

Nexus, crystallographic computing all around the world

Lachlan Michael David Cranswick,^{a*} William Bisson^b and Jeremy Karl Cockcroft^b

^aNational Research Council of Canada, Chalk River Laboratories, Chalk River, Ontario K0J 1P0, Canada, and ^bDepartment of Chemistry, University College London, Christopher Ingold Laboratories, 20 Gordon Street, London WC1H 0AJ, UK. Correspondence e-mail: lachlan.cranswick@nrc.gc.ca

Crystallographic Nexus CD-ROMs, containing a range of free crystallographic software for single-crystal and powder diffraction available on the Internet, have been distributed on request since 1996. The free CD is made in the form of a 'virtual Internet' with the main intent of benefiting crystallographers with inadequate Internet access. The IUCr funds an annual/biennial update which is distributed to known previous recipients. Feedback from current recipients indicates the CD is still useful. The most current IUCr-funded CD is being produced by the CCP14 project at University College London and The Royal Institution UK for distribution to the ECM 2007 and AsCA 2007 conferences.

© 2008 International Union of Crystallography
Printed in Singapore – all rights reserved

1. Introduction

For more than a decade, the Internet has allowed access to a range of free, modern, crystallographic analysis software. This software can help build an effective software toolkit for crystallographic research and teaching. In the mid 1990's, Internet use in the far reaches of the globe was described as 'booming' (Butler, 1996). However, information from crystallographers indicated otherwise, that Internet access for academics and students in less technically advanced regions was generally unavailable, inadequate, costly; and, if available at all, often restricted to e-mail. As computational analysis is crucial in crystallography, there was, and still is, a challenge to ensure access to a range of crystallographic analysis tools.

2. Nexus CD creation and distribution

To help mitigate poor Internet access for affected crystallographers and students, a free CD-ROM was initiated in mid-1996 that contained a variety of crystallographic software and Internet resources. The free CD-ROM was regularly updated and air-mailed on request irrespective of the person's geographic location. The aim of the CD was to put relevant parts of the crystallographic Internet into a form suitable for scientists and students with poor Internet access. The CD provides recipients with modern free crystallographic tools and information for structure analysis and teaching.

Around the mid 1990's in Australia, home- and small-office-based CD writing hardware was becoming generally affordable, enabling the creation of CD-ROMs without professional assistance. For initial versions of the Nexus CD, it was a challenge using a 28000 baud modem-based link to the Internet to fill up the then massive CD-ROM space of 650 MB with useful crystallographic material. As years progressed,

Table 1

Approximate costs in USD for computer hardware as a function of year.

Original costs in Australian and Canadian currency have been converted into USD using February 2007 conversion rates (AUD 1 = USD 0.77; CAD 1 = USD 0.85).

Equipment	June 1996	June 1997	December 2006
CD writer	1550	620	26
Fast hard disk	970	540	34
Internet modem	500	155	50
	(28 kB baud)	(28 kB baud)	(768 kB DSL)

with broadband Internet, more powerful computer hardware and software distributions of much larger size, the problem changed to one of 650 MB becoming an increasingly small space in which to fit a range of crystallographic software and resources.

Current grabbing of programs and web content is performed with the program *Grab-a-Site* for MS-Windows 95 (Blue Squirrel, 1998), using a residential 768 kB DSL connection and personal laptop PC computer with Intel CPU running Microsoft Windows XP. Downloading content for the CD-ROM, CD creation and burning is reliable and routine. The time and cost to create CDs has reduced considerably since the mid-1990's (Tables 1–3).

3. Software included on the CD-ROM

The content on the CD-ROM varies to fit within CD-ROM size constraints, with emphasis on including multiple packages that perform similar crystallographic analyses. In the 2006 version of the CD, small-molecule single-crystal suites

Table 2

Approximate times required to download and generate a Nexus CD-ROM image, as a function of year.

	June 1996	June 1997	December 2006
CD content download time and file manipulation	200 h (28 kB modem and manual download under Microsoft Windows 3.1x)	40 h (28 kB modem using <i>Get-a-Site</i> under Microsoft Windows95)	4 h (768 kB DSL using <i>Get-a-Site</i> for Microsoft Windows95 running under Microsoft Windows XP)

Table 3

Approximate costs in USD and times for burning an individual Nexus CD as a function of year.

Original costs in Australian and Canadian currency have been converted into USD using February 2007 conversion rates (AUD 1 = USD 0.77; CAD 1 = USD 0.85).

Time/Cost	June 1996	June 1997	December 2006
Writable CDs	USD 12 (2× writable)	USD 7 (4× writable)	USD 0.50 (48× writable)
Padded envelopes	USD 0.77	USD 0.77	USD 0.85
Air-mail cost	USD 3.80	USD 3.80	USD 3.40
Set-up time for writing CDs	90 min	45 min	2 min
Time to write each CD	50 to 90 min	25 to 50 min	3 to 8 min

included *Crystals*, *WinGX* and *PLATON*. Single-crystal structure solvers included *Crunch*, *DIRDIF*, *SuperFlip* and programs available within *Crystals*, *WinGX* and *PLATON*. Freestanding powder indexing programs on the CD were *Treor*, *Ito*, *Dicvol2006* and *McMaille*. Powder indexing suites were *Crysfire*, *Fullprof-Winplotr* and *Chekcell*, with powder structure-solution programs *Fox* and *ESPOIR*. A variety of Rietveld, structure drawing and utility programs were included, as well as a portion of the IUCr website including **Crystallography Online**. The source code within Armel Le Bail's Crystallography Source Code Museum is also included (Le Bail, 2002). A list of software on the CD-ROM is provided in Table 4.

4. Distribution of the CD-ROM

Numbers of CD-ROMs sent sorted by country are given in Table 5. Some institutes and departments reported further duplication of the CD, followed by redistribution to colleagues in their institute and region.

The current procedure for generating and mailing a Nexus CD is similar to that in 1996. On receiving a request for a CD-ROM, a current version of the CD is burnt and sent *via* air-mail. Availability of the CD was advertised in the relevant Internet newsgroups, IUCr newsletters, conferences and by word of mouth from prior recipients. The rate at which CDs were sent to new recipients over the last ten years varied from zero to around twenty per month. Current rates at which new requests for CDs are received average around one per month.

Table 4

List of software packages included on the CD-ROM.

<i>Balls and Sticks</i>	(Ozawa & Kang, 2004)
<i>BGMN</i>	(Bergmann <i>et al.</i> , 1999)
<i>CAMERON</i>	(Watkin <i>et al.</i> , 1996)
<i>Celref</i>	(Laugier & Bochu, 2004)
<i>Chekcell</i>	(Laugier & Bochu, 2004)
<i>CMPR</i>	(Toby, 2005)
<i>ConvX</i>	(Bowden, 2000)
<i>Crunch</i>	(de Gelder <i>et al.</i> , 1993)
<i>Crysfire</i>	(Shirley, 2002)
<i>Crystals</i>	(Betteridge <i>et al.</i> , 2003)
<i>Dicvol2004/2006</i>	(Boultif & Louer, 2004)
<i>DIRDIF</i>	(Beurskens <i>et al.</i> , 1996)
<i>Discus</i>	(Proffen & Neder, 1999)
<i>Dispano</i>	(Laugier & Bochu, 2004)
<i>DRAWxtl</i>	(Finger <i>et al.</i> , 2007)
<i>EFLECH/INDEX</i>	(Bergmann & Kleeberg, 1998)
<i>ESPOIR</i>	(Le Bail, 2001)
<i>EXPGUI</i>	(Toby, 2001)
<i>Fox</i>	(Favre-Nicolin & Cerný, 2002)
<i>Fullprof</i>	(Rodríguez-Carvajal, 2001)
<i>Getspec</i>	(Altermatt & Brown, 1987)
<i>Gretep</i>	(Laugier & Bochu, 2004)
<i>GSAS</i>	(Larson & Von Dreele, 2004)
<i>Ideal</i>	(Gould <i>et al.</i> , 1988)
<i>Jana</i>	(Petricek <i>et al.</i> , 2000)
<i>Koalariet</i>	(Cheary & Coelho, 1992)
<i>Marching Cubes ELD</i>	(Rohlíček & Hušák, 2007)
<i>Maud</i>	(Lutterotti <i>et al.</i> , 1999)
<i>McMaille</i>	(Le Bail, 2004)
<i>Orient Express</i>	(Laugier & Bochu, 2004)
<i>ORTEP3</i> for Windows	(Farrugia, 1997; Burnett & Johnson, 1996)
<i>PLATON</i>	(Spek, 2003)
<i>Poudrix</i>	(Laugier & Bochu, 2004)
<i>PowderCell</i>	(Kraus & Nolze, 1996)
<i>Rietan</i>	(Izumi, 2003)
<i>Rietquan</i>	(Lutterotti <i>et al.</i> , 1998)
<i>SuperFlip</i>	(Palatinus & Chapuis, 2007)
<i>UnitCell</i>	(Holland & Redfern, 1997)
<i>Variable Count Time</i>	(Madsen & Hill, 1994)
<i>Wgetspec</i>	(Laugier & Bochu, 2004)
<i>WinGX</i>	(Farrugia, 1999)
<i>WinFIT</i>	(Krumm, 1997)
<i>WinPlotr</i>	(Rodríguez-Carvajal & Roisnel, 1998)
<i>Xfit</i>	(Cheary & Coelho, 1998)
<i>Xlat</i>	(Rupp, 1988)

5. Yearly distribution of an updated CD-ROM

Since 2000, the IUCr (*via* the Committee for Electronic Publishing, Dissemination and Storage of Information) has funded regular annual or biennial updates of the CD-ROM, distributed *via* air-mail to all previous recipients. The intent has been to achieve one version per year, preferably timed to coincide with a suitable crystallographic conference to achieve extra distribution. The most recent IUCr-funded distribution was in June 2007, being produced by the CCP14 project at University College London and The Royal Institution,

Table 5

Distribution by country of Nexus CD-ROMs distributed since 1996.

Country	Recipients Nos.	Country	Recipients Nos.
Algeria	41	Oman	1
Argentina	3	Pakistan	3
Australia	5	Peru	19
Bolivia	1	Philippines	1
Brazil	13	Poland	8
Cameroon	9	Portugal	4
Canada	5	Republic of Macedonia	1
China	41	Romania	9
Columbia	3	Russia/Russian Federation	17
Costa Rica	1	Saudi Arabia	2
Côte d'Ivoire	1	Senegal	2
Croatia	2	Serbia	2
Cuba	7	Singapore	2
Czech Republic	3	Slovak Republic	3
Egypt	13	Slovakia	1
Eritrea	1	South Africa	4
France	13	South Korea	9
Germany	16	Spain	2
Greece	4	Sri Lanka	1
Hungary	3	Sweden	3
India	126	Switzerland	2
Indonesia	5	Syria	3
Iran	2	Taiwan	2
Israel	4	Tanzania	1
Italy	7	Thailand	4
Jamaica	1	Tunisia	23
Japan	5	Turkey	28
Latvia	1	Ukraine	16
Malaysia	7	United Kingdom	9
Mexico	13	USA	27
Morocco	4	Venezuela	4
Netherlands	5	Vietnam	1
New Zealand	3	Yugoslavia	3
Nigeria	1	Zimbabwe	1

London, UK. This timing was for distribution to the ECM 2007 conference in Morocco and AsCA 2007 conference in Taiwan, as well as the usual air-mailing distribution to previous recipients.

6. Internet accessibility and CD-ROM usage

As there has been no requirement for recipients to report usage of the CD-ROM, a questionnaire was sent in January 2007 to the e-mail addresses of CD-ROM recipients. The questions and responses are given in Table 6. Questions were multiple choice to minimize time needed to answer, with options for more elaboration if required. To encourage accurate negative responses, a preamble to the questionnaire emphasized that replies should admit to no longer requiring the CD-ROM if that was currently the case.

Of the 402 unique e-mail addresses to which the questionnaire was sent, e-mails to 121 of the addresses bounced and 43 responses were received. The number of bounced e-mails is not necessarily that surprising as one of the authors (LMDC) is on his sixth new e-mail address since 1996, previous e-mail addresses being defunct due to changes of employer, Internet Service Providers or an account being overwhelmed with junk e-mail.

Table 6

Answers and edited responses, with original questions, received *via* e-mail in January 2007.

The questionnaire was sent to all recipients of Crystallographic Nexus CD-ROM from 1996 to 2006. The first and second sections of the questionnaire do not sum to the 43 received sets of answers due to some respondents selecting multiple preferences.

Questions and respondent elaborations	Responses
Local Internet for downloading scientific/crystallographic software is:	
(a) routine and easy	14
(b) problematic but do-able with enough effort	21
(c) not practical due to problematic/low bandwidth Internet connectivity	12
(d) other (please elaborate)	2
(i) Cost is a problem here. Chinese Yuan (about 3/8 dollar) per MB	
(ii) Computer centres are not willing to download the software and store in their computers	
Nexus CDs are:	
(a) no longer required due to good Internet links	4
(b) no longer required due to change of research interests	
(c) Internet is adequate for software download but CDs are a convenient back-up	21
(d) required due to problematic Internet accessibility	21
(e) other (please elaborate):	
(i) Internet access speed is so bad that at University levels [Nexus] CDs are a must	
(ii) Internet accessing facilities are available	
(iii) CDs are good for passing the information to students and other college teachers who are interested	
Nexus CDs are used for (select multiple if required):	
(a) providing crystallographic software for PhD degree research	33
(b) providing crystallographic software for Postdoc research	27
(c) providing crystallographic software to tenured academic research	25
(d) other research (please elaborate)	2
(e) providing software/resources for undergraduate teaching	14
(f) providing software/resources for PhD/postgraduate teaching	24
(g) providing software/resources for teaching workshops	18
(h) other teaching (please elaborate)	
(i) X-ray diffractometer instrument is not available in our institution. So at least with this CD people can gain some sort of knowledge	
(ii) CD content is made available to all research groups: from colleagues of other areas – chemistry, engineering – through PhD, MSc to training undergrad students. The CD format (instead of Internet) is particularly important to allow students (since their access to Internet is not always suitable) to explore and apply, or at least browse, through the latest achievements in this area. I also would like to state that this initiative was quite welcomed by the members, particularly students.	
Nexus CDs are used for (select multiple if required):	
(i) single-crystal diffraction	20
(j) powder diffraction	35
(k) other diffraction (please elaborate)	1

Of the 43 responses, powder diffraction usage was almost double that of single-crystal diffraction. The majority of respondents indicated that downloading of crystallographic software *via* the Internet ranged from 'problematic but do-able' to 'not practical'. Of the 14 respondents that indicated downloading of crystallographic software *via* the Internet was 'routine and easy', 12 indicated a preference for still receiving the Nexus CDs in future as a convenient back-up of crystal-

lographic software. 13 respondents were from India and six from China. Within India and China, responses varied from the Internet accessibility being 'routine and easy' to 'not practical'. This could indicate that difficulties with academic and student access to the Internet may involve regional issues and types of scientific facility.

7. Conclusions

While requests for CDs from new recipients have reduced markedly over recent years, feedback indicates Nexus CD-ROMs have been, and still are, a benefit for recipient crystallographers.

The following are thanked for suggestions, permissions and assistance in producing the Nexus CD-ROMs. Web content owners and custodians for permission to include material on the Nexus CD-ROM: Dr Armel Le Bail of the University of Le Mans, France; Dr Alan Hewat of ILL, Grenoble, France; Dr Howard Flack of the University of Geneva, Switzerland; and Mr Tony Sanderson of CSIRO Division of Minerals, Australia (deceased) for suggestions and encouragement of the initial versions of the CD-ROM. Dr Stephen Fletcher of CSIRO Division of Mineral Products, Melbourne, Australia (currently Professor of Inorganic Chemistry at the University of Loughborough, UK) for recommending the name 'Nexus' for the CDROM. Professor I. David Brown of McMaster University, Ontario, Canada, for assistance in distributing current versions of the CD-ROM, and comments on an initial draft of the text. Dr Richard Stephenson, previously of the CCP14 Project, University College London, UK, for arranging duplication and distribution of the 2005 batch-produced version of the CD.

References

- Altermatt, U. D. & Brown, I. D. (1987). *Acta Cryst.* **A43**, 125–130.
- Bergmann, J., Friedel, P. & Kleeberg, K. (1999). *IUCr Commission on Powder Diffraction Newsletter*, No. 21, p. 5.
- Bergmann, J. & Kleeberg, K. (1998). *IUCr Commission on Powder Diffraction Newsletter*, No. 20, pp. 5–8.
- Betteridge, P. W., Carruthers, J. R., Cooper, R. I., Prout, K. & Watkin, D. J. (2003). *J. Appl. Cryst.* **36**, 1487.
- Beurskens, P. T., Beurskens, G., Bosman, W. P., de Gelder, R., Garcia-Granda, S., Gould, R. O., Israel, R. & Smits, J. M. M. (1996). *The DIRDIF96 Program System*, Technical Report of the Crystallography Laboratory, University of Nijmegen, The Netherlands.
- Blue Squirrel (1998). *Grab-a-Site for Windows version 3.0.14*, 686 E. 8400 South Sandy, Utah, 84092, USA, <http://www.bluesquirrel.com/products/grabasite/>.
- Boultif, A. & Louër, D. (2004). *J. Appl. Cryst.* **37**, 724–731.
- Bowden, M. E. (2000). *IUCr Commission on Powder Diffraction Newsletter*, No. 23, p. 21.
- Burnett, M. N. & Johnson, C. K. (1996). Report ORNL-6895, Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA.
- Butler, D. (1996). *Nature (London)*, **380**, 377–381.
- Cheary, R. W. & Coelho, A. (1992). *J. Appl. Cryst.* **25**, 109–121.
- Cheary, R. W. & Coelho, A. A. (1998). *J. Appl. Cryst.* **31**, 862–868.
- Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
- Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
- Favre-Nicolin, V. & Černý, R. (2002). *J. Appl. Cryst.* **35**, 734–743.
- Finger, L. W., Kroeker, M. & Toby, B. H. (2007). *J. Appl. Cryst.* **40**, 188–192.
- Gelder, R. de, de Graaff, R. A. G. & Schenk, H. (1993). *Acta Cryst.* **A49**, 287–293.
- Gould, R. O., Moulden, N. & Taylor, P. (1988). Department of Chemistry, University of Edinburgh, Scotland.
- Holland, T. J. B. & Redfern, S. A. T. (1997). *Mineral. Mag.* **61**, 65–77.
- Izumi, F. (2003). *J. Ceram. Soc. Jpn.* **111**, 617–623.
- Kraus, W. & Nolze, G. (1996). *J. Appl. Cryst.* **29**, 301–303.
- Krumm, S. (1997). *WinFit 1.2.1*, Institut für Geologie, Scholssgarten 5, 91054 Erlangen, Germany.
- Larson, A. C. & Von Dreele, R. B. (2004). *GSAS. Generalized Structure Analysis System. Manual*, LAUR 86-748, Los Alamos National Laboratory, Los Alamos, NM, USA.
- Laugier, J. & Bochu, B. (2004). *LMGP-Suite. Suite of Programs for the Interpretation of X-ray Experiments*, ENSP/Laboratoire des Matériaux et du Génie Physique, BP 46, 38042 Saint Martin d'Hères, France.
- Le Bail, A. (2001). *Mater. Sci. Forum*, **378–381**, 65–70.
- Le Bail, A. (2002). *Crystallography Source Code Museum*, <http://www.cristal.org/museum/>.
- Le Bail, A. (2004). *Powder Diffr.* **19**, 249–254.
- Lutterotti, L., Ceccato, R., Dal Maschio, R. & Pagani, E. (1998). *Mater. Sci. Forum*, **278–281**, 93–98.
- Lutterotti, L., Matthies, S. & Wenk, H.-R. (1999). Proceedings of the Twelfth International Conference on Textures of Materials (ICOTOM-12), Vol. 1, p. 1599.
- Madsen, I. C. & Hill, R. J. (1994). *J. Appl. Cryst.* **27**, 385–392.
- Ozawa, T. C. & Kang, S. J. (2004). *J. Appl. Cryst.* **37**, 679.
- Palatinus, L. & Chapuis, G. (2007). *J. Appl. Cryst.* **40**, 786–790.
- Petricek, V., Dusek, M. & Palatinus, L. (2000). *Jana2000. The Crystallographic Computing System*, Institute of Physics, Praha, Czech Republic.
- Proffen, Th. & Neder, R. B. (1999). *J. Appl. Cryst.* **32**, 838–839.
- Rodríguez-Carvajal, J. (2001). *IUCr Commission on Powder Diffraction Newsletter*, No. 26, pp. 12–19.
- Rodríguez-Carvajal, J. & Roisnel, T. (1998). *IUCr Commission on Powder Diffraction Newsletter*, No. 20, pp. 35–36.
- Rohlfíček, J. & Hušák, M. (2007). *J. Appl. Cryst.* **40**, 600–601.
- Rupp, B. (1988). *Scr. Metall.* **22**, 1.
- Shirley, R. (2002). *The Lattice Press*, 41 Guildford Park Avenue, Guildford, Surrey GU2 7NL, England.
- Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
- Toby, B. H. (2001). *J. Appl. Cryst.* **34**, 210–213.
- Toby, B. H. (2005). *J. Appl. Cryst.* **38**, 1040–1041.
- Watkin, D. J., Prout, C. K. & Pearce, L. J. (1996). *CAMERON*, Chemical Crystallography Laboratory, University of Oxford, Oxford, UK.