Oral Contributions

[MS44-05] Powder data indexation by parallel GPU accelerated grid search method. Michal Hušák,a Ivan Šimeček,b Jan Rohlíček,a a

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Finding the unit cell is a starting and also an unavoidable point of the crystal structure determination process from powder diffraction data. Due to the loss of the 3D information we are unable to reconstruct the 3D reciprocal space directly from the measured data. Therefore, the unit cell has to be found from the measured 1D pattern. This is not a trivial task and, unfortunately, in many cases it is still an unrealizable dream (e.g. large unit cell or one very small unit cell parameter compared to the others).The unsuccessful attempts to determine lattice parameters lead to the impossibility of determining the whole crystal structure. Following study [1] had demonstrated that brute force algorithms based on simulated annealing (McMaille implementation) or systematic search so-called grid search can better solve some complex problems, in comparison to the old fine tuned sophisticated algorithms. Unfortunately there exist a key problem of the grid search method ¬it take a lot of computing time. Existing computer hardware gives us a chance to implement indexation algorithms in a non¬standard way utilizing brute force method. This can make possible to solve several mentioned problematic situations not covered fully by existing methods. We had implemented a grid search based algorithm executing the main part of the calculation by massive parallel processing in multi-core CPU or even faster by GPU calculation on the graphic card shader units. The whole indexation process in the multigrid method is divided into three stages (all are repeated until all possible combinations of direct lattice parameters are evaluated): 1) Procedure GENERATE – it generates all possible combinations of direct lattice parameters with given step until buffer is filled. The buffer contains a large number of sets of tested reciprocal lattice parameters (or a subset of these parameters, depending on the crystal system). In current version, this procedure is single-threaded. 2) Procedure EVALUATE -buffer is sent to CPU or to GPU. The CPU/GPU evaluate the number of indexed lines for all elements in buffer. Results of this procedure are sent back to CPU. In current version, this procedure is executed by GPU using CUDA API or by the multithreaded CPU code. 3) Procedure VERIFY -the promising lattice parameters are optimized by least-squared refinement. The ”figures of merit” (M20 by de Wolff [2], F20 by Smith and Snyder [3]) are calculated and stored into result database. In current version, this procedure is executed by the multithreaded CPU code. The algorithm was tested on multiple examples In comparison to the execution of the grid search on a single core CPU, the speed up during execution on a graphic card (GeForce GTX 590) is in 17x-63x range, in comparison to quad core CPU, the speed up is in the 4x¬16x range. Current code version is available as an executable for Debian Linux and Windows. For the GPU acceleration, a nVidia graphic card with CUDA support is required. We believe that after the code optimization the grid search method executed on GPU can be executed in a reasonable time and become a tool for difficult problems indexations.

[1] Bergmann J., LeBail A., Shirley R., Zlokazov V. (2004). Z. Krystallogr. 219,783-790
[2] Wolff P.M. (1968). J. Appl. Cryst.1,108-113
[3] Smith G.S., Snyder R.L.(1979). J. Appl. Cryst.12, 60-65

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