

OASIS-2004 and Difficult SAD Phasing

Haifu Fan^a, Yuanxin Gu^a, Jiawei Wang^a, Sheng Huang^b, Chaode Zheng^a, Xiaodong Su^c, Yuhe Liang^c, Jie Nan^c, ^a*Institute of Physics, Chinese Academy of Sciences, Beijing 100080, China.* ^b*Institute of High Energy Physics, Chinese Academy of Sciences, Beijing 100039, China.* ^c*Life Science College, Peking University, Beijing 100871, China.* E-mail: fanhf@cryst.iphy.ac.cn

OASIS [1] is a direct-method program for resolving the phase ambiguity in single-wavelength anomalous diffraction (SAD) and in single isomorphous replacement (SIR) of proteins. The new version, OASIS-2004 includes algorithms for automatically tuning the scaling factor associated to the lack-of-closure error and for dynamically incorporating known structure fragment(s) in the iterative direct-method phasing. Details of the phasing strategy will be described. Application to SAD data from a series of known as well as originally unknown proteins will be given. The data sets were collected either with synchrotron radiation or with in-house sources (Cr-K α and Cu-K α) X-rays. Among the applications, an originally unknown protein with more than a thousand amino acids in the asymmetric unit has been solved with Cr-K α sulfur-SAD data. Good quality phases have been successfully derived from sulfur-SAD data at the Bijvoet ratio $\langle |\Delta F| \rangle / \langle F \rangle$ lower than 0.6%. In all cases the combination of programs OASIS-2004, DM, RESOLVE-BUILD and ARP/wARP enabled automatic structure analysis from *ab initio* SAD phasing to model building. All resulted in a model containing more than 90% of the content of the asymmetric unit.

[1] Hao Q., Gu Y. X., Zheng C. D., Fan H. F., *J. Appl. Cryst.*, 2000, **33**, 980-981.

Keywords: SAD phasing, direct methods, proteins