Apply quantum algorithms to protein structure prediction

Qcourse570

Faculty of Computing, University of Latvia | QWorld

19th May 2022

Our Project

- Our Model:
  - Hydrophobic-polar energy model (HP)
  - Tetrahedral Lattice
  - VQE algorithm

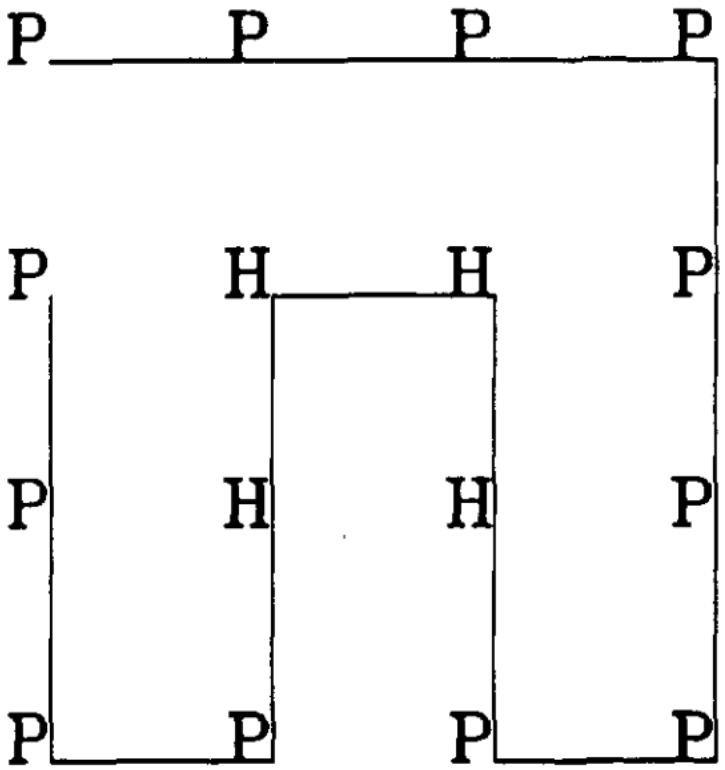
- VQE algorithm
  - ansatz: Real amplitude (Ry gates)
  - optimizer: COBYLA (scipy)

Hydrophobic-polar model (HP)

- Previous works (HP model):
  - Planar lattice
  - Cubic Lattice

- Protein as a linear chain of n amino acids
  - H (Hydrophobic or nonpolar)
  - P (polar)

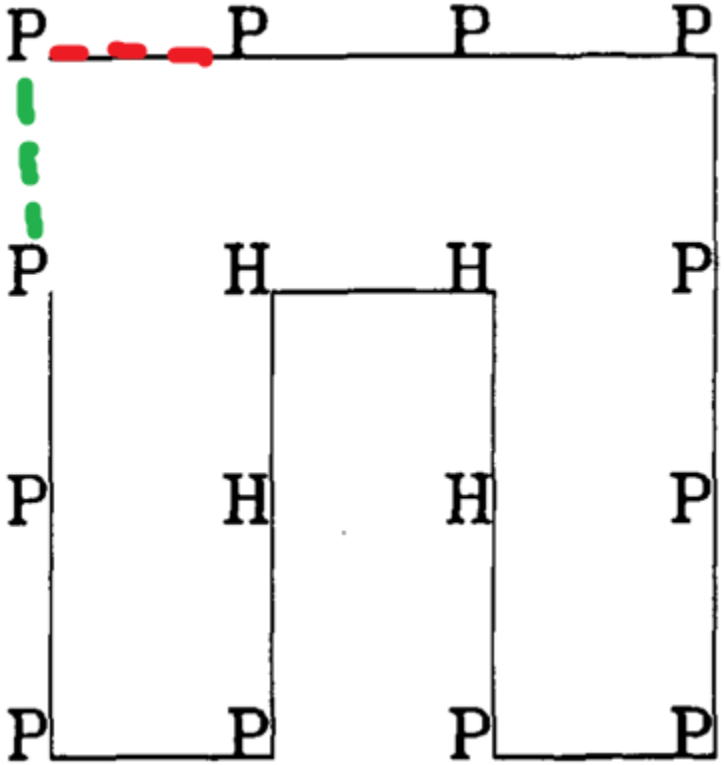
- Example (planar model):
  - PPPPPPPPHHHHPPPP
  - n = 16
  - 4×4 lattice



HP model

- Neighbors:
  - "connected neighbors": units j and j + 1 adjacent along the chain sequence
  - "topological neighbors": those that are adjacent in space (in contact) but are not adjacent in position along the sequence.

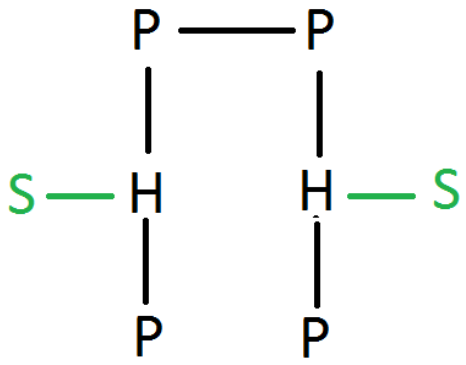
- Energy:
  - Only consider topological neighbor
  - HP and HS interaction (solvent)



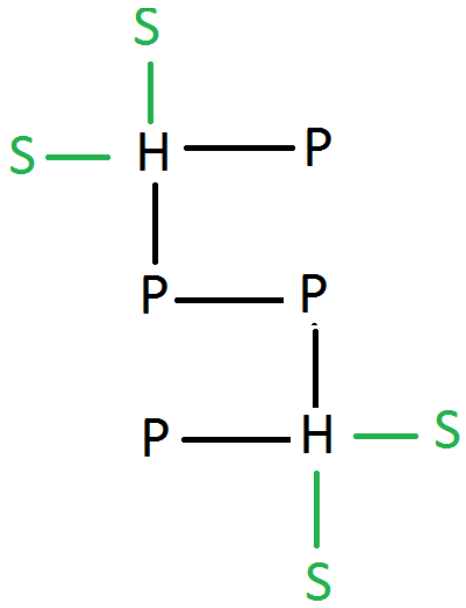
Example

- sequence: PHPPHP
- n = 6
- 3×2 Planar lattice

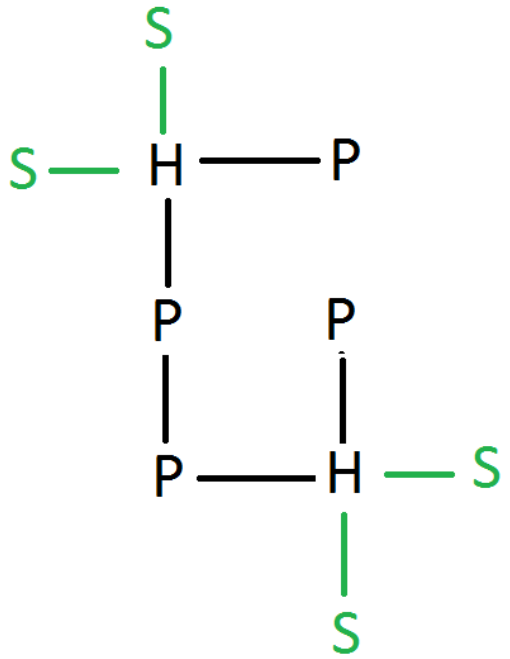
- Possible structures (3 structures)



2 interactions



4 interactions



4 interactions

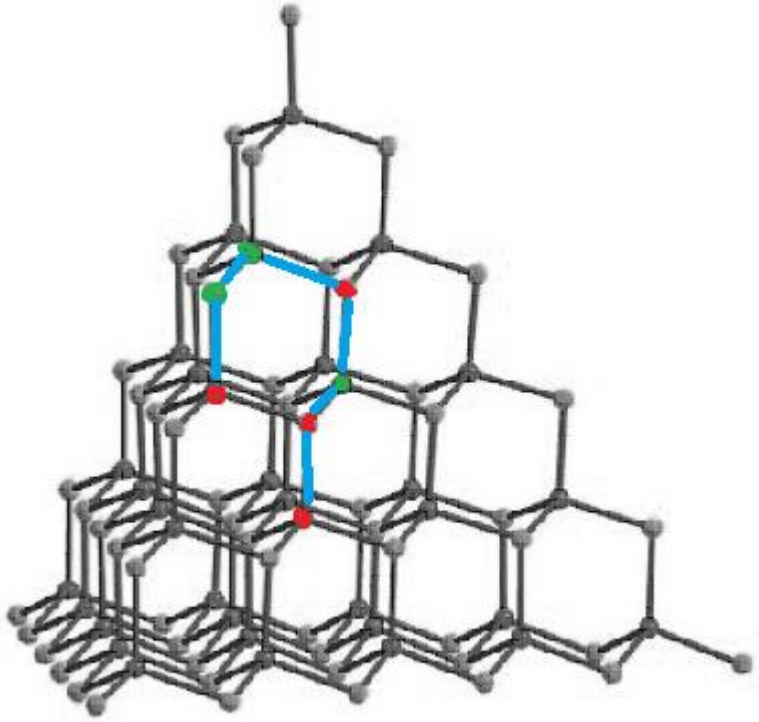
Protein

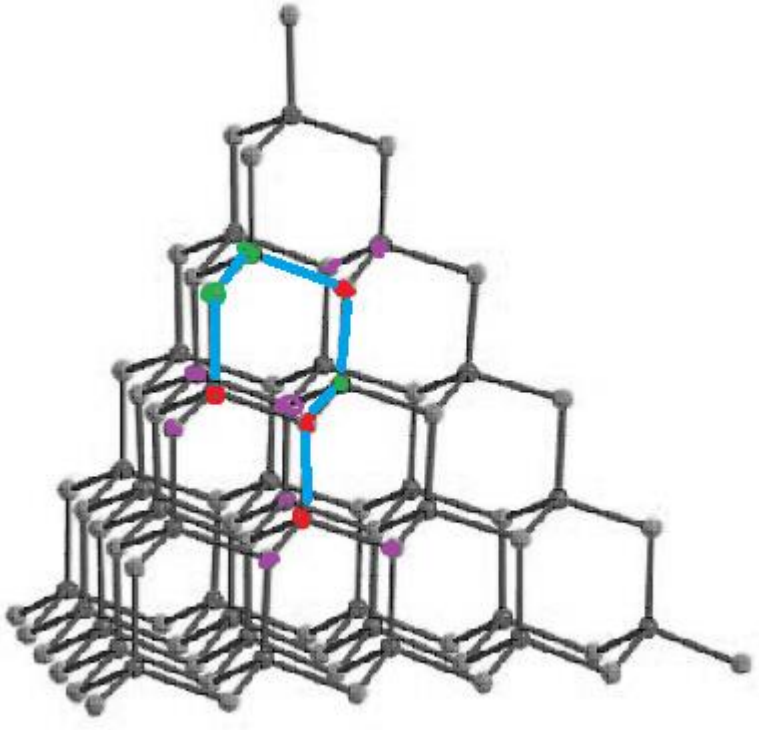
- Example:
  - APRLRFY
  - HPPHPHH

#	Amini acid	3-letter symbols	1-letter symbols	HP
1	Alanine	Ala	A	H
2	Arginine	Arg	R	P
3	Asparagine	Asn	N	P
4	Aspartate	Asp	D	P
5	Cysteine	Cys	C	H
6	Glutamine	Gln	Q	P
7	Glutamate	Glu	E	P
8	Glycine	Gly	G	P
9	Histidine	His	H	P
10	Isoleucine	Ile	I	H
11	Leucine	Leu	L	H
12	Lysine	Lys	K	P
13	Methionine	Met	M	H
14	Phenylalanine	Phe	F	H
15	Proline	Pro	P	P
16	Serine	Ser	S	P
17	Threonine	Thr	T	P
18	Tryptophan	Trp	W	H
19	Tyrosine	Tyr	Y	H
20	Valine	Val	V	H

Tetrahedral Lattice

- Example:
  - APRLRFY
  - HPPHPHH
- H (red) and P(green)
- Goal: minimize the purples (neighbors of H)





Thanks For Attention