Stochastic molecular replacement with powder diffraction data

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Molecular replacement methods that do not rely on the properties of the Patterson function to reduce the dimensionality of the search space appear to offer an advantage in the case of powder diffraction-derived data: In essence, the availability of a complete model of the target crystal structure (ie. the knowledge of both rotational and translational parameters of all of the search models) allows molecular replacement problems to be treated in the context of a stochastic Rietveld-like rigid-body refinement problem. A multidimensional, multimodel approach like the one implemented in the program 'Queen of Spades', retains these advantages even for molecular replacement problems that include several search models per asymmetric unit.
An attempt to modify this program for dealing with powder diffraction data (and using a correlated integrated intensities approach) is currently underway. The availability of this modified version of 'Queen of Spades' would also allow us to test its usability as a heavy-atom search procedure for powder diffraction data [in which case the search model would be just one heavy atom and the dimensionality of the search space would be (3n), where (n) is the number of heavy atoms per asymmetric unit].