Sonderforschungsbereich 1060

The Mathematics of Emergent Effects

Einladung zu einem Vortrag im SFB-Seminar

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spricht zum Thema

Self-Assembly: Variational models, Energy Landscapes, and Metastability

Zeit: Dienstag, den 25. November 2014, 14.15 Uhr

Ort: Raum 0.011, Endenicher Allee 60

Kaffee/Tee: anschl. im Hausdorff-Raum

gez. **Sergio Conti**

Abstract: Self-assembly, a process in which a disordered system of preexisting components forms an organized structure or pattern, is both ubiquitous in nature and important for the synthesis of many designer materials. In this talk, we will address three variational models for self-assembly from the point of view of mathematical analysis and computation.
The first is a nonlocal perturbation of Coulombic-type to the well-known Ginzburg-Landau/Cahn-Hilliard free energy. The functional has a rich and complex energy landscape with many metastable states. I will present a simple method for assessing whether or not a particular computed metastable state is a global minimizer. The method is based upon finding a "suitable"global quadratic lower bound to the free energy.
The second model is a purely geometric and finite-dimensional paradigm for self-assembly which generalizes the notion of centroidal Voronoi tessellations from points to rigid bodies. Using a level set formulation, we a priori fix the geometry for the structures and consider self-assembly entirely dictated by distance functions. I will introduce a novel fast algorithm for simulations in two and three space dimensions.