many nano-materials, or not crystalline at all, such as glasses. In some cases crystalline and amorphous phases coexist making the traditional crystallographic structure refinement difficult or incomplete. The total scattering pattern, however, contains structural information over all length scales [1] and can be used to obtain a complete structural picture of complex materials.

Here we present different applications of this technique including data taken on the new high resolution neutron powder diffractometer NPDF located at the Lujan Neutron Scattering Center at Los Alamos National Laboratory. This instrument is design for total scattering studies using the Pair Distribution Function (PDF) approach. We hope to attract many new users to use total scattering as a tool to fully characterize their materials structurally.

[1] Proffen Th., Billinge S.J.L., Egami T., Louca D., *Z. Krist.*, 2003, **218**, 132-143.
Keywords: pair distribution function, powder diffraction, disorder

P.02.17.4
Structure Determination from a Quantum Mechanical Formulation in Momentum Space
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The proposed method aims at the crystal structure determination by using the theoretical background of quantum mechanics. This is achieved through the quantum mechanical formulation in momentum space by means of the Fourier Transform (FT) of the usual Schrödinger equation in direct space. The key step is the identification of the FT of the potential function $V(r)$ with the expression $E(H)/H^2$ where $E(H)$ is the normalized structure factor. An algorithm has been developed for practical implementation of this new method for direct phasing of x-ray data [1]. In this algorithm a new criterion, based on the crystallographic symmetry, has been introduced. The idea consists of testing the phase calculation, extension and refinement, by deliberately sacrificing the space group symmetry information and using its gradual re-appearance as a criterion of correctness [2].

New theoretical developments relevant to the convergence of this algorithm in different cases have been formulated. An upgraded algorithm for macromolecules has also been developed and tested in phase extension and refinement with promising results.

[1] Bethanis K., Tzamalis P., Hountas A., Tsoucaris G., *Acta Cryst.*, 2002, **A58**, 265-269. [2] Tzamalis P., Bethanis K., Hountas A., Tsoucaris G., *Acta Cryst.*, 2003, **A59**, 28-33.
Keywords: algorithm, phase problem, quantum mechanics

P.02.17.5
Molecular Replacement via Normal Mode Analysis and Homology Modelling on the Web
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Molecular replacement (MR) is the method of choice for X-ray crystallography structure determination when structural homologues are available in the Protein Data Bank (PDB). However, the success rate of MR decreases sharply when the sequence similarity between template and target proteins drops below 35% identical residues. Another reason for MR failure are conformational differences between target and template, induced for example by ligand binding or different crystallogenic conditions. It has been found that screening for MR solutions with a large number of different homology models or models that are perturbed in the direction of one or two low frequency normal modes may still produce a suitable solution where the original template failed [1-3]. Here we present the web tools *elNémo* [2] and *CaspR*, [3] that implement such strategies in an automated manner. *elNémo* is accessible at http://igs-server.cnrs-mrs.fr/elnemo/, *CaspR* at http://igs-server.cnrs-mrs.fr/Caspr/.

[1] Suhre K., Sanejouand Y.H., *Acta Cryst. D*, 2004, **60**, 796-799. [2] Suhre K., Sanejouand Y.H., *Nucleic Acids Research*, 2004, **32**, W610-W614. [3] Claude J.B., Suhre K., Notredame C., Claverie J.M., Abergel C., *Nucleic Acids Research*, 2004, **32**, W606-W609.
Keywords: crystallography, phasing, template perturbation

P.02.17.6
HUNTER: A Package of small Tools to Manipulate FOX
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The HUNTER package consists of a number of small programs for handling the .xml-input files of the simulated annealing program FOX [1]. By use of simple scripts HUNTER allows to set up genetic algorithm techniques [2] for crystal structure determination. In this context the simulated annealing serves as Lamarckian [3] component of the evolution process. The package can also be used to explore possible neighboring minima to a current local minimum of the structure cost function. This is accomplished by sophisticated application of reorientations of randomly chosen molecules or building groups.

The individual tools currently available are: MATE, which produces a new file from two parent files by choosing randomly position, orientation and content of each molecule (or atom) from one of the parent files. ORIENTATION locates the main axes of a random molecule and applies a randomly chosen reorientation of twofold symmetry. DEFORMATION applies a rotation to a randomly chosen group of atoms using a user-defined list of groups and rotation axes. FITNESS extracts the cost function from the files written by FOX and stores it into the .xml-file, using either the current cost minimum or an exponentially extrapolated value. SELECTION sorts structure files by their fitness. Additional programs will complement the package.

[1] Favre-Nicolin V., Černý R., *Z. Krist.*, 2004, **219**, 847. [2] Harris K.D.M., Habershon S., Cheung E.Y., Johnston R.L., *Z. Krist.*, 2004, **219**, 838. [3] Turner G.W., et al., *Chem. Phys. Lett.*, 2000, **321**, 183. **Keywords: structure solution, software, powder diffraction**

P.02.17.7
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".

P2

Keywords: computing method, Monte Carlo treatment, molecular replacement

P.02.17.8
Optimization of Genetic Algorithm Techniques for Powder Structure Solution
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With advances of direct space strategies for structure solution from powder X-ray diffraction data [1,2], and in particular the success of the Genetic Algorithm method [3], structural problems in a variety of fields are being tackled using information from powder data. Applications to study the structures of increasingly complex molecules present new challenges. Increasing the number of degrees of freedom leads to a concurrent increase in the size of the search space. Implementing a combination of other figures of merit, such as energy together with R-factor, provides an opportunity for optimization of the search space, leading to enhanced rates of success of structure solution. Systematic testing results show that the method is both general and applicable to a number of different problems without a simultaneous increase in computational time required.

[1] Harris K.D.M., Tremayne M., Lightfoot P., Bruce P.G., *J. Am. Chem. Soc.*, 1994, **116**, 3543. [2] Harris K.D.M., Tremayne M., Kariuki B.M., *Angew. Chemie Int. Ed.*, 2001, **40**, 1626. [3] Kariuki B.M., Serrano-González H., Johnston R.L., Harris K.D.M., *Chem. Phys. Lett.*, 1997, **280**, 189.
Keywords: powder structure determination, computing in crystallography, crystal structure solution

P.02.17.9
Removal of the Phase Problem by the Atomicity Assumption
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In the late twenties Ott[1] showed that, once the atoms are treated as point-like objects, the positions of the atoms present in the unit cell of an ideal crystal are the roots of a set of polynomial equations whose coefficients are determined by a finite set of unitary structure factors. This result was later generalized by Avrami[2] showing that the positions of the peaks of the infinitely resolved Patterson map are the roots of a system of polynomial equations determined from the knowledge of a finite set of reflection intensities. Ott's results were later rediscovered and generalized[3] within the framework of Goedkoop's vectorial formulation of the phase problem. The point missing in these analyses is the algorithm able to select the (smallest) set of the reflections such that the corresponding intensities determine a resolvent system of polynomial equations. This problem was fully solved recently in the case of x-ray scattering[4] and, in this contribution, the proof is extended to the case of neutron scattering.

[1] Ott H., *Z. Kristall.*, 1927, **66**, 136. [2] Avrami M., *Phys. Rev.*, 1938, **50**, 300. [3] a) Navaza J., Silva A.M., *Acta Cryst.*, 1979, **A35**, 266; b) Navaza A., Navaza J., *Acta Cryst.*, 1992, A **48**, 695; c) Rothbauer R., *Z. Kristall.*, 1998, **213**, 195. [4] a) Cervellino A., Ciccariello S., *Riv. Nuovo Cim.*, 1996, **19**, 1; b) Cervellino A., Ciccariello S., *J. Phys. A: Math.*, 2001, **34**, 731.
Keywords: algebraic approach, basic sets of reflections, resolvent equations