

Re: Protein folding and P = NP

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mike3 wrote:

> *Hi.*

>

> *What would happen if an algorithm capable of performing highly
> accurate protein folding in polynomial time was found? Would it prove
> P = NP? And if it did, what would this lead to?*

The short answer is no, it would not prove P=NP.

The longer answer is that protein folding is not necessarily an NP problem. Many biological proteins fold quickly and reproducibly, indicating a wide, deep, unique basin of attraction and/or helper molecules to guide the folding path. Even proteins, such as the immunoglobulins, which take a long time to fold, do so reproducibly. If there were an exponential number of deep minima, reproducibility could not happen unless there was a much wider, deeper, unique basin of attraction and/or helper molecules guiding the folding sequence.

When biologists talk of the protein folding problem, they are talking about the class of proteins that are biologically relevant, which so far consist of the proteins that fold reproducibly.

For random polymers of amino acids, there is empirical evidence of a random energy landscape that does induce random glassy behavior in the conformational dynamics, but I don't know of any theorems proving that biologically realistic models are NP. You need to prove NP before finding a P folding algorithm and proving P=NP :)

–Mark