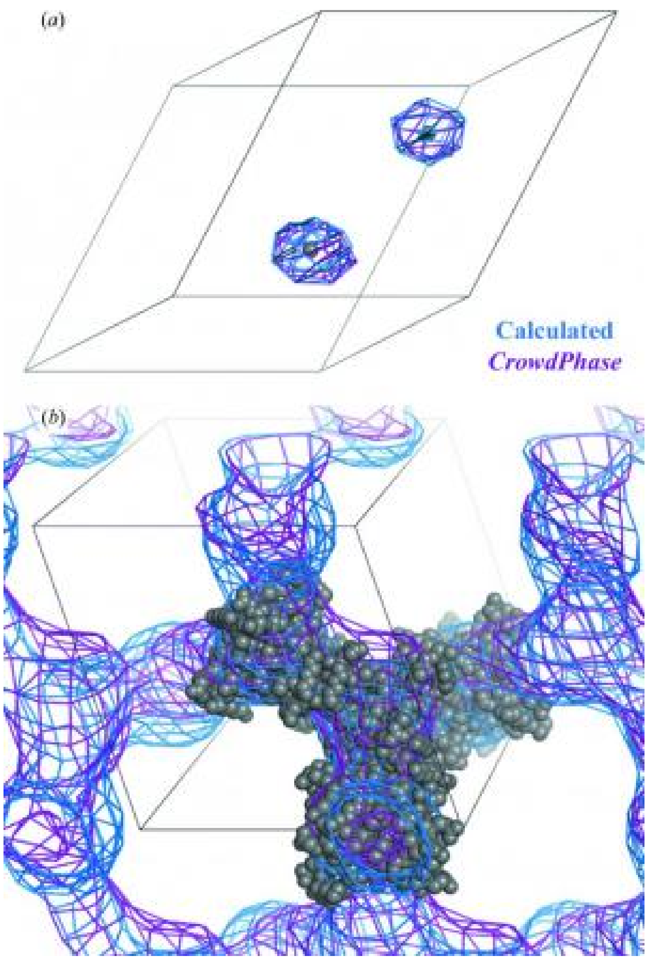
PHYS.ORG

Crowdsourcing the phase problem

June 17 2014, by Jonathan Agbenyega



This is an overlay of electron-density maps calculated from the final crowdsourced phase solutions and the true phases for the two test cases. Credit: Jorda et al./International Union of Crystallography

Compared with humans, computers have the capacity to solve problems at much greater speed. There are many problems, however, where computational speed alone is insufficient to find a correct or optimal solution, for example because the parameter "space" cannot be fully searched in a practical time. In contrast, the human mind can formulate expert knowledge specific for particular problems, providing a capacity to guide more efficient searches, although with more limited processing speed.

The power of the human contribution can be multiplied through the efforts of a greater number of individuals. The term `crowdsourcing', which combines the two domains of human and electronic computing, was coined in 2006 and since then has seen its definition broadened to a wide range of activities involving a network of people.

A challenging problem that might benefit from crowdsourcing is the phase problem in X-ray crystallography. Retrieving the phase information has plagued many scientists for decades when trying to determine the crystal structure of a sample.

In a diffraction experiment, the observed diffraction pattern allows measurement of the amplitudes of the reflection structure factors (as the square root of the intensities) but not their phases. The amplitudes and phases are both needed to reconstruct an electron-density map (by Fourier synthesis) so that a model of the crystallized molecule can be obtained.

There are a number of ways currently scientists try to solve the phase problem, all with varying degrees of success.

Regardless of the particular approach, most attacks on the phase problem can be viewed as having two sub-problems. One concerns how a high-dimensional space (i.e. of phases) can be efficiently searched, while the other concerns how a good solution can be recognized.

Crowdsourcing may be a route to solving these sub-problems [Jorda et al. (2014), *Acta Cryst*. D70, 1538-1548; doi:10.1107/S1399004714006427], here scientists have developed a game based on a genetic algorithm (a powerful search-optimization technique), where players control the selection mechanism during the evolutionary process (by recognising the good solutions). The algorithm starts from a population of "individuals", in this case a map prepared from a random set of phases, and tries to cause the population to evolve towards individuals with better phases based on Darwinian survival of the fittest. Players apply their pattern-recognition capabilities to evaluate the electron-density maps generated from these sets of phases and to select the fittest individuals.

The game called CrowdPhase was applied to two synthetic low-resolution phasing puzzles and it was shown that players could successfully obtain phase sets in the 30 degree phase error range and corresponding molecular envelopes showing agreement with the low-resolution models.

Successful preliminary studies suggest that with further development the crowdsourcing approach could fill a gap in current crystallographic methods by making it possible to extract meaningful information in cases where limited resolution might otherwise prevent initial phasing.

Provided by International Union of Crystallography

Citation: Crowdsourcing the phase problem (2014, June 17) retrieved 24 April 2024 from https://phys.org/news/2014-06-crowdsourcing-phase-problem.html

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