

A Tutorial for TIPSI, and How to Assemble Paths

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8th of July 2016

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Introduction

Who am I?

- Student at the computational science master
- Attended the course on biomolecular simulation
- Enjoyed figuring out TIPSII
- Did a project to write a tutorial that introduces TIPSII over the past months!

Structure

In this presentation I will:

- Give a brief recap of TPS
- Outline my contribution
- Discuss both the examples the tutorial offers
- Discuss the additional documentation

What is TPS again?

What is TPS again?

IMAGE

What is TIPSII?

TIPSII is a script by Tsjerk Wassenaar, which:

- Adaptation of a Perl script
- Written in Python
- It relies on GROMACS version 4.5.4
- Does random shooting moves forwards and backwards
- Reverses time for backward shooting
- A "molecular calculator"

Contributions

I made several minor contributions to this project:

- Bash implementation to assemble paths
- Python script to analyze the paths
- Tutorial with a Python tool

Assembling paths

The problem:

- TIPSI outputs shooting moves only
- Instructions on how the paths are made in dat-files
- Backward shooting moves are the wrong way around
- Negative timestamps

Result: assembling the paths is a minor nightmare...

Assembling paths

The solution:

- Bashscripts that searches for directories with ACCEPTED-file
- Scans dat-file using regular expressions
- Overwrites timestamps
- Creates each path by dumping and appending single frames
- Stores some metainformation in a csv-file

Sadly takes a while for long fragments...

Metainformation paths

We can do some nice things with the metainformation, I wrote a script that:

- Finds the average path length
- Finds the number of decorrelated groups of paths
- Ratio of FW:BW shooting moves
- Draws a tree of all shooting moves

The tree is not extremely pretty though, better to do in OPS probably...

Alanine Dipeptide

Fast

Alanine Dipeptide

PICTURE

Preparing for TIPSI

Running TIPSII

Appended the bashscript to the end of the job

Running TIPSII

Print PARfile

Introduction

Introduction

Introduction

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