Folding of a simplified protein model by a Monte Carlo algorithm

Rousseau Baptiste

M2 BI - Université de Paris Cité

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based on: A replica exchange Monte Carlo algorithm for protein folding in the HP model. Thachuk et al. 2007

The algorithm

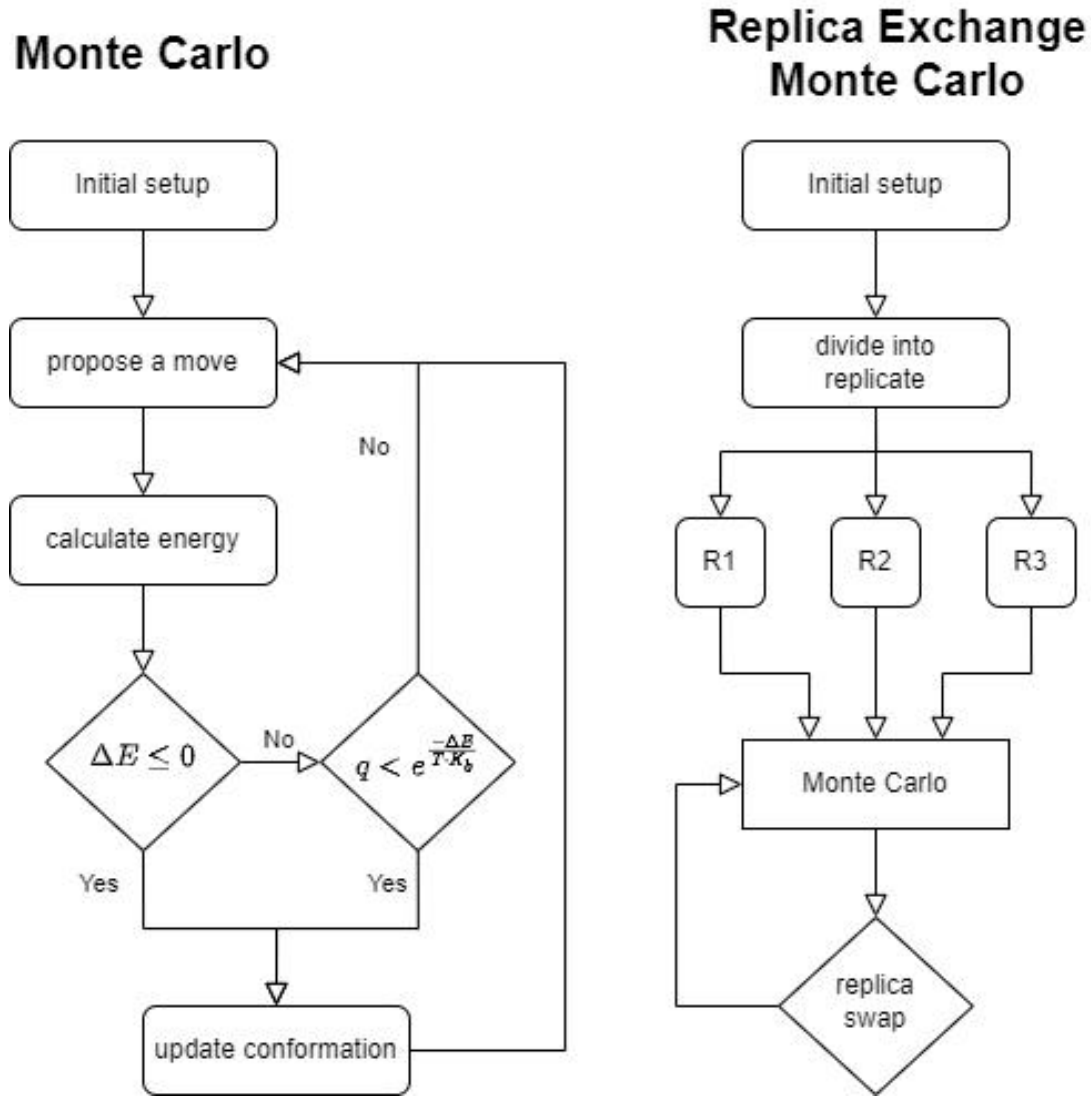

Fig.1: Monte Carlo and Replica Exchange Monte Carlo algorithms

Moves

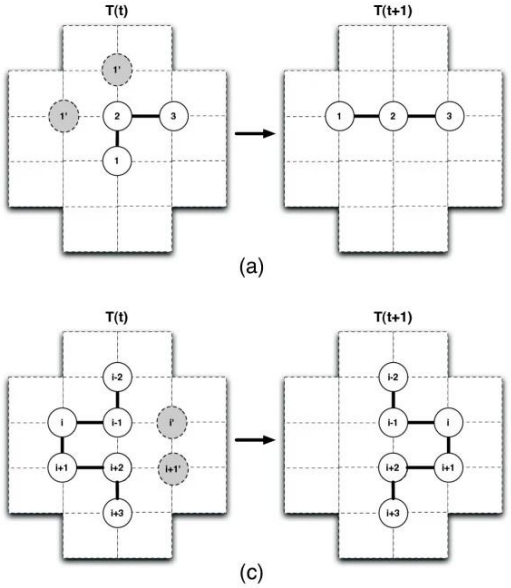

Fig.2: VSHD moves

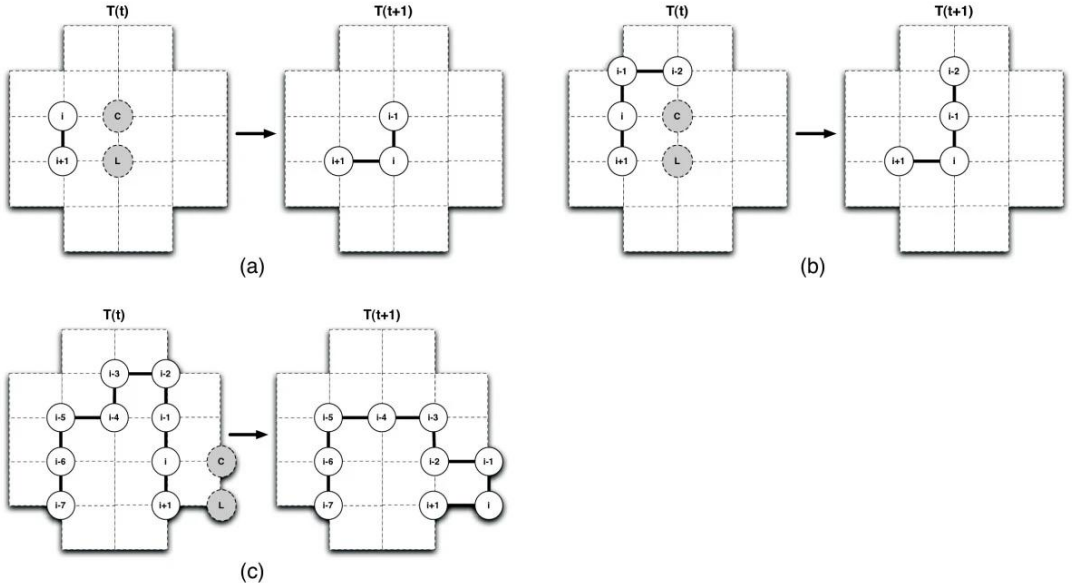

Fig.3: pull moves

from: A replica exchange Monte Carlo algorithm for protein folding in the HP model. Thachuk et al. 2007

Class dependencies

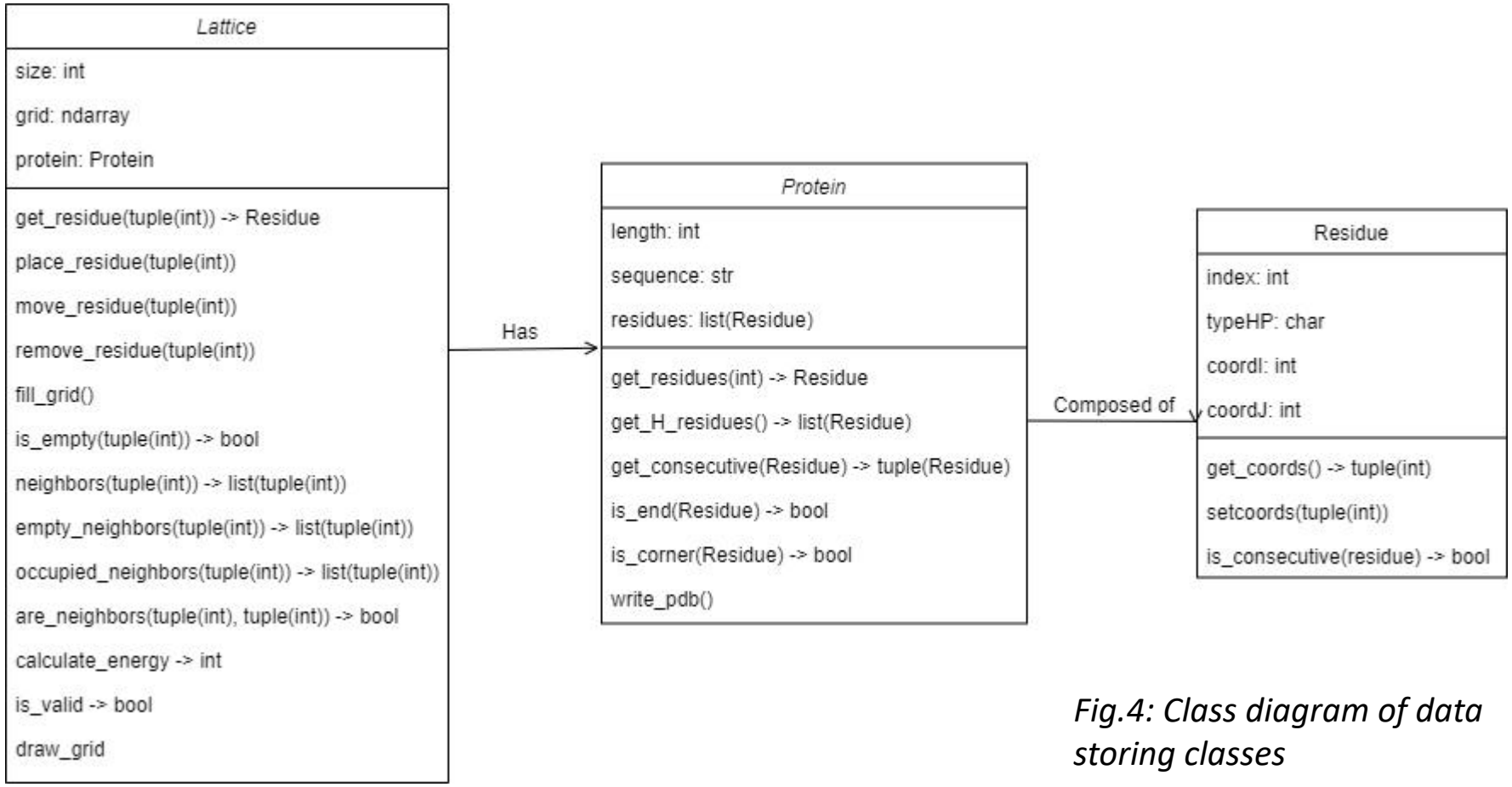

Fig.4: Class diagram of data storing classes

Class dependencies

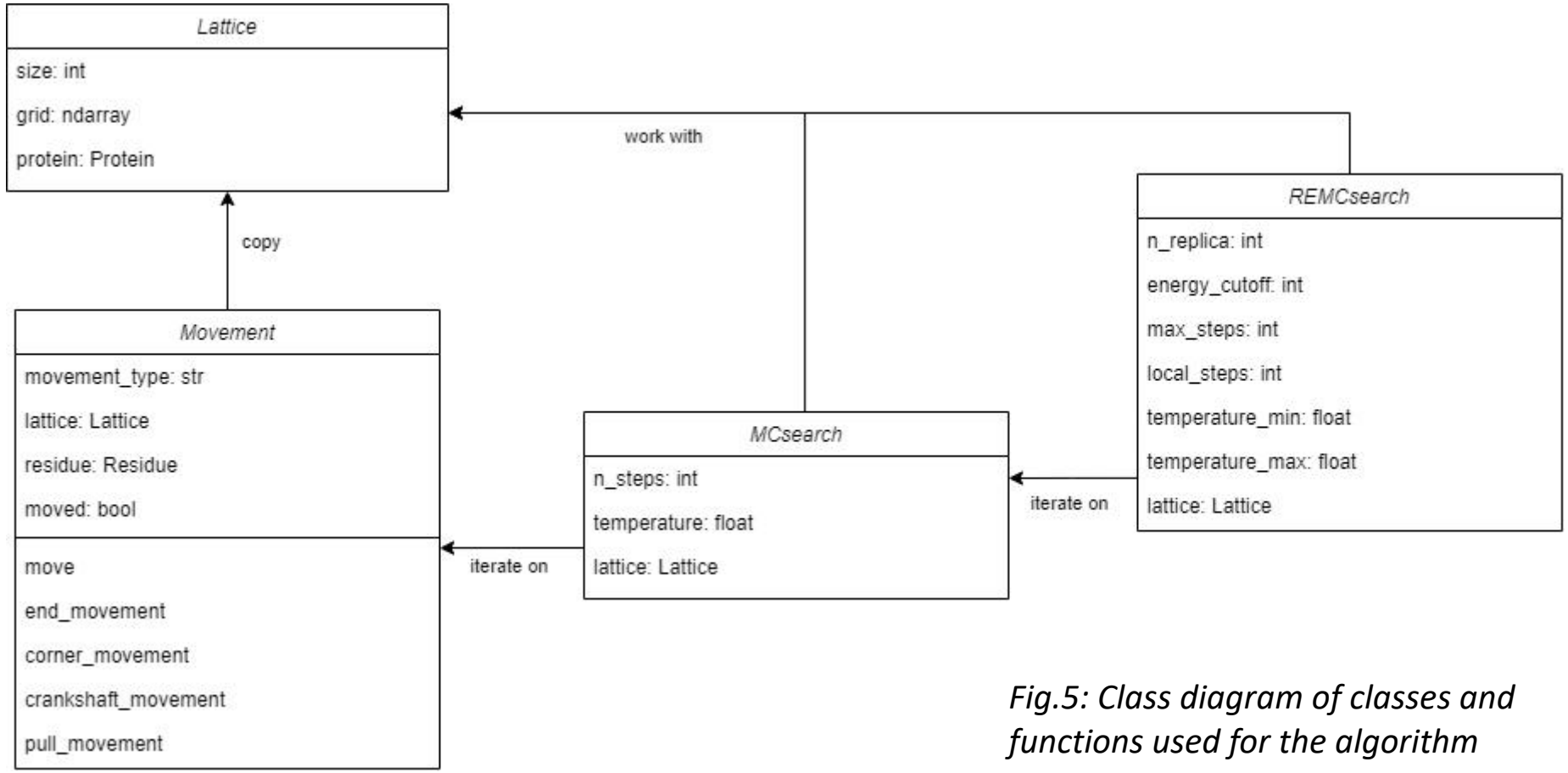

Fig.5: Class diagram of classes and functions used for the algorithm

Results

ID	E^*	MC	REMC
S1	-9	-4	-4
S2	-9	-4	-3
S3	-8	-3	-1
S4	-14	-3	-1

Table 1: Results of runs on benchmarking proteins

```
Running test case: HPHPPHHPHPPHPHHPPHPH with optimal energy: -9
Running MC with parameters: n-steps=5000, temperature=200
Final lattice with energy of -4
+-----------+
|           |
|         PP |
| PH      HH |
| HHHPHHPHP |
| PP  PP  H |
|           |
+-----------+
Running REMC with parameters: n-replica=5, energy-cutoff=-9,
max-steps=1000, local-steps=100, temperature-min=160,
temperature-max=220
Final lattice with energy of -4
+--------------+
|              |
| PH         PP |
| HHHPHPPHPHHH |
| PP         HP |
|              |
+--------------+
```

Fig.6: Example of a run on protein S1

Discussion

Bad performances:

- runs takes a long time
- need a lot of iterations
- obtained energy far from expected optimal energy

Possible improvements:

- add tests (pytest) and reproductible examples (non-random)
- calculate runtime
- the lattice data structure