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Constitution

The Maximum Entropy Method Project on Charge , Spin and Momentum Densities. The Maximum Entropy Method (*MEM*) is rapidly gaining ground in X–ray Crystallography. In the field of Charge, Spin and Momentum Densities we now see increasing use of it. At the last Sagamore conference in Brest, France in 1944, the *MEM* was the subject of a full session and later on it was discussed at the meeting of the Commission on Charge, Spin and Momentum Densities. Under these circumstances, it was decided to start a project on *MEM*, in close cooperation with a project on multipole refinements, following a suggestion made at the open Commission meeting at the Beijing conference in 1993. The aim of the project is to gain information on the usefulness of the Maximum Entropy Method for the study of Charge, Spin and Momentum Densities. All the scientists who are willing to join the project in carrying out the activities of the project are welcome and are requested to contact to one of the steering committee members. If the participants wish to have *MEM* calculation program, it is possible to obtain the program called *MEED* by an anonymous ftp. (ftp://hod.nuap.nagoya–u.ac.jp/pub/ftp.html) There will be no restrictions on methods of *MEM* data analysis or interpretation of the results, and publication of their work by participants will not be restricted in any way. The results of the project will be published and are accessible to all the crystallographers who are interested in the method. To meet the object of the project,we envisage a number of activities. They are as follows.

1. Survey of the work. It is desirable to establish the easy accessible system through which the information concerning the following questions can be obtained such as which results have been obtained as yet or which computer programs exists.

2. A critical analysis of the results. Is the same result obtained when a set of data is analysed by different groups, using different programs and/or applying the programs in different ways? If there is any difference, it is essential to understand how significant the difference is. In order to have better results, many factors must be reconsidered. Through these survey, it is hoped to establish
    1. a weighing scheme,
    2. an appropriate initial density,
    3. suitable experimental conditions for *MEM* analysis

3. Comparison between the algorithm of the computer programs in use. It is highly desirable to understand the most efficient algorithm for the *MEM* calculation. It is also desirable to understand the limitation of the *MEM* computer programs, if it is possible.

4. Further analysis of the *MEM* densities. It is possible to further analyse the *MEM* densities in terms of sophisticated models thus allowing a more quantitative description of the underlying density. Characterization of the density by its topological properties represents a further possibility.

5. Other important questions are:
    1. how to estimate the accuracy of the *MEM*> charge densities,

[1] http://www.iucr.ac.uk/welcome.html
[2] http://www.tuwien.ac.at/theochem/iucr/csmd.html
[3] http://www.nuap.nagoya–u.ac.jp/~sakata/act/MEM.html
[4] http://www.nuap.nagoya–u.ac.jp/~sakata/TOPE.html

2. how to avoid any pitfalls of the method such as artefacts.

6. Theoretical background of *MEM* The MEM project is concerned with *MEM* as a tool for determining Charge, Spin and Momentum Densities from diffraction data. In order to guide the use of MEM in this application, it is desirable to have a better understanding of its theoretical background. Although philosophical discussions of *MEM* are outside the scope of the project, it is hoped that the project will lead to better use of *MEM* as a tool, and that the project results will be useful in many other discussions and applications.

It is hoped the project encourage people to tackle above questions. The members of the steering committee of the project are as follows,

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[MEM project] [[13] Examples] [[14] Reference] [15]

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15 refer.html