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Improved direct-method aided iterative dual-space model completion

Y. He[1], D. Yao[3], S. Huang[4], T. Zhang[1], Z. Lin[2], Y. Gu[1], H. Fan[1]

[1]*National Laboratory for Condensed Matter Physics and Institute of Physics, CAS, Beijing, P. R. China,* [2]*Institute of Biophysics, Chinese Academy of Science, Beijing, P. R. China,* [3]*Institute of Biochemistry and Cell Biology, Shanghai Institutes for Biological Sciences, Chinese Academy of Sciences, Shanghai, P. R. China,* [4]*Shanghai Synchrotron Radiation Facility, Shanghai, P. R. China*

It has been proved that direct methods are efficient in providing phase constraints within the dual-space phase-model iterative framework [1]. The program OASIS is used for the direct-method implementation. Two kinds of iterative direct methods are performed by OASIS. One involves the use of SAD/SIR information [2], while the other dose not [3]. Improvements have been made on both kinds of iterative direct methods. First, the Srinivasan's weighting function replaces previously used Sim's weighting function in the direct-method phase derivation leading to better estimation of phases. This affects both kinds of direct-method iteration. Second, the process of the second kind direct-method iteration has been made multi-threaded and parallel. This significantly speeds up the iteration in multi-CPU systems. Finally, a new figure of merit combining the R factor and Srinivasan's weighting function is used to pick up the best partial structure instead of using the R factor alone. The improved procedure has been tested using a set of SIRAS data from the protein LegC3N with Hg-derivative at 5.0Å resolution and native at 2.1Å resolution. With the previous version of OASIS, SAD phasing at 5.0Å resolution was successful but phases were failed to extend to the 2.1Å resolution native data as is described in §3.2 of [1]. However the new version of OASIS has succeeded in extending 5.0Å resolution SAD phases to 2.1Å resolution native phases leading to a nearly complete structure model.

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