"Government funded central initiatives for encouraging a diversity of freely available crystallographic software;
and the threat of Crystallographic Software Patents

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Talk Aims

- 1st: Elaborate on the UK nationally funded software resources for crystallography

- 2nd: Assert and explain the opinion that Software Patents are a threat to crystallographic software and software development

- Talk notes at:
  - http://www.ccp14.ac.uk/poster-talks/aca2003/

Nationally Funded Crystallographic Software Projects

- A way of getting around haphazard local department and university funding of important soft scientific informational and analytical infrastructure

- Get academics and students the software tools and information resources they need to get the job done effectively.

- Will concentrate on the UK resources and funding.

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UK Central funded and nationally based academic resources

- British academics and students have national access to a wide variety of scientific databases and resources that are centrally funded by the government scientific funding agencies.

e.g. The Chemical Database Service (CDS)

- http://cds3.dl.ac.uk/

- CDS pays to obtain relevant scientific databases and then give "free" UK National access to academics and students.

- Funded by the EPSRC

- Provides databases in: Crystallography, organic chemistry, spectroscopy, physical chemistry

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Chemical Database Service webpage
http://cds3.dl.ac.uk/

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Central support for scientific software: The CCP's

(Collaborative Computational Projects)

- Listed at: http://www.cse.clrc.ac.uk/ccp/

- Have been 14 of them funded so far

- Some have become defunct.

- Depending on the CCP's focus, are funded by the relevant UK research council:
  - BBSRC (Biotechnology and Biological Sciences Research Council)
  - EPSRC (Engineering and Physical Sciences Research Council)
  - PPARC (Particle Physics and Astronomy Research Council)

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What are the CCP's for?

- "The Collaborative Computational Projects (CCPs), assist universities in developing, maintaining and distributing computer programs and promoting the best computational methods."

Current CCP's

- ## Listed at: http://www.cse.clrc.ac.uk/ccp/
    - CCP1 - The electronic structure of molecules
    - CCP2 - Continuum states of atom and molecules
    - CCP3 - Simulation of physical and electronic properties of surfaces and interfaces
    - CCP4 - Protein crystallography
    - CCP5 - Computer simulation of condensed phases
    - CCP6 - Heavy particle dynamics
    - CCP7 - Analysis of astronomical spectra
    - CCP9 - Computational studies of the electronic structure of solids
    - CCP11 - Biosequence and structure analysis
    - CCP12 - High-performance computing in engineering
    - CCP13 - Fibre and polymer diffraction
    - **CCP14 - Powder and small molecule single crystal diffraction**

How do CCP's Run

- Depends on the project grant holders and the resources available to that particular CCP

- This means they don't operate the same way. E.g., they might do one or all of the following:
    - Further development of publicly available source code
    - Training workshops
    - Develop new flagship software
    - Provide linking programs for existing code
    - Archive and promote existing software

The CCP14 – http://www.ccp14.ac.uk/
CCP for Single Crystal and Powder Diffraction

- To help provide the academic community with freely available small-molecule single crystal and powder diffraction crystallographic software.

- Promote existing software and encourage the development of new software to fill existing analytical problems.

- Mirrors and supports existing software programs and authors via Internet facilities.

- Is officially only meant to benefit the UK academic community.

CCP14 webpage
http://www.ccp14.ac.uk/

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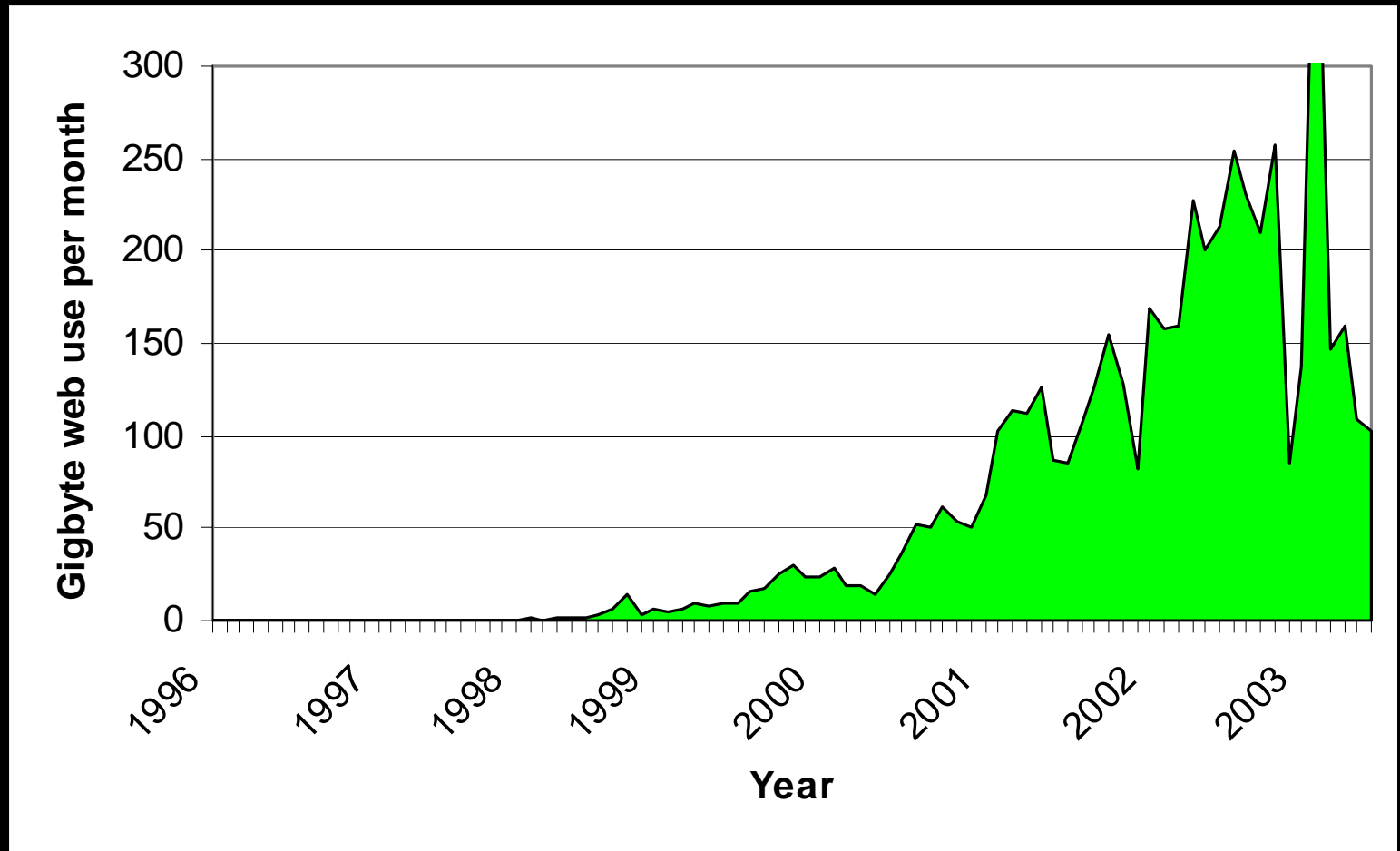Lachlan M. D. Cranswick (lachlan.cranswick@nrc.ca) http://neutron.nrc.ca/

How the CCP14 works

- Has a limited set of resources - and has to operate within those resource constraints:
  - One permanent staff member/post doc
  - Some web-servers and user of UK academic internet bandwidth
- User feedback to optimize the direction of the project. (no fixed plan – go where the users take it – in directions that are useful to them)
- If user direction is lacking, create some promotional initiatives so that users have something to use as a starting point for feedback. Examples in the past:
  - Seeking out new powder indexing programs and methods.
  - Powder peak profiling programs and methods.
  - Single Crystal suites
  - Structure solution from powder X-ray diffraction data

Encouraging Software Diveristy

- CCP14 has a policy of letting users decide what is useful, so tries to mirror and make available as wide a variety of crystallographic software as possible.
    - Multiple powder indexing programs and suites
    - Multiple single crystal suites
    - Multiple Rietveld refinement programs
    - Multiple
    - Etc, etc

Usage of the CCP14 website
(http://webstats.ccp14.ac.uk/)

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History of funding the CCP14

- **Proposed in 1994 by Bob Cernik (Daresbury Laboratory).**
  - First round of grant funding by EPSRC (1995 to 1997) with J. Ian Langford (Birmingham) as the first Principal Investigator of the grant.
  - Second round of grant funding by EPSRC (1998 to 2000) Grant renewal with Jeremy Cockcroft (Birkbeck College) as Principal Investigator ; Bob Cernik and David Watkin as co-investigators.
  - Third round of grant funding by EPSRC (2001 to 2006) Jeremy Cockcroft (Birkbeck College) as Principal Investigator ; Bob Cernik and David Watkin as co-investigators.

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Keeping end user focused

- It is concerned and interested academics that provide the focus for these initiatives, not secretive government mandarins.

- It is obvious that if the grant holders do not focus on the needs of its academics users, grant renewals are less likely to occur.

- Renewal occurs via the standard grant proposal system.

- Creating these projects not a big problem – providing the funding bodies support these initiatives.

The Threat of Software Patents

- Give an overview of Software Patents (also called "computer-implemented business method patents") and assert that they threaten crystallography and crystallographic software development.

- The emphasis of this talk is that Software Patents threaten the freedom in i) using existing crystallographic algorithms and ii) developing new crystallographic algorithms and software.

First Amendment Rights

- This talk is only the personal opinions of the author

- ''Non-qualified'' non-lawyers perspective – as would I be slumming it at ACA2003 if I was on a lawyers wage?

- Opinions generalized and condensed - ''as life is short''

Why be concerned about Software Patents

- A quote attributed to the crystallographer Prof. Alan Mackay, (FRS):

"Americans are not scared of the secret police, but they are of lawyers".

- With software patents, you are up against lawyers chilling your right of free speech and expression (on ideas algorithmic and scientific), not the secret police.

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Some Patent History

- Originally a patent was based around "grants of privilege" (also called "royal privilege"), giving monopolies to manufacturers and traders by a monarch.

- As can be expected, patents were subject to abuse.

- Queen Elizabeth I of England was most noted in this regard, having granted patents to various people including "royal favourites" on such things as:

  – "soap, saltpetre, alum, leather, salt, glass, knives, sailcloth, sulphur, starch, iron and paper"

Thomas Tallis
(1505 - 1585)

- "the Father of English Church Music"

- "most influential English composer of his generation"

- "In 1575, Queen Elizabeth granted a monopoly on printing music to Thomas Tallis and William Byrd."

- "the music-patent was one of the factors which hampered the full flowering of musical publishing in England in the sixteenth and in the beginning of the seventeenth centuries."

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Philosophy behind the modern patent system

- Most appropriate to quote the American Constitution:
  - http://www.house.gov/Constitution/Constitution.html
  - Article. I., Section. 8., Clause 8: "To promote the Progress of Science and useful Arts, by securing for limited Times to Authors and Inventors the exclusive Right to their respective Writings and Discoveries"

- Patents do not exist to benefit the inventor, they exist to get information into the public arena by providing an incentive for the inventor to disclose information. Benefiting the inventor by granting a temporary monopoly is a means to that end. If the information was already getting into the public arena – no point for issuing a patent.

In theory - no patenting of ideas

- In theory, the patenting of "ideas" (and the ideas as implemented in software) are not allowed, only of "inventions". Recent US Patent law seems to have become rather confused in differentiating between what is an "idea", and what is an "invention". European law is clearer:

- The European Munich Convention states that the following shall NOT be regarded as inventions:

  - discoveries, scientific theories and mathematical methods

  - aesthetic creations

  - schemes, rules and methods for performing mental acts, playing games or doing business, and programs for computers

  - presentations of information

Why not allow patenting of ideas?

- To allow the patenting of ideas, one argument would be the infringement of First Amendment rights:
  - "Congress shall make no law respecting an establishment of religion, or prohibiting the free exercise thereof; or abridging the freedom of speech, or of the press; or the right of the people peaceably to assemble, and to petition the Government for a redress of grievances."
  - http://www.house.gov/Constitution/Amend.html

- In the case of software patents, infringing how others may wish to express ideas: algorithmic and scientific.

- With the patenting of "ideas", any scientific principle can be legally monopolized: gravity, diffraction, mathematical formulae, etc, etc, etc – which would restrict the free expression and development of these ideas by others.

In application - now anything goes(?)

- US Patent Office used to not allow software patents – as they were not officially inventions.

- But there was a lack of qualified patent assessors and an apparent criterion of USPTO success being the Number of New Patents, irrespective of their quality.

- USPTO started passing lots of garbage patents, including software patents, (allegedly) under the logic that the courts could then figure out what is a good patent or a bad patent. An easy examples of patenting the trivial or ridiculous is:

  – US Patent 6,368,227 titled "Method of swinging on a swing" (Filed: November 17, 2000)

  – "Licenses are available from the inventor upon request."

    • http://patft.uspto.gov/netacgi/nph-Parser?patentnumber=6,368,227

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Passing Patents of the absurd

- There are claims that patent assessing has become so lax or under-qualified that almost anything can pass: US Patent 5,533,051: "Method for data compression" (July 2, 1996)
  - http://patft.uspto.gov/netacgi/nph-Parser?patentnumber=5,533,051

- This "should be invalidated" as it would seem that "patent 5,533,051 claims something mathematically impossible, and therefore should not have been issued." . . "It took three years to the patent office to ascertain the validity of such a patent. A person with basic knowledge in mathematics and data compression can find the flaws immediately upon first reading."
  - http://www.bustpatents.com/invalid.htm

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Many Software Patents involve triviality, obviousness or prior art

- Possible example: US Patent 6,108,401 (Date of Patent: August 22, 2000). Titled "Method of standard-less phase analysis by means of a diffractogram"

  – "Using an estimate of the dispersive power of the individual atoms in the unity cells of the constituents"

- Sounds like(?) Quantitative Rietveld analysis (developed in the late 1980's (Hill and Howard - 1987; Bish and Howard - 1988))?

- But in the case of patents, that would be for the lawyers and courts to decide (not scientists) – assuming you have the funds to "defend" against claims of infringement ($10,000's to $100,000's).

Claiming obvious areas(?)

- E.g., US Patent Number: 6,192,103 (Publication Date: February 20, 2001) Titled "Fitting of X-ray scattering data using evolutionary algorithms" (genetic algorithms)

- Please note the definition of "scattering":

  - "The present invention relates to X-ray metrology, and more particularly to the fitting of simulation models to X-ray scattering data for the purpose of determining parameters that characterize the structure of a material being tested." . . .

  - "Examples of these methods include X-ray absorption, diffraction, fluorescence, reflectivity, scattering, imaging and fringe analysis. In the context of the present invention, the term "X-ray scattering" is employed as a generic term which collectively encompasses any known X-ray technique that is applied to materials characterization."

Applying the obvious to Crystallography

- Many software patents take an idea in the public view and apply it software – then patent it as something "new". Or take an idea in the public view and quickly apply it to crystallography:

- US Patent Number: 5,577,239 (Publication Date: November 19, 1996) Titled "Chemical structure storage, searching and retrieval system"

- From the patent abstract:
  - "The present invention is a chemical structure search system and method which expands the capabilities of existing systems by capitalizing on the strengths of relational database technology."

Patenting the Obvious

- According to an 1882 U.S. Supreme Court Decision:
  - "It was never the object of patent laws to grant a monopoly for every trifling device, every shadow of a shade of an idea, which would naturally and spontaneously occur to any skilled mechanic or operator in the ordinary progress of manufactures." . . . "It creates a class of speculative schemers who make it their business to watch the advancing wave of improvement, and gather its foam in the form of patented monopolies," . . "It embarrasses the honest pursuit of business with fears and apprehensions of unknown liability lawsuits" . .
    - --U.S. Supreme Court, Atlantic Works vs. Brady, 1882

Some of many crystallographic software "inventions"

- US Patent: 5,249,137 (September 28, 1993); "Computer-aided chemical illustration system"

- US Patent: 6,411,676 (June 25, 2002); "Method for determining parameters of a unit cell of a crystal structure using diffraction"

- US Patent: 6,438,205 (August 20, 2002); "System and method for reducing phase ambiguity of crystal structure factors"

- US Patent: 4,991,191 (February 5, 1991); "Quantitative analysis of the active table ingredient by powder x-ray diffractometry"

- World Patent: WO9906824 (February 11, 1999); "Method and apparatus for determining molecular crystal structures"

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Some more crystallographic software "inventions"

- US Patent Application: 20020111761 (August 15, 2002); "Method for determining multi-dimensional topology"

- US Patent: 5,235,523 (August 10, 1993); "Apparatus and methods for identifying and comparing lattice structures and determining lattice structure symmetries"

- US Patent: 5,353,236 (October 4, 1999); "High-resolution crystallographic modelling of a macromolecule "

- United States Patent: 6,326,619 (December 4, 2001); "Crystal phase identification "

- United States Patent: 5,884,230 (March 16, 1999) and 5,557,535 (September 17, 1996) both titled: "Method and system for protein modelling"

- US Patent: 6,582,233 (June 24, 2003); "Apparatus and method for monitoring the validity of a molecular model"

More crystallographic software "inventions"

- US Patent: 5,200,910 (April 6, 1993); "Method for modelling the electron density of a crystal"

- US Patent: 6,014,449 (January 11, 2000); "Computer-implemented system for analyzing rigidity of substructures within a macromolecule"

- US Patent: 5,752,019 (May 12, 1998); "System and method for confirmationally-flexible molecular identification".

- US Patent: 5,557,104 (September 17, 1996); "Method and apparatus for determining crystallographic characteristics in response to confidence factors".

- US Patent Application: 20020107643 (August 8, 2002) (Filed January 22, 1999); "Process for pan-genomic determination of macromolecular atomic structures".

Even if you are not infringing any crystallographic software patents, that still leaves other non-crystallographic software patents :

- Applying Fast Fourier Transforms in Crystallographic Software? This could be infringing multiple software patents:
  - United States Patents: 6,434,583 (issued August 13, 2002) and/or 5,371,696 (issed December 6, 1994) and/or 6,430,587 (issued August 6, 2002) and/or 6,058,409 (issued May 2, 2000), etc, etc
- Many "trivial" computer algorithms have already been patented; compression, sorting routines, display routines, etc.
- Refer: "Archive of bad software/Internet patents" and "European Software Patents Horror Gallery"
  - http://www.bustpatents.com/main.htm#BAD
  - http://swpat.ffii.org/vreji/pikta/mupli/index.en.html

In theory: challenging patent applications

- In theory, anyone can challenge a patent application (US and Europe) if they think it has problems due to a number of criteria including:

  – prior art

  – obviousness to a practitioner

  – lack of an inventive step

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In practise: challenging patent applications

- In practice (Europe patent system), for an individual to challenge an obviously ludicrous patent:
    - The challenge must be done no more than 9 months after the patent has been granted
    - The time required for the opposition process goes from 1 to more than 2 years after filing the opposition. The last step is a hearing in Munich.
    - You need a specialist recognised by the European patent office to represent you in front of the EPO.
    - The total cost to the challenging individual is in the order of 10,000 to 15,000 Euros

- Thus ludicrous (European) software patent applications have little to fear from individuals with the scientific knowledge that could show them to be nonsense.

Searching the US Patent system via the web

- Very easy to display and search for US patents and patent applications via the USPTO website:
  - http://www.uspto.gov/patft/
  - Example of a US patent search form

Searching the US Patent system via the web

- Be wary that it is easy to miss some patents due to non-obvious key words in the subject or content.

    - US Patent: 6,453,246 (September 17, 2002); "System, method, and computer program product for representing proximity data in a multi-dimensional space"

    - "proximity data in a multi-dimensional space" – possibly(?) being the alias you need to know for a "crystal structure"

Finding relevant Patent keywords

- Useful features on the USPTO web system are the [Referenced By] and [References Cited] options:
  - E.g., while viewing patent 5,572,439 (November 5, 1996) titled "Molecular design support system" - using the [Referenced By] option, points to a newer patent that was missed by conventional keyword searching: patent 6,582,233 (June 24, 2003) – "Apparatus and method for monitoring the validity of a molecular model"
  - This can also help you make up a list of keywords that crystallographic software patents are using without first having to know the keywords in advance. "molecular model" being a new synonym for "crystal structure" to add to you search list – keywords that may not seem obvious at the time.

Patent it all?: Just call all "ideas" - "inventions"(?)

- A practice of Software Patents is to couch terms in "legalese" and give things different "uncommon" names to try and make everything and every idea sound like a profound, novel "invention".

  – A "Powder indexing program" (well known in the powder diffraction community) has a name change to "unit cell analyzer" – thus, as if by magic, it has become a complex new invention - now worthy of patenting.

- It looks like this strategy is very common in most areas of software patents to try and hide triviality.

Effects of applying software patents

- It is not improbable that is software patents were widely applied en-masse, that patent law would most likely collapse due to its absurdity and the widespread chaos it would cause.

- But many scientists and academics could get minced in the machinery of law while this sorts itself out.

- If you are doing any crystallographic software development (any software development at all), you are most likely at risk from Software Patents (at least if you step or live on US soil)

Policy of a European crystallographic programmer "if" Software Patents become law in Europe

Vincent Favre Nicolin on the Fox software website at
http://objcryst.sourceforge.net/

> "As an individual I cannot take the risk of being prosecuted because some company patented a simple principle used in Fox or ObjCryst++ (use of integrated R-factors, the description of molecules using a Z-Matrix, genetic algorithms..). Therefore, I will still continue the Fox/ObjCryst++ development privately, but I will not be able to distribute it myself anymore."

The practical effect of software patents is not to encourage innovation, but to scare off academic and scientific rivals – using blackmail and threat (real or implied) of legal entanglement and personal financial bankruptcy in attempting to defend themselves.

Software Patents are not just being used as wallpaper

"BT Sues Prodigy Over Hyperlink Patent" - December 2000
US Patent 4,873,662

"Amazon sues Barnesandnoble.com over patent" – October 1999
US Patent 5,960,411

Also used to try and silence critics of software patents:

"When a company sues a notorious critic for infringement, is it just business or intimidation?" – (December 2000) over the Techsearch "Remote Query Communication System" patent.

In this instance, a software patent holder did not claim libel against its critic (Greg Aharonian) but patent infringement. First Amendment rights are generous for defendents, so people attempting libel cases face large risks of being counter sued for frivolous or malicious prosecution.

Surely commonsense will prevail?

- In the US alone, patent law is a multi-billion dollar earner for the legal industry. It is unlikely that the legal industry would like to give up a significant chunk of their earnings to aid the public or scientific good in the matter of software patents.

- "lawyers, whose trade it is to question everything, yield nothing, and talk by the hour"
    - Thomas Jefferson (Autobiography, 1821. ME 1:87)

Summary

- UK centrally funded government initiatives have been highly beneficial in developing and distributing crystallographic software and related resources to academics performing teaching and scientific research. There is potential for academics in other countries to benefit from this approach.

- This talk also asserts the opinion that Software Patents (also titled "Computer-Implemented Business Methods Patents") are a scam and a threat to science and crystallography.
  - "We cannot stand on the shoulders of giants if the giants wear spiked shoulder pads" (same goes with "patent trolls")

- Check this out for yourself - links:
  - CCP14: http://www.ccp14.ac.uk/maths/software-patents/
  - "The Threat of Patents on Crystallographic Algorithms and Software" by Vincent Favre-Nicolin, IUCr Commission on Crystallographic Computing, Compcomm Newsletter No 1. Jan 2003 (http://www.iucr.org/iucr-top/comm/ccom/newsletters/2003jan/)