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Crowdsourcing the Phase Problem: Progress in Low Resolution Ab Initio Phasing

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Solving molecular structures from X-ray diffraction data without knowledge of the phases is an example of an inverse problem. Solving such problems requires searching a potentially high dimensional parameter space (e.g. of phases) and recognizing when a correct solution is encountered. Computers are good at performing rapid searches, whereas teaching a computer to recognize subtle patterns is generally challenging. Humans are naturally better at the latter task, but lack the search speed required for many scientific problems. We have begun experiments to 'crowd-source' the ab-initio phase problem in crystallography by harnessing the pattern recognition capabilities of a large group of human game players to drive a computational search for good phase sets given only low resolution structure factor magnitudes [1]. The search framework is based on a genetic algorithm; each 'individual' in a population has a genome that encodes a set of (initially random) phases for the given diffraction magnitudes. In an iterative procedure of Darwinian evolution (i.e. survival of the fittest), human gamers use a multi-player web-interface (CrowdPhase) to select the most fit individuals for survival based on the qualities of their corresponding electron density maps. Through mutation, recombination, and selection, the population then evolves over many generations toward a final solution. Preliminary experiments with groups of users numbering around 20 show that good phases can be obtained for very low resolution test problems. New results on more challenging test cases will be discussed.

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