

Folding solution

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Abstract

A drone-and-stick folding solution

An I-swarm of connected (using sticks) millimetric submarine spherical drones - like a variable ball-and-stick structure - could be used to simulate coronavirus enzymes.

If an I-swarm (colored spherical millimetric drones) is contained in a transparent viscous fluid, and the drones are propelled in the interaction with other drones using the measured distance (with drone sensors and the right propulsion force) to simulate the interactions, then the final configuration is the tertiary enzyme structure.

The tension in the sticks of the tertiary structure could be measured, so that the weakness of the enzymes could be explored for drug structures.

The macroscopic model could be made public, for drug research, using a standard for the tertiary structure and stick tensions.

The drone propulsion could be randomly varied (like the thermal fluctuation in the enzyme interactions) to overcome the local minima, in the search of the global minima: the NP folding problem is solved by the nature, so that an equivalent analog system could be a solution; if this is true, then each NP natural problem could be solved in the same way, simulating the system analogically.

The solution is not perfect¹ so that this could be an initial approximation for a numerical method.

The drones need to be robust, fault-tolerant and they must have an error control: they must be redundant, with multiple propulsion, multiple chipset and multiple sensors, so that an error in a component does not cause an error in the structure; it is conceivable that an incorrect drone could be automatically replaced with another drone (with an automatic movement of an efficient drone and an exchange), or with a manual procedure using a unveiling of the incorrect drone from the structure by associating a high (virtual) repulsive covalent charge to open the tertiary structure.

The rous sarcoma virus has 3500 base pairs, so that could be possible a complete simulation of the virus tertiary structure, with a number of atom-drones almost 35 times bigger.

¹the propulsion flow deforms the tertiary structure because of action-reaction law, but the viscosity disperses the flow, reducing the effect from the structure to the containment tank