Poster

QCrBox: Unlocking (Quantum) Crystallography

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In the crystallographic community refinement using the independent atom model is ubiquitous while more sophisticated methods of describing the aspheric electron density are largely ignored. The slow but consistent adoption of Hirshfeld atom refinement implemented in Olex2 [1] in the form of NoSpherA2 [2] has shown that if the experience of using more sophisticated models is sufficiently streamlined, adoption is possible. However, current implementations of quantum crystallographic methods often lack this streamlined experience due to several issues, which QCrBox aims to solve:

- *Complex Software Workflows*: The integration of disparate software solutions often leads to cumbersome and error-prone workflows.

- *Lack of Interoperability*: Variability in file formats and program interfaces impedes effective communication between different (quantum) crystallographic software, complicating the standardisation of data processing and analysis. While established software is less prone to this, this issue occurs especially in more niche applications, which are often tightly coupled to files created with specific software used by the developer for previous processing steps.

- *Difficulty in Managing and Reproducing Workflows*: The sensitivity of the charge density refinement (in the form of multipolar or wavefunction refinement) to details of data processing in earlier steps necessitates a systematic exploration. By manually exploring multiple different settings across various pieces of software, combined with the conversion between file formats, reproducibility can be compromised if the exploration is not done with the utmost care.

- *Software Installation Hurdles*: The diverse ecosystem of software frequently presents installation challenges, with certain software packages only strongly supported on specific operating systems. This further compounds reproducibility issues when processing steps in a computational workflow require the use of different computers.

- *Challenges in Reporting Procedures*: While reporting the results of data processing is done in a standardised format, namely CIF, reporting data processing details is often inadequate, which can obscure critical influences in evaluations and reduce the ability to reproduce, reuse or learn from successful studies in the field.

We will solve these problems by providing tooling for an ecosystem of containers which allow accessing existing crystallographic applications interactively through a web browser. This eliminates the need for manual installation by the user or having to use a specific operating system, significantly reducing the barrier to entry. Applications can exchange data using the CIF format and the user can build up computational workflows via a unified web interface. Any workflow can be created and reproduced with parameters recorded and the resulting data appropriately managed under the hood. Any (and all) crystallographic software can be accommodated, and we invite contributions.

[1] Dolomanov, O. V.; Bourhis, L. J.; Gildea, R. J.; Howard, J. A. K.; Puschmann, H. (2009). J. Appl. Cryst., 42, 339.

[2] Kleemiss, F., Dolomanov, O. V., Bodensteiner, M., Peyerimhoff, N., Midgley, L., Bourhis, L. J., Genoni, A., Malaspina, L. A., Jayatilaka, D., Spencer, J. L., White, F., Grundkötter-Stock, B., Steinhauer, S., Lentz, D., Puschmann, H., Grabowsky S. (2021). Chem. Sci., 12, 1675.