Monte Carlo Search with Many CPUs: Application to 6 dim. Molecular Replacement

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Monte Carlo search is the simple method that the solution is searched by iterating the many trials for given random parameters. By randomness, every trial is assured that the searching region is different from that of the rest. And, all the trials are completely independent, that is, it is not necessary to wait the result of the other trials at all. With this method, we are able to flexibly use the whole power of many CPUs without losing its efficiency.

It is able to use a lot of computers by a modern internet technology. If it is a calculation to which the Monte Carlo search method can apply, it is possible to achieve it comparatively easily even by an enormous calculation.

We applied this method to search the six dimensional parameters at once for rotation and translation of the molecular replacement method. An initial model was obtained for the unknown protein molecular structure: SHPS-1. It was hard to find solutions by traditional way, because the peaks of the correct solutions for rotation functions are low as about two sigma level of random noises.

Space group of the crystal is P622 and the size of the cell is long as about 100 angstrom. There are two molecules in asymmetric unit. To find the correct solutions, it took about 10 days by using at most 30 various kinds of CPUs "non-exclusively".

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