Small Molecule Crystallographic Computing – What is the future?

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A well known proverb amongst programmers is 'If it's not broken, don't mend it'. This is good advice, but what should be done if it is clear that very soon something is going to stop working?

In recent years small molecule crystallographic programs have disappeared one by one. This usually happens when there is no one left who really understands the program, and who can support it in a changing environment. For a short while after the programs become unavailable, old crystallographers bore young crystallographers by repeating 'I remember when it was easy to do …. with program X'. Then people forget that it was ever possible, and then some one re-discovers the process. The wheel is re-invented.

All of the well-loved program systems have their roots in ideas formed about 30 years ago, and have evolved slowly under the care and attention of individuals or small groups. These programs ***express*** the knowledge held by these people, but they do not document it.

The equation $A^T.A.\delta x = A^T.\Delta F$ sums up what happens in least-squares, but it requires a lot of code to convert this into even a simple useable program, and a massive amount of understanding of the problem and environment to turn it into a user-friendly program.

The principal writers and care-takers of the most popular programs are now in the final phases of their careers. When they shuffle off their mortal coils, devotees may be able to keep some of the programs running for a short while, as a kind of working museum. Every thing in not broken yet, so there is nothing to fix. However, if the community is to avoid re-inventing very may wheels in the future, there is urgent need to properly document current knowledge, and use it to create better wheels.

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