Solvation Experiments with Tangled Tubes

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In this talk I will present a computational tool developed to perform energy minimisation experiments on classes of curves. Each curve of the class, imagined as the centre line of an embedded tube, is of the same length and representative of the same knot. For our purposes, think of these objects as some what loosely tied knotted rope with fused ends. We perform computational experiments, which imagine these physical objects dissolving in a liquid, with the aim of investigating curve embeddings which minimise the thermodynamic potential energy of the fluid. Such an investigation is made possible by a simple geometric approach to the thermodynamics of solvation, which enables investigation of complicated solute geometries like knotted tubes. These are in turn simple models for long, much more complicatedly entangled soluble biomaterials, like proteins, which exist in the fluid environment of living cells. The interaction of the fluid and protein, a process which strives to decrease the thermodynamic potential energy of the system, is decisive for the protein's functionality. Here is our main motivation, to probe the interplay between form a function: How may entanglement influence the thermodynamically ideal embeddings of the dissolved tube?

This is joint work with my PhD supervisor Prof. Myf Evans of Potsdam Universitaet and our collaborator Prof. Roland Roth of the Universitaet Tuebingen.