Knots in proteins and polymers: some recent developments

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I will present several bridging algorithms which are suitable for simulation of globular phases of single polymers [1]. In this context, the determination of knots provides a measure for entanglement which allows us to gauge the efficiency of the move sets. The algorithm is applied to study semi-flexible polymers in spherical confinement as a model system for DNA in viral capsids and to random copolymers in globular states to study aspects of protein-like systems. We also predict entanglements of single polystyrene molecules in mini-emulsions which are currently investigated in ongoing experiments.

In the second part of my talk I will give a short overview of knots in proteins with a focus on structures discovered in the past three years [2].

[1] D. Reith, P. Virnau, Comput Phys Commun **181**, 800 (2010)
[2] D. Bölinger, J. Sulkowska, H.-P. Hsu et al, PLoS Comp Biol **6**, e1000731 (2010)