Monte Carlo Simulations with ProtoMS

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Monte Carlo Simulations with ProtoMS

Workshop Outline

14:30-14:45	Monte Carlo Simulation and the ProtoMS Code Dr Chris Cave-Ayland
14:45-16:00	ProtoMS Exercise 1 Simulating a protein-ligand system
16:00-16:15	Introduction to GCMC Hannah Bruce Macdonald
16:15-17:30	ProtoMS Exercise 2 GCMC Calculations for Water Binding

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Development History

v1.0

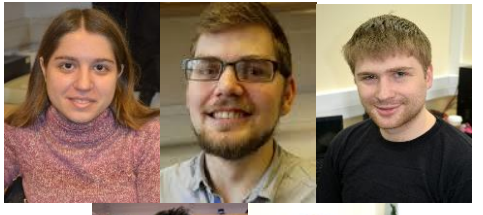
2002

2006

v2.1

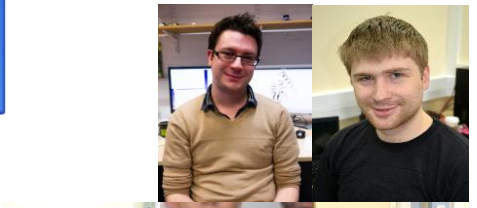
v2.4

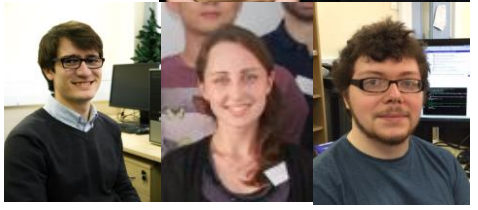
2013



v3.0

2014





v3.3

2017

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Execution Outline

Setup

- Parameterise small molecules
- Create input files
- Modular tools
- Master script
- Setup wizard

Simulation

Fortran 77

- Metropolis Monte Carlo
- Alchemical Transformations
- Grand Canonical Ensemble

Analysis

- Extract system properties
- Calculate free energies
- Clustering

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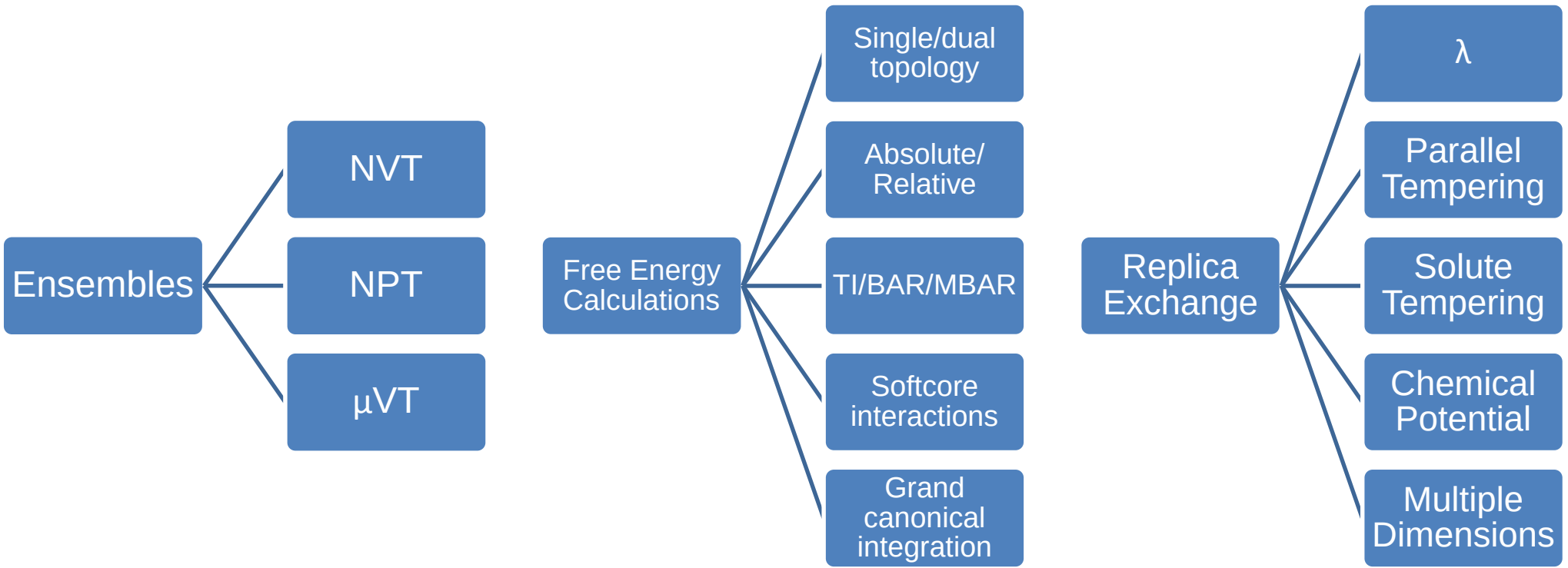
Code Capabilities



Monte Carlo Simulations with ProtoMS
Development Processes

- Developed with Mercurial, hosted on Bitbucket
- Bamboo continuous integration server
- SSI Collaboration
  - Test Suite
  - Usability review
- Licenced under GPL v2
- www.protoms.org
- ~10 publications – application note in preparation

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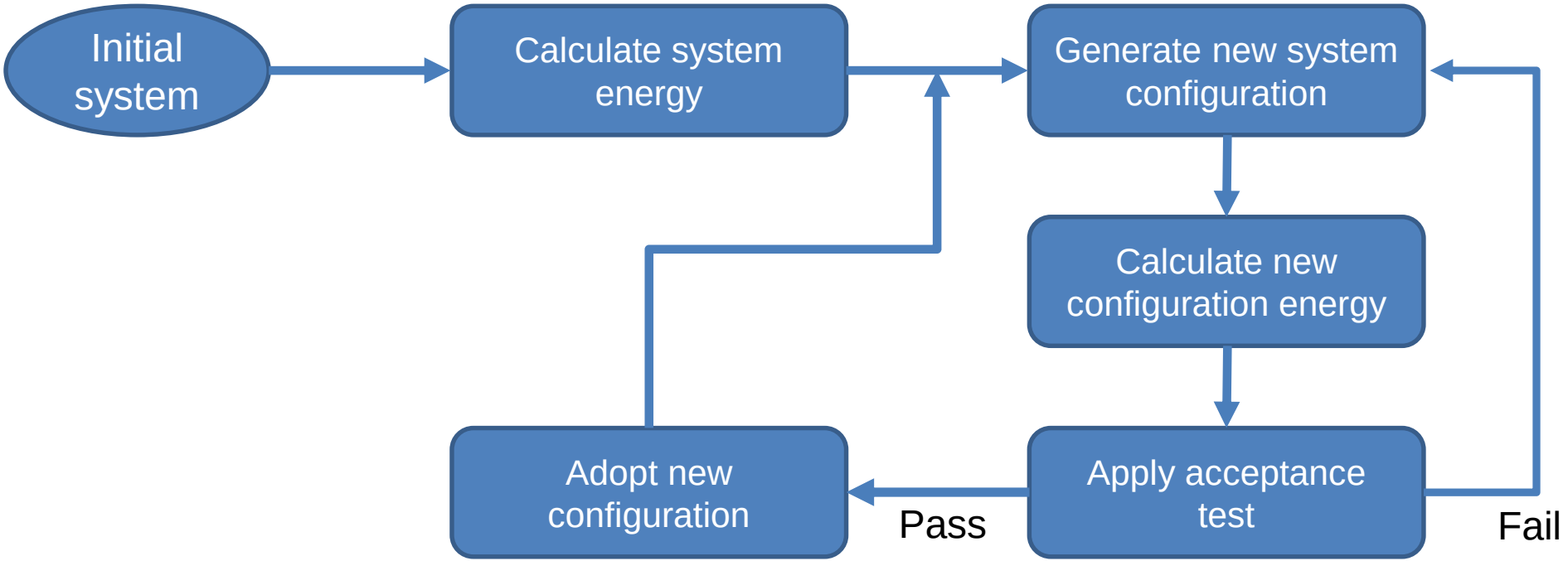
Metropolis Monte Carlo Algorithm



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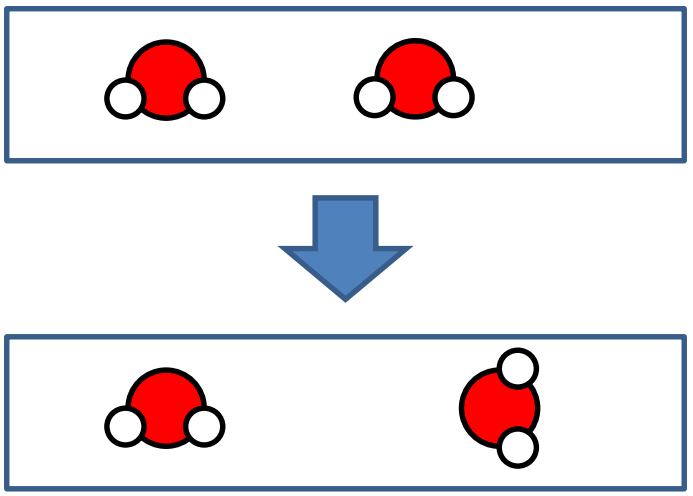
Move Types - Displacement



Test:

$$P_{accept} = \min(1, \exp[-\beta \Delta E])$$

- Single or multiple atoms
- Test assumes symmetric proposal distributions

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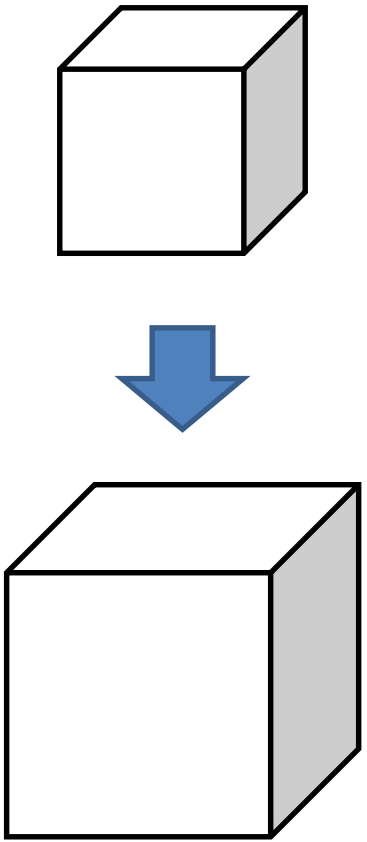
Move Types - Volume



Test:

$$P_{accept} = \min(1, \exp[-\beta(\Delta E + p\Delta V) + N \ln\left(\frac{V_{new}}{V_{old}}\right)])$$

- Usually displace particles as well

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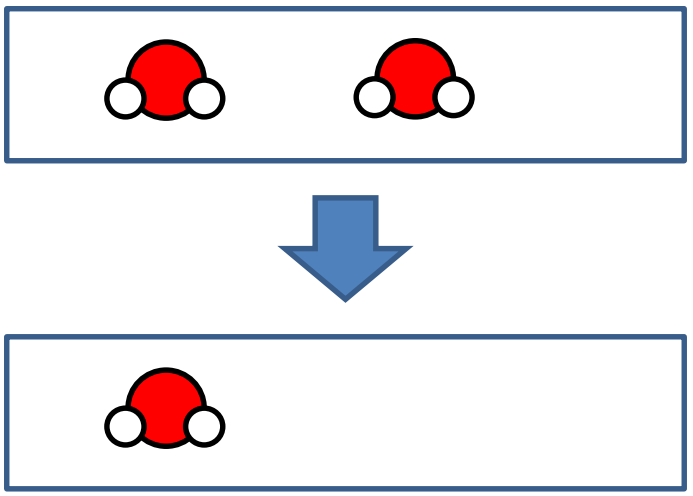
Move Types – Insertion/Deletion



Test:

Depends

- Variable particle number – GCMC

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MC Overview

Advantages

- Only evaluate energy terms that change
- Free choice of move proposal distributions
- Can focus sampling on interesting parts
- Easy to impose constraints
- Vary particle number

Disadvantages

- Parallelisation
- Need to define move proposal distributions
- Non-pairwise interactions

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To get started:

https://ccpbiosim.github.io/gcmc_protoms_workshop/