TEMPLE UNIVERSITY
Department of Mathematics

Applied Mathematics and Scientific Computing Seminar

Room 617 Wachman Hall

Wednesday, 25 February 2017, 4:00 p.m.

Approximate Global Minimizers to Pairwise Interaction Problems Through a Convex/Non-Convex Energy Decomposition: With Applications to Self-Assembly

by David Shirokoff
New Jersey Institute of Technology

Abstract.

A wide range of particle systems are modeled through energetically driven interactions, governed by an underlying non-convex and often non-local energy. Although numerically finding and verifying local minima to these energies is relatively straight-forward, the computation and verification of global minimizers is much more difficult. Here computing the global minimum is important as it characterizes the most likely self-assembled arrangement of particles (in the presence of low thermal noise) and plays a role in computing the material phase diagram. In this talk I will examine a general class of model functionals: those arising in non-local pairwise interaction problems. I will present a new approach for computing approximate global minimizers based on a convex/non-convex splitting of the energy functional that arises from a convex relaxation. The approach provides a sufficient condition for global minimizers that may in some cases be used to show that lattices are exact, and also be used to estimate the optimality of any candidate minimizer. Physically, the approach identifies the emergence of new length scales seen in the collective behavior of interacting particles.