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Borrowing HEP algorithms for detector alignment in photon science

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Accurate and precise information about the position of the detector is critical to the success of many types of experiment in photon science. This is particularly true for serial crystallography, which is sensitive to detector misalignments of less than one pixel's width. However, serial crystallography data is also very useful for refining the detector geometry, consisting of sharp, bright Bragg peaks in regular and geometrically simple patterns. Several methods have been developed for this process over the last decade. The current state of the art involves refining the "global"detector geometry parameters along with the "local"crystal orientation parameters, in one very large least-squares refinement. The joint refinement of local and global parameters is needed to avoid a biased fit and slow convergence. Unfortunately, with a typical serial crystallography dataset consisting of many tens of thousands of crystals, only a fraction of the data can be used before the refinement becomes too computationally demanding.

The "Millepede"algorithm was developed in high energy physics to address exactly this problem. The relevant matrix equations can be rearranged such that the full calculation can be performed, without approximations but with vastly reduced memory and CPU requirements. This makes a full joint refinement using tens or even hundreds of thousands of crystals practical.

In this contribution, I will describe the ongoing experience of applying the Millepede algorithm to serial crystallography data, and the potential for other applications in photon science.

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