Towards controlled self-assembly of curved surfaces

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Inverse design problems are ubiquitous in material science as well as in complex biological and biologically inspired systems. In soft materials, designing of interactions for self-assembly allows for precise tuning of material structure, properties, and even kinetics. On the other hand, self-assembly of mesoscopic particles, such as synthetic hard particles, proteins or larger biological building blocks, is often affected by the curvature of the substrate. The particles themselves can influence this curvature or even assemble into curved structures on their own. Understanding how to manipulate the curved geometry of assemblies can elucidate new ways of tuning properties of functional soft materials.

In this seminar, I will discuss how we can target self-assembly into surfaces with specified curvature in systems of model patchy particles. I will start by presenting the automatic differentiation-based approach to inverse design that allows us to determine parameter gradients by differentiating through self-assembly kinetics. I will discuss challenges that arise when we differentiate through long time sequences, such as exploding gradients, and possible ways to mitigate them. Finally, I will show some preliminary results of controlled assembly into curved structures.