Gero Friesecke

Crystallization in classical particle systems

The emergence of crystalline order is ubiquitous in physics, biology, and mathematics: atoms self-assemble into three-dimensional crystals; messy-looking proteins assemble into perfectly regular two-dimensional virus shells; densest sphere packings appear to be crystalline. Related effects appear in continuum models (vortex lattices in nonlinear Schroedinger equations; periodic Voronoi tesselations in optimal transport). Mathematically, these phenomena are subtle. Previous understanding for 2D classical particle systems by pioneers like Heitmann, Radin, Theil, Mainini, Stefanelli relies on highly technical, puzzlingly detailed, model-specific estimates. After a general introduction, I present a new viewpoint inspired by continuum mechanics which rigorously and exactly decomposes discrete 2D many-particle energies into elastic, surface, defect, and topological contributions, via methods from discrete differential geometry (used for the first time in crystallization problems). This approach, developed jointly with Lucia De Luca (Rome), yields a much simpler proof of the Heitmann-Radin crystallization theorem, and appears to be very promising for future research.