

pyDiSCaMB: enabling the use of multipolar scattering factors in Phenix

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Multipolar scattering factors expand upon the established Independent Atom Model (IAM) used when calculating scattering factors in Phenix [1]. The DiSCaMB software library [2] was written with multipolar scattering in mind, and supports e.g. Transferrable Aspherical Atom Model (TAAM) and Hirshfeld Atom Refinement (HAR). However, as Phenix is written in a mix of Python and C++, and Discamb is written independently in C++, multipolar calculations with DiSCaMB have thus far remained unavailable in Phenix.

To facilitate integration with Phenix, we developed pyDiSCaMB, a Python wrapper for DiSCaMB. This wrapper is designed to interface with *cctbx*, the underlying library of Phenix. pyDiSCaMB can be used as a standalone library, but its implementation within *cctbx* lets users leverage the extensive toolkit available for e.g. structure refinement. As an example, the control flow when using *phenix.refine* with pyDiSCaMB as the backend for TAAM structure factor calculations is presented in Fig. 1, showing how pyDiSCaMB acts as a translation layer between the two libraries. Developer versions of *cctbx* and Phenix already support TAAM calculations via pyDiSCaMB, and will soon be publicly available.

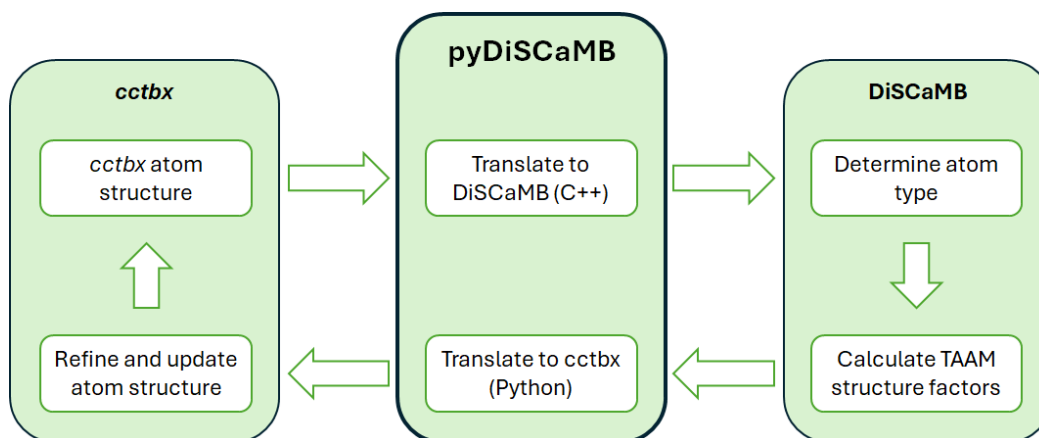


Figure 1. Control flow when running *phenix.refine* with TAAM scattering factors using pyDiSCaMB.

[1] Adams, P. D., Afonine, P. V., Bunkoczi, G., Chen, V. B., Davis, I. W., Echols, N., Headd, J. J., Hung, L.-W., Kapral, G. J., Grosse-Kunstleve, R. W., McCoy, A. J., Moriarty, N. W., Oeffner, R., Read, R. J., Richardson, D. C., Richardson, J. S., Terwilliger, T. C. & Zwart, P. H. (2010). *Acta Cryst.* **D66**, 213-221.

[2] Chodkiewicz, M. L., Migacz, S., Rudnicki, W., Makal, A., Kalinowski, J. A., Moriarty, N. W., Grosse-Kunstleve, R. W., Afonine, P. V., Adams, P. D. & Dominiak, P. M. (2018). *J Appl Cryst* **51**, 193-199.