Master 2 BI

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

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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

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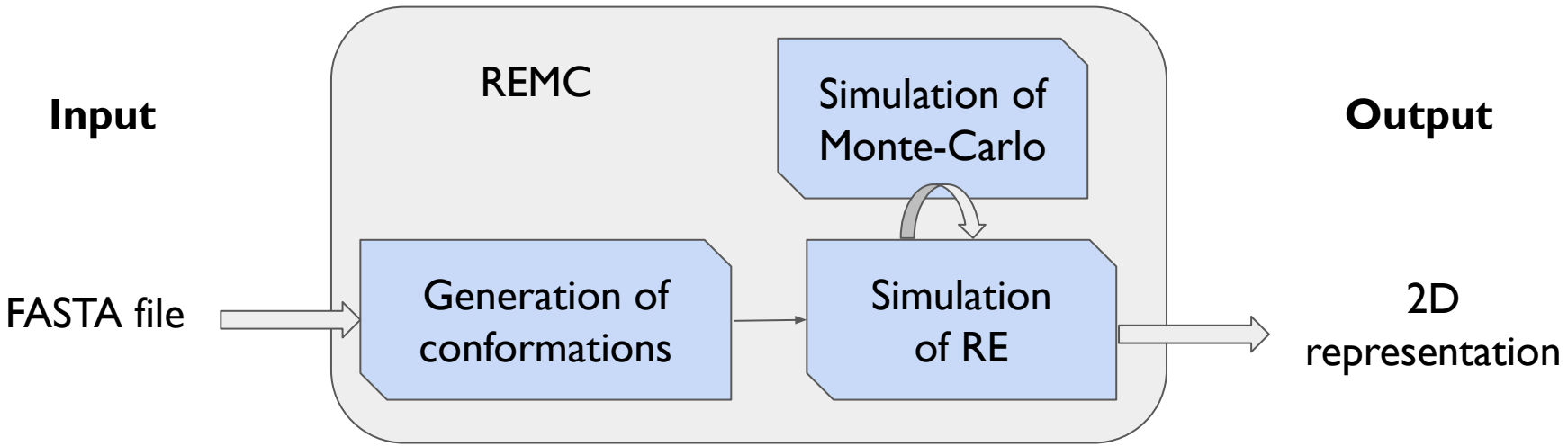
Pipeline



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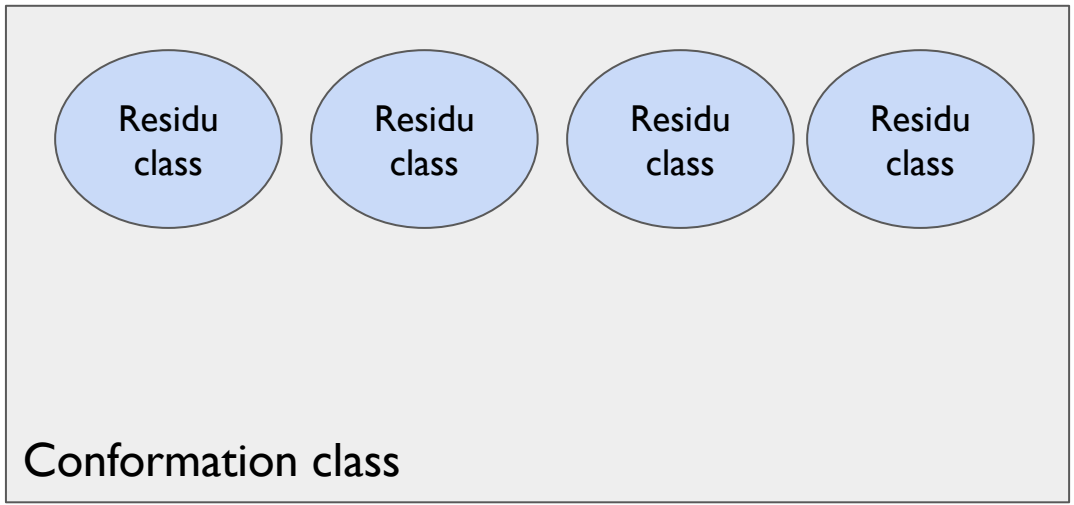
OOP



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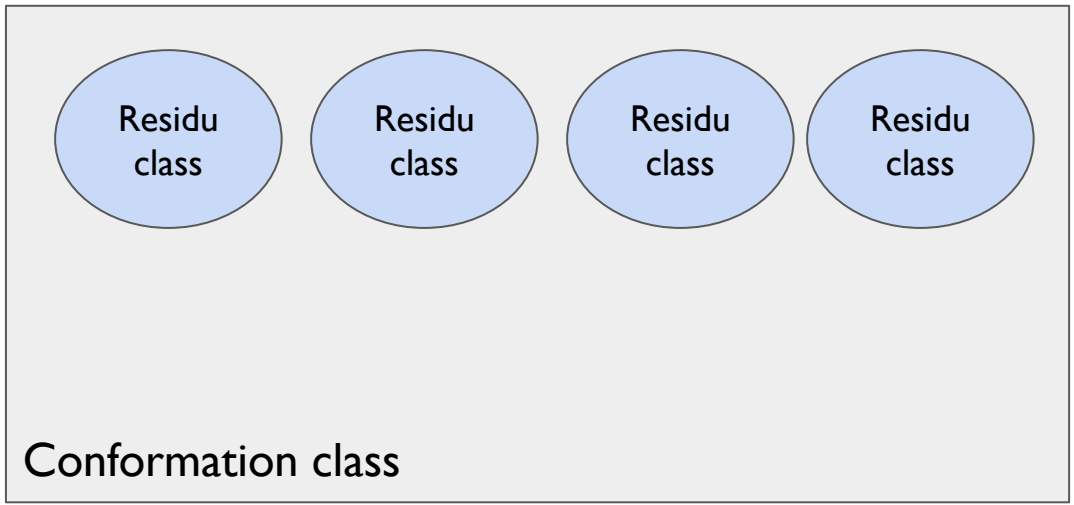
OOP



REMC simulation functions

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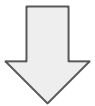
HP model (Dill and al. 1985)

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



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

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

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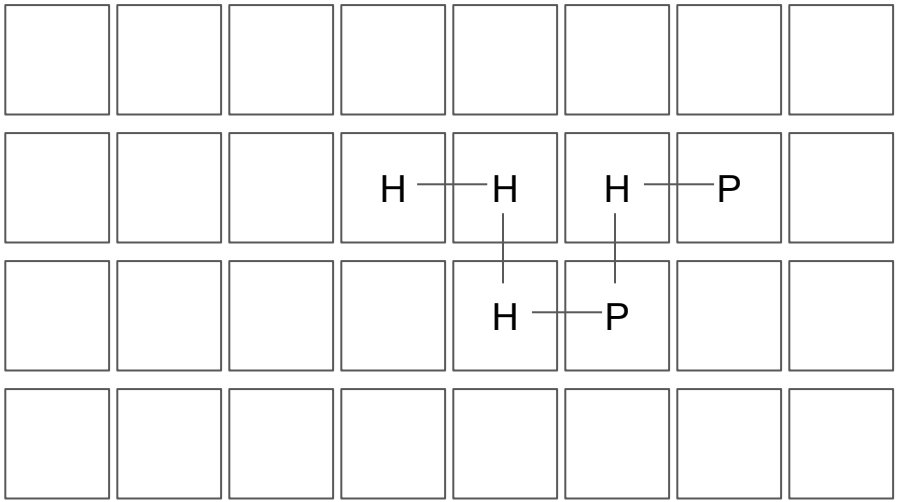
Placement of residues on trellises

H-H-H-P-H-P



2D representation

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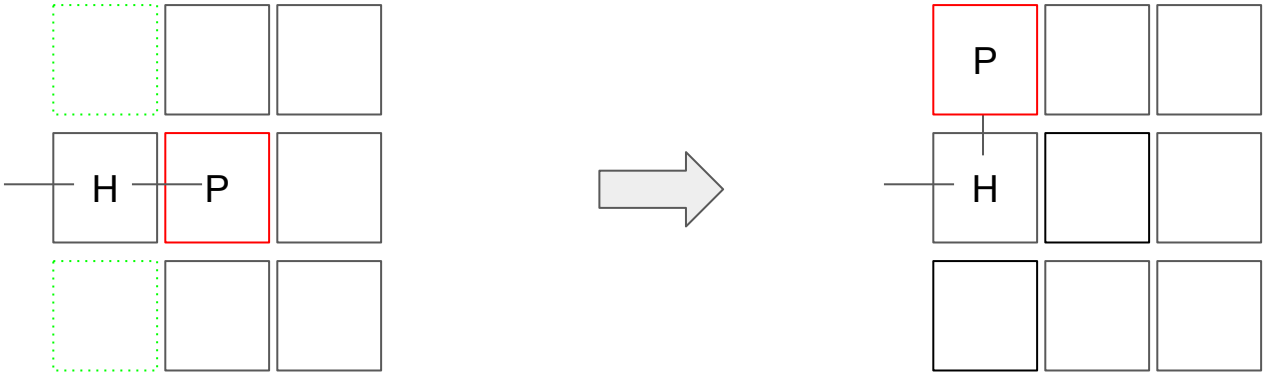
Movements

End move



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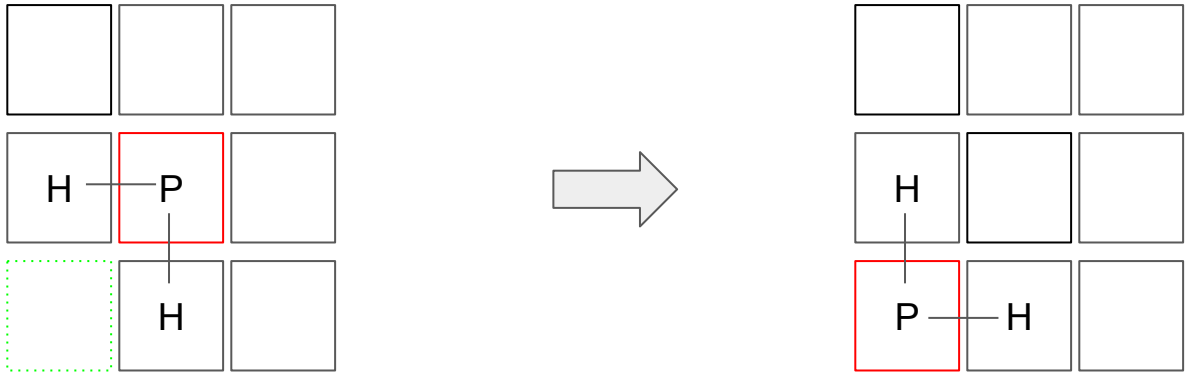
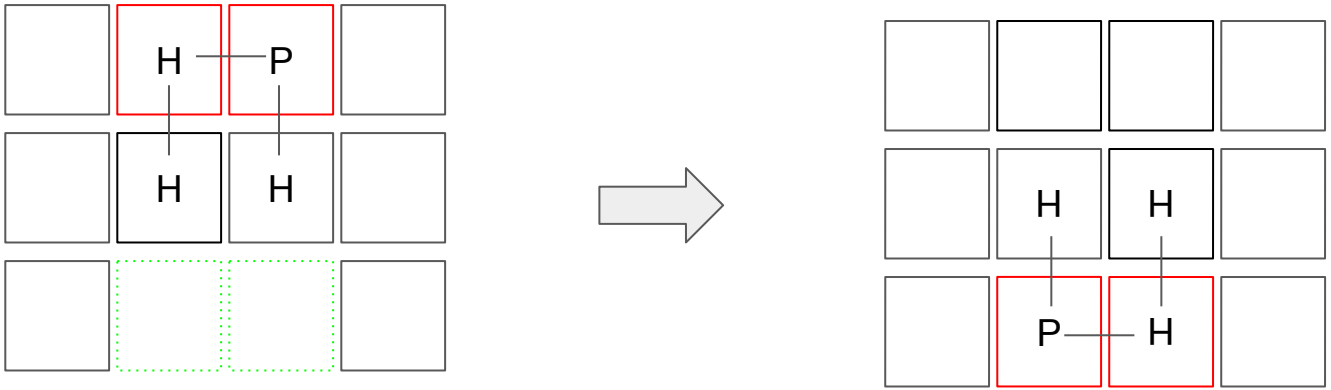
Movements

Corner move



Crankshaft move



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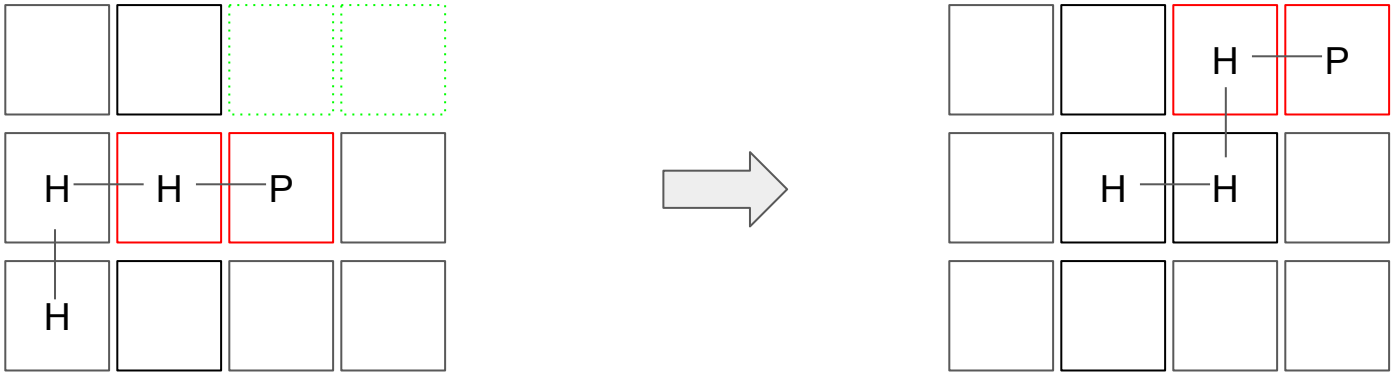
Movements

Pull move



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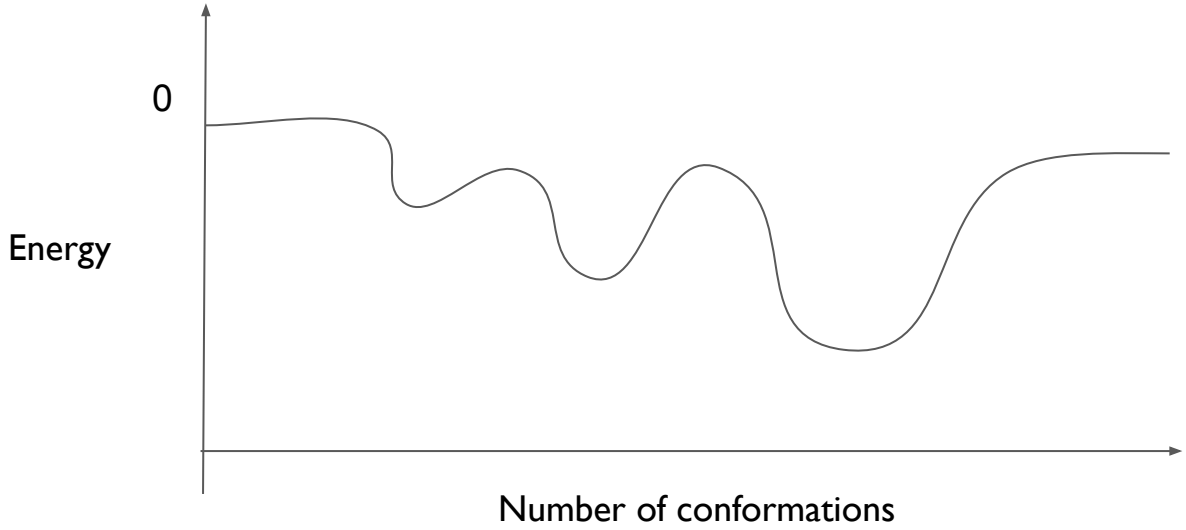
Monte-Carlo simulation



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

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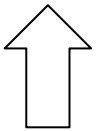
Replicas exchange simulation

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

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Replicas exchange simulation

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

230 C 220 C 240 C 250 C

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Replicas exchange simulation

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Results

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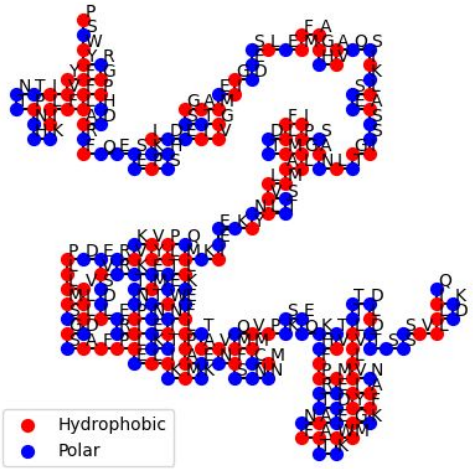
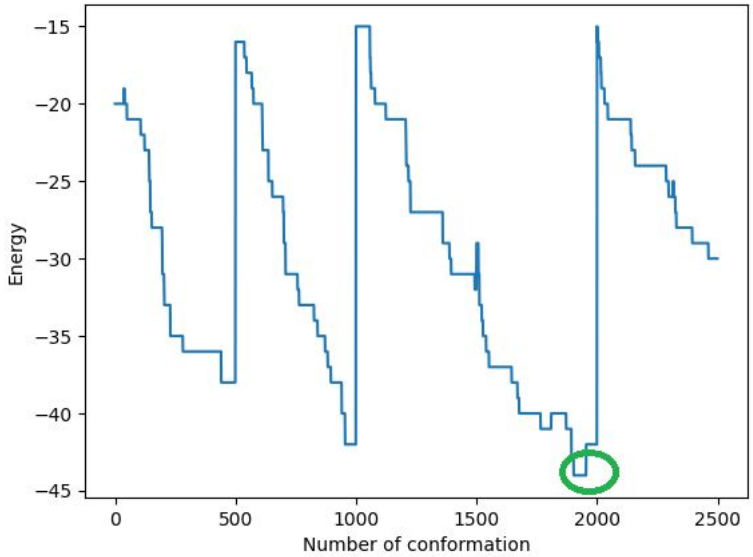


Threshold : -30, 500 iterations Monte-Carlo



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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

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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

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