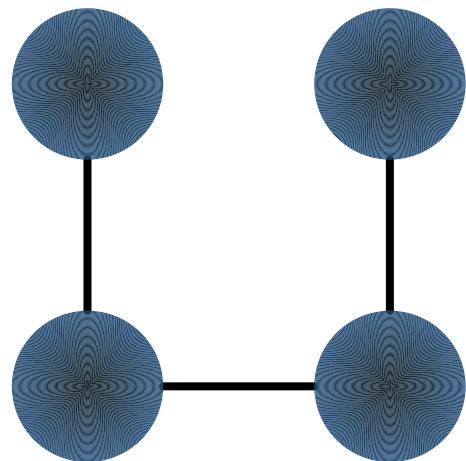


Implementation of a Replica Exchange Monte Carlo algorithm using Python

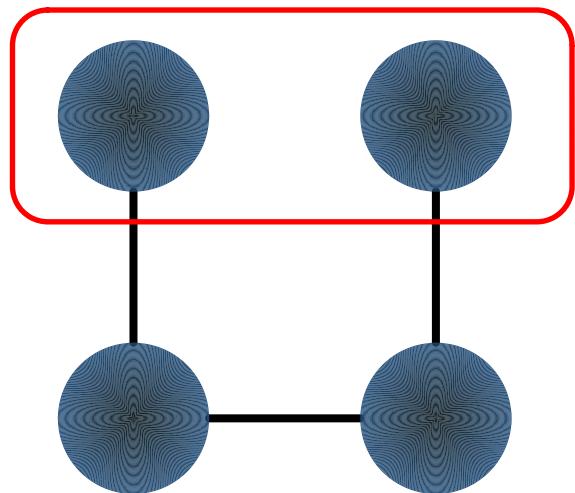
ROUAUD Lucas
Master 2 bio-informatique

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>.

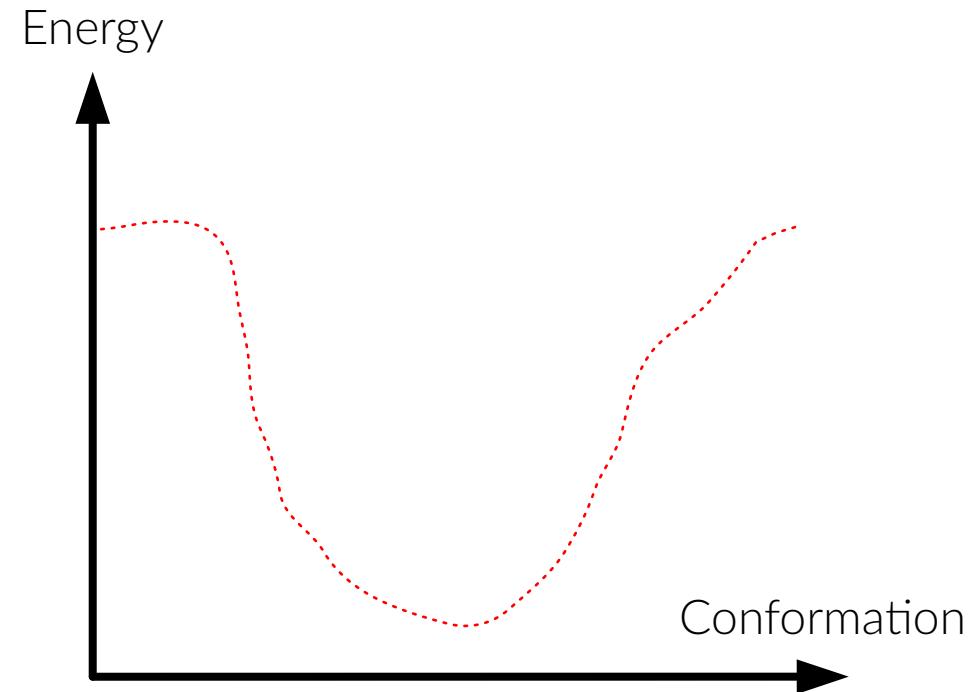
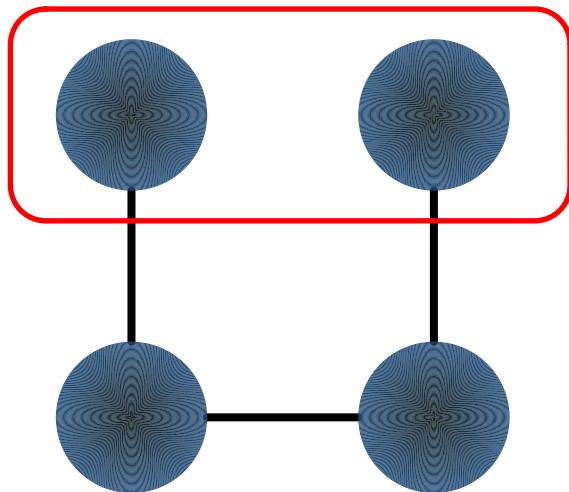
Introduction



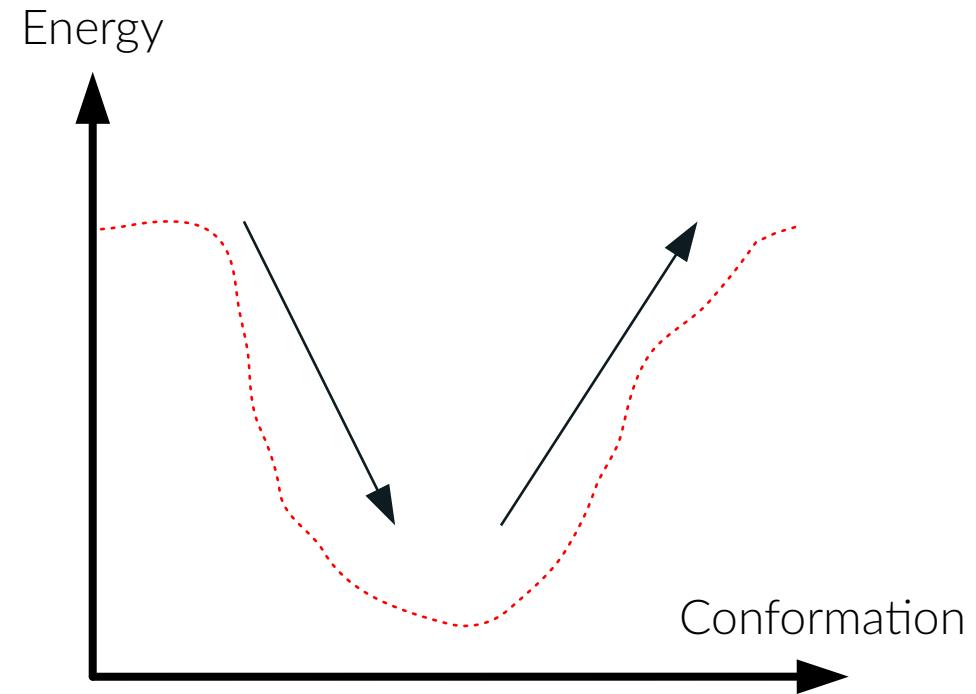
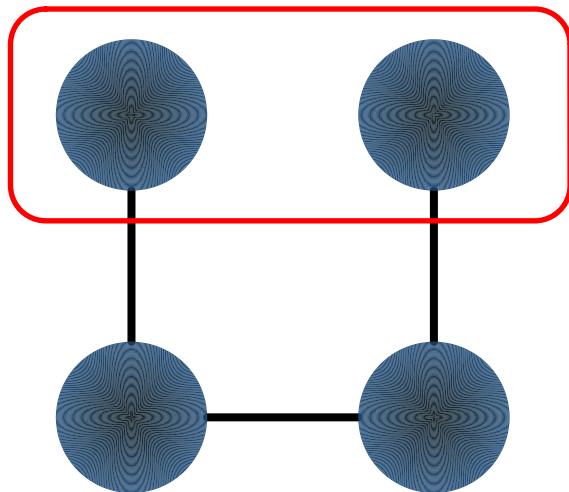
Introduction



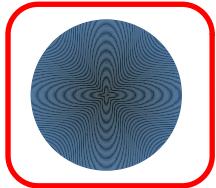
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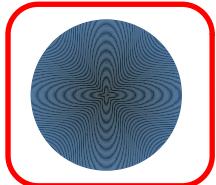
Introduction



Implementation

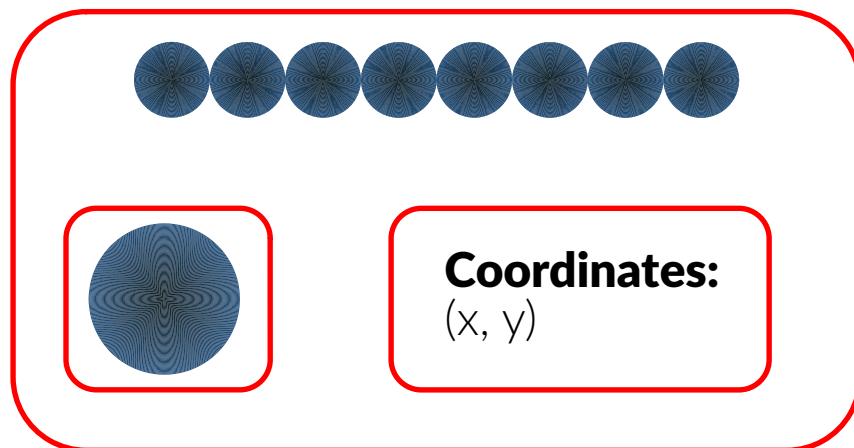


Implementation

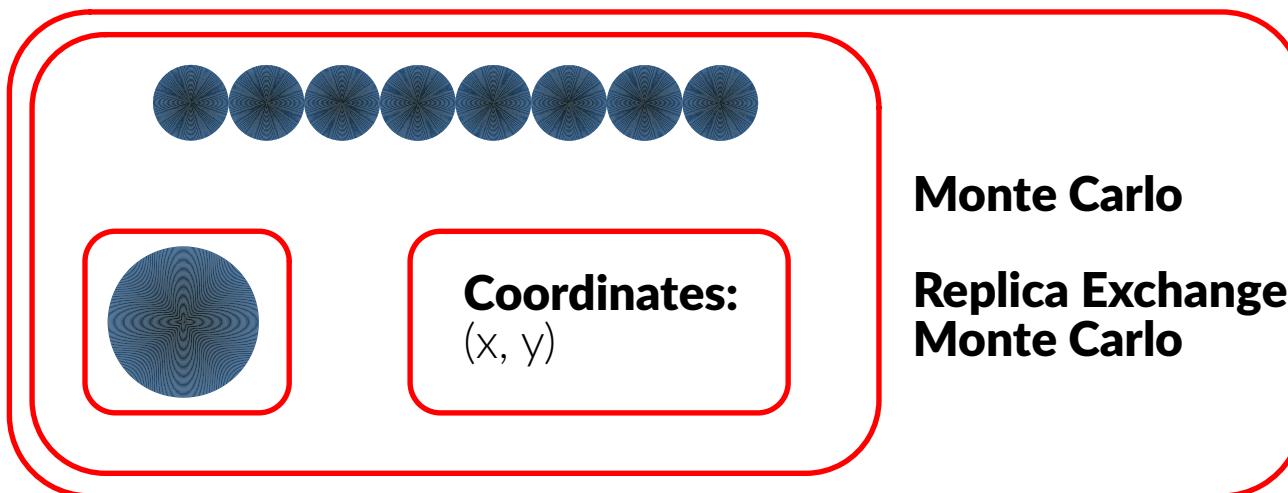


Coordinates:
 (x, y)

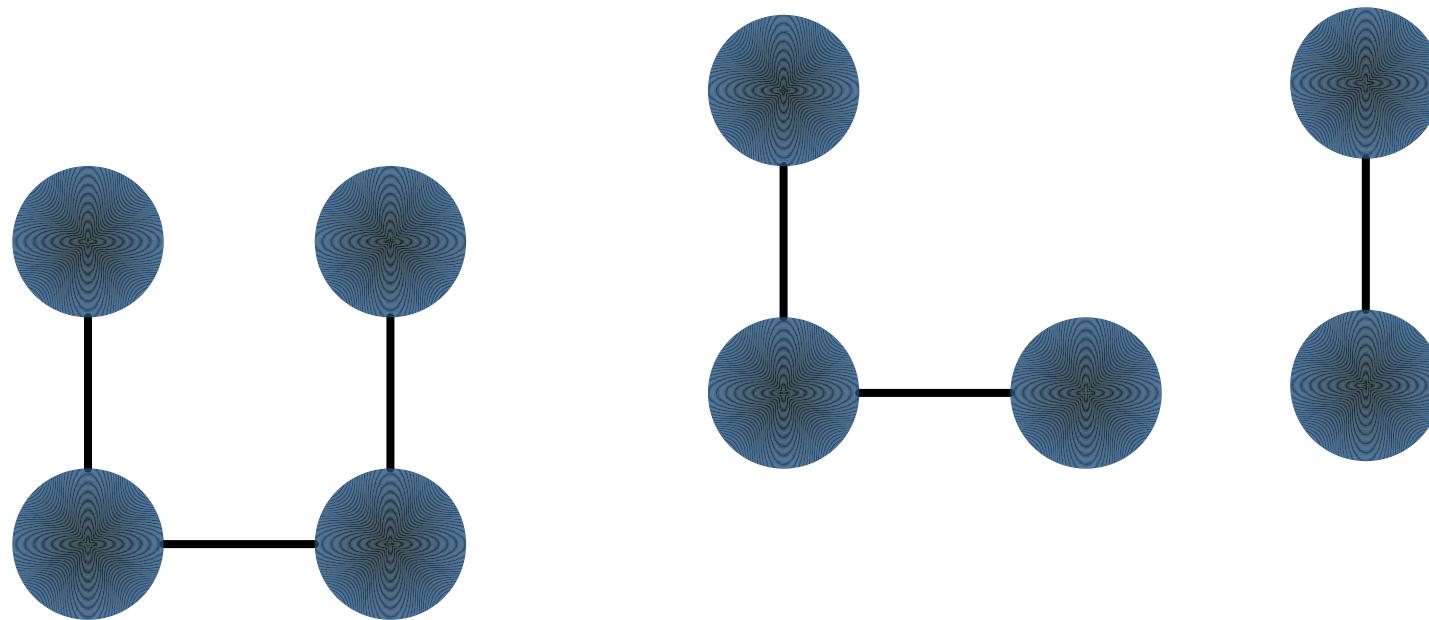
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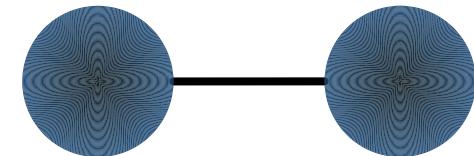
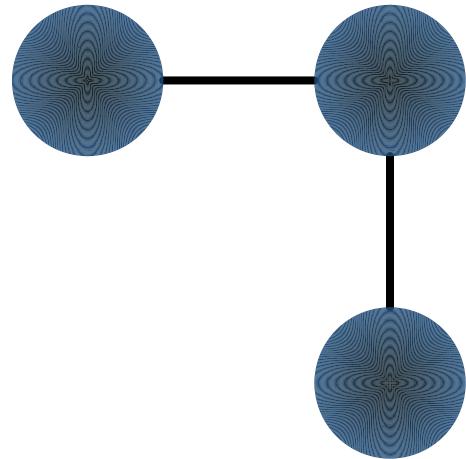
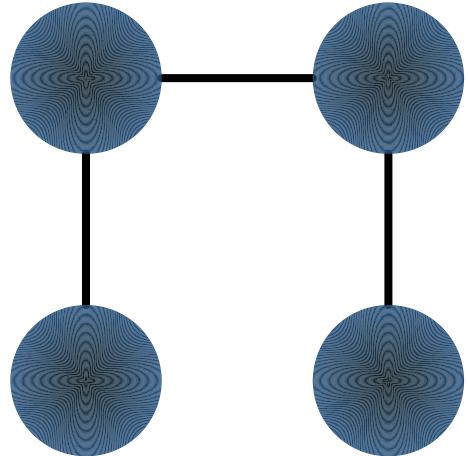
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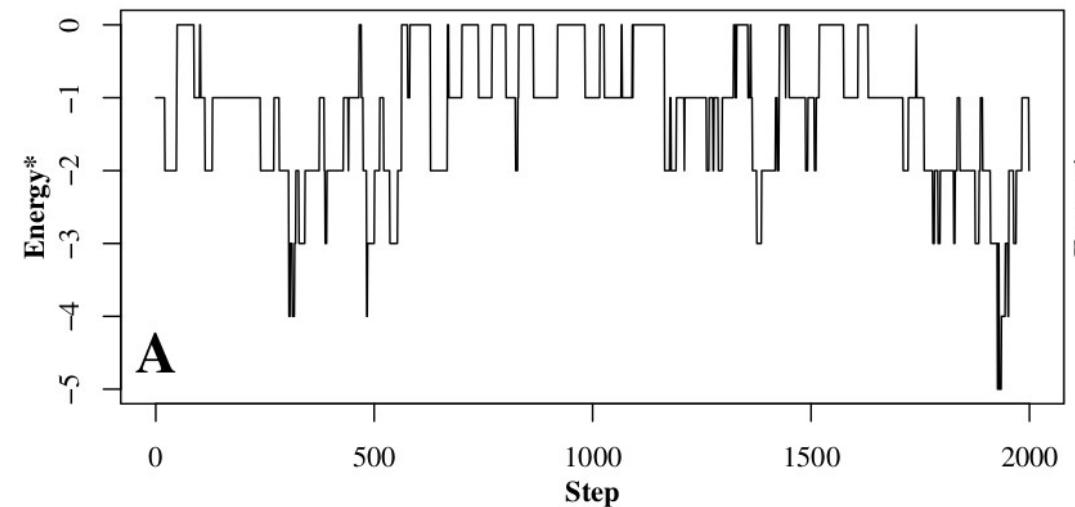
Implementation



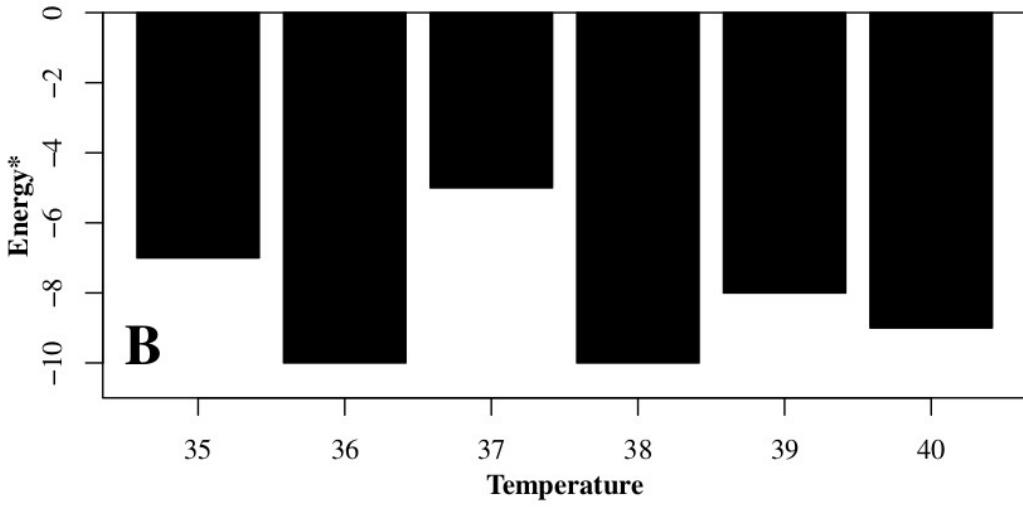
Implementation



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.
- Upagrade OOP implementation.



THANKS FOR
YOUR
ATTENTION