streamlines analysis of MD simulations
  - Provide location of simulation and list of analyses
  - Figures out what needs to be done
  - Splits analyses across multiple cores
  - Stores results in HDF5 database

- Wraps around existing tools, provides simple interface

- Written in Python for Linux/OSX
- Version controlled
Goals for Capstone Project

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3. Analyze either internal or external coordinates (6 weeks)
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  4. Copy binary restart file to allow simulation extension (2 weeks)
Project Management

• Work with myself, Nick Rego, and Professor Lillian Chong
  – Weekly meetings
  – Collaboration via BitBucket

• If interested of have questions contact me at ktd3@pitt.edu

• Check out code at https://bitbucket.org/karl_debiec/molecular-dynamics-analysis-toolkit