

Position available for a Software Specialist in C++ and Modern Fortran programming.

The availability of this position arises in the context of a planned effort to modernise and update the CCP4 coordinate manipulation library ("MMDB"). This effort is funded by CCP4 and is being undertaken jointly by the CCP4 Core group ("STFC") in the Research Centre at Harwell, UK ("RCaH") and Global Phasing Ltd ("GPhL") in Cambridge, UK.

Background

The CCP4 Project is 37 years old and has produced software for macromolecular crystallography (MX) that has around 20,000 users worldwide. Its coordinate manipulation library (MMDB) is used in some 40% of about 200 CCP4 applications, including major programs such as REFMAC and Coot. In view of the move in 2015 by the wwPDB from PDB to PDBx/mmCIF for the format and content of all PDB depositions, and of the planned extensions to the contents of such files (e.g. to include the handling of CIF restraint dictionaries), MMDB needs a major upgrade to enable it to continue fulfilling its current role and to play its expected pivotal role in future-proofing the use of this evolving PDBx/mmCIF standard as a working format by CCP4 applications. This will include the restructuring of its code to modern standards of C++ programming, and the provision of a comprehensive interface to an equally modern standard of Fortran for use in REFMAC, in software (esp. BUSTER) from GPhL, and in Fortran-based software from other parties.

STFC and GPhL have been awarded CCP4 funding for jointly carrying out this modernisation of MMDB - the results of which will be incorporated into the CCP4 Suite - as outlined below.

Specific Aims

1. Development of a thoroughly modernised version of MMDB, based on the PDBx/mmCIF paradigm instead of the PDB-centred one it currently uses, while maintaining compatibility with the old PDB format where still applicable. This will entail the adoption of modern C++ programming standards such as the use of the Standard Template Library (STL) instead of raw pointers, and error handling through the exception mechanism rather than return codes. A binary format capability will also be provided.
2. Development of high-quality Modern Fortran and Python APIs to this modernised MMDB, aimed at giving programmers in Modern Fortran and Python access to all MMDB capabilities available to C++ programmers. Compatibility with the old PDB format and old applications will be achieved through a "legacy version" of the C++ API. Detailed documentation for these APIs will be produced throughout, both to support the liaising between the various groups of developers and to open up its use to third parties in the future.
3. Development of new specialised tools to create a comprehensive toolkit for querying, inspecting and manipulating PDBx/mmCIF files, together with documentation aimed at general software developers working in the areas of structural biology and bioinformatics.

Description of Software Specialist position

In order to bolster this team effort, STFC and GPhL are seeking to recruit, for a period of 3 years, a Software Specialist – specifically, a software engineer experienced in scientific code development in both C++ and Fortran. Essential skills and experience for this position are fluency in C++, Python and modern Fortran, familiarity with creating language bindings between C/C++ and other languages, experience with thread-safe developments, as well as a verifiable track of successful software development projects with personal contribution above 30,000 lines. Desirable further skills and experience include writing parsers for PDB/mmCIF/PDBx files, knowledge of MX coordinate file formats, and knowledge of crystallography.

This position will be at a level equivalent to Band E of the STFC Salary Scale. The Software Specialist will be employed by GPhL and seconded to the CCP4 Core group at RCaH. Regular communication and visits will ensure coordination with the development teams for REFMAC, BUSTER and C++-based CCP4 applications in the definition, development and testing of the new MMDB and its Fortran API.

Applications for this position should be sent to Dr Gerard Bricogne at gb10@globalphasing.com and should include a CV and a covering letter. The closing date for applications is February 26th 2016 and the expected starting date is early April 2016.