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Conic programming of a variational inequality for self-assembly

In this talk we examine a class of non-local, non-convex functionals that describe pairwise interactions in systems with a large number of particles. Although finding and verifying local minimizers to these energies is relatively straight-forward, the computation and verification of global minimizers is much more difficult, Here the global minimum is important as it is the most likely observable state in the presence of low thermal noise. We discuss how minimizing the energy functional can be viewed as testing whether an associated bilinear form is co-positive. We then examine sufficient conditions for global optimality which are obtained through a convex relaxation of the cone of co-positive functionals. The sufficient conditions are (i) sometimes sharp (for instance, in the case of a lattice minimizer), (ii) provide an optimal decomposition of the original energy functional into a convex/non-negative energy decomposition, and (iii) can also be used as a heuristic (with rigorous lower bounds) to compute the emerging shapes of self-assembled structures. It is conjectured that the solutions to the heuristic equations are also, in some cases, globally optimal.