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Computational Mathematics Seminar Series

Approximate Global Minimizers to Pairwise Interaction Problems Through a Convex/non-convex Energy Decomposition: With Applications to Self-assembly**David Shirokoff, New Jersey Institute of Technology**Lockett Hall 233
February 13, 2017 - 03:30 pm**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.

Speaker's Bio:

David completed his undergraduate degree at the University of Toronto, followed by a Phd in applied mathematics from MIT under Rodolfo Ruben Rosales. Prior to arriving at NJIT, he was a postdoctoral fellow in the mathematics department at McGill university with J-C. Nave and Rustum Choksi.

