FA4-MS12-P01

A Further Improved Structure Matching Algorithm. N. David Brown[a], James Haestier[a], Mustapha Sadki[a], Amber L. Thompson[a], David J. Watkin[a]. [a]*Chemical Crystallography, Inorganic Chemistry Department, University of Oxford.*
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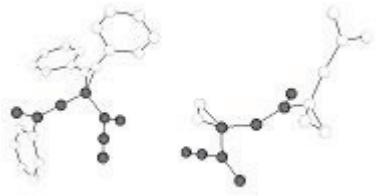
Since publication of the classic Ullmann algorithm for subgraph isomorphism [1], a variety of works have successfully augmented the algorithm's behaviour for graph matching, such as that presented by Cordella *et al*. [2]. Their paper describes a generic implementation of Ullmann with emphasis on an efficient implementation utilising linear data arrays rather than the matrices Ullmann originally specified.
As part of "Age Concern", a joint project between the crystallography laboratories in Durham and Oxford, funded by the EPSRC (grant EP/C536282/1), Oxford team members have developed an improved version of the Cordella algorithm, to be used for chemical structure matching. We explore the problem by considering graph and chemical theory in parallel, and allowing tailoring of the algorithm's behaviour to perform structure matching bespoke to any context via parameters specified prior to execution.



The state tree for any chemical structure matching algorithm is a search space of all possible atom-to-atom mappings between two input structures. Through parameterisation of our algorithm, we are able to winnow choices at every stage of our state search and maximise pruning of the state tree, as much as is possible for any given chemical context, according to the knowledge of the user. Pre-specified similarity conditions for both individual atoms as well as atom environments can be considered during matching, allowing 'chemically similar' fragments and molecules to be rapidly identified, as well as those which are 'structurally similar'. We provide distinct definitions of 'graph isomorphism' and 'chemical isomorphism' to clarify our proposal.
Additionally, by leveraging the arbitrary mapping of certain single-degree atoms within any input chemical structure, we are able to further improve the efficiency of the original graph matching algorithm [2]. A working demonstration of the algorithm will be available at the poster presentation.

[1]J.R. Ullmann, **1976**. *Journal of the Association for Computing Machinery*, 23, 31-42 . [2] L.P. Cordella, P. Foggia, C. Sansone, M. Vento, **2004**. *IEEE Trans. On Patt. Anal. & Mach. Intell*., 26, 10, 1367-1372.

Keywords: crystallographic analysis; computing methods in crystallography; structural similarity

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OLEX2 News. Oleg V. Dolomanov[a], Luc J. Bourhis[a], Richard J. Gildea[a], Judith A. K. Howard[a], Horst Puschmann[a]. [a]*Department of Chemistry, Durham University, Durham, DH1 3LE, UK.*
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OLEX2 is a portable open-source program for structure analysis and visualisation which provides a workflow driven user interface to manipulate crystal structures [1]. The workflow seamlessly links all aspects of the structure solution, refinement and publication process. Numerous built in functions, such as space group determination, void calculation, hydrogen atoms placement, electron density maps and structure alignment help the user with the structure solution, refinement and analysis. Our current work on the small molecule toolbox smtbx [2] and its integration with OLEX2 provides new potential for the development of small molecule refinement software. This poster presents new developments on the interface and structure analysis sides which have taken place since previous presentations at IUCr conferences.

[1] O.V. Dolomanov, L.J. Bourhis, R.J. Gildea, J.A.K. Howard and H. Puschmann **2009**. *J. Appl. Cryst.*, 42, 339-341. [2] L.J. Bourhis, R.W. Grosse-Kuntsleve, P.D. Adams **2007**. *IUCr Commission on Crystallographic Computing Newsletter*,8, 74-80.

Keywords: structure analysis; structure visualisation; open-source

FA4-MS12-P03

Harnessing the Power of the CCTBX with OLEX2. Richard Gildea[a], Luc Bourhis[a], Oleg Dolomanov[a], Judith Howard[a], Horst Puschmann[a]. [a]*Department of Chemistry, Durham University, UK.*
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The Computational Crystallography Toolbox (cctbx) [1] is an open-source portable library of reusable crystallographic algorithms. Whilst much of the current development of the cctbx is driven towards macromolecular crystallography, the core of the cctbx is completely general to all aspects of crystallography.
As a part of the cctbx, we are developing the small molecule toolbox (smtbx) module [2], which contains algorithms specifically for small molecule work. The algorithms developed within the smtbx will be made accessible through the OLEX2 software [3]. Currently available are a charge-flipping structure solution routine [4], and a refinement routine using an LBFGS minimiser [5].
Recent development involves the implementation of restraints and constraints specific to small-molecule work in the refinement module, and final structure report generation. Currently we use OLEX2 as the main interface to formulate the restraints and constraints and all other aspects of the refinement model, however, the library is designed to be easily reused in building or extending other crystallographic software.

[1] The Computational Crystallography Toolbox **2009**. http://cctbx.sourceforge.net. [2] L.J. Bourhis, R.W. Grosse-Kuntsleve, P.D. Adams, *IUCr Commission on Crystallographic Computing Newsletter*, **2007**, No. 8, 74-80. http://www.iucr.org/resources/commissions/crystallographic-computing/newsletters/8. [3] O.V. Dolomanov, L.J. Bourhis, R.J. Gildea, J.A.K. Howard & H. Puschmann, *J. Appl. Cryst.*, **2009**, 42, 339-341. [4] G. Oszlányi & A. Sütö, *Acta Cryst.*, **2008**, A64, 112-122. [5] C. Lui & J. Nocedal, *Mathematical Programming*, **1989**, 45, 503-528.

FA4-MS12-P04

Crystals: Refinement and Validation Tools. David J. Watkin[a], Richard I. Cooper[b], Amber L. Thompson[a]. [a]*Chemical Crystallography, Department of Inorganic Chemistry, Oxford.* [b]*oXray Ltd., Oxford.*
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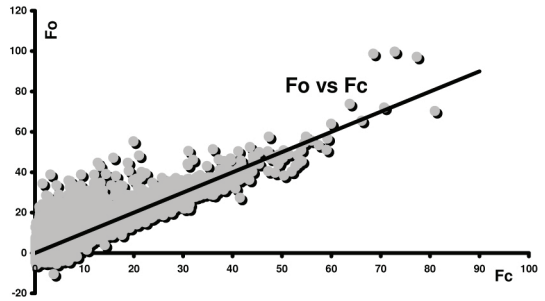
The basic technology for the refinement of small molecule structures has remained largely unchanged for 30 years. A standard refinement program will use a least-squares method to optimise parameters and have a range of constraints and restraints available to deal with troublesome problems. The programmers' task includes providing tools to help the users identify and resolve problems.
One kind of troublesome problem is that in which the R-factor is inexplicably high for what appear to be fair diffraction images. The crystallographer is faced with the task of deciding whether the data is in fact faulty, or whether the structural model is inadequate. The web-service checkCIF/PLATON [1] will pinpoint some sources of difficulty. However, there are cases where crystallographic experience is needed. In these cases, graphical displays can be exploited to make use of human pattern recognition abilities. Histograms, scatter-plots and iso-surfaces can draw the eye to trends or outliers which might not be evident in a simple table of values.



The powerful refinement tools available in CRYSTALS [2] are now being supplemented by a wide variety of graphical and statistical diagnostic and validation tools. The summer 2009 release of CRYSTALS will include these tools and examples of their use.

There will be a live demonstration of Crystals at the ECM25 Software Fair.

[1] PLATON. A.L. Spek **2005**, A Multipurpose Crystallo-graphic Tool, Utrecht University, Utrecht, The Netherlands.[2] Betteridge, P.W., Carruthers, J.R., Cooper, R.I., Prout, K., & Watkin D.J. **2003**. *J. Appl. Cryst.*, 36, 1487.

Keywords: computer software; data vali-dation; small-molecule crystallography

FA4-MS12-P05

Handling of Cell Errors and Their Effect on Derived Parameters. James Haestier[a], N. Dave Brown[a], Mustapha Sadki[a], Amber L. Thompson[a], David J. Watkin[a]. [a]*Chemical Crystallography, Inorganic Chemistry Department, University of Oxford.*
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Area diffractometers output standard uncertainties (s.u.s) on cell parameters that are an order of magnitude smaller than those on atomic coordinates. Herbstein[1], referring to area diffractometers, reported "little (or no) reliance can be placed on currently reported s.u.s from such diffractometers" yet area diffractometers continue to output cell parameter s.u.s with much the same magnitude now as then. The real uncertainties could be up to an order of magnitude greater, but as a consequence of the current output, it is generally felt that their effect on dependent parameters can be neglected. This means that the standard uncertainties of most derived parameters are underestimated. In addition, Kennard and Taylor[2] suggest that the s.u.s on atomic parameters derived by Normal Matrix Least Squares refinement are also underestimated. For calculations of s.u.s of the dihedral angle, Shmueli[3] revealed that the omission of covariances can cause discrepancies as large as 20-25%. Currently there is no cif definition for the variance-covariance matrix (VcV) for the atomic parameters, so programs attempting to compute uncertainties for derived parameters from a published cif have only the isolated parameter s.u.s to work with.

Part of the brief of the Age Concern Software Project is to re-visit common calculations and either reformulate them in a clear and consistent way or, if the published algorithms were incomplete, to put them on a sound mathematical basis. Since rigorous derivation of the standard uncertainties of derived parameters has been consistently neglected, it was felt useful to provide a general analysis that includes all sources of error in the anticipation that some day proper treatment of the data would yield valid VcV matrices.

Our experience from deriving the effect of cell parameter s.u.s on the TLS calculation[4] leads us to believe that if the atomic-parameter VcV in crystal space and the unit cell VcV matrix could be combined to give an augmented parameter VcV matrix in orthogonal space, the computation of valid s.u.s on any derived parameter would be greatly simplified. This manipulation has currently been achieved for all systems except triclinic. The work is on-going.

[1] F. H. Herbstein **2000**. *Acta Cryst*., B56, 547-557. [2] R. Taylor & O. Kennard **1985**. *Acta Cryst*, A41, 85-89. [3] U. Shmueli (1974). *Acta Cryst*, A30, 848-849. [4] J. Haestier, M.Sadki, A.L. Thompson and D. Watkin **2008**. *J. Appl. Cryst*, 41, 531-536.

Keywords: software; uncertainties; analysis