

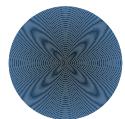
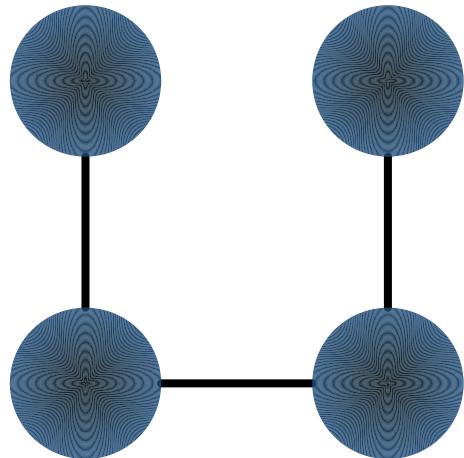
Implementation of a Replica Exchange Monte Carlo algorithm using Python

ROUAUD Lucas
Master 2 bio-informatique

Thachuk, C., Shmygelska, A. & Hoos, H. H. A replica exchange Monte Carlo algorithm for protein folding in the HP model 8, 342. URL: <https://bmcbioinformatics.biomedcentral.com/articles/10.1186/1471-2105-8-342>.

Introduction

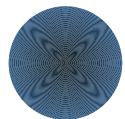
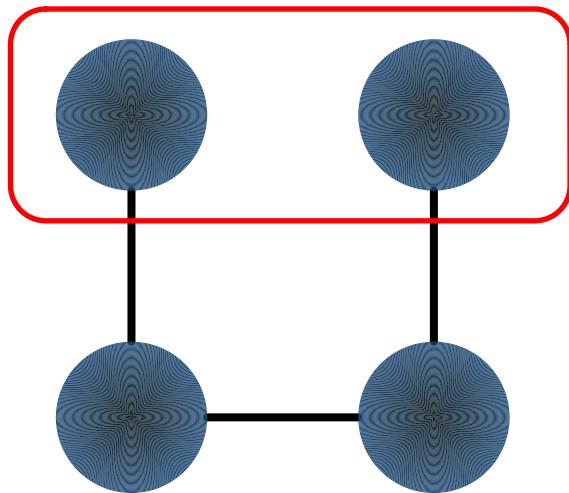
HP model



Hydrophobic

Introduction

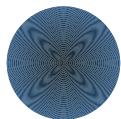
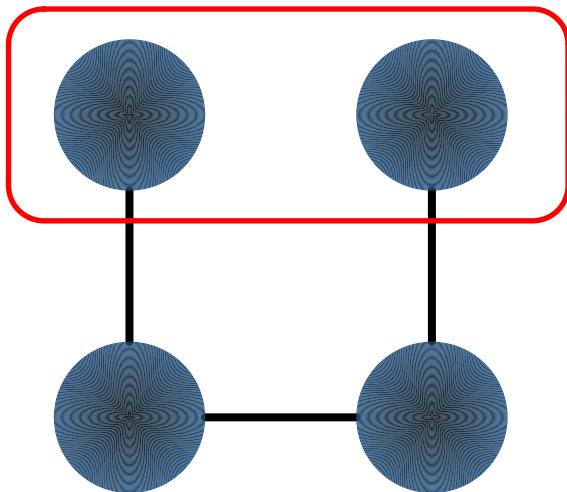
HP model



Hydrophobic

Introduction

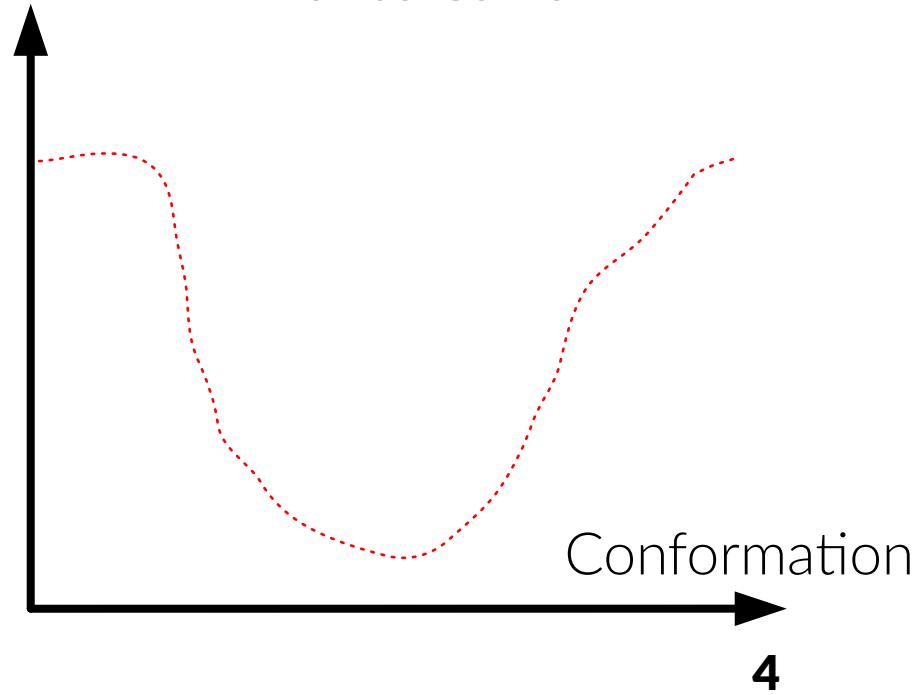
HP model



Hydrophobic

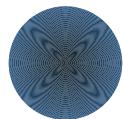
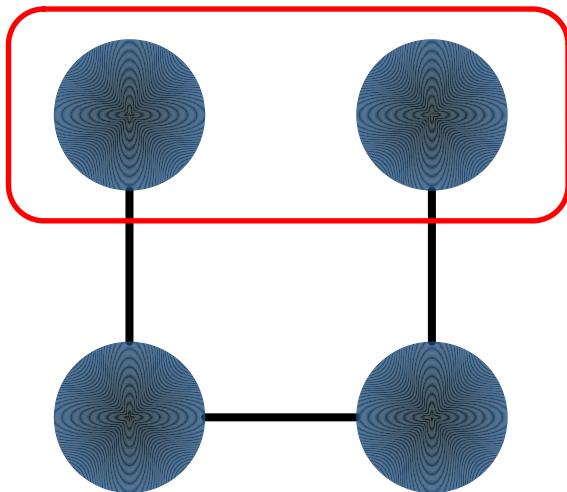
Energy

Monte Carlo



Introduction

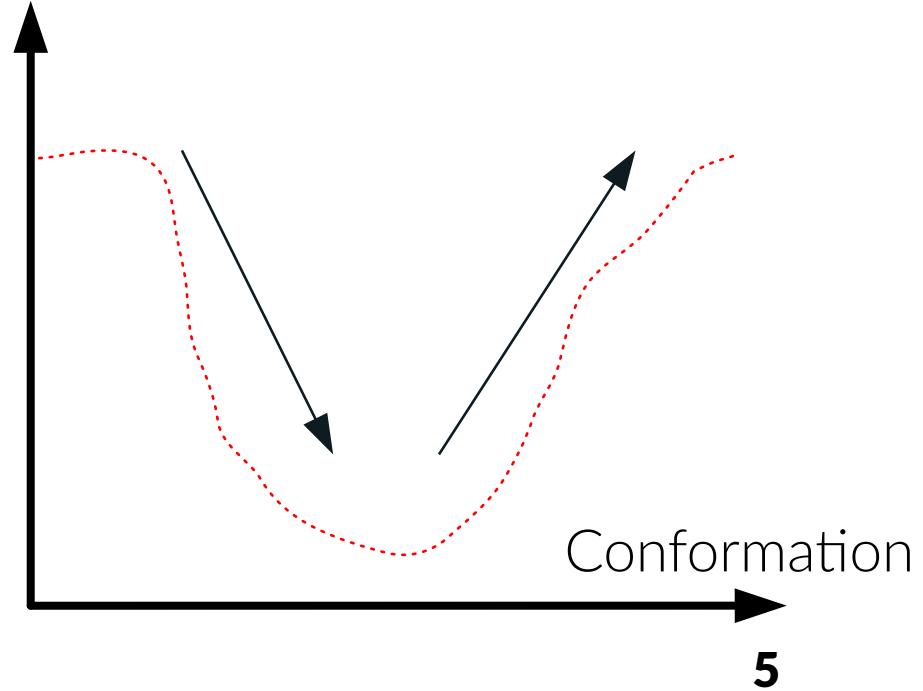
HP model



Hydrophobic

Energy

Monte Carlo



Introduction

REMC

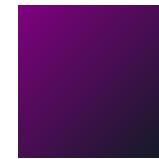
37



38

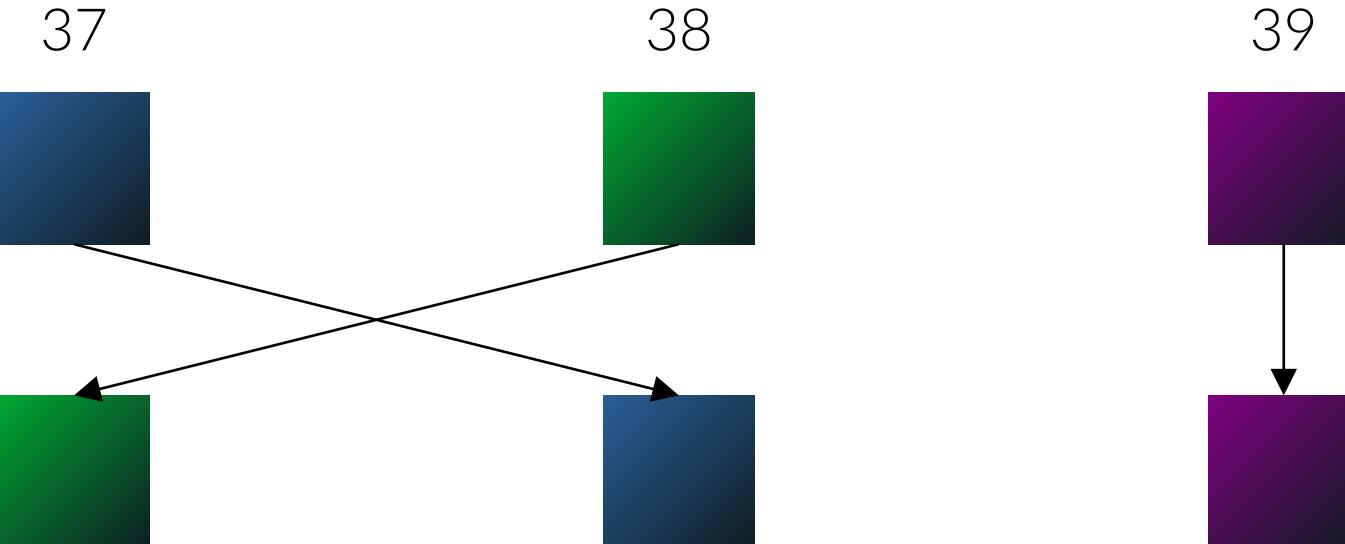


39



Introduction

REMC



Pipline

FASTA sequence

ATWVER

Pipline

FASTA sequence → HP model

ATWVER

HPHHPP

Pipline

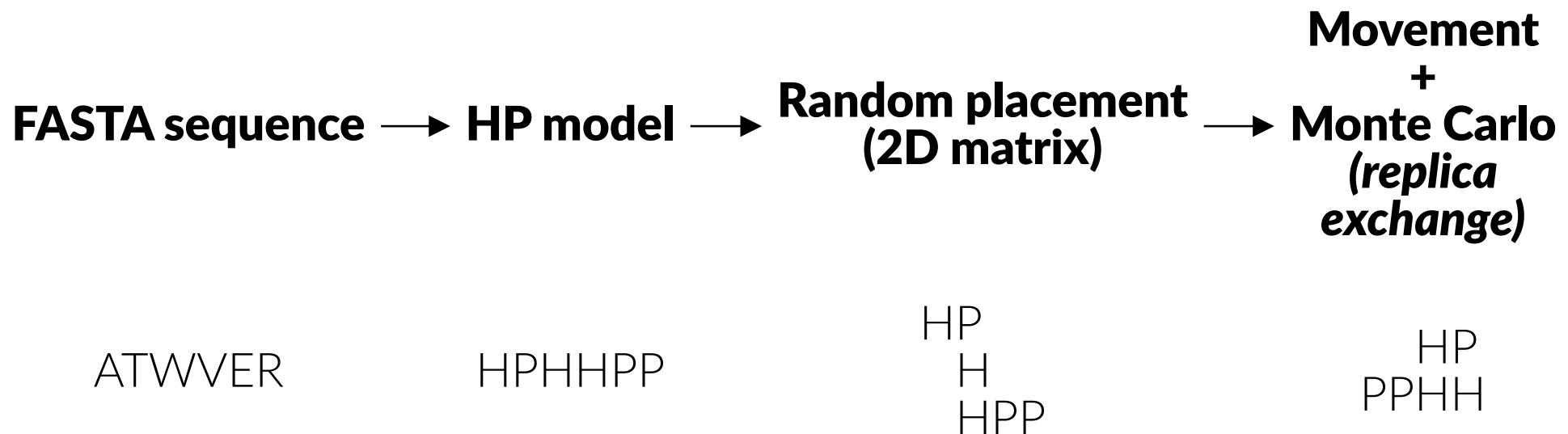
FASTA sequence → **HP model** → **Random placement
(2D matrix)**

ATWVER

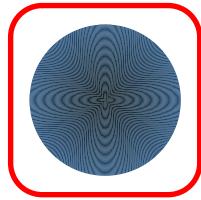
PHHHPP

HP
H
HPP

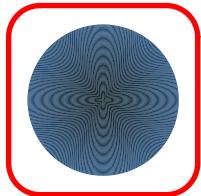
Pipline



Implementation

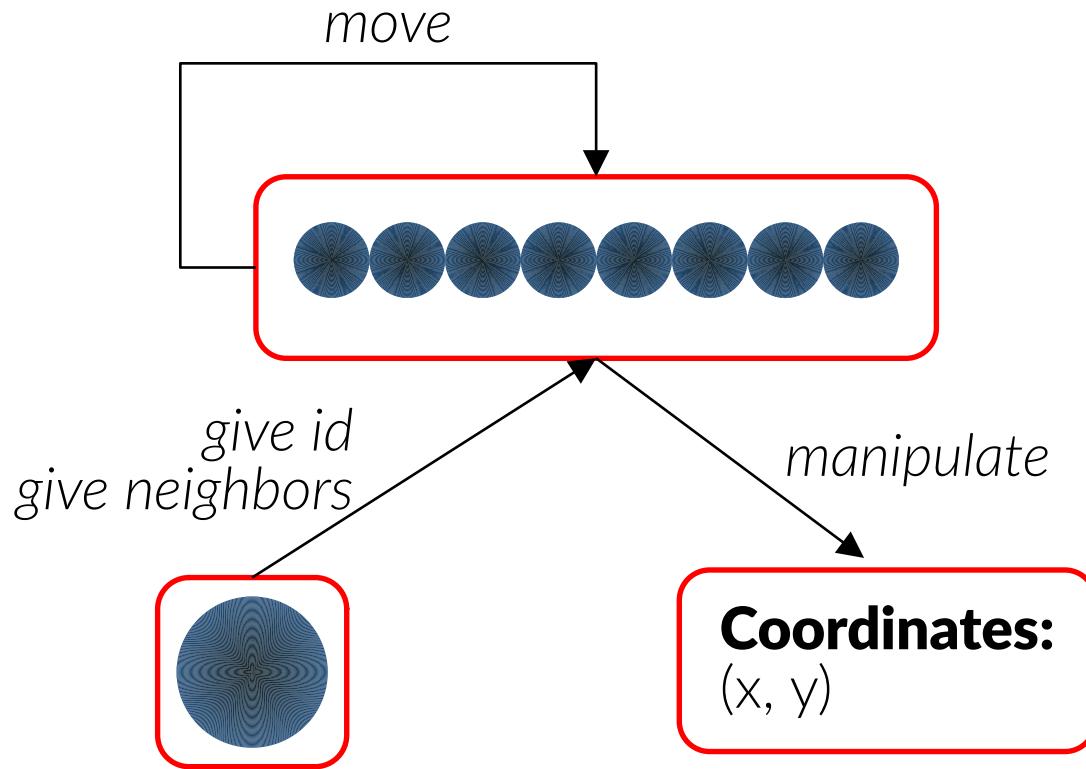


Implementation

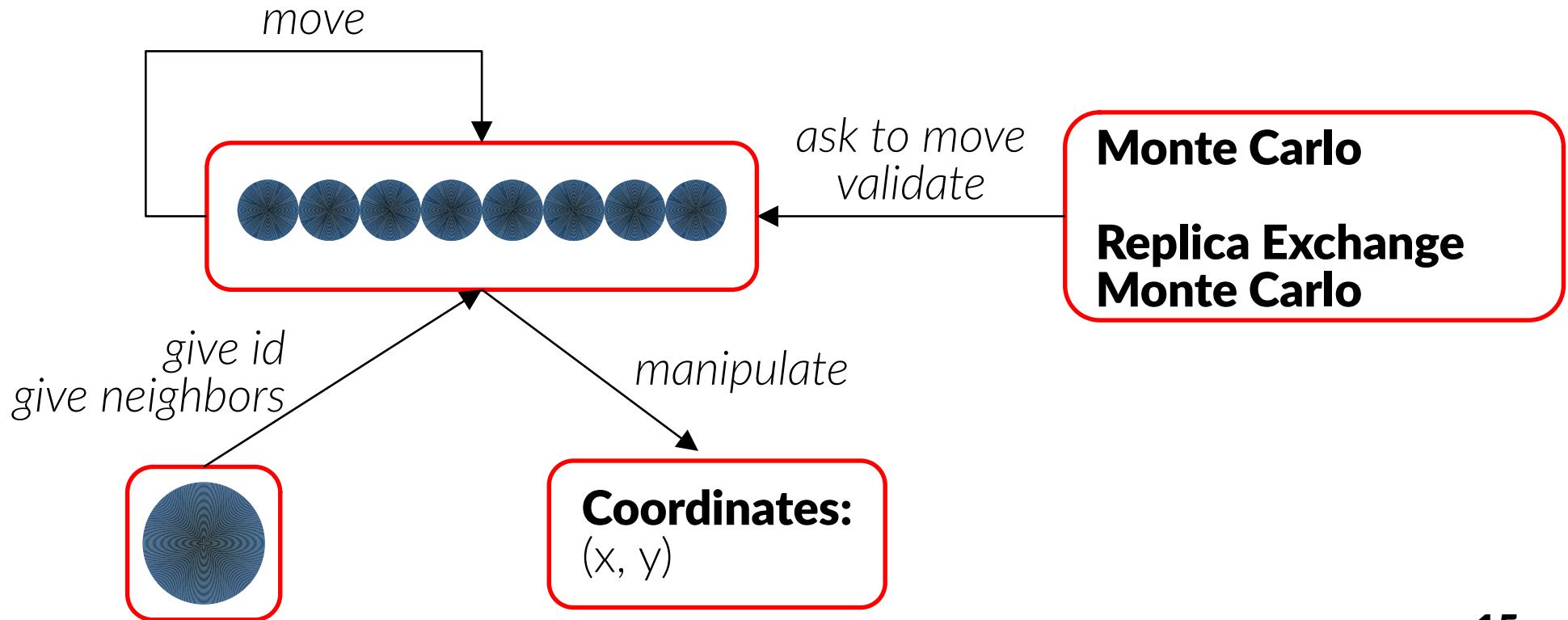


Coordinates:
 (x, y)

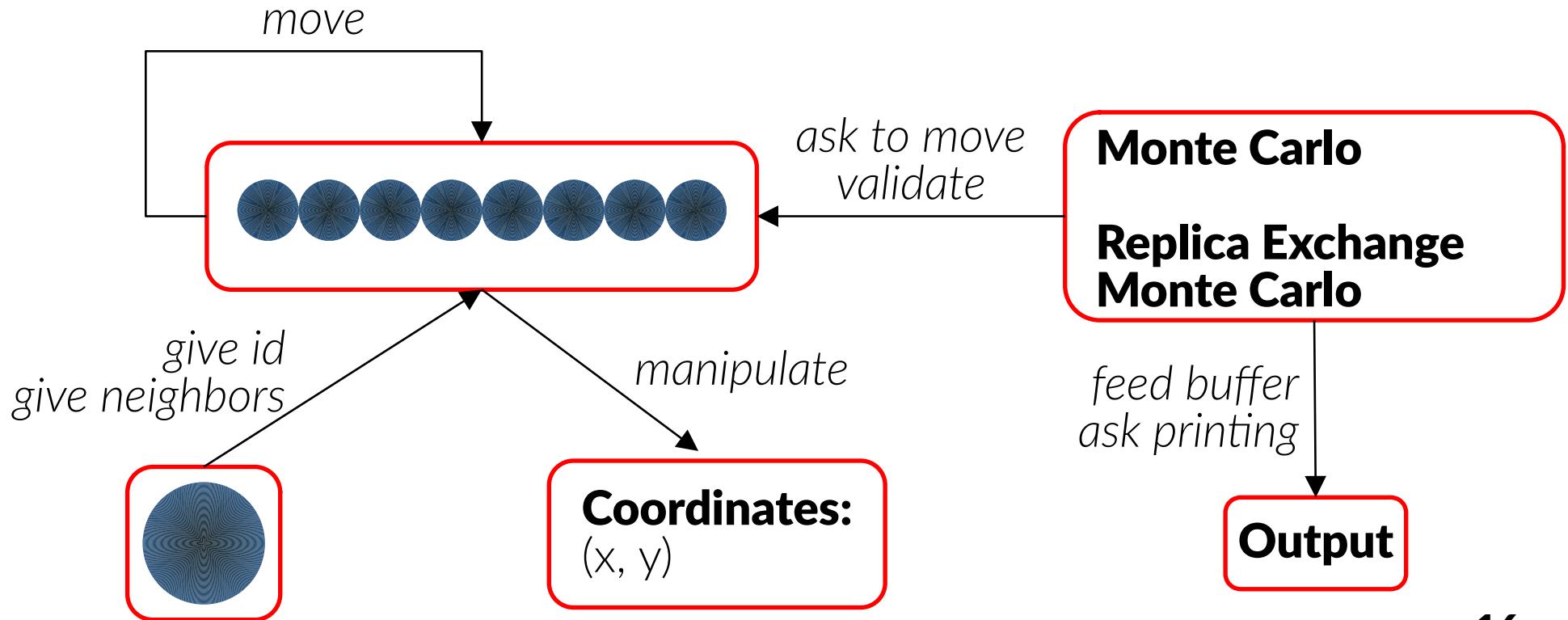
Implementation



Implementation

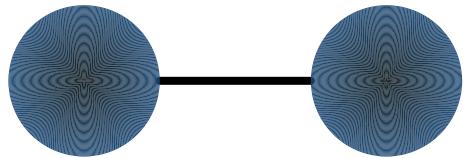


Implementation



Implementation

END MOVE



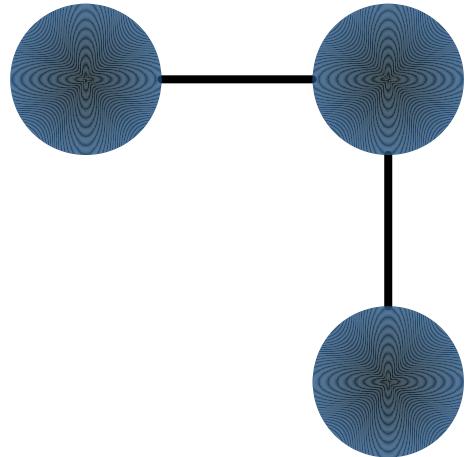
Implementation

END MOVE



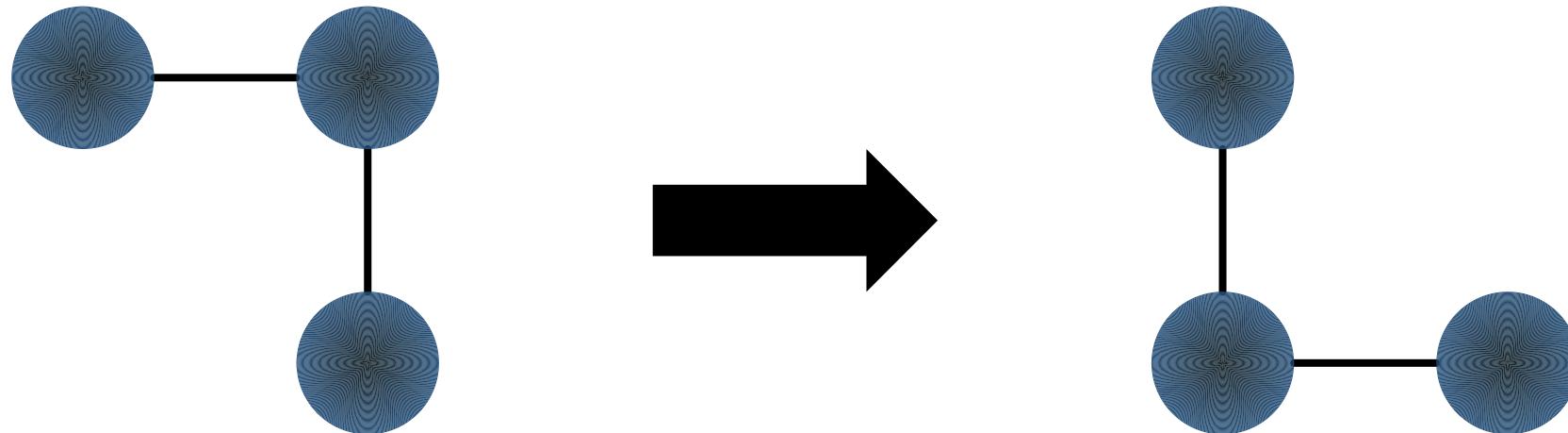
Implementation

CORNER MOVE



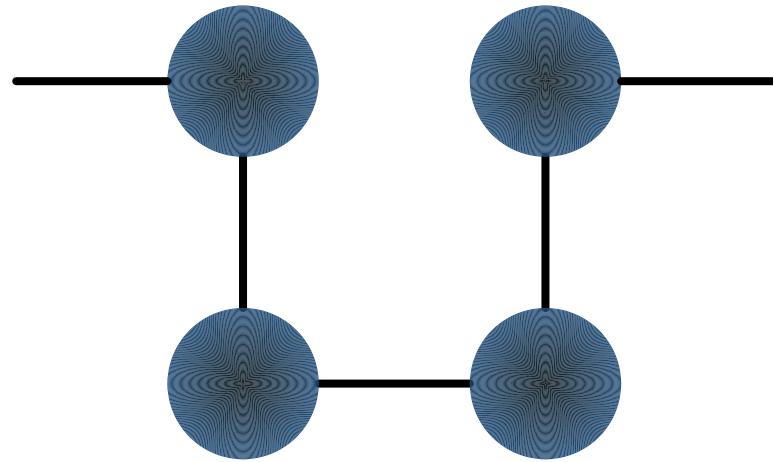
Implementation

CORNER MOVE



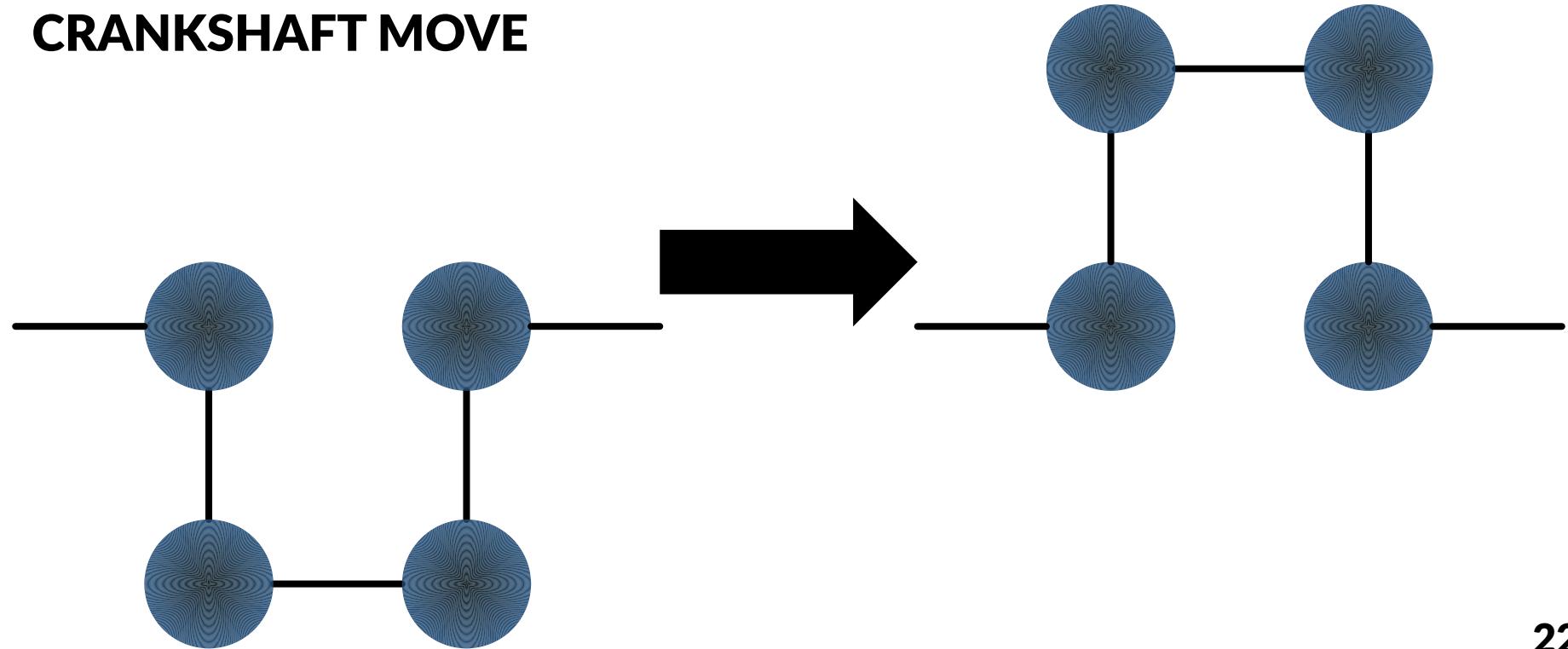
Implementation

CRANKSHAFT MOVE

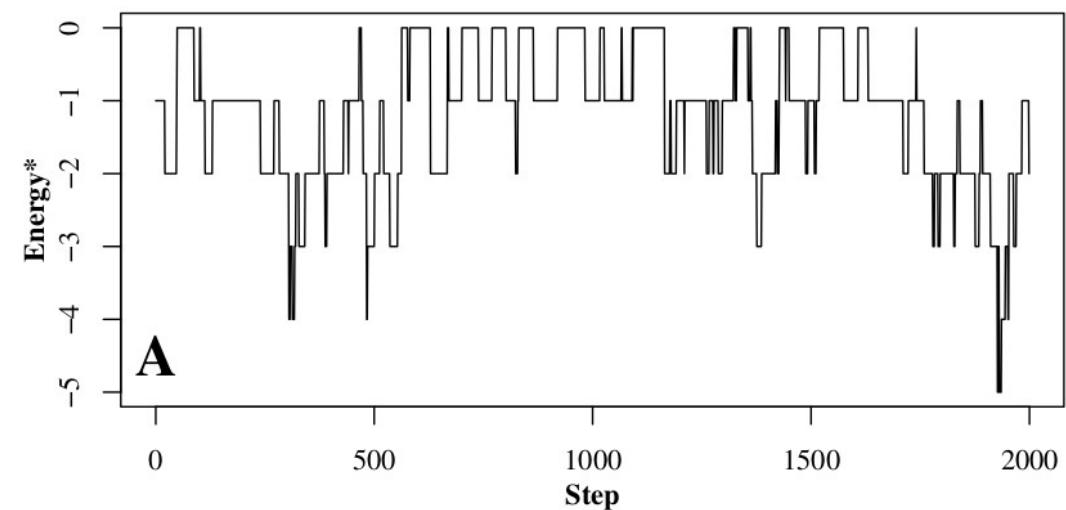


Implementation

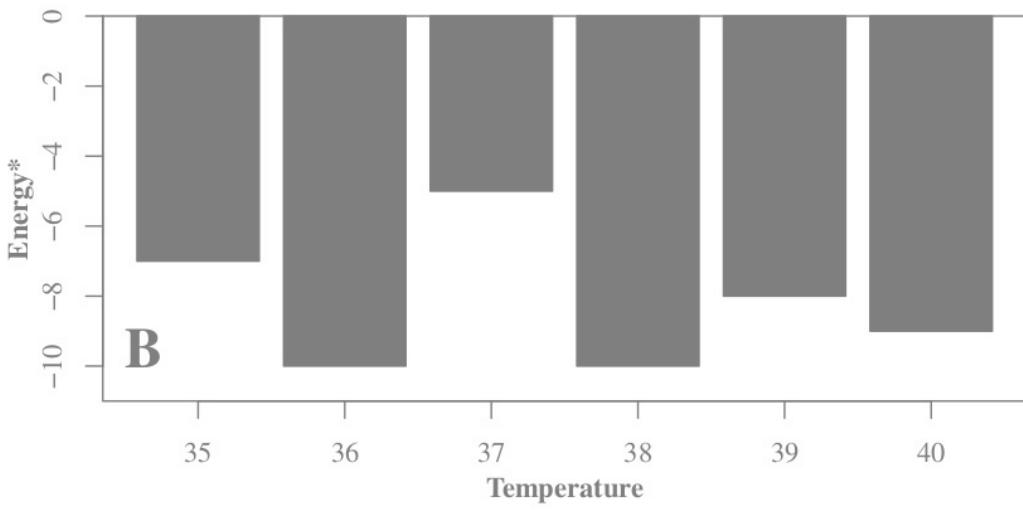
CRANKSHAFT MOVE



Results

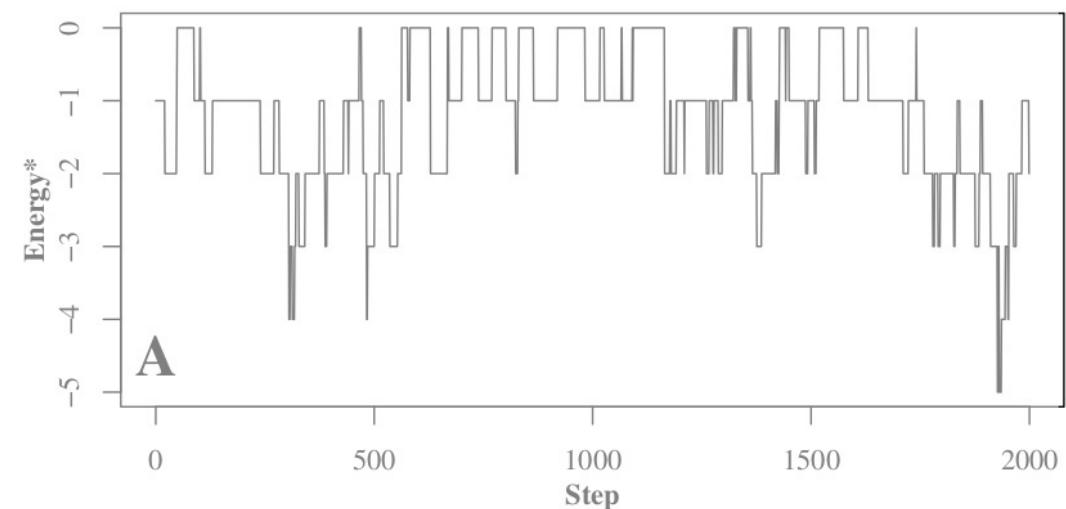


Energy in function of the step, obtain with the sequence in the original paper.

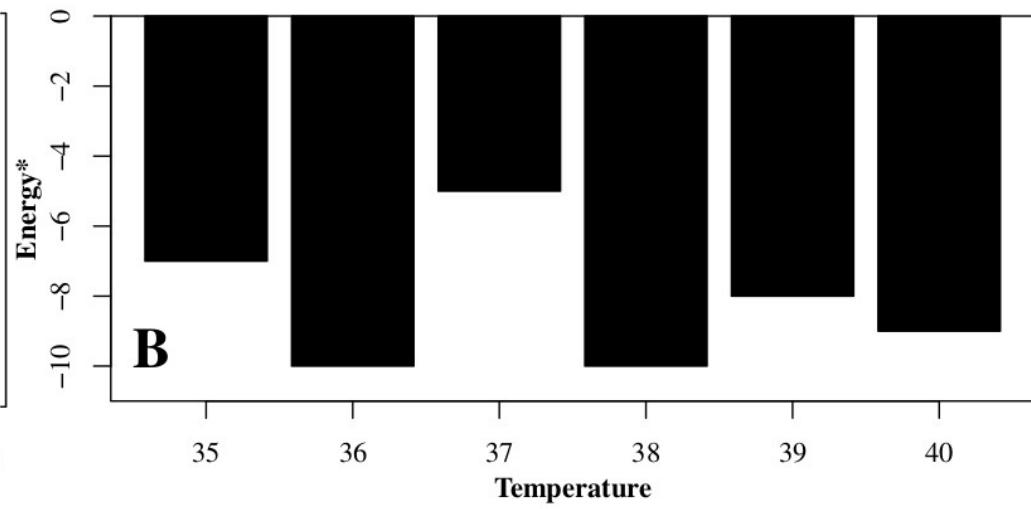


Energy in function of the temperature.
Only minimal energy are show here.

Results



Energy in function of the step, obtain with the sequence in the original paper.



Energy in function of the temperature.
Only minimal energy are show here.

Conclusion

What have been done:

- Program implementation in Oriented Object Programmation.
- Accelerate the program by not using matrix.
- Implemented Monte Carlo and Replica Exchange Monte Carlo.
- Use all VHSD move.

Perspective:

- Adding the pull move.
- Parallelize the program.
- Upgrade OOP implementation.
- Use C++/C.



THANKS FOR
YOUR
ATTENTION