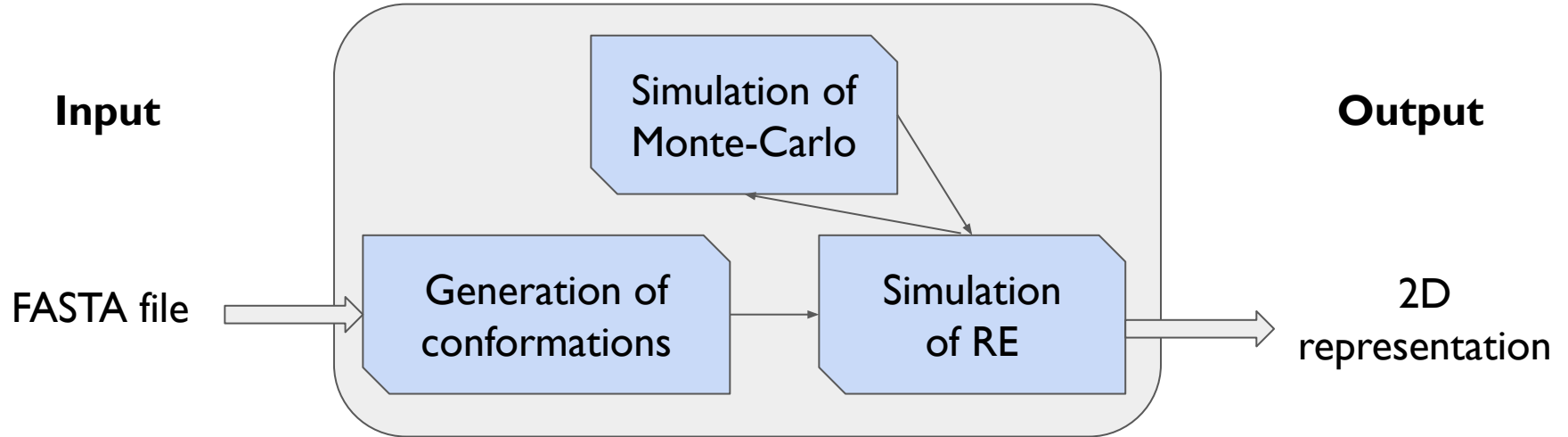


A REPLICA EXCHANGE MONTE CARLO ALGORITHM DEVELOPMENT FOR PROTEIN FOLDING IN THE HP MODEL

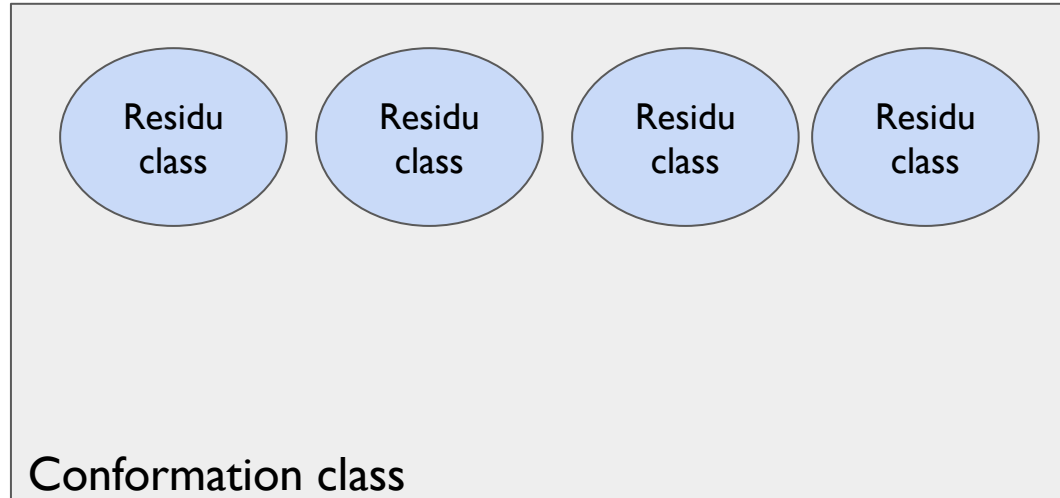
Autor : OUSSAREN Mohamed

16 Septembre 2022

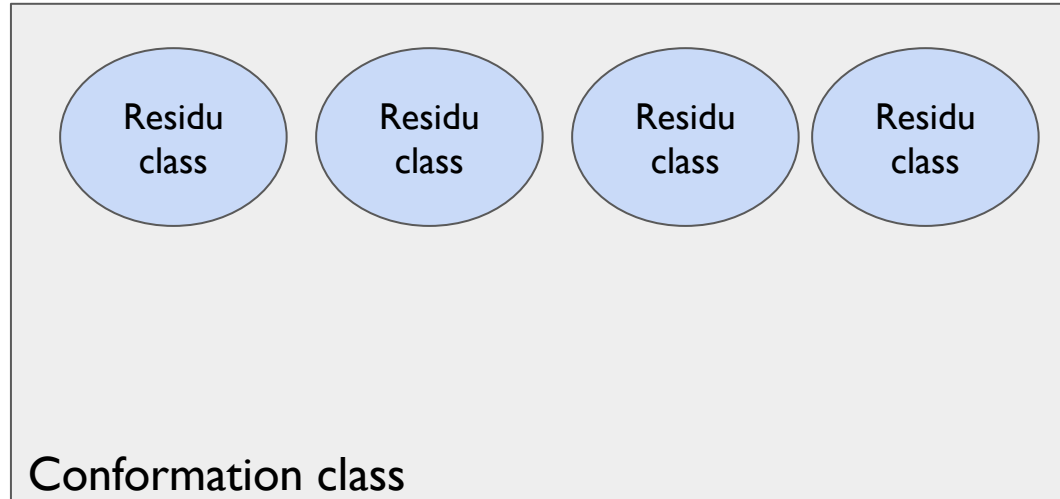
Pipeline



OOP



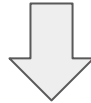
OOP



REMC
simulation
functions

HP model (Dill and al. 1985)

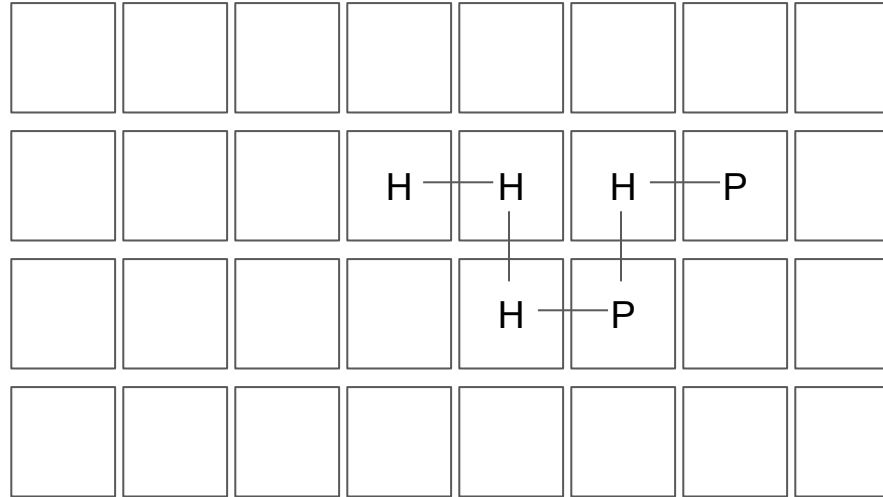
Primary structure: Basic sequence : A-P-V-T-L-K



Sequence containing only H and P : H-H-H-P-H-P

Placement of residues on trellises

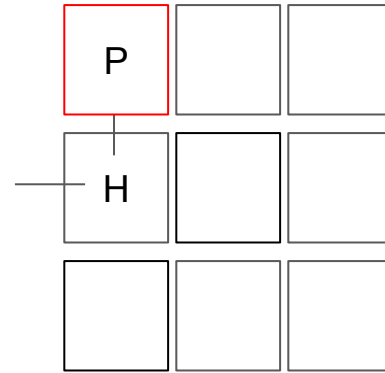
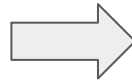
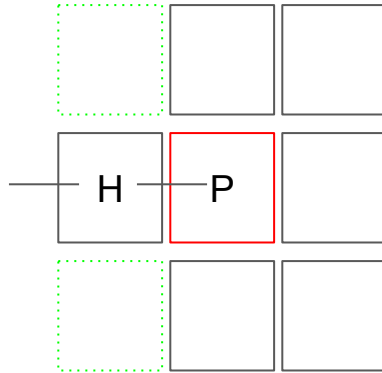
H-H-H-P-H-P



**2D
representation**

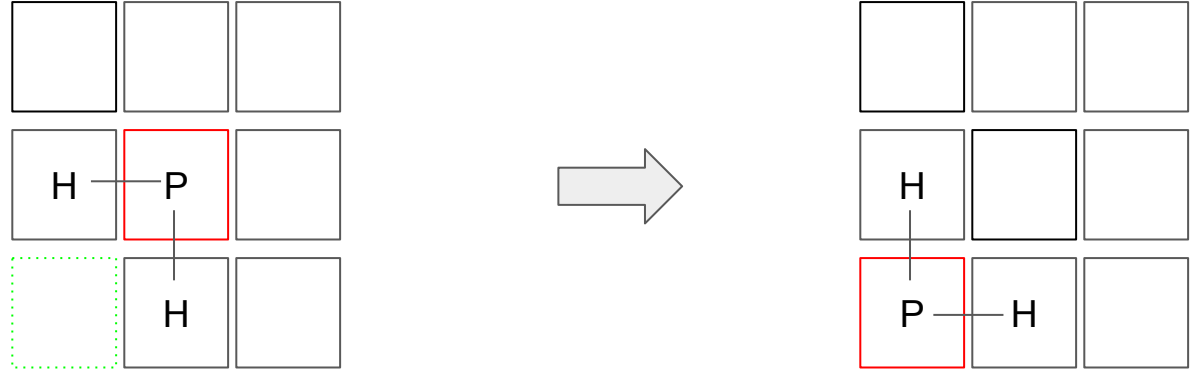
Movements

End move

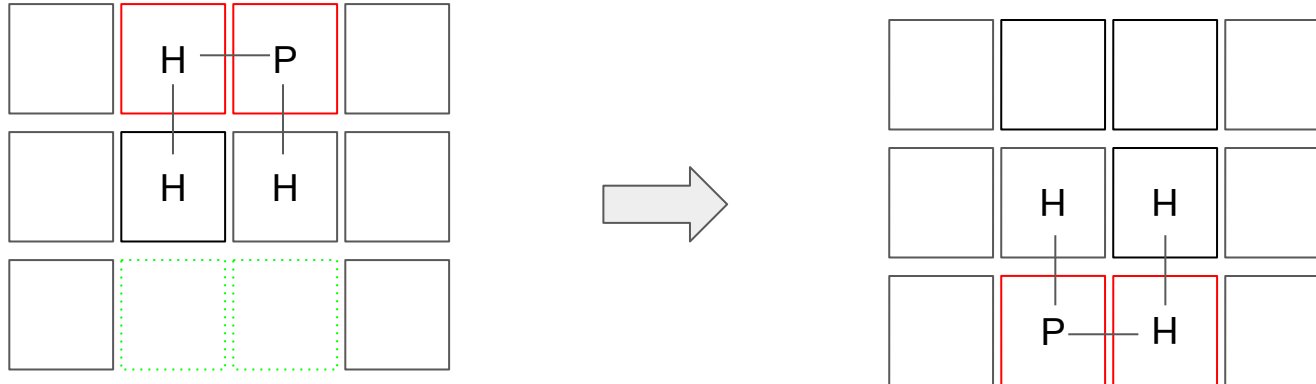


Corner move

Movements

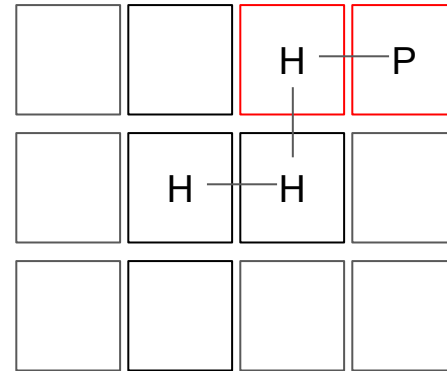
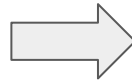
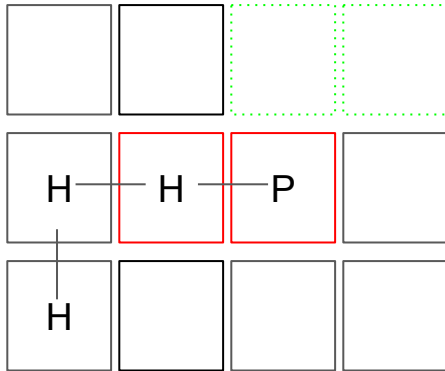


Crankshaft move

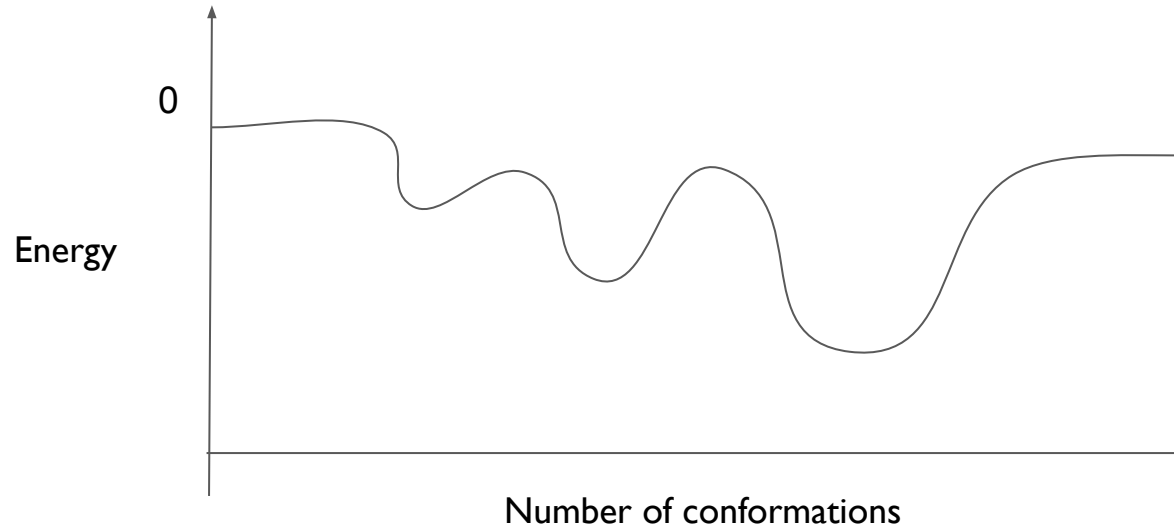


Movements

Pull move



Monte-Carlo simulation



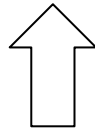
Explore protein conformation to block on global minimum by leaving local minimum

Replicas exchange simulation

220 C



230 C



240 C



250 C



Replicas exchange simulation

220 C



230 C



240 C



250 C



Replicas exchange simulation

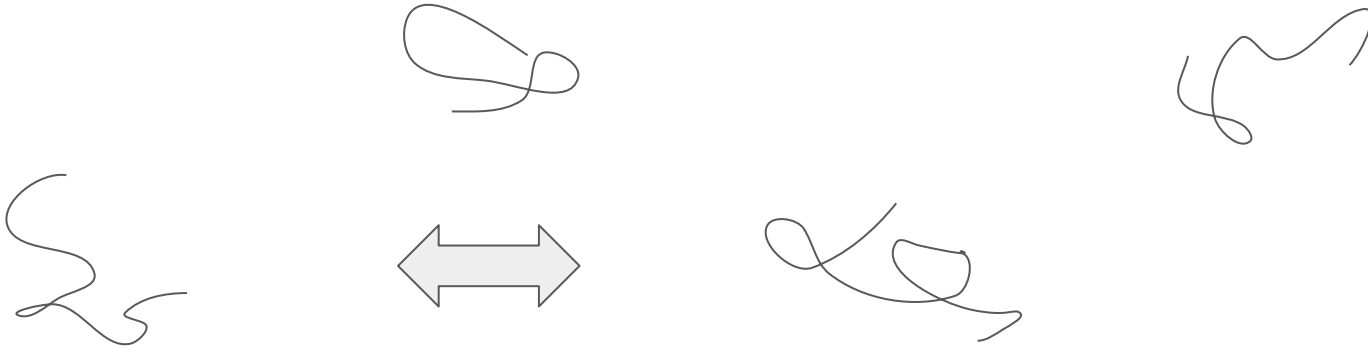
If the proportion of energy difference and temperature between 2 replicas is high then there is temperature exchange

220 C

230 C

240 C

250 C



Replicas exchange simulation

240 C



230 C



220 C



250 C



Replicas exchange simulation

240 C



230 C



220 C

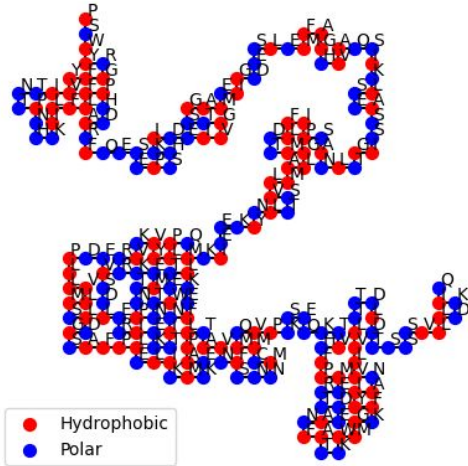


250 C

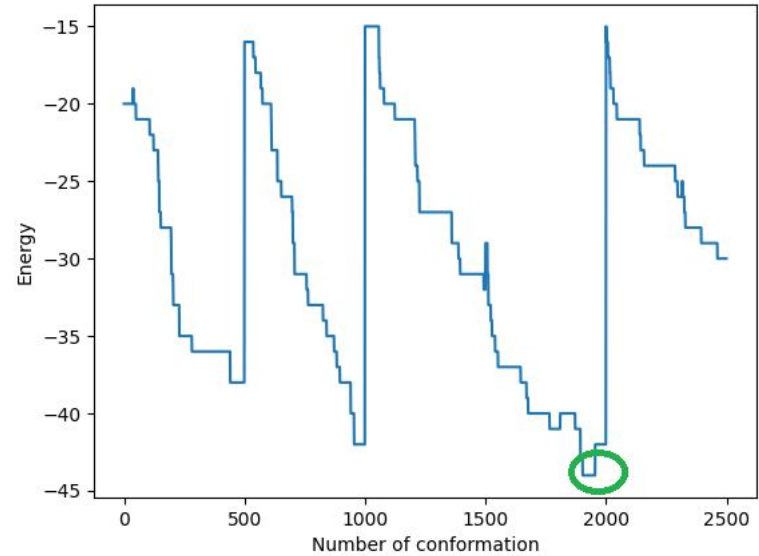


Results

P01013



Threshold : -30, 500 iterations Monte-Carlo



Conclusion

Conclusion :

Development of a REMC method in Python 3 based on a HP model representation, movement system and energy minimization. A polynomial time algorithm.

Perspectives :

- Revaluation of results
- Multiprocessing
- Transcription of the code into C/C++ to optimise the code

References

- Thachuk, C., Shmygelska, A. & Hoos, H.H. A replica exchange Monte Carlo algorithm for protein folding in the HP model. *BMC Bioinformatics* 8, 342 (2007). <https://doi.org/10.1186/1471-2105-8-342>
- Dill KA. Theory for the folding and stability of globular proteins. *Biochemistry*. 1985 Mar 12;24(6):1501-9. doi: 10.1021/bi00327a032. PMID: 3986190