PS02.06.19 MOLECULAR REPLACEMENT METHOD USING A PARALLEL PROCESSING MACHINE. V.S.Yadava and K.K.Kannan Solid State Physics Division,Bhabha Atomic Research Centre,Bombay-400 085,INDIA.

The molecular replacement method involves six parameters - three rotational and three translational and the correct orientation and position is identified by calculating R-factor at each grid point.

Time requirement: The six-dimensional search requires very large amount of computer time. For a moderate size protien like Carbonic Anhydrase with about 2000 atoms in the molecule and 2000 reflections to 5A requires 20 minutes of cpu time on a Landmark 860 machine for structure amplitude calculations at 1.5Å resolution along the axes for each orientation. For a coarse search with steps of 5 degree in Eulerian angles there are 46656 orientations which require 648 days of computer time. However, with a 64-node parallel-processing system the time required is10 days of the machine time and can be further reduced by using more nodes and faster machines. Program implementation: As the calculations for each orientation are independent of that for others, the different orientations are equally distributed between different nodes. Each node has all the information for calculating structure amplitudes and Rvalue.

Results: The method has been tested first with Human Carbonic Anhydrase (HCA) I data and the same protein as model structure. Next HCA II was used as the model structure for obtaining structure of HCA I. Lowest R-value corresponded to correct orientation and position in both the cases.